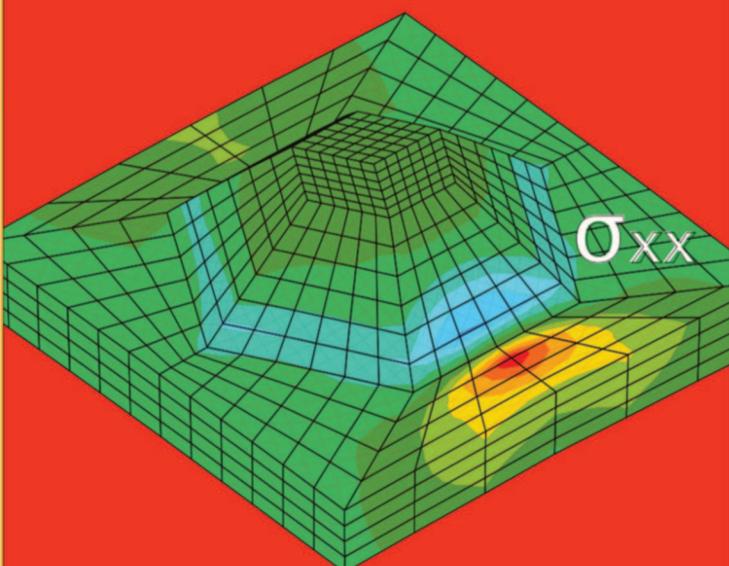
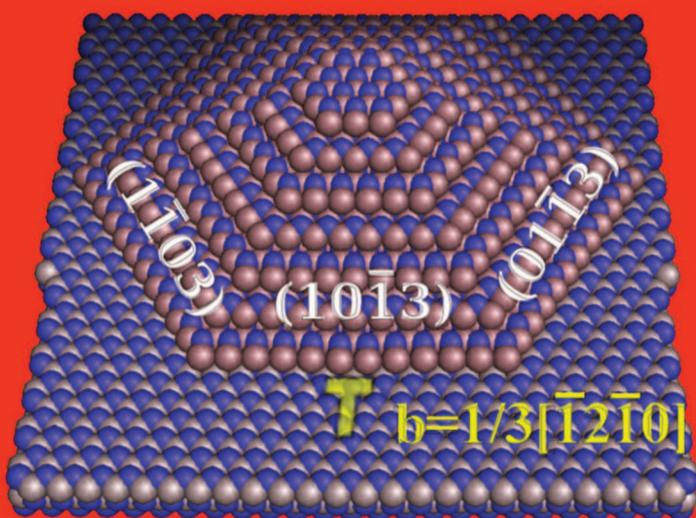


*Paweł Dłużewski,  
Grzegorz Jurczak,  
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(editors)*

## *Book of abstracts*

*3<sup>rd</sup> International  
Conference  
on Material Modelling  
incorporating the  
13<sup>th</sup> European  
Mechanics of Materials  
Conference*

*September 8<sup>th</sup> - 11<sup>th</sup>, 2013  
Warsaw, Poland*



Paweł Dłużewski, Grzegorz Jurczak, Toby D. Young (editors)

Book of Abstracts

**Third International Conference on Material  
Modelling**

incorporating the

**Thirteenth European Mechanics of Materials  
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# Preface

The International Conference on Material Modelling (ICMM) is a conference series dedicated to the modelling of materials and with the purpose of consolidating and exchanging information on new developments and discussing open questions related to the many facets of material modelling. In these conferences, information and ideas are freely discussed and openly shared and new learning and research collaborations are fostered. The third International Conference on Material Modelling, held at the Old Library of Warsaw University, from the 8th to the 11th of September, 2013, continues in the tradition of the first conference held in Dortmund (2009) and the second held in Paris (2011). This year ICMM attracted the attention of over two hundred and seventy-five scientific researchers from forty-three countries of five continents and incorporated twenty-three topical sessions held in parallel. As in previous meetings of ICMM, there is a continued high interest in sessions devoted to elasticity, plasticity, viscoplasticity and material theory. Additionally, this year showed an increase of participation in atomistic modelling and fields directly related to more technical aspects of computational modelling. It is the combined contribution of the participants and others that made this event a success. The organisers gratefully thank the following institutions for their support in organising ICMM3 2013: The European Mechanics Society (EUROMECH) which co-organised the thirteenth European Mechanics of Materials Conference (EMMC13) incorporated within ICMM3, and the European Collaborative dissemination of Aeronautical research and application project (E-CAero).

Warsaw, August 2013

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Session 1

Material theory



## On the generalization of uniaxial thermoviscoplasticity with damage to finite deformations based on enhanced rheological models

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In recent publications [1, 3], an enhanced concept of rheological networks has been proposed for the material modeling of thermoviscoplasticity. By introducing new basic elements, the depiction of nonlinear isotropic and kinematic hardening as well as an improved description of energy storage and dissipation during plastic deformations are enabled by means of the rheological models including damage representation as well—see [4]. Satisfying the thermomechanical consistency, the yield function and the flow rule are deduced from the equilibrium of stresses and the kinematics of the rheological network by means of simple algebraic calculations. Moreover, different approaches are proposed to improve the energy storage behavior by relating storage of inelastic work to ideal plasticity. The subsequent validation agrees well with the experimental test data.

However, the enhanced concept of rheological modeling, as presented in [3], is restricted to the uniaxial case only, but already requires a complex structure. Hence, the question consequently arises: How can the one-dimensional constitutive equations be systematically generalized for the spatial application for both small and large deformations. The former task is treated in [1, 2].

The present contribution introduces a representation of rheological networks for finite deformations as a straightforward generalization of the enhanced concept of rheological models in [3]. The basic components such as springs, dashpots, friction elements etc. are individually defined as tensor-valued bodies on either the reference or current configuration, which allows for assembling a rheological network of thermoviscoplasticity for finite strains by means of series and parallel connection of the elementary components and, hence, generates the free energy of the entire model. This arrangement of ideal bodies and the concept of dual variables [5] form the basis for the derivation of the constitutive material equations in finite deformation viscoplasticity with continuum damage, providing the yield function and the flow rule in an analogy procedure as in the uniaxial case [3]. In this process, the thermomechanical consistency of the model is satisfied.

**Acknowledgments** The authors thankfully acknowledge the financial support of the German Research Foundation (DFG) through grant number Ma1186/5.

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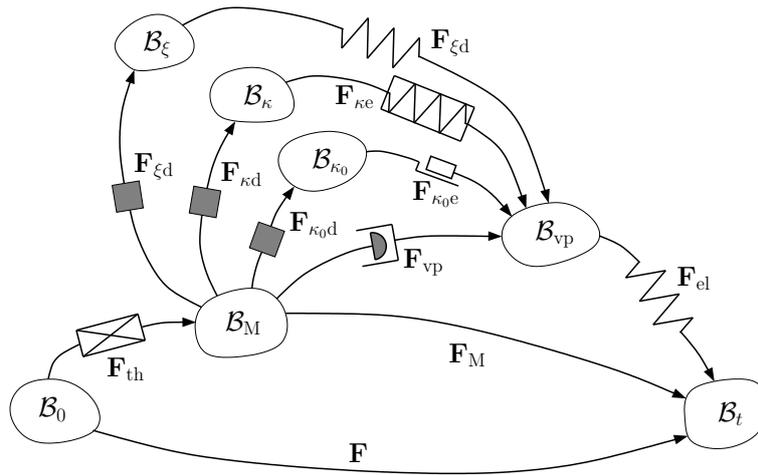


Figure 1: Rheological network representation for finite strain thermoviscoplasticity model with several multiplicative and parallel decompositions of deformation gradient  $\mathbf{F}$  and resulting intermediate configurations as motivated by the uniaxial model in [3]

## Non-Fickian Diffusion in Amorphous Polymers

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The diffusion of vapours and liquids in glassy polymers may deviate significantly from classical, i. e. Fickian, diffusion behaviour due to the restricted molecular mobility around and below the glass transition temperature. These deviations manifest in an alteration of penetrant uptake kinetics and can be macroscopically visible in, e. g., swelling or a glass transition caused by the penetrant.

The slow relaxation rates in glassy polymers inhibit the solvent uptake. If the relaxation is so slow as to dominate the diffusion process, the ensuing behaviour is referred to as Case II diffusion. Case II is a limiting case for anomalous diffusion characterised by the formation of a well-defined, sharp front between the unpenetrated glassy and the swollen regions, as opposed to the smooth concentration profiles observed for Fickian diffusion.

Fick's laws assume proportionality of the diffusion flux and the gradient in concentration. Their formulation implies an infinite propagation speed. While this theory has been very successful in describing a multitude of diffusional processes it is obviously unsuited for Case II diffusion. There has been considerable effort in finding an adequate formulation in the past decades. An overview over different models is given in [1] and in [2, 4] a general description of anomalous diffusion in the framework of non-linear continuum mechanics is presented.

In this contribution, the focus is on the modelling of pure diffusion in three spatial dimensions with a suitable extension of Fickian diffusion that accounts for the complex uptake kinetics observed in Case II diffusion, i. e. the sharp front and its wave-like propagation. Furthermore, the change in the material properties associated with the glass transition is taken into account.

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## Notes on the Geometry of Dislocations

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We present, see [1], a mathematical description of dislocations in crystalline solids having the following two features: (1) Formulated on a body manifold with no particular Riemannian metric, it specifies the geometry of dislocations independently of the configuration of the body in space. (2) It applied to both continuous distributions of dislocations as well as discrete dislocations.

A continuous body  $B$  is modeled as an  $n$ -dimensional differentiable manifold. We conceive a layering structure in the body which is analogous to the crystallographic planes structure. In the continuous case, the layering structure is specified by a differential 1-form, the layering form, in  $B$ . The value of the layering form at a point in the body is a co-vector which is analogous to the Miller indices for the corresponding crystallographic planes. If the layering form is the gradient—exterior derivative—of a real valued function  $u$  on the body,  $u$  can be used to label the various crystallographic  $(n - 1)$ -dimensional surfaces that serve as level sets for  $u$ . The condition for such integrability of the layering form is that its exterior derivative vanishes. Thus, the exterior derivative of the layering form, a differential 2-form, describes the obstructions to integrability—the dislocations in the body. We will therefore refer to the exterior derivative of the layering form as the dislocation form. Being an exterior derivative of a form, the dislocation form is exact and it follows that its exterior derivative should vanish identically. This identity provides the Frank's rules for the continuous distribution of dislocations.

In order to generalize the preceding framework to singular distributions of dislocations, we consider its weak form. Thus, using the theory of de Rham currents, we take as the basic object is an  $(n - 1)$ -current. If a layering differential form is given, such a current  $T$  is induced as follows.  $T$  acts on an  $(n - 1)$ -form by integrating over  $B$  the exterior product of the layering form and the  $(n - 1)$ -form. However, one may consider, as we propose to present, examples of currents that are not induced by smooth forms and are relevant to singular dislocations, e.g., non-coherent interfaces and edge dislocations. We will refer to such currents as layering currents. The generalized integrability condition for a layering current is that its boundary vanishes. It is recalled that the boundary operator for currents is the dual of the exterior derivative operator. Thus, the boundary of the layering current—the dislocation current—describes the geometry of singular dislocations. Being a boundary of the layering current, the boundary of the dislocation current vanishes identically. This provides the version of Frank's rules for the singular case.

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## Energy-Based Method in Phenomenological Description of Mechanical Properties of Nonlinear Elastic Material for Flat State of Stress

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Energy-based methods in solid mechanics are interesting and useful way for mathematical description of phenomena in material under external load program. Attention to the important of energy rule in modelling of mechanical properties of material was paid in a lot of papers just like [1] – [9]. The present work is a trial of phenomenological description of mechanical properties for nonlinear elastic material in flat state of stress, with using of energy-based method, what is continuation of investigations carried out in [9], where the flat state of strain was taken under account. The strain energy density function is formulated on the base of approximations of mechanical characteristics of material and geometrical interpretation of deformation process. The extraction of its volumetric part was made using hydrostatic pressure interpretation. The strain energy was used to formulation the material stability assumptions due to plastic flow and determination the regions of stability. The analytical form of stability assumptions is modified (in comparison to these known from [7]) on the ground of volumetric part of energy. All theoretical investigations are illustrated on the example of aluminium and steel for flat state of stress.

**Keywords:** energy-based method, strain energy density function, material characteristics, Sylvester's theorem.

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## On the phenomenological equations of elastic quasicrystals

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In recent years many papers have been published concerning the elasticity of quasicrystals (which admit usually forbidden symmetries such as a five-fold one [1]-[2]). The present study has for main purpose to replace the presently proposed formulations into the framework of the modern thermo-mechanics of continua. Two types of modelling are envisaged in small deformations, those inspired by the physical descriptions proposed by Bak [3] on the one hand and by Lubensky and co-workers [4] on the other. While the first one fits well in a traditional variational formulation, the second one seems to be best accommodated in the frame of the thermomechanics of internal variables of state, the newly introduced "phason" field being then interpreted as such a vector variable. The inclusion of these two models in the theory of configurational forces - useful for the study of the expansion of defects frequent in such crystals - and the possibilities of including the effects of nonlinear elasticity and plasticity are briefly discussed. Important symmetry conditions are however left aside.

**Note** The study reported in this work was kindled while the author acted as editor and/or referee of several papers on the elasticity of quasicrystals. It results from a specific effort from the author to comprehend the basis of this elasticity, as in particular exposed in a recent book by Fan [5], and to replace its two basic formulations in a more familiar thermo-mechanical framework, as nowadays accepted in continuum mechanics.

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## A thermoelastic beam theory *via* Virtual Power Principle

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A method to obtain from three-dimensional elasticity *lower-dimensional* theories for thin structures is to lay down a *restricted* version of the Principle of Virtual Powers: the first restriction concerns the special shape of the three-dimensional bodies considered; the second restriction consist in choosing as admissible a special class of body parts; third and last concerns in selecting the special class of virtual velocities, consistent with the representations of admissible displacements [3, 7]. When applied to beams, this method yields the balance equations in terms of force and moment resultants, defined as cross-sectional averages of the three-dimensional stress field.

On the other hand, in [8] it is shown that a Virtual Power format more general than usual can be employed to deduce all balance laws of three-dimensional thermomechanics, regarded as an example of a *multiphysics* theory, that is a composition of two material body structures, the one mechanical the other thermal.

Several models for thermomechanics of beams have been proposed in literature, some of them direct [1, 2, 4–6], others induced by three-dimensional thermomechanics [9]. We here propose a model consistent with the three-dimensional parent theory and deduced by means the application of the Principle of Virtual Powers, employed as an instrument to simultaneously obtain dimensional reduction and multiphysics. An essential role is played by the notion of thermal displacement, which is given a convenient *a priori* representation, just as the mechanical displacement.

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## Continuum Surface Energy from a Lattice Model

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We investigate some connections between the continuum and atomistic descriptions of deformable crystals, using certain interesting results from number theory. The energy of a deformed crystal is calculated in the context of a lattice model with pair interactions in two dimensions. A new bond counting approach is used, which reduces the problem to the lattice point problem of number theory. When the crystal shape is a lattice polygon, we show that the energy equals the bulk elastic energy, plus the boundary integral of a *surface energy density*, plus the sum over the vertices of a corner energy function. The surface energy density is obtained *explicitly* as a function of the deformation gradient and boundary normal, that involves the interatomic potential. The result is then generalized to three dimensions and more general regions with possibly curved boundary [1].

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## Chemical Affinity Tensor and Chemical Reaction Front Kinetics in Deformable Solids

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We consider a stress-assist chemical reaction front propagation in a deformable solid undergoing a chemical reaction between solid and gas constituents. The reaction is localized at the reaction front and sustained by the diffusion of the gas constituent through the transformed material. For simplicity sake we accept a solid skeleton approach assuming that the gas diffusion does not affect the solid constituent [1]. We find a chemical transformations strain tensor that relates two reference configurations of solid constituents. Then mass, momentum and energy balances and the the entropy inequality for the case of the reaction front propagation in a solid with arbitrary constitutive equations are written down. As a result, the expression of the chemical affinity tensor is obtained. A quasi-static part of the expression of the chemical affinity tensor takes the form similar to the expression of the classical chemical affinity (see, e.g., [2]) if replace scalar chemical potentials of the solid constituents by the Eshelby stress tensors determined with respect to the reference configurations of solid constituents and divided by the reference mass densities. Earlier such a formula was derived for the case of the reaction in a non-linear elastic solid [3].

The chemical affinity tensor determines the configurational force. We formulate the kinetic equation that relates the reaction front velocity with the normal component of the chemical affinity tensor and compare the conditions at the chemical reaction front and interphase boundary.

Having in mind the notion of chemical equilibrium [2], we introduce the notion of the equilibrium gas concentration as the concentration at which the normal component of the chemical affinity tensor equals zero. This allows us to formulate the kinetic equation in terms of chemical potentials of the gas constituent calculated at the current gas concentration at the reaction front and at the equilibrium concentration that depends on stresses. Analytical (see e.g. [4]) and numerical solutions of some coupled problems of mechanochemistry are demonstrated. The influence of stresses including locking effects (blocking the reaction by stresses) and stability problems are discussed.

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## Dual variational problems and limit analysis for masonry bodies

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The paper deals with the questions of the statics of masonry bodies modeled as bodies made of no-tension materials. The characteristic feature of no-tension materials is that the stress tensor in the body must be negative semidefinite. Because of this, no-tension bodies cannot sustain all loads, certain loads lead to the collapse of the body. To determine which loads are safe and which lead to collapse, the static and kinematic theorems are conventionally invoked. These theorems involve the choices of the function spaces for stresses and for strains. The paper discusses the validity of the static and kinematic theorems from the viewpoint of the function spaces. It is generally pointed out that the static and kinematic theorems can give different predictions and examples are given to this effect.

Specifically, the paper formulates the kinematic and static problems of limit analysis of no-tension bodies. The kinematic problem involves the infimum of kinematically admissible multipliers, and the static problem the supremum of statically admissible multipliers. The central question of the paper is under which conditions these two numbers coincide. A whole ordered scale of function spaces for stresses and strains is presented. The mentioned problems are formulated as convex variational problems considered by Ekeland and Temam. The static problem is unconditionally shown to be the dual problem of the kinematic problem. A *necessary and sufficient condition*, the normality, guarantees that the kinematic and static problems give the same result. The normality is not always satisfied, as examples show. The qualification hypothesis of Ekeland and Temam, *sufficient* for the equality of the static and kinematic problems, is never satisfied in the spaces of admissible displacements of bounded deformation or of functions integrable together with the gradient in the power  $p$ ,  $1 \leq p < \infty$ . In the cases of Lipschitzian displacements and of smooth displacements, the qualification hypothesis is equivalent to simple conditions that can be satisfied in the case of the pure traction problem. However, it is shown that then the space of admissible stresses must be enlarged to contain stressfields represented by finitely or countably additive tensor valued measures.

## Residually stressed beams by $\Gamma$ -convergence

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The theory of linear elasticity with residual stress goes back to Cauchy (1829), but for a long time the attention of researchers was almost exclusively given to the so-called linear theory of elasticity. In recent years, instead, the theory with residual stress has been studied and used quite extensively. As in the case of the derivation by  $\Gamma$ -convergence of thin structures without residual stress, initiated 20 years ago, also the corresponding asymptotic analysis for a material with residual stress started in 2006 from the simplest case of a plate with the paper of Paroni [3]. After that, in 2009, Della Longa and Londero [1] have considered the case of a thin-walled beam with a rectangular cross-section. The most difficult case of a slender rod, which is the subject of this talk, has been recently studied in [2].

The presence of residual stress introduces in the constitutive equation for the Piola-Kirchhoff stress tensor a dependence from the displacement gradient and not simply on the strain as in the case without residual stress. Precisely, the Piola-Kirchhoff stress tensor  $S$  is given by

$$S = \mathring{T} + Du\mathring{T} + \mathbb{L}Eu,$$

where  $Du$  denotes the gradient of the displacement  $u$ ,  $Eu$  is the symmetric part of  $Du$ ,  $\mathring{T}$  is a second order symmetric tensor representing the residual stress in the reference configuration and  $\mathbb{L}$  is a fourth order tensor called incremental elasticity tensor. The term  $Du\mathring{T}$ , that comes into play because of material frame indifference, makes the theory quite different from the elastic theory without residual stress; for instance, the elastic energy density is no longer convex.

In our analysis we do not impose any material symmetry on the incremental elasticity tensor  $\mathbb{L}$  and we allow it to depend on the longitudinal variable  $y_3$ , i.e., the cross-sections of the beams are assumed to be homogeneous. By assuming the rod to be clamped to one of its bases, we find that the elastic energy of the limit problem is

$$I_{1d}(\xi, \theta) = \frac{1}{2} \int_0^\ell Q(y_3, \xi_1'', \xi_2'', \xi_3', \theta') + \text{tr}\langle \mathring{T} \rangle \theta^2 + \langle \mathring{T} \rangle (\xi_1', \xi_2') \cdot (\xi_1', \xi_2') dy_3,$$

where  $\xi$  is a Bernoulli-Navier displacement and  $\theta$  is a scalar field representing the twist of the cross-section around the longitudinal axis. The energy density  $Q$  is defined by a minimum problem on the cross-section involving the incremental elasticity tensor, and

$$\langle \mathring{T} \rangle := \int_\omega \begin{pmatrix} \mathring{T}_{11} & \mathring{T}_{12} \\ \mathring{T}_{21} & \mathring{T}_{22} \end{pmatrix} dy_1 dy_2,$$

where  $\omega$  denotes the cross-section.

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## **Asymptotic theories for thin-walled beams**

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Geometrically, a thin-walled beam is a slender structural element whose length is much larger than the diameter of the cross section which, in turn, is larger than the thickness of the thin wall. These beams have been used for a long time in civil and mechanical engineering and, most of all, in flight vehicle structures because of their high ratio between maximum strength and weight.

From a mathematical point of view, these beams present *two scaling factors*: one is the ratio between the diameter of the cross-section and the length of the beam, the other is the ratio between the wall thickness and the diameter of the cross-section.

In this talk, starting from the three-dimensional linear theory of elasticity we shall deduce one dimensional models for these kind of beams by means of an asymptotic analysis in which the two scaling factors go to zero.

## Modelling the curing process for magneto-sensitive elastomeric materials

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In this paper, a phenomenologically motivated coupled finite strain elastic framework for simulating the curing process of polymers in the presence of magnetic field is proposed. This approach is in line with our previously published finite strain curing modelling framework for pure (mechanical) polymer curing. The thermodynamically consistent approach is independent of any particular free energy function that has been used for fully-cured magneto-sensitive polymer modelling, i.e. any phenomenological or micromechanical-inspired free energy can be inserted into the main modelling framework. For preparation of magneto-sensitive polymers, micro-size ferromagnetic particles are used in the uncured stage. The particles will align in a preferred direction with the application of a magnetic field during the curing process. Polymer curing process is a complex (visco) elastic process that transforms a fluid to solid with time. Such transformation process can be modelled by an appropriate constitutive relation which takes into account the temporal evolution of material parameters appearing in a particular energy function. For demonstration in this work, two different energy functions have been chosen, i.e. the Neo-Hookean model and the Mooney-Rivlin model. Several representative numerical examples have been demonstrated that prove the capability of our approach to correctly capture common features in polymers undergoing curing processes in the presence of a magnetic field.

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In the context of rheology, linear elastic materials can be modelled using bunch of networks of linear springs each having certain stiffness. Using similar analogy, the continuous cross-linking within a curing polymer can be conceptualised as the addition of more and more springs to the network, cf. Fig (1). Keeping this fact in mind, a magneto-elastic coupled free energy function is proposed in the form of convolution integral for the curing process in the presence of a magnetic induction as

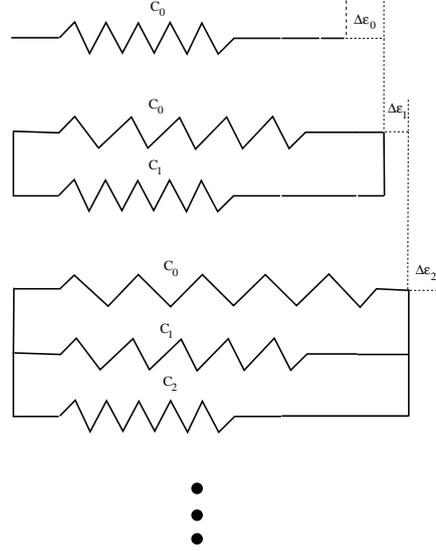


Figure 1: Formation of new chains during curing process

$$\begin{aligned} \Phi(t) &= \frac{1}{2} \int_0^t [\mathbb{A}'(s) : [\mathbf{F}(t) - \mathbf{F}(s)]] : [\mathbf{F}(t) - \mathbf{F}(s)] ds + \frac{1}{2} \int_0^t [\mathcal{K}'(s) \cdot [\mathbb{B}(t) - \mathbb{B}(s)]] \cdot [\mathbb{B}(t) - \mathbb{B}(s)] ds \\ &+ \int_0^t [\mathcal{C}'(s) \cdot [\mathbb{B}(t) - \mathbb{B}(s)]] : [\mathbf{F}(t) - \mathbf{F}(s)] ds \end{aligned} \quad (1)$$

where  $\mathbb{A}'(s) = d\mathbb{A}(s)/ds$ ,  $\mathcal{K}'(s) = d\mathcal{K}(s)/ds$  and  $\mathcal{C}'(s) = d\mathcal{C}(s)/ds$ . To derive the relations for these time-dependent stiffness tensors, a coupled energy potential is necessary which relates the three stiffness operators in the following way

$$\mathbb{A}(t) = \frac{\partial^2 \Omega(t)}{\partial \mathbf{F} \partial \mathbf{F}}, \quad \mathcal{C}(t) = \frac{\partial^2 \Omega(t)}{\partial \mathbf{F} \partial \mathbb{B}}, \quad \mathcal{K}(t) = \frac{\partial^2 \Omega(t)}{\partial \mathbb{B} \partial \mathbb{B}} \quad (2)$$

where  $\Omega(t)$  is a coupled energy function for magneto-elastic polymers with time dependent material parameters.  $\Omega(t)$  is nothing but an appropriate free energy that has been used for modelling a fully-cured magneto-sensitive polymer and available in the literature. The second law of thermodynamics in the form of Clausius-Duhem inequality for the isothermal process can be written in the case of magneto-elastic problem as

$$\mathbf{P} : \dot{\mathbf{F}} + \mathbb{H} \cdot \dot{\mathbb{B}} - \dot{\Phi} \geq 0 \quad (3)$$

Finally after some simplifications, the evolution of the stress and the magnetic field yield

$$\dot{\mathbf{P}}(t) = \mathbb{A}(t) : \dot{\mathbf{F}}(t) + \mathcal{C}(t) \cdot \dot{\mathbb{B}}(t), \quad (4)$$

$$\dot{\mathbb{H}}(t) = \mathcal{C}^t(t) : \dot{\mathbf{F}}(t) + \mathcal{K}(t) \cdot \dot{\mathbb{B}}(t). \quad (5)$$

## Session 2

# Elasticity and viscoelasticity



## Damping behavior of an Al-Cu alloy with 20% of SiC fibers.

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The aim of this study is the characterization of the mechanisms that contribute to damping phenomena observed in the Metal Matrix Composite 2024 - 20% SiC fibers.

To highlight the contribution of the added whiskers to the 2024 aluminum matrix, two samples of 2024 aluminum alloys without and with 20% SiC whiskers have been studied by isothermal mechanical spectroscopy.

Experiments were performed in a very large frequency range ( $10^{-4}$  Hz – 50 Hz) between room and solidus temperatures. During heating, for each temperature of measurement, experiment started after a hold time long enough for a complete stabilization of the microstructure. Indeed the sample has reached stability such that its hardness does not evolve.

The obtained results are quite different, in fact:

- A non-thermally activated effect was highlighted on the matrix material; the maximum of its peak is at about 0.2 Hz. It has been linked to the  $\theta$  precipitates.

-A relaxation peak has been evidenced at high temperature for the reinforced sample. This peak has been attributed to the movements of dislocation segments within clusters surrounding each whisker. These dislocations derive from the difference between the coefficients of expansion of the 2024 alloy and the SiC fibers. Then, the interface fiber - matrix is the origin of the observed internal friction.

Furthermore, this comparison clearly confirms that the introduction of whiskers modifies significantly the precipitation process in the matrix. Indeed, the Al-SiC interfaces will play the wells gaps role, which induces an excessive segregation of alloying elements and depletes the matrix of solute atoms. This depletion will lead to a minimum saturation in solute which therefore tends to reduce the precipitation process in the composite.

We can then conclude that this comparative study shows that the strengthening of the 2024 aluminum matrix by SiC whiskers plays a key role in the anelasticity of the CMM.

**Keywords:** Internal Friction, Isothermal Mechanical Spectroscopy, Aluminum alloy, Metal Matrix, Composite Materials, Whiskers, precipitates, non-thermally activated effect, relaxation peak, high temperature.

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## Boundary integral method in the theory of thermoelasticity for solids with double porosity

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The quasi-static theory of elasticity for materials with double porosity in the framework of mixture theory was proposed in [1]. This theory unifies the earlier proposed models of Barenblatt's for fluid flow through undeformable porous media with double porosity and Biot's for deformable porous media with single porosity. The theory of thermoelasticity for materials with double porosity is presented in [2, 3]. The double porosity model of poroelasticity is effective and useful model for deformation-driven bone fluid movement in bone tissue [4, 5]. The basic properties of plane harmonic waves are studied and the existence of eigenfrequencies of the internal boundary value problems (BVPs) of steady vibrations in the 3D theory of elasticity for materials with double porosity is established in [6, 7]. The basic BVPs in this theory are investigated by the boundary integral method (potential method) and the theory of singular integral equations in [8, 9].

In this paper the 3D theory of thermoelasticity for materials with double porosity [2, 3] is considered and the following results are obtained. The fundamental solutions of the systems of quasi-statics and steady vibrations equations of this theory are constructed by elementary functions. The representations of general solutions and Green's formulae in the considered theory are obtained. The basic properties of surface (single-layer and double-layer) and volume potentials are established. The uniqueness and existence theorems of solutions of the external BVPs of quasi-statics and steady vibrations in the 3D theory of elasticity for materials with double porosity are proved by the boundary integral method and the theory of singular integral equations.

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## Boundary value problems in the theory of thermoviscoelasticity for Kelvin-Voigt materials with voids

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Viscoelastic materials play an important role in many branches of engineering, technology and, in recent years, biomechanics [1]. One of the simplest mathematical models constructed to describe the viscoelastic effects is the classical Kelvin-Voigt model [2]. The basic boundary value problems (BVPs) of the classical theories of viscoelasticity and thermoviscoelasticity for Kelvin-Voigt materials are investigated in [3].

The modern theories of viscoelasticity and thermoviscoelasticity for materials with microstructure have been a subject of intensive study in the last decade [4, 5]. The theory of thermoviscoelasticity for Kelvin-Voigt materials with voids is presented in [6]. Recently, the theory of thermoviscoelasticity for Kelvin-Voigt microstretch composite materials is introduced in [7]. The uniqueness and existence theorems of the BVPs of steady vibrations in the theory of viscoelasticity for Kelvin-Voigt materials with voids are proved in [8].

In the present paper the linear theory of thermoviscoelasticity for Kelvin-Voigt materials with voids [6] is considered and some basic results of the classical theory of thermoelasticity are generalized. Indeed, the fundamental solution of the system of equations of steady vibrations is constructed by means of elementary functions. The Green's formulas in the considered theory are obtained. The uniqueness theorems of the internal and external basic BVPs are proved. The representation of Galerkin type solution is obtained and the completeness of this solution is established. The formulas of integral representations of Somigliana type of regular vector and regular (classical) solution are obtained. The basic properties of thermoelastopotentials and singular integral operators are given. Finally, the existence theorems for classical solutions of the basic BVPs of steady vibrations are proved by using of the potential method (boundary integral equations method) and the theory of singular integral equations.

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## Micromechanical modelling of the thermo-mechanical behaviour of oriented semicrystalline polymer foils

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In flexible electronics, polymeric materials may replace conventional substrate materials as silicon, providing flexibility, and potentially enabling roll-to-roll manufacturing. Polymeric foils that are used as a substrate for flexible electronics and which usually have a strongly oriented semicrystalline microstructure, need to satisfy a number of requirements, among which good dimensional stability, also at elevated temperature. This dimensional stability is highly dependent on the internal macromolecular orientation.

This work aims at understanding and predicting the effects of the microstructure, as well as loading conditions as time, stress, temperature and humidity on the mechanical response of thin semicrystalline polymer foils. For this purpose, a micromechanical thermo-elasto-viscoplastic model is developed to predict the dimensional stability of foils when exposed to these loads. The model considers the material to consist of an aggregate of two-phase layered domains, where different constitutive laws are used for the phases [1,2]. The crystalline phase is modelled with crystal viscoplasticity and the amorphous phase is described as an elasto-viscoplastic glassy polymer, taking account material ageing [3,4].

The micromechanically-based model is used to describe the mechanical behaviour of amorphous and semicrystalline polyethylene terephthalate (PET) under uniaxial compression and uniaxial tension up to large strains and at different temperatures. The model is used to describe the anisotropic elastic and viscoplastic response of oriented PET foils, that is experimentally observed, based on their microstructure. Using information about the orientation distribution of the crystalline phase, the local thermo-mechanical behaviour is predicted. To demonstrate the applicability of the model to describe the long-term response, the creep behaviour is simulated and compared to experimental data.

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## Damping, Dispersion and Classification

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Common description of the damping behavior of viscoelastic material is based on the combination of one or more spring and dashpot elements in a specific construction. Such rheological models are widely in use for the description of both, the structural behavior as well as in the case of fluid dynamics and acoustics. It is also common to describe the stress-strain relationship by an ordinary differential equation and by using the so-called viscoelastic correspondence principle.

Important for the analysis of the mathematical and physical structure of the above mentioned applications are the corresponding partial differential equations in terms of the unknown displacement, which in addition one achieves by means of the Eulerian equation of motion and the kinematic relation between the spatial derivative of the displacement and the strain parameter. On this level dispersion phenomena will be discussed, which leads to a physical classification. A pure mathematical classification will also be performed. The latter one yields to different hyperbolic and mixed parabolic-hyperbolic classes of the partial differential equations.

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## Thermo-mechanical Modelling for Visco Elastic, Visco Plastic Polymers; Application to fatigue

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A 3D Visco elastic model is discussed and validated using a rich and rigorous data base obtained on PA66 above T<sub>g</sub> [1].

In this constitutive model [1] inelastic phenomena are accounted for as an evolution of internal variables assumed to be related to entanglements. Inelastic strain-rate is deduced from energy balance between elastic and dissipative phenomenon. The stress is written in the framework of Irreversible Processes Thermodynamics (IPT) and in the frame of large strain approximations.

The concept allows introducing time effects in any energy potential. It is combined with Edward-Vilgis' model [2]. Revisited model allows reproducing most of the linear and non-linear visco-elastic phenomena in polymer: strain rate dependence, hysteretic effects and relaxation.

An accounting for temperature and strain-rate by an "a priori" uses of time temperature superposition principle is also proposed.

The three concepts result in an original and attractive model of high efficiency with only a small number of parameters.

In this paper ability of the model to model uploading – unloading, uploading-relaxation/unloading relaxation cycles and even fatigue experiments using one unique set of parameters will be illustrated.

Physical meaning of parameters will be discussed

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## Asymptotic modeling of a piezoelectric layered assembly

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In the last decades the use of intelligent materials, like piezoelectric materials, has deeply increased in several domains of aeronautical, mechanical and civil engineering. For instance, piezoelectric transducers, in the form of piezo-patches, are commonly employed in structural monitoring, in the active/passive dumping of high frequency vibrations and in the eliminations of undesired vibrations. An important example is given by the actuated rotating blades of the helicopters. The present work is aimed at deriving a mathematical model of the mechanical behavior of a piezo-patch, which is constituted by a thin piezoelectric plate between two conductor films, glued to a structural member, as a helicopter blade, or surrounded by the structure that needs to be monitored. This particular structural assembly gives rise to a complex multi-material characterized by a high contrast between the thickness of the piezo-plate and the actual dimensions of the structure and, also, among the mechanical properties and physical behaviors of its constituents. This important difference in the geometrical and electromechanical properties creates remarkable numerical instabilities in a FEM analysis and justifies the need of looking for a simplified model. The successful application of the asymptotic methods to obtain a mathematical justification of the most used models of elastic and piezoelectric plates (see [2,4]) has stimulated the research toward a rational simplification of the modeling of complex structures obtained by joining elements of different dimensions and/or materials of highly contrasted properties. For example, Bessoud et al. in [1] have studied the behavior of elastic shell-like inclusions with high rigidity immersed in a three-dimensional body; concerning with piezoelectric multimaterials, Geis et al. in [3] derive an asymptotic model of a piezoelectric stack actuator with metal inclusions. In this case we consider a simplified situation in which the assembly is made by a transversely isotropic linearly piezoelectric plate included in two three-dimensional linearly elastic and conductor bodies. By defining a small real parameter  $\varepsilon$ , which represents the thickness of the plate-like domain, we perform an asymptotic analysis, following the approach of [2]. Then we derive a limit model in which the piezoelectric plate between the two bodies in some way “disappear”: its contribution in the limit model is given by a specific surface energy defined over the middle plane of the plate, which generates some appropriate electromechanical transmission conditions at the interface of the two bodies. The obtained model is then mathematically justified by a variational convergence argument.

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## Multi-scale modeling of nano-clay reinforced polymers

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New multi-scale representation of nano-clay-reinforced polymer will be considered. Nano-clay platelets with adjacent polymer will be represented as bi-layered sandwich. Depending on the exfoliation degree of the material the morphology will be represented as dispersed bi-layered (exfoliated) or a stack of bi-layered sandwich (intercalated). The polymer will be considered isotropic whereas the nano-platelets are anisotropic. To predict the macroscopic elastic properties, two approaches will be used; hybrids ([7]) and matrix-inclusion models ([5], [6]). Each approach has its limitations due to the stated hypothesis ([2], [4], [1], [3]).

In this study we link these different models; hybrid and matrix-inclusion, to take into account possible micro-structure : exfoliation, intercalation and aggregation. The comparison with the experimental data shows that length scale sensitive models allow to represent elastic behavior of nano-composite considering particularities of the morphology.

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## **Green's Function in Plane Anisotropic Bimaterials with Imperfect Interface in Plane Elasticity**

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The fundamental solutions or Green's functions for two or three-dimensional anisotropic media with imperfect interface remains a challenging problem. In this paper, a general method is presented for the rigorous solution for the two-dimensional Green's function in an anisotropic elastic bimaterial subject to a line force or a line dislocation. Most significant is the fact that the bonding along the bimaterial interface is considered to be homogeneous imperfect. Specifically, the tractions are continuous but the displacements are discontinuous and proportional, in terms of interface stiffness parameters, to their respective traction components.

Using complex variable techniques the basic boundary value problem for two analytic vector functions is reduced to a coupled linear first-order differential equation for a single analytic vector function defined in the lower half space. The coupled linear differential equation for the single analytic vector function can be subsequently decoupled into three independent linear first-order differential equations for three newly defined analytic functions. Closed-form solutions for the two-dimensional Green's function are derived in terms of the exponential integral. Unlike previous works which involve some sort of inverse transform method to obtain the physical quantities from the transform domain, the key feature of the present method is that the physical quantities can be readily calculated without the need to perform any inverse transform operations.



## Session 3

# Finite elasticity



## Transversely isotropic finite deformation thermo-hyperelasticity in the framework of p-version finite elements

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In this contribution, the constitutive modeling of transversely isotropic thermo-hyperelasticity for the case of finite deformation is presented. The formulation is based on the multiplicative decomposition of the deformation gradient into thermal and mechanical parts. The thermal part is purely transversely volumetric. The mechanical part is further decomposed multiplicatively, in order to distinct the deformation in the direction of anisotropy from the remaining deformations, see [1]. This clearly attributes the deformation and resulting stress states to the fiber orientation and the remaining material. The proposed model is investigated and studied in the framework of three-dimensional high-order finite elements, which are based on hierarchical-shape functions combined with high-order time-integration, see, for example, [3]. The influence of anisotropy on the accuracy of the problem is studied in detail. Moreover, the resulting system of the system of differential-algebraic equations, where the algebraic part stems from the discretized weak form of the equilibrium condition and the differential part follows the non-linear heat conduction, has to be computed. This fully coupled system is solved using a monolithic approach, where the time integration is done using high-order stiffly accurate, diagonally implicit Runge-Kutta methods, see [2]. A particular focus in the examples lies in the investigation of the sensitivity of anisotropic media to the resulting boundary-value problem.

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## Internally Balanced Solid Response in Compressible Hyperelasticity described by a Deformation Gradient Product Decomposition

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In finite deformation continuum mechanics, the multiplicative decomposition of the deformation gradient

$$\mathbf{F} = \hat{\mathbf{F}} \mathbf{F}^*$$

has been used to treat mechanical effects such as plasticity, swelling, and biological growth and remodeling. In such modeling this response is characterized by the part  $\mathbf{F}^*$  of the decomposition. Then  $\hat{\mathbf{F}}$  is an elastic follow-up that is governed by hyperelastic considerations. For equilibrium problems this elastic follow-up can then be formulated in terms of a variational procedure with an associated stored energy density  $W(\hat{\mathbf{F}})$ . Recently the mechanical behavior of incompressible soft solid materials has been modeled using this deformation gradient decomposition where both  $\mathbf{F}^*$  and  $\hat{\mathbf{F}}$  have been treated as hyperelastic in nature. Then the energy density is regarded as a function of both  $\mathbf{F}^*$  and  $\hat{\mathbf{F}}$ , and the decomposition of  $\mathbf{F}$  into  $\hat{\mathbf{F}} \mathbf{F}^*$  is itself determined on the basis of an additional balance principle that emerges naturally from the variational treatment. This additional principle can be interpreted as a requirement of internal balance. The resulting theory naturally describes certain strain localization phenomena that are not readily modeled in the context of the standard hyperelastic treatment. In this presentation we discuss the implications of this modeling for compressible soft solid materials. The theoretical framework naturally retrieves classical compressible hyperelasticity for certain limiting forms of the stored energy  $W(\hat{\mathbf{F}}, \mathbf{F}^*)$ . The framework shows promise for modeling the development singular surfaces that serve as locations of concentrated microstructural rearrangement.

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## On Geometrical Foundations of the Theory of Growing Solids

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A vast majority of objects around us arise from some growth processes. Many natural phenomena such as growth of biological tissues, glaciers, blocks of sedimentary and volcanic rocks, and space objects may serve as examples. Similar processes determine specific features of many material processing technologies which include crystal growth, various types of deposition, melt solidification, electrolytic formation, polymerization, *etc.* These processes are rather dissimilar in their physical nature but have much in common from viewpoint of continuum mechanics: they produce solids with structural inhomogeneity that appears due to joining of geometrically incompatible in stress-free state shapes. Mechanical features of such solids differ significantly from those of permanent composition. Particularly the inhomogeneity causes residual stresses that are observable phenomena for the growing solids.

There are various approaches in modelling of growing solids. We use the geometrical one. In the framework of this approach the residual stresses appears due to special non-Euclidean properties of reference (material) representation of the growing solid. Under the assumptions that the material of growing body locally is simple and the process of growing is continuous this properties may be described completely by a special kind of affine connection on the tangent bundle of material manifold. Thereby the growing bodies can be viewed as a special class of inhomogeneous bodies whose inhomogeneity is caused by junction of incompatible stressed parts. In that respect, mechanics of growing solids has much in common with the theory of continuously distributed defects. One may give the interpretation of growing process as couple of complementary processes: the continuous influx of material and the continuous influx of defects. Note that actually these defects play role of the elements of predefined structure specified by the scenario of accretion but not of imperfections.

In the framework of the geometrical mechanics of growing solids one have to describe global and local intrinsic non-trivial properties of material manifold. The global (topological) structure may be described by the representation of a material manifold as a bundle over one- or two-dimensional base (not to be confused with tangent bundle). In order to describe local properties we use the concept of a body as an abstract smooth manifold equipped with a special *material connection*. The notion of *material connection* formalizes the idea of a local uniform reference configuration that brings an infinitesimal neighborhood of a material point into some uniform, typically natural strain state. In general one cannot simultaneously bring infinitesimal neighborhoods of all material points of growing solid into a uniform state by a smooth mapping. From the mechanical viewpoint, such bodies have no residual stress-free shapes embedded into Euclidean space. The only way to return the neighborhoods of all material points to a natural state and thus relax the residual stresses is to cut the body into infinitely many parts and allow them to deform independently. This fictitious process is in a sense the inverse of the growth process. At the same time one may “deform“ space and arrive at non-Euclidean description of reference stress free material manifold. This line of reasoning evolve to the Cartan machinery of exterior calculus and permit to formulate governing field equations in rather elegant way.

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## **On the use of a four-dimensional formalism to build linear or non-linear isotropic hypo-elastic behaviors using the Lie derivative**

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In the present work, we are interested in discussing covariance issues in continuum mechanics, in relation with material objectivity. The covariance principle was first introduced by A. Einstein and corresponds to frame-indifference within a 4D description of physics. Objectivity is equivalent to the concept of frame-indifference when considering its classical 3D definition (because it is linked to rigid body motions). The present paper is focused primarily on the application of these concepts to material constitutive models [1-5]. The aim is to place the mathematical framework of these constitutive relations within the four-dimensional formalism of general relativity theory.

The covariance principle of differential geometry within a four-dimensional space-time ensures the validity of any equations and physical relations through any changes of frame of reference, due to the definition of the 4D space-time and the use of 4D tensors, operations and operators. This formalism enables to separate covariance (i.e. frame-indifference) and material objectivity (i.e. invariance under superposition of any rigid body motion).

First, the behavior of different hyper-elastic materials has been investigated. Indeed, it is possible to demonstrate that potentials can be constructed, whose variation leads directly to material constitutive relations. It is possible to obtain some of the classical 3D relations when extracting the space components. However, some new elastic behaviors could be also obtained with this 4D formalism. Moreover, it has been proved that the present approach enables to encompass the classical Eulerian and Lagrangean approaches, as the description of the same relation, but considering different frames of reference. All these different elastic models are tested through the application of different mechanical loads.

Second, this 4D approach enables to obtain a variational form for these constitutive relations. This formulation enables to propose interesting hypo-elastic models and new constitutive models. Thus, it has been applied to structure calculations in order to see the benefits of this approach. Calculations have been performed for different elementary loads linked to adapted geometries of the tested specimens.

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## Necessary and Sufficient Conditions for Strong Ellipticity of Special Classes of Compressible Nonlinearly Elastic Materials

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In the framework of the nonlinear theory of elasticity, the strong ellipticity condition plays an important role in a number of problems of mechanical interest. For instance, the modelling of deformation fields with discontinuous gradients for solids undergoing phase transformations necessarily requires the loss of strong ellipticity for the elasticity tensor (see, e.g., [1]). Furthermore, when studying bifurcation problems within the theory of elliptic systems, the fulfilment of the strong ellipticity is an essential condition if one attempts to show the existence of branches of diffuse bifurcating modes (see, e.g., [2]).

Here, starting from a general result by Rosakis [3] based on a direction-dependent decomposition of the deformation gradient, we determine necessary and sufficient conditions for the strong ellipticity of some widely used constitutive models for compressible isotropic nonlinearly elastic materials, namely the generalized Blatz-Ko [4] and the Levinson-Burgess [5] materials. These models share a similar structure of the strain energy function; furthermore, they are characterized by the same material moduli: the referential shear modulus  $\mu$ , the referential Poisson's ratio  $\nu$ , and a modulus  $\alpha$ , which is usually related to the volume fraction of voids when dealing with foam-rubbers. The above underlined common structure allows us an unified approach to the analysis of the strong ellipticity condition.

As a main result, for the above classes of materials we find necessary and sufficient conditions for strong ellipticity at a given deformation, which hold regardless of the choices either of the referential shear modulus  $\mu$  or the modulus  $\alpha$ . Consequently, the fulfilment of such conditions determines restrictions only on the value of the referential Poisson's ratio  $\nu$ , which depend on the relative amount of the principal stretches.

Finally, we discuss the implications of our results for a variety of mechanical problems where the above constitutive models are usually employed.

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## Session 4

# Viscoplasticity



## A Finite Element Simulation on Effect of Intermediate Configuration in Multiplicative Decomposition of Deformation Gradient for Single Crystal TRIP Steel

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Strain-induced martensitic transformation occurs inside steel with metastable austenitic phase when the steel undergoes plastic deformation. The steel manifests excellent mechanical properties such as not only strength because of the generation of harder phase but also high ductility and toughness due to this transformation. A phenomenon with the high performances by the transformation is called Transformation-induced Plasticity (TRIP), and the steel with TRIP is called TRIP steel.

Generally, since the martensitic phase transforms obeying crystallographic orientation relationship between the phases, the theory with martensitic transformation in the length scale of single crystal should be considered to estimate and predict the transformation behavior.

Levitas[1] defined the configuration in multiplicative decomposition of deformation gradient based on an idea martensitic transformation promotes the plastic deformation surrounding the nuclei of martensite from the thermodynamic point of view. Obeying Levitas[1], Iwamoto and Tsuta[2] established the model including the martensitic variant into crystal plasticity theory. They introduced the model into FEM and the FE simulation is performed under a symmetric periodic boundary condition. Tjahjanto et al. [3] proposed the crystal plasticity model considering the martensitic transformation at different intermediate configuration for multi-phase TRIP assisted steel as similar to the proposition by Iwamoto and Tsuta [2]. As above-mentioned, several models have been proposed under a framework of crystal plasticity including phase transformation, however, the comparison of these models is not carried out and it is necessary to confirm the validity of the model.

Here, the constitutive models for single crystal TRIP steel with different intermediate configurations by martensitic transformation are derived based on the multiplicative decomposition of deformation gradient due to elasticity, plasticity and phase transformation. The FE simulation is performed by introducing the constitutive models under periodic boundary condition in 2D space. Finally, the effect of a configuration in the decomposition of deformation gradient on the deformation behaviour of single crystal TRIP steel is studied.

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## Analysis of a Superheater Component Made from Advanced Chromium Steel Under Temperature and Cyclic Load

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Advanced chromium steels are used in superheater components. Due to their application range up to 600<sup>0</sup>C and their excellent mechanical properties this steel is used for critical components and the failure of these components can have devastating consequences. Furthermore economical needs lead to more flexible operation programs, so that the components face more fatigue load because of start-up- and shut-down-processes. Finally, from the ecological point of view an increased efficiency reduces the CO<sub>2</sub>-emission but consequently an increase of efficiency implies higher mechanical and temperature load. Concluding from these demands and safety requirements it follows that a reliable material model is an essential part in the design process of superheaters.

To meet this challenge we follow the idea of fraction modeling by [1]. We utilize the idea to set up a continuum which consists of an inelastic hard and an inelastic soft fraction. The idea of this two fractions is based on the initial microstructure of the steel and the evolution of the microstructure. Regions of high dislocation density, subgrain boundaries, precipitates etc., restrain the movement of dislocations and can be therefore treated as inelastic hard regions. Because of the distribution in the volume and the evolution of the distribution, e.g. subgrain coarsening, the inelastic deformation will be non homogeneous. The macroscopic behavior with complex processes on the microscale can be described with the help of a fraction model. The advantages of this this approach was shown, for example, in [2, 3].

Therefore we calibrate and verify a fraction based material model with the help of experimental data for T91-steel from the literature. Finally we analyze a superheater component with the help of the material model and a realistic temperature load taken from a fluid-structure-interaction simulation.

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## Micromechanics of the deformation and failure kinetics of semicrystalline polymers

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The elasto-viscoplastic behaviour of semicrystalline polymeric materials is strongly dependent on the underlying microstructure consisting of both amorphous and crystalline domains. A micromechanically-based model for the constitutive behaviour of semicrystalline polymeric material based on layered two-phase inclusions has previously been developed [1, 4]. The present work is directed towards the prediction of the stress-dependence of the rate of plastic deformation, referred to as the yield kinetics, for semicrystalline polymers based on the underlying microstructure. A critical factor is the stress-dependence of the rate of plastic deformation, the slip kinetics, which is the mechanism underlying time-dependent, macroscopic failure. As a first step in achieving this goal, an Eyring flow rule is used for each slip system. In order to predict the response in both tension and compression, a non-Schmid effect (i.e. a dependence on the normal stress acting on the slip system) is included in the slip kinetics. The re-evaluation of the slip kinetics is performed using a combined numerical/experimental approach taking into account uniaxial compression and tension data of isotropic HDPE, for different strain rates and temperatures [2].

The mechanical response of extruded and drawn semicrystalline materials, in which a stacked lamellar morphology is commonly observed, depends on the direction of loading with respect to the direction of flow. Plastic deformation and failure are, therefore, both anisotropic. The predictive ability of the micromechanical model, including the characterization of the kinetics of crystallographic slip and amorphous yield based on isotropic material, is next evaluated for oriented high-density polyethylene [3]. The initial morphology of the material is generated based on pole figures from wide-angle X-ray diffraction experiments, which show a strong alignment of molecular chains with the drawing direction for specimens produced with a large draw ratio. Uniaxial loading of this aggregate shows the potential of oriented systems for unambiguously determining the yield kinetics of individual slip systems. In doing so, however, also the presence of a potentially oriented amorphous phase should be dealt with. Finally, the macroscopically anisotropic response of oriented polyethylene is described using an elasto-viscoplastic formulation, incorporating different physical sources of anisotropy.

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## A Multi-Mechanism Model for Cutting Simulations Combining Visco-plastic Asymmetry and Phase Transformation

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We develop a multi-mechanism model for strainrate- and temperature-dependent asymmetric plastic material behavior accompanied by phase transformations, which are important phenomena in steel production processes. To this end the well-known Johnson-Cook model is extended by the concept of weighting functions [1], and it is combined with a model of transformation-induced plasticity (TRIP) based on the Leblond's approach [2]. The bulk model is formulated within a thermodynamic framework at large strains, and it will be specialized and applied to cutting processes in steel production. In this prototype situation we have: Transformation of the martensitic initial state into austenite, then retransformation of martensite. For incorporation of visco-plastic asymmetry two variations of the classical Johnson-Cook model are presented: In "Model A" we introduced a rate dependent flow factor with a rate independent yield function. In "Model B" we introduce a rate independent flow factor with a rate dependent yield function. In the examples parameters are identified for the material DIN 100Cr6, and we illustrate the characteristic effects of our multi-mechanism model, such as strain softening due to temperature, rate dependence and temperature dependence as well as the SD-effect. A finite-element simulation illustrates the different mechanisms for a cutting process.

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## Flow Rules for Amorphous and Semi-crystalline polymers

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When polymers are subject to large deformations, molecular orientation ensures that they become anisotropic. Any constitutive model should reflect this. When plasticity is involved, this can be achieved by the use of an appropriate flow rule. Most commonly, flow rules used are isotropic, as exemplified in the Levy-Mises formulation. An alternative is Hill's flow rule [1] for anisotropic material. In a series of studies involving experiments on polymers in non-uniaxial states of strain [2-4], we have shown the necessity for an anisotropic flow rule for semi-crystalline polymers in both compression and tension and at both room temperature and forming temperatures. We have used Hill's formulation with the coefficients dependent on strain to reflect the evolution of anisotropy from an initially isotropic state. The strain dependence is in the form of a power law function of the principal extension ratios defined by the exponent  $m$

$$\begin{aligned}\mathbf{L}_1^p &= \dot{\mathbf{e}}_p \left[ (\lambda_3)^m (\sigma_1 - \sigma_2) + (\lambda_2)^m (\sigma_1 - \sigma_3) \right] / 3\tau \\ \mathbf{L}_2^p &= \dot{\mathbf{e}}_p \left[ (\lambda_1)^m (\sigma_2 - \sigma_3) + (\lambda_3)^m (\sigma_2 - \sigma_1) \right] / 3\tau \\ \mathbf{L}_3^p &= \dot{\mathbf{e}}_p \left[ (\lambda_2)^m (\sigma_3 - \sigma_1) + (\lambda_1)^m (\sigma_3 - \sigma_2) \right] / 3\tau\end{aligned}\quad (1)$$

in equation (1). Here the flow rule is defined along principal axes 1, 2 and 3.  $\mathbf{L}_1^p$ ,  $\mathbf{L}_2^p$  and  $\mathbf{L}_3^p$  are principal components of the plastic strain rate tensor and  $\dot{\mathbf{e}}_p$  is the scalar plastic strain rate as defined by an Eyring process.  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  are the principal stresses,  $\tau$  is a scalar driving shear stress and  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  are the principal extension ratios. When  $m = 0$ , equation (1) reduces to the Levy-Mises rule. In general,  $m$  is determined by experiment, for instance from the ratio of axial to transverse stress in a plane strain investigation.

Compressive plane strain experiments on ultra-high molecular weight polyethylene at room temperature showed that the Levy Mises flow rule gave qualitatively incorrect predictions of stress, but that satisfactory predictions were produced with  $m = 2.5$  [2]. In a very different context, large tensile deformations in sequential plane strain of polypropylene at 160°C were successfully modelled with  $m = 0.8$  [4]. To contrast with these results on semi-crystalline polymer we shall present some investigations of amorphous polymer.

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An example of the application of this approach will now be given (see [4]). Square specimens of polypropylene were stretched using a biaxial testing machine at 160°C, and strain rates of 2.2s<sup>-1</sup>, by first stretching along an axis parallel to the specimen side (the 1 axis) while restraining the specimen in the perpendicular 2 direction. Once an extension ratio of 3 had been achieved along 1, stretching was stopped and immediately commenced in the 2 direction, to achieve a final equibiaxial state (Figure 1). This strain history is a severe test of the constitutive model and of practical significance in stretch blow-moulding.

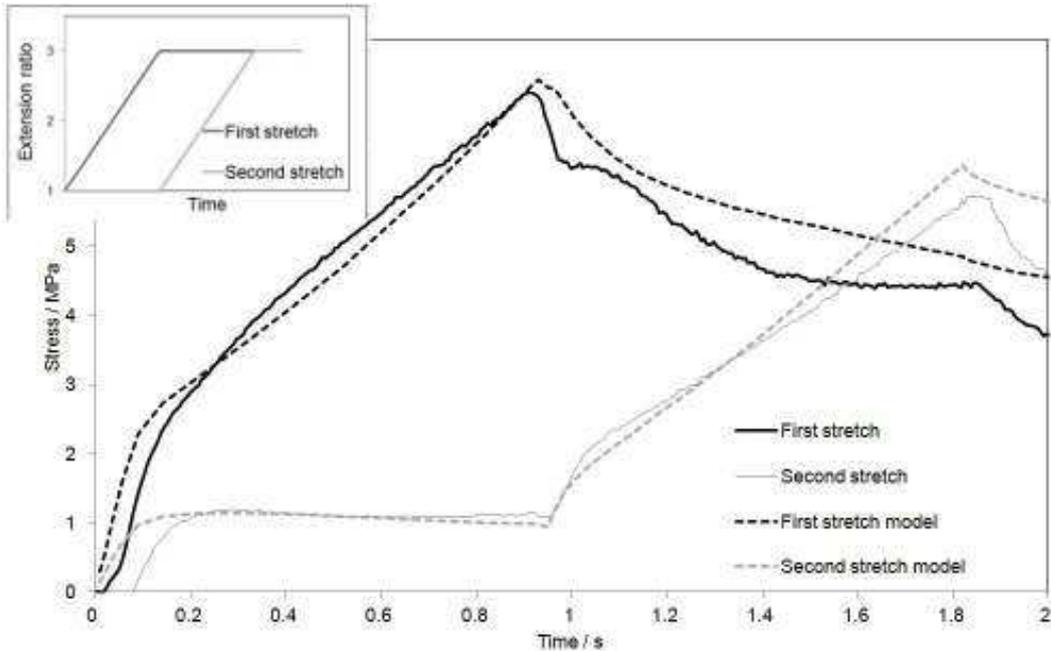
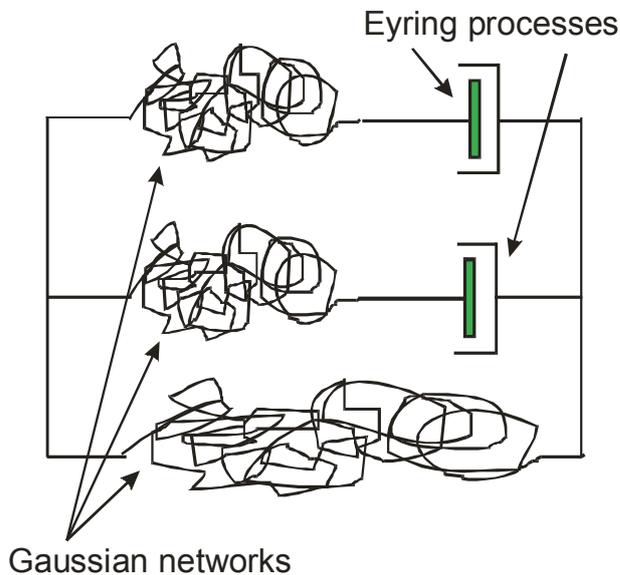


Figure 1 Strain history and short-term response.



The constitutive model is illustrated diagrammatically in Figure 2. The dashpots are Eyring processes subject to the flow rule of equation (1) and the networks are Gaussian. The predictions of the model are shown in Figure 1. The predicted ratio of transverse to axial stress is much lower than would be achievable using the Levy Mises flow rule, and the experimental results are modelled well. The model ran to longer times to give good predictions of stress relaxation to times of 120s.

Figure 2 Constitutive model.

## Formulation a thermomechanical internal state variable constitutive model for elastomers

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Elastomeric materials are widely used in engineering assembly due to their mechanical properties (such as large elongation and energy absorption). Thus the demand for accurate and reliable numerical simulations that adequately represent the time, temperature, and stress state dependent material behavior of elastomers is of prime importance in the development/design of structural components. A large number of constitutive models have been developed to predict the mechanical response of elastomers ([1-5] among others).

In this work, we propose a thermomechanical constitutive model accounting for the time, temperature, and stress state dependent material behavior of elastomers. The formulation follows current internal state variable methodologies and departs from the spring-dashpot representation generally used to characterize the mechanical behavior of elastomers. The model equations were developed within a large deformation kinematics and thermodynamics framework proposed by Coleman and Gurtin [6] in which physically-based ISVs were selected to accurately represent the underlying physics of the elastomer deformation process. The three dimensional equations were then reduced to the one-dimensional case to quantify the material parameters from monotonic compression test data at different applied strain rates and temperatures.

Experimental tests that include compression, tensile, shear, relaxation, and high strain rate loading at different temperatures and strain rates were performed on three different types of commercially available rubbers and elastomers; natural rubber (NR), santoprene, and styrene butadiene rubber (SBR). The model prediction was then compared to the available experimental tests data.

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## Homogenized Elastic-Viscoplastic Behavior of Open Porous Bodies with Two Pore Pressures

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We investigate the homogenized elastic-viscoplastic behavior of anisotropic open-porous bodies with two pore pressures,  $p_1$  and  $p_2$ , as an extension of Ref. [1]. It is assumed that the open-porous bodies considered are periodic and made of metallic materials. Hill's macro-homogeneity condition [2] is then used to show three special cases in which one of  $p_1$ ,  $p_2$  and  $p_m$  entirely affects the homogenized viscoplastic behavior in steady states. Here  $p_m$  indicates the mean of  $p_1$  and  $p_2$ . To verify this finding, we perform finite element homogenization analysis of an ultrafine plate-fin structure with  $p_1$  and  $p_2$ , for which two base metals with different strain-rate sensitivities are considered. It is thus demonstrated that the three special cases typically occur under uniaxial tension and compression in the stacking direction. It is further shown that a macroscopic viscoplastic equation simulates well the homogenized stress-strain relations attained in the homogenization analysis if  $p_1$ ,  $p_2$  or  $p_m$  enters for Terzaghi's effective stress in the macroscopic equation.

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## Plastic Instability Analysis under Biaxial Stress Using Rate Dependent Constitutive Model

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In this study, the adequacy of plastic instability analysis under biaxial stress state with the Marciniak and Kuczyński (M-K) type approach [1] is investigated. Prediction of the ductile fracture of materials is a very important issue in structural engineering as well as in the metal forming field. In sheet materials, it occurs in the form of narrow zones with significant reduction of the thickness, which is often modelled as sheet necking under the assumption of plane stress. As for rate dependent materials, an imperfection analysis can be utilized for predicting the onset of plastic instability when the bifurcation analysis cannot be adopted because it provides unrealistic solution [2]. To predict the formability of ductile sheet materials, the M-K type approach, which is a kind of imperfection analysis, has been extensively employed. The M-K type approach is considered to be one of the most influential contributions of flow localization analysis to the practical metal-forming field. An important advantage of M-K approach in the plastic instability analysis is the computational cost. Only two material points are required to detect the onset of localization. When the necking analysis of sheet specimen is considered as the general full boundary value problem, a numerical method such as the finite element method should be introduced, and it generally requires a huge number of material points. Therefore, the M-K type approach is quite practical and useful way to predict the formability of sheet materials.

In the M-K formulation, it is assumed that a sheet specimen includes a band with an initial inhomogeneity. An essential question of the M-K type approach is if this assumption is adequate because practical materials do not seem to include band-shaped inhomogeneity. To validate the assumption, finite element analyses of sheet which is subjected to biaxial loading of arbitrary strain ratio is conducted. An elasto-visco-plastic model, which is a rate dependent constitutive model, is adopted. The loadings along to two perpendicular directions have to be independently controlled so that the ratio of strains could be kept constant, and a novel arc-length method with two different loading modes is introduced. The finite element analyses up to post-necking stage under biaxial stress are conducted. After the necking occurs, the deformation mode depends on the strain ratio, and it is revealed that the deformation mode in the post-necking stage corresponds to the initial imperfection of M-K type approach.

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## **A new anisotropic model of coupled damage-viscoplasticity – application in electromagnetic forming processes**

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In this paper, we investigate the finite element modelling of the process of quasi-static deep drawing-electromagnetic forming by means of a new coupled damage-viscoplasticity model for large deformations. For this purpose, a recently proposed finite strain anisotropic viscoplastic model, taking combined nonlinear kinematic and isotropic hardening into account, is coupled with ductile damage in the context of continuum damage mechanics. The coupling of damage and plasticity is carried out in a constitutive manner according to the effective stress concept. The damage part is formulated anisotropically using a second order internal variable. A basis for the present material modelling is the concept presented in [1].

In the numerical examples we investigate the potential of the constitutive framework regarding the prediction of forming limits. In particular, the coupled material model is applied to the combined quasistatic-electromagnetic simulation of the cross-shaped cup deep drawing process. For this purpose, the evolution equations for the internal variables of the constitutive model are numerically integrated in an explicit manner and the model is then implemented as a user material subroutine into the finite element package LS-Dyna.

An additional aspect is here the consideration of the process at two different scales. Whereas the above described model represents the macro scale, another aim is to include the microstructure by means of Crystal Plasticity FEM [2]. Defects at the microstructure are modelled by means of cohesive zone finite elements. The overall goal of the research is use the micro model to better understand what happens in the microstructure and to finally improve the macro model for the process simulation.

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## Simulation of Portevin - Le Chatelier effect under cyclic loading

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The Portevin Le Chatelier effect is generally evidenced by the apparition of serrated yielding under monotonic tension loading conditions. It appears at room temperature in some aluminum alloys, around 250C in some steels and in many other metallic materials. This effect is associated with the propagation of bands of plastic deformation in tensile specimens and can in some case leads to unexpected failures. The Portevin Le Chatelier effect has been widely simulated under monotonic condition using finite elements [4] and an appropriate mechanical model able to reproduce serrations and strain localization [2, 3]. The apparition of serrations can be predicted by using an analytical stability analysis [4].

Recently, this serrated yielding has also been observed in specimens made of Cobalt based superalloy under cyclic loading, after a large number of cycles [1]. The mechanical model has then been identified in this case to accurately reproduce this critical number of cycle where serrations appear. The associated apparition of localized bands of deformation in specimens has also been investigated using finite element simulations. Finally these simulations have been compared with an equivalent model without localization in order to compare the local stress values and propose some conclusions on the influence of the Portevin Le Chatelier effect on the life length of components under fatigue conditions.

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## Constitutive relations and evolutive laws in non-smooth elasto/viscoplasticity

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In elastoplasticity constitutive laws are governed by monotone multivalued operators. In their general form yield functions are convex and non-differentiable. In order to derive general elastoplastic constitutive relations among state and associated variables in this paper it is discussed that the appropriate mathematical tools are those of convex analysis and subdifferential calculus which are capable to handle non-differentiable convex functions, see e.g. Hiriart-Urruty and Lemarechal [1], Rockafellar [2] and Moreau [3]. General elastoplastic constitutive relations and plasticity laws are derived within the mentioned theoretical framework. It is then presented a general formulation of the viscoplastic flow rule. The formulation is expressed in subdifferential form and it holds for general non-smooth viscoplasticity. Different generalized forms of plasticity laws are presented within the proposed mathematical treatment. Equivalent generalized forms of the evolutive laws and of the loading/unloading conditions are provided and the equivalence of these forms to the classical well-known expressions is illustrated. The interpretation of the rate dependent phenomenon as a penalty regularization of the rate independent one is then revisited. Non-smooth elasto/viscoplastic models may be interpreted, see e.g. Simo Kennedy and Govindjee [4], by means of regularization techniques, see e.g. Luenberger [5]. Within this context it is then showed how the presented general constitutive viscoplastic relation may be obtained by the optimality condition of a suitably regularized functional representing the viscoplastic dissipation. Finally, connections and relations are described between the general elastoplastic model problem and the general elasto/viscoplastic model problem in such a way that the general treatment is presented in a unitary framework. The presented generalized treatment proves to be well-suited for the appropriate development of variational formulations for structural problems in elastoplasticity and elasto/viscoplasticity.

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## Elastic-Viscoplastic Modelling of Woven Composites Using a Multi-Scale Approach

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In this study, a multi-scale elastic-viscoplastic modelling for woven composite laminates is conducted based on a homogenization theory. For this, a three-scale model of a woven composite laminate is constructed by considering the laminate as a macro structure, fibre bundles and a matrix material in the laminate as a meso structure, and fibres and a matrix material in the fibre bundles as a micro structure. Then, an elastic-viscoplastic constitutive equation of the woven composite laminate is derived by dually applying the homogenization theory for nonlinear time-dependent composites [1] to not only the micro and meso scales, but also the meso and macro scales. To verify the present method, the elastic-viscoplastic behaviour of a plain-woven GFRP laminate with fibre bundles consisting of glass fibres and an epoxy matrix is analyzed. It is shown that the present method is successful in analyzing the strong elastic-viscoplastic in-plane anisotropy of the plain-woven GFRP laminate. Also the method is successful in taking into account the effects of viscoplasticity of the epoxy matrix in fibre bundles on the elastic-viscoplastic behaviour of the plain-woven GFRP laminate.

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## Experimental Studies and Numerical Predictions of Recrystallisation-Assisted Viscoplastic Strain Under Low Stresses After Hot Deformation

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Static and meta-dynamic recrystallisation are known to take place during thermo-mechanical processing, such as the low stress deformation that metallic strips undergo between rolling stages of a hot strip finishing mill [1]. Experimentally, increases in strain rate were recently observed during recrystallisation and corresponding extra viscoplastic deformation is referred to Recrystallisation Induced Plasticity [2]. This work is aimed at understanding the interactions between recrystallisation and viscoplastic deformation when an austenitic alloy (Fe36%Ni) is subjected to low stress levels immediately after hot work.

Recrystallisation kinetics of this alloy was quantified from stress relaxation tests over the 850-1050°C temperature range after pre-straining cylindrical samples to 22-30% in compression at rates ranging from 0.01 to 0.44s<sup>-1</sup>. These results were consistent with those obtained in the double-hit compression and interrupted annealing tests also carried out as part of this work.

One of the original aspects of this work is that the acceleration of the viscoplastic deformation which occurs during recrystallisation immediately after hot work has been quantified for the first time. In particular, the contribution of primary creep to this deformation has been ascertained through creep tests on fully annealed materials under the above testing conditions. The effects of temperature and applied stress on the strain rates and the corresponding microstructural characteristics have been investigated to develop an understanding of the flow mechanisms behind recrystallisation-assisted viscoplasticity.

A novel physically-based constitutive material framework has been developed to predict viscoplastic deformation which accompanies recrystallisation. In this framework, the material is supposed to be composed of two pseudo-phases during recrystallisation: recrystallized and deformed regions. The volume fraction of the recrystallized regions is described using a JMAK relation, which gives good agreement with experimental measurements. A primary creep model is also defined to predict the flow behaviour of both “phases”, having different dislocation densities under both applied and internal stresses. It is shown that this framework is capable of predicting accurately the microstructural evolution and the corresponding viscoplastic deformation during recrystallisation.

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## Stress evaluation during the continuous casting of steel using Viscoplastic model

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Continuous casting process is a technique for the production of steel billets and ingots. The temperature profiles and the stress evolution during the entire process is simulated in this work. A model describing the heat transfer, solidification and the resulting thermal stresses in a solidifying slice is presented. The model simulates a 2D transverse slice of the shell in generalized plane strain as it moves down at the casting speed. The boundary conditions depending on the time and position are imposed on the slice. The model first solves the transient energy balance to obtain the temperature distribution. The known local cooling profiles at each time of the slice are used as boundary conditions for the heat transfer equation. The obtained temperature distribution in the slice at each time is used to calculate the thermal stresses in the solidified steel shell.

Functions depending on temperature and composition are employed for properties such as thermal conductivity, specific heat, thermal expansion and Elastic modulus [2]. A rate dependent viscoplastic model proposed by Anand is used to represent the constitutive behavior of the solidified steel [1]. The effect of liquid pressure at the solid-liquid interface is converted as equivalent nodal force. Generalized plane strain conditions are applied in the casting direction which accounts for the axial strains and strains due to bending and straightening of the shell. The risk of transverse cracking during the bending and straightening of the shell is studied. The model can be effectively used to investigate the issues like mold taper optimization, minimum shell thickness to avoid the breakouts, hot and cold cracks caused by the thermal stresses.

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## Viscoplastic behaviour of Ti-6Al-4V involving phase transformation

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The life prediction of components built by additive manufacturing process, such as Direct Metal Deposition (DMD), implies to know properly their physical states (including metallurgy, residual stresses,...). A robust finite element analysis of the DMD process at a macroscopic scale should then include thermal, metallurgical and mechanical aspects. The present paper shows a comprehensive model, where the metallurgical section is developed in strong connection with the physical process, and the mechanical section introduces a multiscale approach of the cyclic anisothermal behaviour.

In order to reduce the computation time, but preserving the most important physical phenomena, only the relevant interactions are introduced in the model. The latent heat of fusion, the stress induced phase transformations and the heat originating from the viscoplastic dissipation are ignored. This allows us to use a sequential algorithm, where the three models (thermal, metallurgical and mechanical) are weakly coupled and are executed sequentially. Since the microstructural evolutions and the mechanical loading are both generated by the thermal field, the results obtained with this first model are critical. The main assumptions and the results of this computation step were described in a previous paper [1].

The material microstructure is CC- $\beta$  at high temperature, and HCP- $\alpha$  after cooling. The phase transformation is also influenced by the diffusion of vanadium, which is in the solid solution at high temperature, and but not at room temperature. The metallurgical model introduces then as critical variables the volume fraction of  $\alpha$  and  $\beta$ , but also the volume fraction of vanadium in each phase. The evolutions are functions of the thermal history. The equations of the model are derived by solving a diffusion problem at the interface, and using the phase diagrams from the literature.

The mechanical model introduces a different behaviour for each phase, and a scale transition model to link the macroscopic stress and strain fields to the local fields in each phase. The instantaneous behaviour will then derive from the temperature history and from the actual phase volume fraction. The model is implemented in the Finite Element Code Z-Set. A specific strategy is introduced to progressively activate the elements and follow a given fabrication route. The main results of the numerical procedure are the phase distribution, the grain morphology, the residual strain and stress fields.

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## Simulation of viscoplastic material behavior of cast aluminium alloys due to thermal-mechanical loading

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Efficiency increases of combustion engines in automotive development are directly related to higher operating temperatures. Concerning the development of new lightweight alloys detailed information concerning the specific material behavior at elevated temperatures is essential for the design and lifetimes under service conditions. Especially the superposition of complex thermal and mechanical loading occurring mainly in the start and shut-down cycle is considered as the major damaging loading condition. Generally, this thermal-mechanical fatigue behavior (TMF) is characterized by highly complex laboratory experiments.

In this paper the thermal-mechanical deformation behavior of the Aluminium alloy AlSi7Mg is calculated on the basis of a viscoplastic Chaboche-model - with respect to elastic properties, nonlinear isotropic and kinematic hardening and time-dependent material behavior [1, 2]. The experimental analysis of the relevant material parameters (i.e. influences as strain rates, strain amplitudes and viscoplastic relaxation behavior) is performed by isothermal complex low-cycle fatigue testing (CLCF) at specific temperatures.

All material parameters are identified from the measured isothermal CLCF data by computational optimization using a deterministic optimization technique (Levenberg-Marquardt algorithm) [3]. Thus, the temperature dependence of each parameter is obtained. As a result isothermal and thermal-mechanical fatigue under various operating conditions can be predicted. Finally, the accuracy of the model is verified by corresponding experimental TMF testing.

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Session 5

Plasticity



## Multiscale constitutive model of discontinuous plastic flow (DPF) at cryogenic temperatures

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FCC metals and alloys are extensively used in cryogenic applications down to the temperature of absolute zero, because of favourable physical and mechanical properties, including high level ductility. Many of these materials undergo at low temperatures the phenomenon called Discontinuous Plastic Flow (DPF, serrated yielding). The mechanism of DPF is related to formation of dislocation pile-ups at strong obstacles, such as the Lomer–Cottrell (L-C) locks, during the strain hardening process. The back stresses of the piled-up groups block the motion of newly created dislocations. The local shear stress at the head of dislocation pile-up, proportional to the number of dislocations in the pile-up, reaches the level of cohesive strength and the L-C lock collapses by becoming a glissile dislocation. This process takes place below specific temperature ( $T_0$  or  $T_1$ ), where the dislocations have predominant edge character and cannot leave the pile-ups by cross-slip. Such a local catastrophic event can trigger similar effects in the other groups of dislocations. Thus, the final result is massive and has collective character. The physically based, multiscale, 3D constitutive model forms a generalization of the previous uniaxial model [1] that proved efficient in describing the DPF. The model takes into account thermodynamic background, including the phonon mechanism of heat transport and thermodynamic instability caused by specific heat vanishing with the temperature approaching absolute zero. The main function that reflects the readiness of lattice with respect to DPF is the density  $B$  of the dislocation groups (located at the L-C locks). Evolution of dislocations density as a function of deformation at the temperature  $T$  is described by equation containing creation and annihilation terms. The average shear stress in the lattice and the shear stress at the head of dislocation pile-up are computed and constitute, together with  $B$ , the serration criterion. The initial stages of the process reflect the elastic-plastic loading under nearly isothermal conditions. Under these circumstances (low thermal activation) the rate-independent plasticity can be applied. Thus, the yield surface has the standard form expressed by the stress intensity with mixed kinematic/isotropic hardening included. It is assumed that the continuum containing L-C locks obeys the associated flow rule. It is postulated in the present model that in every serration cycle the parameter  $B$  is accumulated de novo from 0, as soon as the DPF is triggered. The fluctuations of temperature corresponding to plastic power dissipated in the course of DPF are computed in the framework of thermo-mechanical coupling. The DPF associated with the proportional and the non-proportional loading paths is studied. Identification of parameters of the constitutive model is based on the experimental data collected during several campaigns of tensile tests carried out on copper and stainless steel samples immersed in liquid helium (4.5 K).

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## A FFT-based approach for solving elastic fields of continuum dislocation mechanics

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In this contribution, a FFT-based approach is developed to solve the static field equations of continuum dislocation mechanics (the so-called Field Dislocation Mechanics theory [1]). Given a spatial distribution of the Nye's dislocation density tensor, the compatible and incompatible elastic distortions are calculated by solving field equations in the Fourier Space using the FFT algorithm. Then, the internal stresses and elastic (lattice) rotations are obtained using inverse FFT for different spatial dislocation density distributions and different material elastic properties. It is also shown that the present approach extends the FFT algorithm introduced in [2] to heterogeneous elastic materials containing lattice incompatibilities due to dislocations. As applications, 2D and 3D FFT grids are used to compute the stress field of single dislocations, dislocation ensembles, dislocation-based fracture densities, assuming isotropic elasticity or anisotropic elasticity within the material. Some comparisons with analytical solutions using Riemann-Graves integral operator for screw dislocations [1] or with finite element approximations [3] are performed to validate the present FFT-based approximation.

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## Modelling martensitic transformation induced by plastic strain: analysis of free energy function

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Mechanically induced martensitic transformation may occur at temperatures higher than the start temperature of spontaneous transformation caused by the temperature variation. Certain types of austenitic steels, called metastable ones, such as high manganese or high nickel steels undergo such transformation. The martensitic transformation affects mechanical properties of austenite structure by increasing the hardening rate and the form of hysteresis loops, generated in the cyclic loading process. Phenomenological constitutive equations for austenitic steel are formulated within the framework of irreversible thermodynamics expressed in terms of internal state variables. The two-phase material is treated as a thermodynamical system in which two irreversible processes occur, that is plastic deformation and phase transformation. The plastic deformation is coupled with the martensite growth which causes an additional plastic deformation (TRIP). The plastic deformation is specified by the associated flow rule and the yield condition dependent on the stress and the back stress which is decomposed into the back stress associated with plastic deformation and the back stress associated with the martensite transformation [1]. The yield condition is assumed in the form:

$$F_{pl} = \sqrt{\frac{3}{2}(s_{ij} - (1 + a(\xi)X^2)X_{ij})(s_{ij} - (1 + a(\xi)X^2)X_{ij})} - R_p \leq 0 \quad (1)$$

where  $X^2 = X_{mn}X_{mn}$ , and  $a(\xi)$  is the monotonically increasing and bounded function of martensite fraction  $\xi$ . Additionally, the transformation condition is formulated in the form:

$$F_{tr} = \beta\sqrt{3J_2} \left( 1 + \nu \frac{J_3}{(3J_2)^{\frac{3}{2}}} \right) + \omega I_1 - \Sigma - R_{tr}(\xi) \leq 0 \quad (2)$$

where  $J_2 = \frac{1}{2}(\mathbf{s} - \tilde{\mathbf{Z}}):(\mathbf{s} - \tilde{\mathbf{Z}})$ ,  $J_3 = \det(\mathbf{s} - \tilde{\mathbf{Z}})$  and  $I_1 = \sigma_{kk} - Z_m$ . Here  $\tilde{\mathbf{Z}}$  is the deviator of back stress in the transformation condition. The specific free energy for isothermal process is assumed in the form:

$$\Psi = \frac{1}{2}\Lambda_{ijkl}\varepsilon_{ij}^e\varepsilon_{kl}^e - \gamma\varepsilon_m^e\theta + \rho c_\varepsilon \left( (\theta - \theta_o) - \ln\left(\frac{\theta}{\theta_o}\right) \right) + \frac{1}{2}C_1(\xi)\eta_{ij}\eta_{ij} + \frac{1}{2}C_2z_{ij}z_{ij} + \rho\varphi_{ch,m} - \rho\Delta\varphi_{ch}(1 - \xi_\sigma) + \rho\Psi_{ir} \quad (3)$$

where  $\Psi_{ir}$  is energy of interaction between austenite and martensite [2],  $\Delta\varphi_{ch} = \varphi_{ch,m} - \varphi_{ch,a}$  is the difference between chemical energy of austenite and chemical energy of martensite and  $\varepsilon_m^e$  is the volumetric strain. The presented model is applied to simulate combined cyclic tension and torsion test with account for martensitic transformation.

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## Sensibility evaluation of rolling with anisotropy

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The present work is devoted to the application of anisotropic plastic models to the analysis of the rolling process. Many models have been developed in recent years for large strain plasticity in connection with metal forming and in particular deep-drawing: anisotropic plasticity with isotropic hardening, Hill's, associated or non-associated. After a brief presentation of these models, their application to the standard rolling model (one dimensional method, Karman equation[1]) is developed; the solution is obtained by determination of the neutral point through a shooting method. These models are then exemplified by a parametric analysis of the influence of the constitutive parameters on the response and a comparison for a given material of different models as identified.

In the rolling process, a very large deformations (>90%) is noticed. Model development requires the use of large deformation formalism which is largely used and applied. However, if the rotation of the principal axes is low and the use of the logarithmic strain tensor (Hencky tensor), a small deformation formalism remains valid without substantial errors [2].

The behavior is defined by the following laws:  $\dot{\epsilon}_{ij}^p = 0$  if  $f(\sigma_{ij}) - Y(p) < 0$  and  $\dot{\epsilon}_{ij} = \lambda \frac{\partial g}{\partial \sigma_{ij}}$

if  $f(\sigma_{ij}, Y) = f(\sigma_{ij}) - Y = 0$ , where  $f(\sigma_{ij})$  is a threshold function.  $g(\sigma_{ij})$  is the plastic potential, ( $f(\sigma_{ij}) = g(\sigma_{ij})$  in associated plasticity), and  $Y(p)$  is the hardening law. In the anisotropic case a quadratic criterion is usually used by the equivalent stresses.

$$\hat{\sigma} = \sqrt{H_{ijkl} \sigma_{kl} \sigma_{ij}} = \sqrt{F(\sigma_2 - \sigma_3) + G(\sigma_3 - \sigma_1)^2 + H(\sigma_1 - \sigma_2)^2}. \text{ Posing } G + H = 1, \text{ we obtain}$$

$$r_1 = \frac{H}{G} \text{ and } r_2 = \frac{H}{F} \text{ so } \hat{\sigma} = \frac{1}{\sqrt{1+r_1}} \sqrt{\frac{r_1}{r_2}(\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 + r_1(\sigma_1 - \sigma_2)^2}$$

The cumulative equivalent strain  $\hat{\epsilon}$ ,  $\hat{\epsilon} = \sqrt{h_{ijkl} \epsilon_{kl} \epsilon_{ij}}$ . In this case the variable of hardening is defined by  $\dot{p} = \lambda$ ,

$$\dot{p} = \frac{\sqrt{\bar{r}_2 + \bar{r}_2 \bar{r}_1}}{\bar{r}_2 \bar{r}_1 + \bar{r}_2^2 \bar{r}_1 + \bar{r}_2 \bar{r}_1^2} \sqrt{(\bar{r}_2 \bar{r}_1^2 \dot{\epsilon}_3 - \bar{r}_2 \bar{r}_1 \dot{\epsilon}_2)^2 + (\bar{r}_2 \bar{r}_1 \dot{\epsilon}_1 - \bar{r}_2^2 \bar{r}_1 \dot{\epsilon}_3)^2 + (\bar{r}_2^2 \bar{r}_1 \dot{\epsilon}_2 - \bar{r}_2 \bar{r}_1^2 \dot{\epsilon}_1)^2}$$

The hardening law used is that of Swift  $Y(p) = K(\epsilon_0 + p)^n$ .

The results of the parametric analysis show the requirement to take into account the anisotropy during rolling. The implementation of the outcomes identified experimentally by A Khalfalla [3] allows to draw some useful conclusions for better control of rolling. It has been confirmed the need to move to non-associated plasticity when the sheets are highly anisotropic.

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## **A Continuum Formulation of Stress Correlations of Dislocations in Two Dimensions**

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The Continuum Dislocation Dynamics theory (CDD) of crystal plasticity, utilizing a second-order dislocation density tensor, is a powerful tool in understanding and modeling the dynamic behavior of dislocations on microscopic scales. Using this model and an integrated, lower dimensional version, a number of benchmark systems have been previously tested, including the one dimensional dislocation pileup and simple torsion. All show excellent agreement with both analytic results, where available, as well as discrete simulations.

While accurate solutions have been found for effectively one dimensional systems, fully two- and three-dimensional systems increase the complexity of the system. In order for the behavior of the continuum density to be accurately predicted, it must be properly understood as an ensemble average over discrete distributions.

In this work, an overview of the CDD method as well as the simplified, integrated form is presented, along with an overview of one-dimensional results compared with both analytic solutions and discrete simulation. Then, the results from CDD for both a fully two-dimensional glide plane and for a distribution of one-dimensional glide planes in a two-dimensional elastic medium is presented. Using comparisons with Discrete Dislocation Dynamics (DDD) in a few simple systems, the multi-component stress field which must be considered for dislocation density motion is derived and demonstrated.

## Thermodynamic consistent modelling of polymer curing coupled to visco-elasticity at large strains

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Our paper concentrates on the development of a macroscopic constitutive model for temperature-dependent visco-elastic effects accompanied by curing of polymeric matrix material, which are important phenomena in production processes. Within a thermodynamic framework we use an additive ternary decomposition of the logarithmic Hencky strain tensor into mechanical, thermal and chemical parts. Based on the concept of stoichiometric mass fractions for resin, curing agent and solidified material the bulk compression modulus as well as the bulk heat- and shrinking dilatation coefficients are derived and compared with ad hoc assumptions from the literature [1,2]. Moreover, we use the amount of heat generated during dynamic scanning until completion of the chemical reactions, to define the chemical energy. As a major result, the resulting latent heat of curing occurring in the heat-conduction equation derived in our approach reveals an ad hoc approach from the literature as a special case. In addition, thermodynamic consistency of the model will be proved, and the numerical implementation of the constitutive equations into a finite-element program is described. In the examples we illustrate the characteristic behaviour of the model, such as shrinking due to curing and temperature dependence [3] and simulate the deep drawing of a spherical part with the finite-element-method.

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## Finite Element Analysis of the Contact Behavior of Rough Surface

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The study of the contact between rough surfaces is of essential significance in many fields (e.g. electrical resistance of contacts). Theoretical approaches analyzing surface contact suffer from limitations, especially for irregular geometries and large deformation with plastic flow. Finite element calculations are attractive for modeling inelastic contact with complex geometries [5]. An experimentally scanned surface measured by a laser profilometer [3] or atomic force microscopy can be used as input to create rough surface, and studied via finite element analysis [1, 4, 6].

In order to analyze the indentation of a rough surface by a rigid spherical indenter, a three-dimensional finite element model is created using the finite element code Z-set. Elastic-plastic materials with different strain-hardening laws (e.g. linear or exponential) are used to investigate effects of material behaviors. Both loading and unloading processes are considered. The contact is normal and frictionless. Parametric studies are carried out to explore effects of material properties (e.g. yield stress, tangent modulus) on the contact responses (e.g. contact area) of rough surfaces. Effect of surface roughness on measurement of effective elastic modulus from the initial unloading of the load-displacement curve is discussed. The simulation results are compared to experimental measurements (e.g. contact area, load-displacement curves).

The numerical computation based on material's elastoplastic constitutive equations is computationally expensive. A hybrid scheme allows direct simulation of the behavior of realistic surfaces at low computational cost [2]. The reduced model [7] based on the contact of one asperity, whose constitutive equations are expressed by load/displacement and contact area/displacement responses, and on the detection technique to locate and characterize asperities, is investigated. The interaction between neighbouring asperities is considered.

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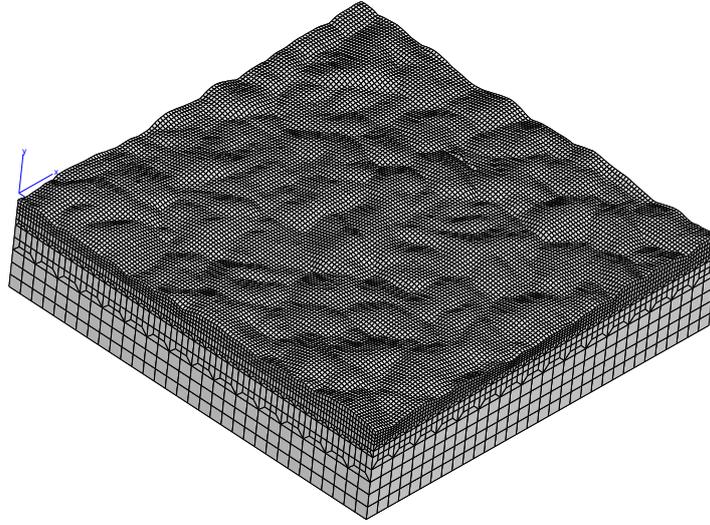


Figure 1: A finite element model with rough surface.

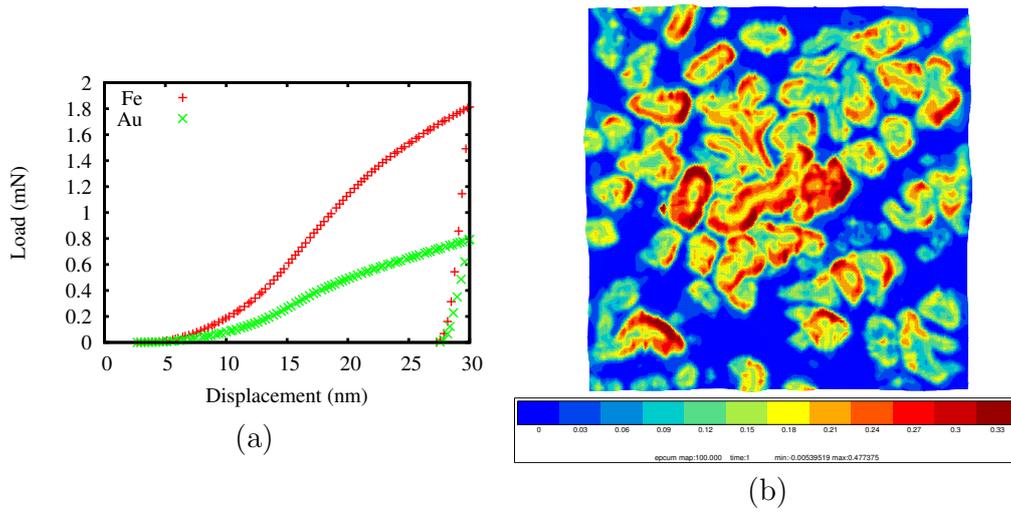


Figure 2: Figures showing (a) indentation load-displacement curves; (b) distribution of the equivalent plastic strain due to contact load (material Au).

## Thermal-Mechanical Modeling of Single Crystal GaN and AlN

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The III-nitrides, such as GaN and AlN, possess some excellent properties including direct energy-band gaps, stability to high temperatures, high thermal conductivity, and low electrical resistivity, making them valuable for the fabrication of high power transistors and optical devices, such as light emitting diodes (LEDs) and laser diodes [2, 3]. However, the cost of these substrate materials remains high as the crystal growth yield and quality is adversely affected by thermal and lattice mismatch stress induced cracks and dislocation defects formed during the manufacturing process. While substantial effort has been devoted to studying the opto-electronic properties of these materials, the thermal-mechanical behavior, especially at high growth temperatures, is not as well understood.

In order to predict cracking and dislocation defect formation, accurate thermal-mechanical models of the material behavior must be used in process modeling. GaN and AlN single crystals have a wurtzite structure (hexagonal). In this work, we develop a thermal-elastic-plastic constitutive model for single crystal GaN and AlN based on underlying mechanisms of dislocation motion, multiplication and interactions. The model is an extension of a model originally developed by Alexander and Haasen [1] for single slip in silicon. The relevant slip systems in AlN and GaN are the basal ( $\langle 11\bar{2}0 \rangle$  (0001)) and prismatic ( $\langle 11\bar{2}0 \rangle$   $\{1\bar{1}00\}$ ) systems. Limited available experimental data from the literature is used to define the models and determine the material properties [4, 5]. The model behavior over a range of temperatures and for different initial dislocation densities will be discussed.

The ultimate goal is to use the model for process design and control in order to improve production yield and reduce costs. The crystal plasticity model is implemented into an advanced finite element framework for thermal-stress analysis during growth processes. The stress and dislocation defect densities resulting for different processing conditions will be presented and discussed.

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## Numerical Simulation of the Formation of the Neck in Heterogeneous Material

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Analyzing the work of structure components undergoing large plastic deformations it is necessary to have the appropriate material parameters. Traditional data obtained from the stress-strain curve is insufficient information. Numerical analysis allow described of the materials with great precision, particularly data describing the heterogeneous material, even at the level of the grain size. The problem is the identification of such material properties on the basis of experimental studies. Data obtained from the stress-strain curve, i.e.  $\sigma - \varepsilon$  are the average values for the entire sample. It seems that a more detailed analysis of stress and strain, especially for large plastic deformations corresponding to the formation and development of the neck will get more valuable material data.

The paper presents a numerical simulation of the formation and development of the neck in a sample consisting of the heterogeneous material. Using FEM with commercial software ANSYS axisymmetric model of cylindrical tensile samples was constructed. The linear triangular elements was adopted. The numerical model consists of over 24 thousands elements and has about 25 thousands equations. Calculations were carried out using a modified Newton-Raphson method and arc-length method. Using a random algorithm, several neighboring elements were combined in homogeneous cluster simulating the grain.

Created three groups of data sets precisely describing stress-strain curve. The material features were the Young's modulus  $E$ , the yield tensile strength  $\sigma_Y$  and ultimate tensile strength  $\sigma_U$ . In each group, only one of the parameters is changed by a few percent to simulate three different materials. Formation of the neck for each of the groups of materials was simulated. In group A, three stress-strain curves differed only in the value of the module  $E$ . In group B, used three different values of  $\sigma_Y$  and in group C the value of  $\sigma_U$  was only changed. The loading was continued until the total strain  $\varepsilon$  reached the value  $\varepsilon_U + 3\%$ .

The obtained results showed that, in the case of group A, deformation process is practically homogeneous throughout the sample. At the end of the loading there is a tendency to the formation of the neck. In group B (change of  $\sigma_Y$ ) neck was formed much earlier. In group C (change  $\sigma_U$ ) neck outlines the earliest and its development is clear. The results show a high heterogeneity of the deformation state even before the appearance of the neck and in the development of course.

**Keywords:** necking, heterogeneity, tensile test

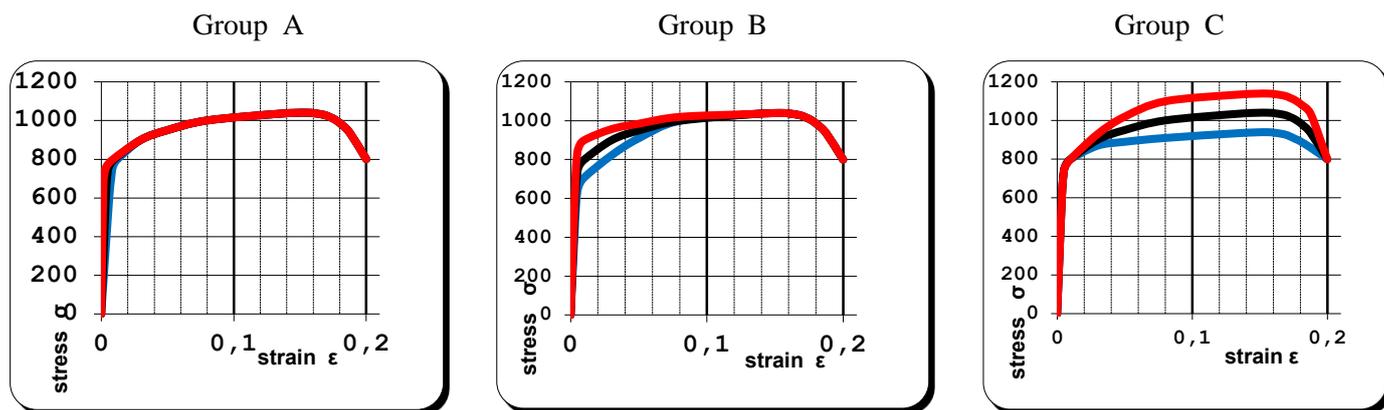


Fig. 1 Basic data for materials. Stress – strain curve.

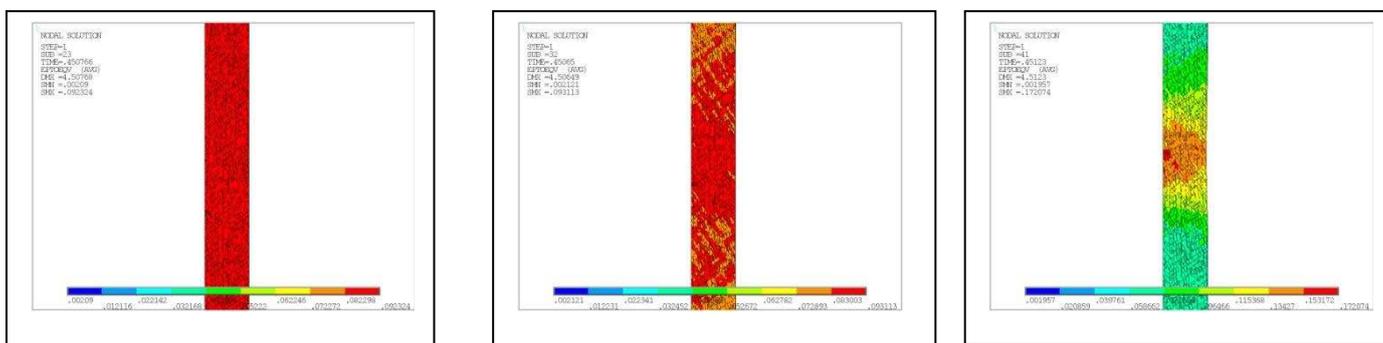


Fig. 2 Equivalent strain for elongation  $u = 4.5$  [mm].

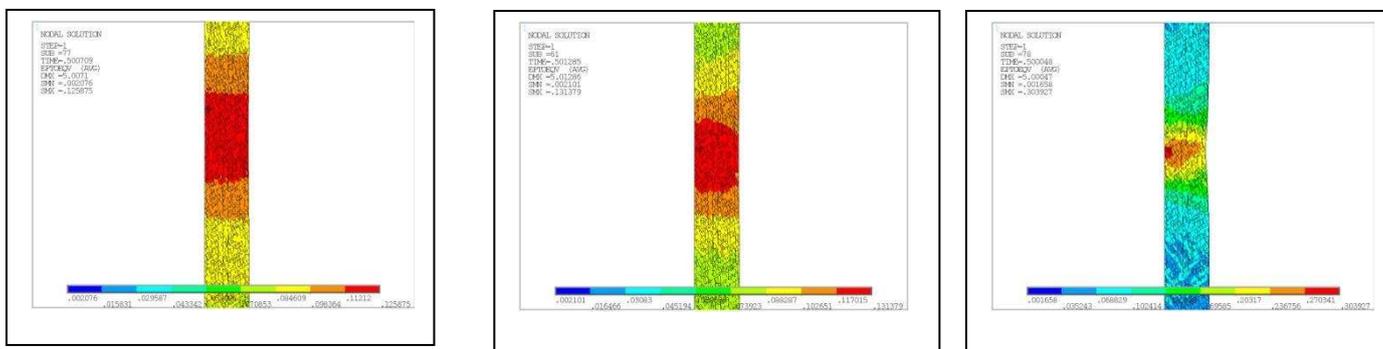


Fig. 3 Equivalent strain for elongation  $u = 5.0$  [mm].

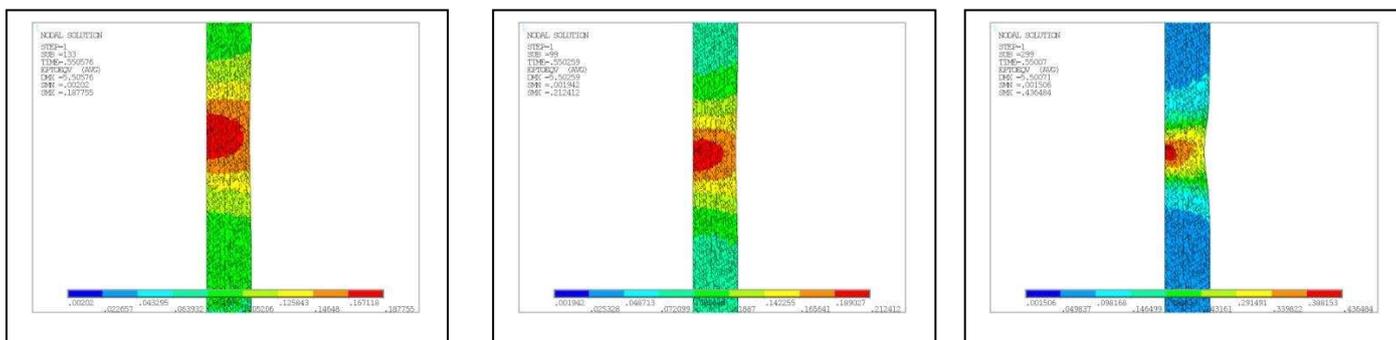


Fig. 4 Equivalent strain for elongation  $u = 5.5$  [mm].

## Crystal plasticity modeling of TWIP steels

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Deformation twins subdivide grains into crystallographically disoriented regions separated by interfaces across which dislocation glide is either impeded or hindered. Twinning may hence contribute significantly to both the strain hardening and the build up of (microscopic) internal stresses or “backstresses”. It for instance is likely to explain the huge work hardening and the formability of TWinning Induced Plasticity steels (TWIP steels).

The commercial TWIP steel grade selected for the present study was investigated using electron microscopy (TEM and SEM) to observe the twin formation, using macroscopic mechanical testing (uniaxial tension, rolling, simple shear) to probe the anisotropic hardening, and using x-ray diffraction and EBSD to measure the texture development and the kinetics of twinning.

A crystal plasticity model was developed that accounts for the co-operative deformation of the very thin (and hence hard) twin lamellae and the parent grains. The meso-to-macro scale transition was computed using either finite element modeling at the grain scale, or using advanced Taylor-type models.

It is demonstrated that the model provides valid prediction of the macroscopic strain hardening and the development of micro and macro texture. The Baushinger effect in reverse shear is properly predicted when one accounts for different sources of internal stresses.

## Dissipative Non-local Models with Dislocations in Finite Elasto-Plasticity

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The paper deals with elasto-plastic materials with crystalline structure, which contain continuously distributed defects, when dislocations are considered as possible lattice defects only. If there are defects inside the body, a global stress free configuration does not exist and the geometry of the material structure with defects is characterized by the so-called plastic distortion and plastic connection. Our model is developed within the constitutive framework of finite elasto-plasticity based on the decomposition of the second order deformation associated with the body motion into elastic and plastic second order deformations. The multiplicative decomposition of the deformation gradient and the transformation rule of the connections are introduced following [1]. We postulate that the plastic connection has zero curvature and non-zero torsion (viewed as a tensorial measure of dislocations, modeling the so-called geometrically necessary defect density tensor). The stress free energy density is assumed to be dependent on the elastic strain, on the Cartan torsion, as well as on the scalar dislocation density (the so called statistically stored dislocation) and its gradient. The non-local evolution equations for plastic distortion and for the scalar dislocation densities are defined to be compatible with the dissipation postulate formulated under the form of the principle of the free energy imbalance. The macro and micro forces are inferred in the internal dissipated power.

We analyze the constitutive restrictions that follow from the supposition that the evolution equation for plastic distortion is described by multislip, like in crystal plasticity and we compare our results with those obtained by Gurtin [2]. We study numerically the influence of the non-local description of the dislocation densities on the elasto-plastic behaviour within a simplified non-local viscoplastic model. The FEM is applied for solving the appropriate variational problem to define the velocity field in the actual configuration, together with a temporal discretization of the differential system to update the current state in the sheet. The sheet is made up from a single fcc-crystal, under in plain stress state.

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## Simple shear flow behavior of advanced high strength steel sheets

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In the present study, a recently developed simple shear test device was used to measure the monotonic and forward-reverse simple shear stress-strain curves for dual-phase (DP980) and transformation-induced plasticity (TRIP780) steel sheet samples. A new simple shear test device was developed specifically to measure the simple shear curves up to large shear strains for high strength materials. A special gripping system was designed to prevent specimen slipping and distortion of the longitudinal direction. This device includes a hydraulic clamping system allowing a maximum pressure of 28 MPa. The device was mounted on a 500 KN MTS universal tension-compression testing machine and the load reversal was achieved by inverting the direction of the cross-head velocity. The load reversal was conducted for different amount of forward loading. The full displacement field was measured with a digital image correlation (DIC) technique using a speckle pattern applied to the specimen prior to testing.

In order to model the observed behavior, the so-called homogeneous yield function-based anisotropic hardening (HAH) model, described in Eqns. (1) and (2), was employed. This is a distortional hardening model that captures the Bauschinger effect in metals although it is not based on kinematic hardening. The HAH model was proposed in a previous investigation [1] and was refined later to account for effects that occur during cross-loading [2]. Although it was developed based on the mechanical behavior of sheet material subjected to single or double loading changes, the HAH approach can be applied to any loading history, including a continuously changing stress state. For proportional loading, the HAH model reproduces exactly the behavior resulting from an anisotropic yield surface expanding isotropically. A tensor variable, the microstructure deviator  $\hat{\mathbf{h}}$ , tracks the loading history, while two scalar state variables  $g_1$  and  $g_2$  distort the yield surface as deformation proceeds. All these variables evolve as a function of the specific plastic work. Additional state variables were added to improve the predictions, in particular, to account for permanent softening after stress reversal and stress overshooting after cross-loading.

In spite of the high strength level, the monotonic stress-strain behavior of TRIP780 and DP980 was measured satisfactorily in monotonic deformation up to shear strains of about 0.6 and 0.8, respectively, and for reversal at various amounts of strain. The HAH model was able to reproduce the behavior of these two materials within a reasonable tolerance margin (Figs. 1 and 2).

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**Equations**

$$\bar{\sigma}(\mathbf{s}) = \left[ \phi^q(\mathbf{s}) + f_1^q \left| \hat{\mathbf{h}} : \mathbf{s} - \|\hat{\mathbf{h}} : \mathbf{s}\| \right|^q + f_2^q \left| \hat{\mathbf{h}} : \mathbf{s} + \|\hat{\mathbf{h}} : \mathbf{s}\| \right|^q \right]^{1/q} = \sigma(\bar{\boldsymbol{\varepsilon}}) \quad (1)$$

with

$$f_k = \left[ 1/g_k^q - 1 \right]^{1/q} \quad (2)$$

**Figures**

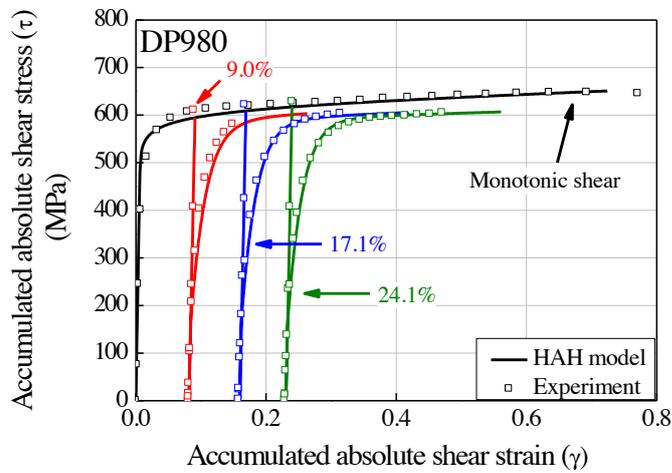


Figure 1. Simple shear stress-strain curves for DP980 for monotonic loading and with stress reversal.

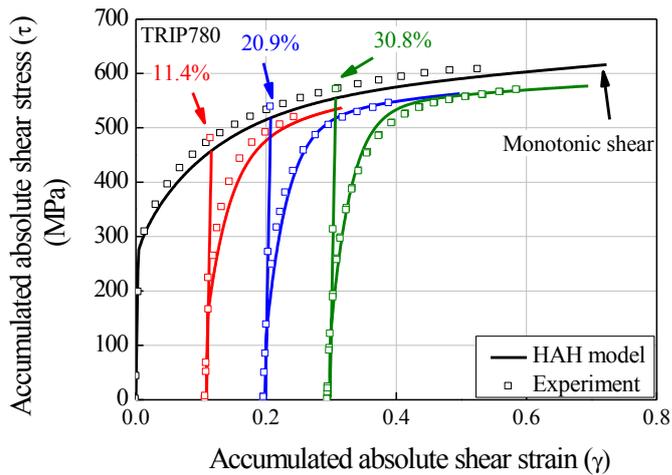


Figure 2 Simple shear stress-strain curves for TRIP780 for monotonic loading and with stress reversal.

## Influence of dislocations on a crystal density: Atomistic and continuum modelling

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The density of metals usually decreases with cold work. Zener first explained the origin of this phenomenon in 1942 [4]. Zener connected the change of crystal volume with two facts: the crystal contains some amount of internal stresses and the crystal lattice is "stiffer" for compression than for extension. In the next years, the observation of Zener was confirmed by three methods:

- *experiment* – correlation between dislocation density, stored energy, and volume change suggested that dislocations decrease material density;
- *continuum mechanics analysis* – the second order nonlinear elasticity analysis and the principle of force equilibrium lead to the formula for increase of material volume in a state of self-stresses. According to the Toupin and Rivlin formula [3], every dislocation decreases crystal density;
- *atomistic simulation* – results of atomistic simulations also confirm that crystal density is changed by dislocations, e.g. [2]. An edge dislocation increases volume by  $0.25\text{--}1.0 |b|^2$  per unit length of the dislocation line.

However, the above view is inconsistent with results of Bell's experiments [1]. He showed that plastic deformation may contract a crystal. The current theories and available computational results do not explain the results of Bell's experiments. **The results reported in this communication prove that the current view on crystal density changes caused by dislocations is incomplete.**

The analysis explores the Kröners continuum theory of dislocations with the finite element method and, as a second methodology, molecular simulations. The obtained results of continuum and atomistic simulations confirm Bell's results. It is shown that edge dislocations may contract the crystal. Additionally, the origin of the contraction is identified. In the current communication the physical interpretation is proposed to explain why in some cases nucleation of dislocations leads to crystal contraction, while in others leads to dilatation. The obtained results suggest that the general formula of Toupin and Rivlin is incorrect in some cases of self-stressed bodies.

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## Scale free phase field theory of dislocations

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With the advance of technology the characteristic size of the microstructure of crystalline materials reached the submicron level. As a consequence, the role of boundaries (sample surface, grain boundary, etc.) became even more important than earlier. So, to model the plastic response of submicron sized sample it is crucial to determine the dislocation distribution near the boundaries. In the paper a continuum theory of the time evolution of an ensemble of parallel edge dislocations with uniform Burgers vectors is presented. Since the dislocation-dislocation interaction is scale free, apart from the dislocation spacing the phase field theory of an uniform edge dislocation system cannot contain any length scale parameter. It is argued, in a continuum theory dislocations this unique feature largely determines the possible terms caused by dislocation-dislocation correlation. It is shown, to recover the dislocation distribution near boundary obtained by discrete dislocation dynamics simulation one has to step beyond the simple gradient type "back stress" assumption commonly used in earlier models. One has to introduce appropriate higher order derivatives with corresponding boundary conditions.

## Plasticity of crystalline solids treated as material flow through adjustable crystal lattice

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Considering severe plastic deformation experiments as a motivation, plastic behaviour of crystalline solids is treated as a highly viscous material flow through an adjustable crystal lattice space [3].

We present thermodynamic derivation of the model of rate dependent crystal plasticity including evolution of Cauchy stress. Unlike the standard approach [1, 4] we follow [5] which is not purely phenomenological.

Moreover we extend our approach to rate independent model by implicit constitutive relation between slip rate and resolved shear stress.

Inspired by numerical methods of fluid dynamics FEM Eulerian representation is formulated and applied in a solution of a flow adjustment boundary value problem of equal channel angular extrusion. We compare our results to [2] considering compressible case.

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Session 6

Nano- to macromechanics



## Oscillations of graphene membranes

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Nowadays there a lot of papers devoted to the NEMS based of graphene membranes. However, there is a lack of experimental data as the experimental nanotechnology of graphene is extremely hard. Hence it is hard to check whether the classical mechanical models can describe the mechanical behaviour of such membranes.

This work contains comparison of several graphene models. The frequencies of graphene films with and without pretension were estimated analytically using the beam and string models. The beam model takes the bending rigidity of graphene into account. An approach to determine this rigidity was proposed. It was shown that if the length of the film is more than 1  $\mu\text{m}$  the string model gives the higher frequencies; otherwise the beam theory gives the higher frequencies with the values up to several THz.

The molecular dynamics simulations of graphene resonator were performed. It was shown that analytic, computational and experimental results correspond quite well. The computational results are close to those obtained with the beam theory for the small membranes. For the big membranes (more than 100  $\mu\text{m}$ ) the computational results tend to the string theory.

The thermoelasticity problem for the graphene film was formulated. The film demonstrates the contraction at the instantaneous heating due to the negative Poisson ratio. The solutions were obtained with molecular dynamics and finite element methods. It was shown that both methods give similar results.

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## Calculations of Strain Induced Energy Gap Variation in ZnTe/ZnMgTe Core/Shell Nanowires

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Optical properties of semiconductor nanowires attract a great interest because of emerging applications of these structures in the field of nano-photonics [1] and photovoltaics [2]. Te-based nanowires are especially promising in this respect because II-VI semiconductors are characterized by direct energy gaps with values covering the entire visible light spectral range, from 1.6 eV (CdTe) to 3.5 eV (MnTe).

Recently ZnTe nanowires embedded in ZnMgTe coating shells are fabricated using gold catalyst assisted molecular beam epitaxy [3]. An intense emission from the nanowire cores at energies corresponding to the energy gap of ZnTe is observed. Depending on the thickness and the Mg content in the shell this emission exhibits a considerable energy shift. This effect may be explained in terms of strain induced energy gap variation of ZnTe, whereas the strain originates from the lattice mismatch between the ZnMgTe nanowire shells and ZnTe nanowire cores.

The aim of this work is to confirm quantitatively, whether the observed energy gap variation as large as 80 meV can be attributed to strain effects only, or some additional effects such as, e.g., intrinsic electric fields, must be taken into account.

The both synthesised materials, ZnTe (core) and ZnMgTe (shell), have the same zinc blende cubic crystal structure, the same spacial orientation of crystal axes, but differ by the lattice constant. This is 6,1034Å in ZnTe, and some percent greater in ZnMgTe.

To find the state of deformation of this system a continuous medium approximation was applied and to determine the strain and stress fields a thermoelastic analogy was proposed. Namely, to account the difference of lattice constants, the structure was considered as a homogeneous one, but subject to a hypothetical non-homogeneous thermal field. First, the both materials were treated as isotropic, and a problem of an elastic cylinder in non-homogeneous thermal field with axial symmetry was considered. The continuity of suitable displacement and stress fields at the interface was assumed. Even in this crude approach, the deformation field in the cross-section of the core was found uniform in agreement with the experiment. Next, the realistic cubic anisotropy of the medium was accounted for and the generalized displacement, Navier's equation were derived. In this case any axial symmetry of the problem can be observed.

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## Energy-Based Approach to Computation of Finite Sized HCP-Metal Specimens Elastic Properties

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On the base of atomistic statics approach the elastic moduli of finite sized metallic hexagonal close packed (HCP) monocrystal are computed. The form of specimen corresponds to HCP-lattice symmetry. The Mie interatomic potential is chosen for potential energy calculation. The initial configuration of HCP-crystal is defined to satisfy the density of potential energy minimization condition. It is shown that using Mie power interatomic potential allows getting different values of ratio for two HCP-lattice parameters, which is different for different HCP-metals. The implied deformational gradient transforms the initial crystal into the actual configuration. The full potential energy of the deformed specimen divided by its volume is calculated to compute the elastic moduli. Quadratic items of its Taylor series in terms of deformational parameters are assumed to be equal to elastic potential in the general non-symmetric form. Energy minimization procedure guarantees that linear items of series are equal to zero. This trick allows finding the HCP-monocrystal elastic moduli. In non-symmetric case a material with HCP-lattice possesses 8 independent non-zero components of elastic properties tensor  $\mathbf{C}$  instead of 5 elastic moduli in symmetric approximation. From the energy-based approach only 6 moduli could be found in general case. It is obtained that under independent computation of the following components:  $C_{1111}$ ,  $C_{1122}$  and  $C_{1212}$ , they are turned out to be in strict connection  $C_{1212} = (C_{1111} - C_{1122})/2$ , which corresponds to the symmetric form of tensor  $\mathbf{C}$ . It is shown that HCP-lattice, which is combined from two simple sub-lattices, could not be homogeneously deformed under the prescribed affine deformation. For supporting minimum of potential energy density for HCP-monocrystal in deformed configuration it is necessary to impose a vector of relative shift between sub-lattices depending on deformational parameters. The components of sub-lattices relative shift vector are considered as additional degrees of freedom for HCP-lattice. The elastic moduli of HCP-lattice are obtained to be symmetric and depending on specimen size as well as lattice parameters. The latter dependencies have got a horizontal asymptotes letting identification of interatomic potential parameters by known macroscopic properties. The procedure of macroscopic properties computation based on introducing periodic interatomic potential is realized. The way of identification of Mie potential parameters is demonstrated with the example of Mg and Ti.

All computations were performed in the symbolic manner using the Wolfram Research "Mathematica" program.

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## Statistical properties of micron-scale crystal plasticity

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Plastic deformation of small scale single crystalline specimens is accumulated by large intermittent strain bursts (dislocation avalanches). As a result, the stress-strain curves of such specimens are characterized by random steps corresponding to these bursts. This behaviour makes, for example, the conventional yield stress definition unusable in the sense, that it does not provide a material- and size-specific value, rather it varies from specimen to specimen. In order to understand this fluctuating behaviour a detailed statistical analysis of the deformation curves and the underlying collective dislocation dynamics is necessary. In this talk we give such a description by analysing the results of discrete dislocation dynamics simulations in 2 and 3D [2] and compression experiments performed on a large number of identical Cu micropillars. First we show that in each studied case the stress levels corresponding to a given strain value are Weibull-distributed suggesting that there is an underlying weakest link phenomenon behind micron-scale plasticity. This finding is supported by the fact that long-range dislocation stress fields are screened [1] in dislocation networks and that spatial correlations are short-ranged [3]. After giving a detailed overview on these effects we discuss the system size dependence of our results and the implications of these findings.

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## Plasticity and High Toughness of CNT Nanosprings

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The presence of defects in the hexagonal network of carbon atoms usually degrades the extraordinary mechanical properties of graphitic nanomaterials. Here we report via atomistic simulations unexpectedly plasticity and high toughness found in nanosprings of coiled CNT with intentionally incorporated non-hexagonal defects, in addition to well-recognized extreme elasticity of the material. The obtained toughness approaches to 5,000 J/g with decreasing spring dimension. The high toughness originates from the plastic nano-hinge deformation as a result of partial fractures distributed in the nanosprings, which are initiated and arrested by the defects required to coordinate the spring curvature. We would thereby provide an atomistic principle for toughness enhancement in mechanical design of carbon-based nanomaterials.

**KEYWORDS:** CNT single/multi-strand nanospring, defects, partial fracture, high toughness, size effect, nano-hinge deformation.

## General Theory of Statics of Micropolar Elastic Multilayered Thin Shells

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Currently development of mechanics of solids is connected with construction of generalized mathematical models, considering the element of the body not as a point but as a complex object, which has special properties, concerning with micro- and nano structure of material. Micropolar (asymmetric, momental) theory of elasticity or Cossera's continuum is one of the theories of deformation of elastic bodies with consideration of internal structure of the material, which has final form. The influence of the micropolarity of material is important in case of thin bodies (thin plates, shells). From this point of view the construction of mathematical models of statics and dynamics of micropolar elastic isotropic and anisotropic, single and multilayered thin plates and shells is actual. In paper [1] on the basis of hypotheses method, which has asymptotic justification [2], general theory of static deformation of micropolar isotropic elastic thin shells is constructed. In this paper this approach is developed and for the whole package applied theory of statics of multilayered orthotropic elastic thin shells with free fields of displacements and rotations is constructed. Main equations and boundary conditions of statics are introduced for micropolar multilayered shells of rotation and cylindrical shells.

Models of two and three-layered micropolar orthotropic shells of symmetric structure are also introduced as private cases.

Problem of determination of stress-strain state of two and three-layered micropolar orthotropic cylindrical shells of symmetric structure is studied. On the basis of numerical analysis effective properties of micropolar orthotropic material are revealed.

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## **The interval lattice Boltzmann method for transient heat transport in two-dimensional silicon thin film**

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In the paper the description of numerical analysis of heat transfer process proceeding in a two-dimensional silicon thin film is presented. It is assumed that some parameters (relaxation time, internal heat generation rate related to an unit of volume and boundary temperatures) appearing in the mathematical model of the problem analyzed are given as intervals. The problem discussed has been solved using the interval form of the lattice Boltzmann method applying the rules of the directed interval arithmetic [2].

In dielectric materials and also semiconductors the heat transport is mainly realized by quanta of lattice vibrations called phonons. Phonons always “move” from the part with the higher temperature to the part with the lower temperature. During this process phonons carry energy. This process can be described by the Boltzmann transport equation (BTE). The BTE is one of the fundamental equations of solid state physic. In order to take advantage of the simplifying assumption of the Debye model, the Boltzmann transport equation can be transformed to an equation on carrier energy density [1].

The interval lattice Boltzmann method (ILBM) is a discrete representation of the interval Boltzmann transport equation [3]. The ILBM discretizes the space domain considered by defining lattice sites where the phonon energy density is calculated. The lattice is a network of discrete points arranged in a regular mesh with phonons located in lattice sites. There are a few possibilities for spatial position of the particles. In the paper the D2Q9 lattice, which has two dimensions and nine velocities, has been applied. Phonons can travel only to neighboring lattice sites by ballistically travelling with a certain velocity and collide with other phonons residing at these sites. In the ILBM it is needed to solve nine interval equations supplemented by the boundary and initial conditions allowing to compute interval phonon energy in different lattice nodes. The total interval energy density is defined as the sum of discrete interval phonon energy densities in all the lattice directions. After subsequent computations the interval lattice temperature is determined using the formula describing the relation between interval phonon energy and interval lattice temperature.

As a numerical example the heat transport in 2D silicon thin film has been analyzed.

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## Session 7

# Scale transition and homogenization



## Micromechanics based constitutive modeling of martensitic transformation in metastable materials subjected to torsion at cryogenic temperatures

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Special class of multi-phase structural members with graded microstructure can be obtained at cryogenic temperatures as a result of controlled transition from the parent phase to the secondary phase. The required features are obtained via the mechanism of diffusionless plastic strain induced phase transformation from purely austenitic to martensitic lattice ( $\gamma \rightarrow \alpha'$ ). Many ductile materials are known to behave in metastable way when strained at extremely low temperatures. Among them the austenitic stainless steels are often used to construct components of superconducting magnets, cryogenic transfer lines and other cryogenic systems. The constitutive model developed to describe the plastic strain induced phase transformation at very low temperatures involves plastic hardening where two important effects play fundamental role: (1) interaction of dislocations with martensite inclusions and (2) increase of resultant tangent stiffness due to the evolution of harder martensite within the softer austenite. The micro-mechanism of interaction of dislocations with martensite inclusions is based on the Orowan scenario. The other mechanism takes into account constantly evolving proportion between the primary and the secondary phase and involves the relevant homogenization scheme. Both effects contribute to strong nonlinear hardening that occurs as soon as the phase transformation process begins. The constitutive model has been used in order to obtain a new closed form analytical solution for the case of torsion of round bars at extremely low temperatures. Moreover, numerous experiments involving quasistatic and cyclic loads were carried out in order to trace the profile of phase transformation. An ultimate prove is presented that a functionally graded structural member, characterized by the required profile of volume fraction of both phases, can be obtained. The profile of volume fraction of secondary phase (martensite) is checked by means of 2 independent methods: hardness measurements and verification by using a ferriscope (magnetic induction). Theoretical prediction of linear distribution of the volume fraction of martensite in circular rods subjected to torsion at cryogenic temperatures has been obtained by Skoczeń [1]. A 3 dimensional constitutive model of metastable material undergoing phase transformation has been developed. The advantage of the constitutive model developed in the present paper is founded on the assumption that all the parameters used have to be thoroughly identified at cryogenic temperatures. This implies reduction of the number of parameters to the necessary minimum. However, all the basic mechanisms that govern the phase transformation process as well as the description of isotropic and kinematic hardening are included. The originality of the model starts from the observation that at extremely low temperatures the plastic strain induced  $\gamma \rightarrow \alpha'$  phase transformation occurs in very fast way and follows nearly linear transformation path in terms of the volume fraction of martensite as a function of plastic strains. For the mixed (isotropic/kinematic) strain hardening, that reflects the effect of phase transformation on the stress-strain curve, the same principle has been adopted. Thus, the most important contributions to the hardening process were taken into account: micromechanics and evolution of tangent stiffness corresponding to the evolution of proportion between phases. A comparison of the experimental and the numerical results indicates that the model performs correctly in a wide range of temperatures.

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## Homogenization schemes for elastic-viscoplastic heterogeneous materials based on an “affine” extension of the “Translated Fields” method

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An “affine” extension of homogenization schemes for elastic-viscoplastic materials with Maxwellian phases and based on the so-called “translated fields” method initiated in [1] is presented. The main steps of the “translated fields” method will be first presented for linear composites. Then, the extension to elastic-viscoplastic composites with non linear viscoplasticity will be shown in the case of the Mori-Tanaka approximation and two Self-Consistent schemes assuming a linearization of the constituent’s behavior of the “affine” type [2]. This extension gives a new theoretical interaction law between mean fields within phases and overall ones, which contains the coupling between elastic- and viscoplastic- mechanical interactions and the phase stress histories. In order to check the validity of the approach, the results are reported for two-phase composites and are compared to other existing analytical and numerical approaches (e.g. [3]).

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## Fluctuation-based viscoplasticity and the issue of dissipation potentials

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The motivation for this work is the modelling of the viscoplasticity of anisotropic solids. In a fully 3D elasto-viscoplastic setting (e.g. [1]), the key task is to model the flow rule, i.e. the relation between the stress tensor and the plastic strain rate tensor. In a wider context, the challenge consists in formulating constitutive relations between thermodynamic forces and thermodynamic fluxes. In the field of solid mechanics, such relations are often established on the basis of dissipation potentials [2], in order to ensure thermodynamic admissibility.

In this contribution, we demonstrate that fluctuation-based approaches to formulating the flow rule, i.e. the force-flux relation, are advantageous in several respects. Specifically, the fluctuation-based approach establishes a relation between the fine-scale rapid motions and the coarse-scale dissipative dynamics, in the form of fluctuation-dissipation relations [3,4,5,6]. The fluctuation-based approach has a number of advantages. For example, it can be shown that the fluctuation-based approach encompasses a wider class of constitutive relations than what can be covered by the dissipation-potential. This is due to the fact that fluctuation-dissipation relations result in quasi-linear force-flux relations, which in turn are more general than the ones based on a dissipation-potential [7]. In addition, the relation of the coarse-scale constitutive relation to the underlying fine-scale dynamics in the fluctuation-based approach is of practical use even if the fine-scale dynamics is not fully calculated in all detail. Specifically, we demonstrate using the example of transversely isotropic viscoplastic materials that symmetry considerations on the fluctuations are sufficient to severely constrain the form of the plastic strain rate tensor [6]. By application to experimental data for polypropylene [8], it is shown that the so-derived flow rule is superior to conventional approaches in modelling the anisotropic rate-dependent yield behaviour [9].

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## Effects of the local resonance in periodic reticulated materials

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Numerous materials and structures of various sizes can be considered as periodic reticulated (or cellular) systems, that is to say they are obtained by repeating a unit cell made up of interconnected beams (or plates). Examples include the microstructure of foams, plants, bones, the sandwich panels, stiffened plates and truss beams used in aerospace and marine structures, buildings. As beams are much stiffer in tension-compression than in bending, the propagation of compressional waves with wavelengths much greater than the cell size and the bending modes of the elements can occur in the same frequency range. Thus reticulated materials can behave as metamaterials and exhibit unusual dynamic properties [1].

The consequences of this phenomenon are investigated by considering the archetypal case of frame materials. Since the condition of scale separation is respected for the compressional waves, the homogenization method of periodic discrete media [2,3] is used to rigorously derive the macroscopic behavior at the leading order. The main advantages of the method are the analytical formulation and the possibility to study the behaviour of the elements at the local scale. This provides a clear understanding of the mechanisms governing the dynamics of the material.

In the presence of the local resonance, the form of the equations is unchanged but some macroscopic parameters depend on the frequency. In particular, this applies to the mass leading to a generalization of the Newtonian mechanics. As a result, the compressional waves are dispersive and there are frequency bandgaps. The longitudinal modes of reticulated beams can also be affected by the local resonance. In that case, the same macroscopic modal shape is associated with several resonant frequencies (but the deformation of the elements at the local scale is different). These atypical behaviours are first established theoretically and then, they are confirmed by numerical simulations.

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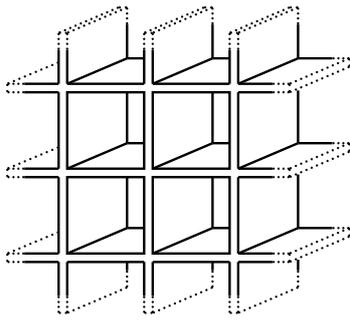


Figure 1: Studied material

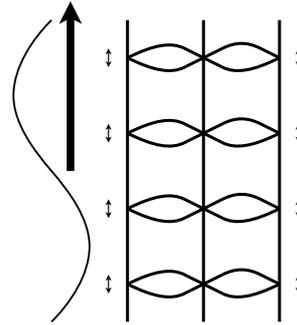


Figure 2: Resonance in bending of the horizontal elements induced by a compressional wave traveling in the vertical elements

Expression of the effective mass:

with  $m$  the mass of the elements experiencing tension-compression,  $m_r$  the mass of the resonating elements,  $\omega_f$  the ratio between the circular frequency and the circular frequency of the first bending mode of the resonating elements

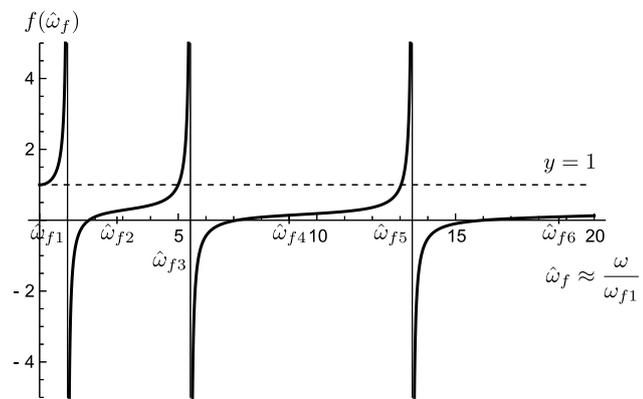


Figure 3: Variations of the effective mass according to the frequency

13.76	64.83	35.99	74.22	45.46	97.37	48.28	127.0	49.76	157.5
(14.00)	(65.14)	(36.73)	(74.35)	(46.42)	(97.68)	(49.36)	(127.8)	(50.49)	(158.9)

Figure 4: Modal shapes and resonant frequencies calculated with the code CESAR-LCPC and comparison with the resonant frequencies (into brackets) obtained thanks to homogenization.

## Modelling of Deformation Banding in Grains of Polycrystalline Metals

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The phenomenon of spontaneous formation of deformation bands in single crystals or grains of ductile metals deformed plastically by crystallographic multislip has been widely observed experimentally. In distinction to strain localization, deformation banding is not a localized phenomenon as the bands cover the whole domain of a crystal or grain with alternating lattice orientation. It affects mechanical properties of a grain and, after performing scale transition, also of a polycrystalline aggregate. For instance, intragranular differences in lattice orientation can result in less sharp textures at the macroscopic level.

Quantitative effect of deformation banding within grains on overall properties of polycrystals represents an actual problem in modelling. A difficulty appears at the level of adequate modelling of grain subdivision. It is shown that the lack of symmetry of the matrix of geometric interaction between slip-systems can invalidate the approach based on incremental energy minimization unless special measures are undertaken. Recently, the energy criterion for deformation banding in rate-independent single crystals has been developed [1] that requires selective symmetrization of the interaction matrix between active slip-systems only [2].

In this lecture, main features of the modelling of deformation banding based on the energy criterion are discussed and illustrated by examples calculated for copper crystals. An algebraic equation is provided whose solutions define deformation banding modes preferable to uniform straining of a crystal for any positive excess of latent hardening over self-hardening of slip-systems. The algorithm for tracing the development of deformation bands with automatic selection of active slip-systems is outlined, and difficulties related to subsequent subdivision of bands are discussed. Predictions of lattice misorientation evolution within grains are presented along with the resulting effect on deformation textures.

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## Periodic homogenization of an anisotropic elastic-plastic compressible material: application to cellular core sandwich structures

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Thanks to their outstanding mechanical specific properties, such as structural strength and impact absorption, cellular architected materials are well-suited for the aeronautic industry. These materials exhibit three characteristic length scales: the macro-scale of the structure, the meso-scale associated to the internal structure of the material and the micro-scale linked to the base material. Modeling large structures is difficult because of the computational cost of the FE models. A multi-scale modeling strategy based on the identification of a macroscopic constitutive model is therefore proposed [1]. The work here focuses on sandwich structures with a stacking of tubes as cellular core. The tubes are brazed following two patterns, a square one and a hexagonal one.

The core is considered to be periodic and its multi-axial behavior is obtained by a periodic homogenization scheme on one unit cell. This method gives the macroscopic mechanical response on which an anisotropic compressible Homogeneous Equivalent Laws is fitted [2, 3]. The core of a sandwich structure is then replaced by a Homogeneous Equivalent Medium.

Quasi-static loadings are applied to finite sandwich structures to study the influence of the edge effects on the macroscopic behavior depending on the stacking pattern, the sandwich structure size and the load case. This approach gives satisfactory results but the hypothesis of scales separation is not satisfied in the general case of complex load cases, therefore the extension of the method to generalized continua is considered. The large deformation framework combined to non local media provides a better model taking into account the strain localization induced by the softening behavior of the collapsed cells. A numerical / experimental comparison will be carried out to discuss the quality of the proposed models.

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## **Transient computational homogenization for locally resonant acoustic metamaterials**

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Locally resonant acoustic metamaterials (sonic crystals) with random arrangement of inclusions are crucially important for solving noise shielding problems due to their unique property to attenuate acoustic waves with large wavelengths without forming resonant transmission peaks [1]. Though the properties of these materials were discovered experimentally more than ten years ago, there is still a lack of theoretical methods to predict frequency band gaps for sonic crystals specifically under transient conditions of excitation, which are expected in applications and typically used for obtaining experimental data [2].

In this work, the transient computational homogenization scheme is proposed to model the effective response of sonic crystals with randomly distributed composite inclusions subjected to a longitudinal pulse loading. This procedure is an extension of the classical (first-order) computational homogenization framework by taking into account the inertia for the inclusions leading to the negative effective mass density effect. Key aspects are the enriched description of the micro-macro kinematics and the generalized Hill-Mandel condition to ensure a consistent solution of the balance of linear momentum at micro- and macroscales [3]. Consistency of the framework is confirmed by a good agreement of the calculated frequency band gaps with experimental data [1] and with results obtained by means of direct numerical simulations. The dispersion properties of a rubber-coated particle reinforced heterogeneous material were investigated by varying the frequency of the loading pulse, the size of the inclusions, thickness of the rubber coating and particle distribution. The dependences of the values of dip frequencies on these microstructural parameters are analysed in detail. The obtained results are of importance for a deeper understanding of the physical properties of sonic crystals as well as for their future practical applications.

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## Modelling of the cyclic behavior of elasto-viscoplastic composites by a Mori Tanaka approach and validation by Finite Element Calculations

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This work deals with the prediction of the macroscopic behavior of two-phase composites, based on a Mori Tanaka scheme recently proposed in Mercier and Molinari (2009), see also K. Kowalczyk-Gajewska and H. Petryk (2011). Cyclic tension–compression loading and relaxation process are investigated in the present work to further validate the approach.

The composite is made of spherical inclusions dispersed in a matrix. Both materials have an elastic-visco-plastic behavior described by a Perzyna overstress type of law. Since the inelastic behavior of the two materials accounts for strain rate and strain hardening, it is well known that no closed form solution can be found to evaluate the overall behavior of such composite.

In a second part, finite element calculations are performed using ABAQUS/STANDARD software in order to validate the proposed homogenization technique. As in Pierard and Doghri (2006), the representative volume element is made of a spherical inclusion embedded in a cylinder filled with the matrix material. These simulations allow the determination of the local strain and stress fields in the composite and the mean value of the corresponding fields within the matrix and the inclusion.

Comparisons between Mori-Tanaka scheme and finite element calculations are made for different volume fractions of inclusion (from 15% to 40%). A parametric study is also conducted by varying material parameters such as Young modulus, hardening parameters, viscoplastic modulus and viscoplastic exponent. Tests are conducted at strain rates of  $10^{-6}$  s<sup>-1</sup>– $10^{-3}$  s<sup>-1</sup>. These comparisons demonstrate the efficiency of the proposed homogenization scheme in terms of the macroscopic response. It is also shown that the average stress and strain in the two phases are correctly predicted by the Mori-Tanaka approach when compared to numerical results.

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## Homogenisation towards grain size and structural size dependent plasticity

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The macroscopic inelastic response of polycrystalline materials is strongly influenced by heterogeneities in the microscopic plastic slip. Well-known is the effect of grain boundaries on the yield stress of metals. The constraint on plastic slip imposed by them causes the classical Hall–Petch effect: a dependence of the yield stress on grain size. A second type of size dependence, i.e. on the specimen size, is caused by gradients of the plastic strain at a scale which is larger than the individual grains. Our study aims to clarify how these two influences contribute to the macroscopically observed response and, in particular, how the length scales associated with them propagate to the macro-scale. In the interest of transparency we limit ourselves to a simple, laminar grain structure and either single slip or symmetric double slip. We adopt the single crystal plasticity model by Cermelli and Gurtin [1] and propose a homogenization theory to translate this mesoscopic crystal plasticity formulation to a macroscopic one in a thermodynamically consistent manner. The work done and energy stored at the mesoscale are formulated in terms of macroscopic quantities. A homogenized micro-force balance is obtained. When grain boundary resistances are present, the homogenized (macro) solution is able to predict the additional hardening due to the micro-fluctuations within a unit cell and it thus exhibits grain size dependence. The second type of size dependence, i.e. on the specimen size, enters via gradients of the macroscopic quantities. The resulting equations thus allow us to study the interaction of these two length scales.

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## The size of the representative volume element and its effect on the averaged properties of materials

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Representative Volume Element (RVE) is an important, yet not precisely defined, concept in the mechanics of heterogeneous materials, which is used in problems of estimating the effective macroscopic properties of such materials. Strictly speaking, an RVE of finite size does not exist for non-periodic materials. In the usual stochastic descriptions of microstructures, random fluctuations of material properties within a given volume element can always lead to large variations in its averaged properties, forbidding their determination with certainty. A true RVE has to be infinite in size; for practical reasons though, it is usually assumed that it has dimensions greater than 100 average grain sizes for a given microstructure.

For the above reasons, the concept of Stochastic Volume Element (SVE) has been introduced; the averaged material properties for this volume have been called *apparent* (as opposed to effective). For an SVE of a given size over a given stochastic microstructure, its apparent properties can only be defined to within a certain accuracy, and with a certain probability. As the size of an SVE gets larger, the probability that its apparent properties lie in near proximity of the effective properties for the given material becomes close to 1.

Much progress has been made towards establishing hierarchies of bounds for material properties computed on SVE's of different sizes, for different types of materials ranging from linear elastic to visco-elastic and elasto-plastic [1]. One of the important problems concerned with the SVE, and still largely unsolved, is the determination of statistical characteristics of the apparent properties for a given random material, and a given size of the SVE [2].

In the present work, the connection between the size of the SVE, the characteristics of the heterogeneous material, and the resultant apparent properties will be explored in more detail. Also the effect of other microstructural features like constant-width grain boundaries in small-grained microstructures [3], less frequently considered in the context of the SVE and effective properties, will be taken into account.

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## On Variationally Consistent Homogenization and the Role of a Generalized Hill-Mandel condition

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The classical setting of model-based homogenization is considered in this presentation. For the standard quasistatic stress problem based on subscale elasticity, the Hill-Mandel (or macrohomogeneity) condition can be expressed as the "equivalence of virtual work of the fine-scale and the macroscale". How to generalize this condition to a more general class of nonlinear and/or time-dependent coupled field problems involving selective homogenization of the pertinent fields (and balance equations) is not obvious; however, a possibility is offered by the paradigm of Variationally Consistent Homogenization in the spirit of the Variational Multiscale Method, originally proposed by Hughes [1] in a quite different context. The corresponding macrohomogeneity condition is then associated with a Galerkin property of the homogenized problem: We consider the particular situation that a RVE-potential exists, whose stationary point defines the fluctuation solution. The Galerkin property then states that the homogenization of the stationarity condition for the RVE-potential equals the stationarity condition for the homogenized potential. As a result, symmetry of macroscale tangent operators is preserved. For example, this situation arises for stress analysis if any model of Standard Dissipative Material type is assigned to the micro-constituents, and the incremental response is obtained upon using Backward Euler integration of the pertinent evolution equations.

Two types of problems are chosen to illustrate the fundamental idea: Firstly, (selective) homogenization of incompressible Stokes' flow in a rigid porous medium leads to Darcy-type of seepage. Only the continuity equation is homogenized, whereas the momentum balance remains completely local, Sandström and Larsson [4]. Secondly, we consider a class of gradient-enhanced dissipative mesoscale material models that are relevant for the modeling of grain-size effects in polycrystalline metals. The adopted homogenization strategy results in the classical equilibrium equation on the macroscale, whereas the internal variables "live on the mesoscale" only, Runesson et al. [3]. For both problem types, we adopt (as the point of departure) the concept of weakly periodic/antiperiodic boundary conditions on the RVE, cf. Larsson et al. [2], for which the pertinent macrohomogeneity condition is satisfied. Moreover, we discuss how to establish a "macroscale pseudo-elastic strain energy" that serves as the potential for the macroscale (homogenized) "fluxes" and, thereby, guarantees symmetry of the macroscale tangent operators.

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## Session 8

# Inverse problems and optimisation in multiscale modelling



## Evolutionary optimization of bone scaffolds geometry

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The paper is devoted to the geometry optimization of bone scaffolds. The multiscale approach with use of computational homogenization method is used [1,2]. The scaffolds [4] are used as an artificial filling of bone defects in the human skeletal system. Their application allows bones to rebuild even if much of the bone tissue has been removed by surgery. The paper presents a method for scaffolds geometry optimization, so the remodeling of bone tissue is possible. For this purpose, scaffolds material properties needs to be similar to the material properties of the surrounding bone tissue. Comparison of the materials is performed using a computational homogenization method. The averaged orthotropic material properties for bone tissue are determined in the first stage. The cubical specimen of trabecular bone, extracted from head of the human femur bone is used as an example. Basing on the experimental and simulation data, and by using the artificial intelligence methods, bone trabeculas material parameters were determined [3]. The average material parameters for bone specimen are then obtained with use of numerical homogenization method. The objective function of the optimization process is formulated as a norm of the difference between homogenized material parameters of scaffold and bone. The design variables describes the shape of the scaffold. The evolutionary algorithm is used in optimization process. The real coded chromosomes contains genes with design variables. The fitness function of the evolutionary algorithm is equal to the objective function of optimization problem. The evaluation of the objective function value leads to the analysis of multiscale problem. The geometry of representative volume element (RVE) for scaffold is created on the basis of genes values. Then the boundary value problems are solved six times to obtain stress-strain relation with use of the computational homogenization method. The averaged material properties are used in the fitness function value computation. The analyses of scaffolds RVEs and reference bone RVE are performed with use of the finite element method.

**Acknowledgments** The research is financed as a research project no. BK-214/RMT4/2012.

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## Numerical material representation using proper orthogonal decomposition and diffuse approximation

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Recently, image-based microstructure modeling and analysis have attracted the interest of more and more researchers [4]. However, access to microstructural images is economically expensive by experiments or time-consuming by numerical simulations [1]. Therefore, there is a great demand for an economical and efficient approach to generate microstructure images.

Techniques of model reduction have been widely used in the fields computational mechanics and multidisciplinary optimization [2]. To the knowledge of the authors, the literature reveals little investigation into developing microstructure image generation approach using model reduction techniques. In [3], Principal Component Analysis (PCA) has been applied to reduce the parametric space constructed by a large-dimensional data set using the so called *method of snapshots*.

Suppose we have means to generate microstructure representations for instants by varying processing parameters (numerical or experimental, etc.), the goal of this work is to establish a parameterized geometrical description from learning the set of given instances. Using the *method of snapshots*, microstructure snapshots are represented in terms of a POD basis, where the number of modes retained is decided after taking both the image reconstruction errors as well as the convergence of the effective material constitutive behavior obtained by numerical homogenization into consideration. The geometry and topology of individual phases of a parameterized snapshot is given by a series of response surfaces of the projection coefficients using the method of Moving Least Squares (MLS), also called *diffuse approximation* [5]. Two cases are considered:

- a) when the parameters  $\mathbf{v} = [v_1, v_2, \dots]^T$  of the RVE are known *a priori*, the parameterized microstructure representation is given by a series of response surfaces of the projection coefficients in terms of  $\mathbf{v}$ ;
- b) when the parameters are unknown *a priori*, a set of pseudo parameters  $\boldsymbol{\eta} = [\eta_1, \eta_2, \dots]^T$  corresponding to the detected dimensionality of the set of  $M$  snapshots are locally taken from learning the manifolds of the projection coefficients, and then represent the parametric space using the approximated manifolds with respect to  $\boldsymbol{\eta}$ .

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Consider a set of discrete 2D  $N \times N$  RVE snapshots  $\mathbf{S}_k$  generated corresponding to instants by varying parameters  $\mathbf{v}_k \in \mathbb{R}^P$ ,  $k = 1, \dots, M$ . Storing each  $\mathbf{S}_k$  is stored in a column vector  $\mathbf{s}_k$ , by standard POD approach we have:

$$\tilde{\mathbf{s}}_k = \bar{\mathbf{s}} + \sum_{i=1}^m \alpha_{ik} \phi_i \quad (1)$$

where  $\bar{\mathbf{s}} = \sum_{k=1}^M \mathbf{s}_k / M$  is the average and  $\alpha_{ik} = \phi_i^T (\mathbf{s}_k - \bar{\mathbf{s}})$ .

In cases where  $\mathbf{v}$  are known *a priori*, we approximate the projection coefficients in terms of  $\mathbf{v}$  directly:  $\tilde{\alpha}(\mathbf{v})$  using approximation techniques such as Radial Basis Functions (RBF), Kriging, MLS and etc. Fig. 1 gives an illustration of the interpolation approach. For a considered set of  $\mathbf{s} \in \mathbb{R}^3$  corresponding to  $M = 7$  instances, the truncated space is of dimensionality  $m = 2$  where the “true” parametric dimensionality is  $p = 1$  as is indicated by the red solid line.

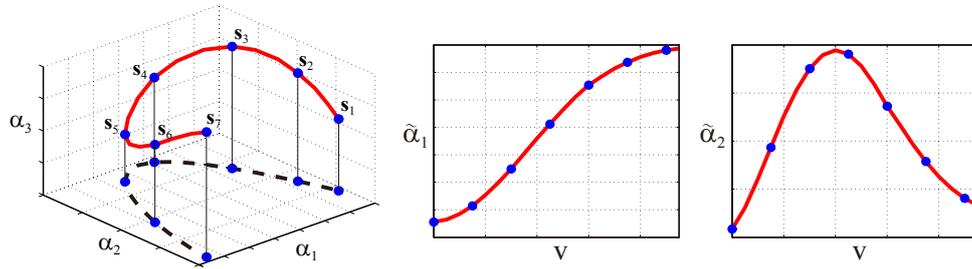


Figure 1: Illustration of the interpolation approach of Eq. (1):  $\mathbb{R}^3 \rightarrow \mathbb{R}^2 \rightarrow \mathbb{R}$ .

An illustrative flowchart of this interpolation approach is given in Fig. 2. As can be seen, once the approximations have been constructed, a corresponding RVE snapshot may be interpolated for any given admissible value of  $\mathbf{v} = \mathbf{v}^*$ .

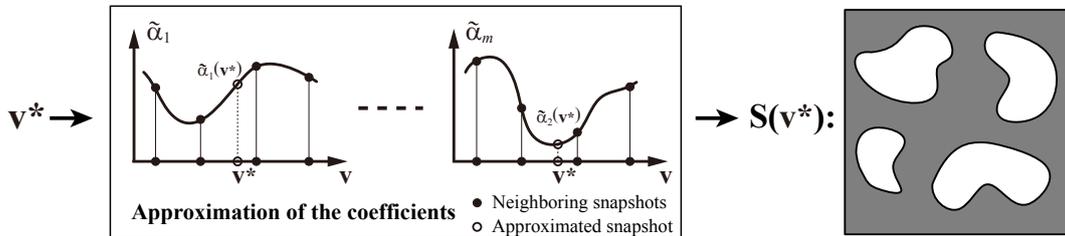


Figure 2: Flowchart of MLS-based microstructure parametrization.

When the parameters are unknown, the intrinsic dimensionality of the set of snapshots has to be detected in advance. Assume that the dimensionality is  $p$ , the projection coefficients in Eq. (1) are implicitly interrelated as:  $f_j(\alpha_1, \dots, \alpha_m) = 0$ ,  $j = 1, \dots, (m - p)$ . By performing *diffuse approximation*, the input parametric space can be reparametrized using pseudo parameters  $\boldsymbol{\eta} = [\eta_1, \dots, \eta_p]^T$ . The interpolation is developed in a similar manner as former case using the pseudo parameters:  $\tilde{\alpha}(\boldsymbol{\eta})$

Note that the coordinate system in which  $\boldsymbol{\eta}$  is defined is locally fixed. The overall interpolation technique here is nonlinear, and is constrained to produce only microstructure representations from an abstract manifold in shape space induced by learning.

## Reconstruction of the properties of heterogeneous materials

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Creation of more effective engineering constructions in different areas of production requires the development of new materials. At present time artificially created functionally gradient and composite materials are the most demanded. By production of structural elements of such materials, very important problem is to determine the mechanical properties. Traditional experimental methods for evaluating the properties of such materials in the framework of the homogeneity hypothesis are rather rude. Therefore it is necessary to develop the alternative nondestructive methods of identification of heterogeneous characteristics. These methods rely on the acoustic sounding methods and apparatus of the inverse problems.

In this paper two problems are examined. First problem is considered for determining three heterogeneous characteristics of the elastic rod: the Young modulus, shear modulus and density. The following scheme is proposed to determine the unknown functions: at the first stage, on the basis of combined analysis of longitudinal and bending oscillations, we determine the functions that characterize the laws of variation for the Young modulus and density; at the second stage, from analysis of torsional oscillations for a known density function, we determine the function characterizing the law of variation for the shear modulus. Second problem is the inverse problem of reconstruction the heterogeneous elastic modulus of the layer. Identification is made on the basis of data on the fields of displacements measured at the surface layer. With the help of integral Fourier transformation original problem is reduced to the solution of two unbound problems concerning averaged displacement characteristics.

For solving these problems an iterative process that uses consistent solution of Fredholm integral equations of the first and second kind is proposed [1, 2]. Solution of Fredholm integral equation of the first kind is an ill-posed problem. In this work for the construction of numerical solutions the Tikhonov regularization method is used. Several computational experiments in the problems of identifying of the mechanical characteristics of the rod and the layer for different types of heterogeneities were carried out. The experimental results showed that the proposed method can effectively restore smooth heterogeneity laws. Computational experiments for finding the singular values of the operator in the equation of Fredholm of the first kind were carried out. It is shown that the set of singular values can be divided into two subsets. The number of singular values, which are in the first subset, is associated with a number of frequencies of observation. The number of singular values in the second subset is defined by the dimension of the discretized problem.

**Acknowledgments** This work was supported by the President of Russian Federation (grant MK-6213.2012.1).

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## Inverse approach to the design of controlled cooling of rails

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Improvement of the rails wear resistance is important for passengers safety and for materials saving. For pearlitic steels the wear resistance depends on hardness, which is controlled by microstructural parameters: pearlite grains size, colony size and interlamellar spacing [1]. Required properties of the are obtained by heat treatment after rolling [2], in which head is subject to subsequent cycles of cooling in air and in the polymer solution. The objective of the paper was to develop computer system, which will support design of heat treatment of rails.

The model describes kinetics of transformation and morphology of pearlite. Transformation begins with nucleation of cementite lamellas at the carbon concentrations on grain boundaries. Carbon diffuses from the austenite (0.74%C) to the cementite (6.67%C) and ferrite nucleates in the areas, which which had lost carbon. During ferrite grain growth carbon is pushed to austenite, which leads to the formation of cementite plates, and the whole cycle is repeated. At the higher undercoolings the distance of carbon diffusion is small and the finer pearlite is formed, which increases the hardness and strength of steel.

The model, which calculates parameters of the pearlitic microstructure, was combined with the FE code, which simulates temperature during cooling. This multiscale model was used to solve direct problem formulated as operator equation  $\mathbf{K}\mathbf{x} = \mathbf{y}$ , where:  $\mathbf{K}$  - operator,  $\mathbf{x}$  - cooling process parameters,  $\mathbf{y}$  - parameters describing pearlitic microstructure.

The cooling cycle composed of 3 cycles of cooling in air and in the polymer solution was considered. The inverse task was formulated as follows: Given  $\mathbf{y}$  and an operator  $\mathbf{K} \Rightarrow$  solve  $\mathbf{K}\mathbf{x} = \mathbf{y}$  for  $\mathbf{x}$ . In other words, calculate the parameters of the thermal cycle, which will give the required microstructure of the rail head. Since finding  $\mathbf{K}^{-1}$  is not possible, the problem was solved using optimization technique. The microstructural parameters, which are included in the objective function, were interlammellar spacing and average hardness. The following schedule was obtained: 10s A  $\Rightarrow$  32s P  $\Rightarrow$  15s A  $\Rightarrow$  12s P  $\Rightarrow$  15s A  $\Rightarrow$  8s P (A - air, P - solution).

**Acknowledgments:** Financial support of the NCBiR, project no. R07 0006 10, is acknowledged..

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Illustration of the one cycle of the cooling process is shown in Fig. 2. Scheme of the multiscale model used to solve direct problem is shown in Fig. 3. Parameters, which are exchanged between macro and micro scale are given in the arrows. Equations describing microstructural parameters, which further allow to calculated mechanical properties, are also give in Fig. 3.

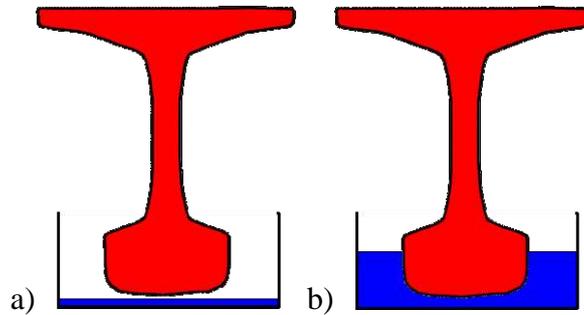


Fig. 2. Schematic illustration of one cycle of controlled cooling of rail head, a) head above the level of the solution, b) head immersed in the solution.

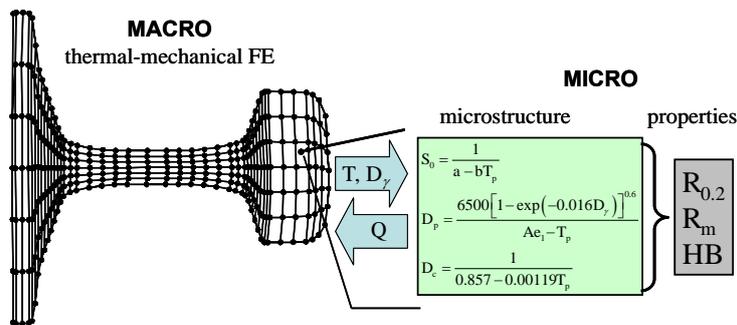


Fig. 3. Schematic illustration of the multiscale approach used in the present work.

Optimization was performed using simplex method. Selected examples of distributions of microstructural parameters and mechanical properties obtained for the optimal cooling schedule are shown in Fig.4.

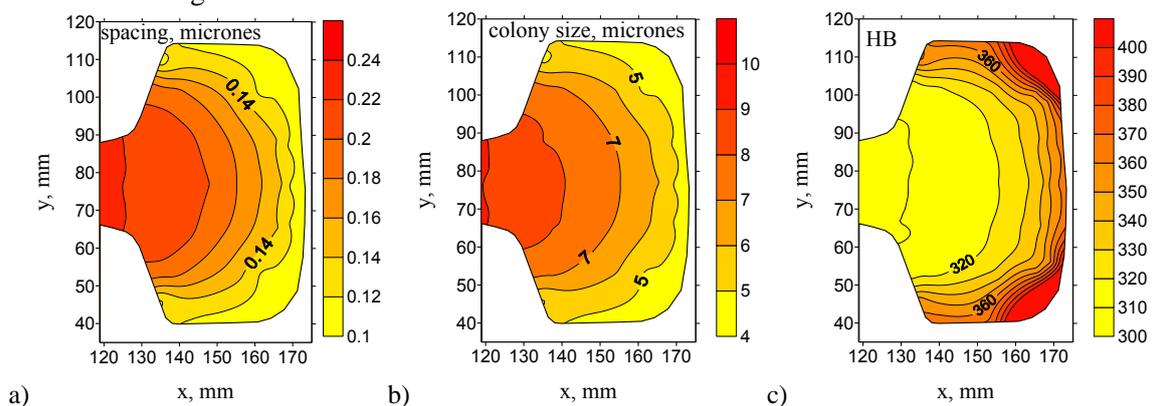


Fig. 4. Calculated distribution of the interlamellar spacing (a), pearlite colony size (b) and hardness (c) at the cross section of the rail head after the optimal cooling schedule.

## The Free Material Design leads to the Locking Material Problem

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The problem of maximization of the overall stiffness of a structure can be formulated in several manners. One can assume that two or three materials are at our disposal, the amount of them being given. The aim is to find the optimal placement of these materials. Majority of papers in this vein are targeted at the shape design and base on the relaxation by homogenization method. The alternative method is FMD (free material design approach) where all the anisotropic properties are treated as design variables of non-uniform distribution, see e.g. [1-3]. The Hooke tensor encompasses all these properties. In FMD no point-wise conditions are imposed on this tensor, instead an integral isoperimetric condition is assumed. The present paper puts forward a new version of the FMD in which the Kelvin moduli and the eigen-states are design variables. We refer here to the theory of spectral decomposition of Hooke's tensor. The isoperimetric condition is imposed on the trace of the Hooke tensor, the trace being equal to the sum of the Kelvin moduli. Both a single load case and multiple load case are dealt with. A special attention is put on the two loading conditions. The merit function is the weighted sum of the total compliances corresponding to the loading conditions. The departure point is stress-based. This makes the formulation a minimum problem with respect to: statically admissible stress fields and design variables. The problem discussed brings about local minimization problems which turn out to be solvable by relatively elementary methods. By solving the local problems explicitly, the main problem is rearranged to the stress based form of an equilibrium problem of a hypothetical body with locking properties. These equations are inverted to the primal form thus disclosing the locking loci. By using SVD decomposition and un-constrained optimization methods the stress based formulation is numerically solved. The aim of the article is to discuss the numerically found optimal solutions for various problems in 3D and 2D for a single load case (see [4]) and multiple load cases.

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## Evaluation of possibility of application of various metamodels to inverse analysis of material tests

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Continuous progress in numerical modelling of metals processing is observed. The accuracy of numerical simulations depends mainly on the correctness of the description of boundary conditions and properties of processed materials. The latter problem is the subject of the work. A number of material models can be found in the scientific literature. Potential extensive predictive capabilities of these models are useful only when proper identification was performed on the basis of experiments. Interpretation of results of various tests is the main part of the identification, which usually uses inverse analysis with FE simulation of the test and allows to eliminate influence of various disturbances, such as friction or heating due to deformation or phase transformation. Various inverse algorithms were developed in 1990s [1,2]. The published results show that this method improves accuracy of interpretation of experimental tests. On the other hand, in a conventional inverse analysis FE model is combined with optimization, what involves long computing times. Therefore, a lot of effort is put into searching for more efficient inverse calculations. Application of the metamodel in the optimization was proposed in [3]. The metamodel substituted the FE solution and significantly reduced the computing costs.

The objective of the work was exploring capabilities of various metamodels as direct problem models in inverse analyses of material tests. Two types of tests were investigated: plastometric test used to identify rheological model and dilatometric test used to identify phase transition model. Material models of various complexity of formulation were considered. Rheological models accounting for an influence of temperature, strain and strain rate (4 coefficients) and additionally for softening due to recrystallization (5 coefficients) and for softening and saturation (7 coefficients) were investigated. Phase transformation models describing kinetics of ferritic, pearlitic, bainitic and martensitic transformations in steels (up to 23 coefficients) were considered, as well. Kriging approximation and artificial neural networks were used as metamodels. Following aspects were evaluated: accuracy of metamodels depending on a number of training data, capability to be used in the optimization procedure depending on the complexity of the model and accuracy of the inverse solution with the metamodel were made. The use of metamodelling approach allows reduction of computational time of the inverse analysis. Moreover, performed analysis shows, that Kriging metamodelling technique requires much less number of the experimental points than ANN metamodelling to achieve good accuracy.

**Acknowledgments:** Financial assistance of the NCN, project N N508 629 740, is acknowledged.

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The schematic flow chart of the inverse analysis for plastometric test with the metamodel is shown in Fig. 1 [3]. Interpretation of plastometric tests was performed first. Typical responses of metallic materials to deformation are shown in Fig. 2, together with the equations which allow to describe these responses. Identification of coefficients in these equations on the basis of the inverse analysis with the metamodel was the objective of the paper.

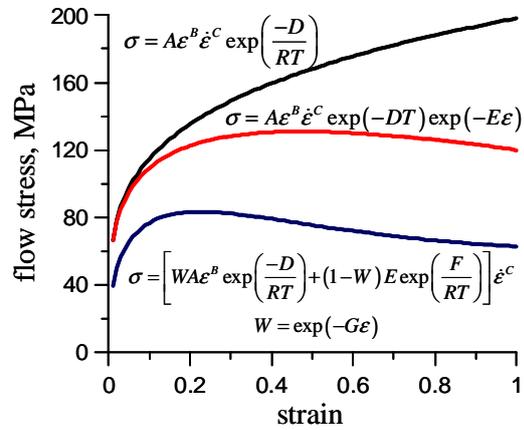
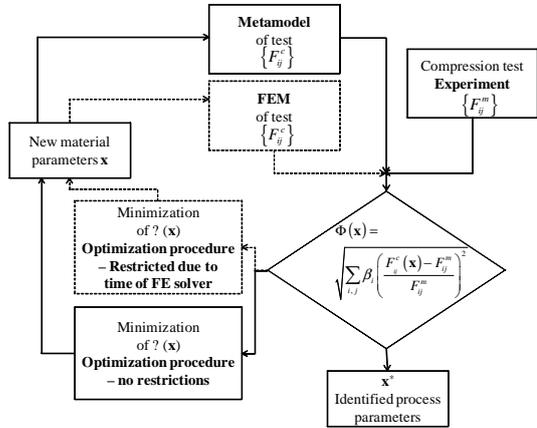


Fig. 1: Flow chart of the inverse algorithm with metamodel (solid line) and FE model (dotted line);

Fig. 1: Typical responses of metals subjected to deformation and equations used to describe these responses.

Artificial neural network and kriging approximation were used as metamodels. Data for training the metamodels were generated using FE code developed by the Authors.

A number of various materials including steels and non-ferrous alloys were tested and inverse analysis of results was performed. Very good results were obtained for the simple function with 4 coefficients. ANN performed better for 5 coefficients, see selected results of comparison of flow stress of bainitic steel predicted by the conventional inverse approach with the FE model and by the inverse approach with the metamodel shown in Fig. 3.

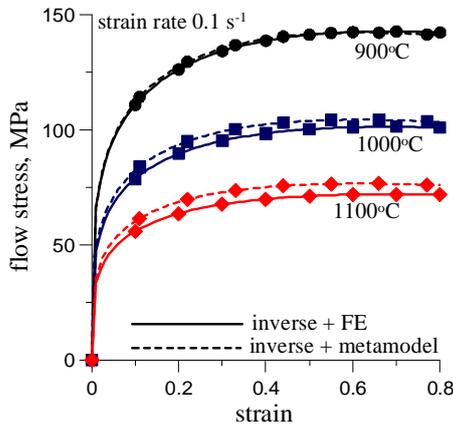


Fig. 3: Flow stress calculated by inverse with FE and with metamodel

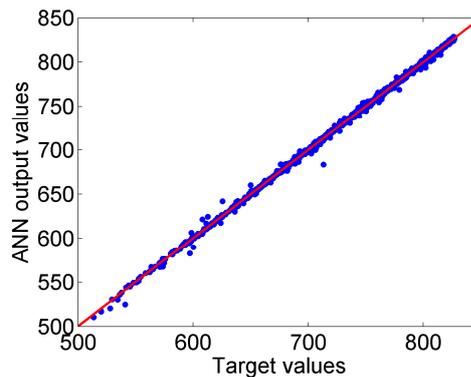


Fig. 4: Results of training of the ANN for start temperature of ferritic transformation

Metamodels were applied next to identification of phase transformation model. Separate metamodels were developed for temperatures of start and end of all transformations and for volume fractions of phases. Dilatometric tests were performed for various steels and metamodels were trained (Fig.4).

## **Dedicated computer system for comparison of ANN and Kriging-based metamodels for identification of material models.**

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Conventional inverse analysis based on sophisticated numerical models uses time consuming procedures and costly computations. Therefore, approach based on metamodels implemented by using artificial intelligence methods was developed [1]. The most widely used solutions for this purposes are Artificial Neural Networks (ANN) and Kriging, which offer satisfactory reliability and acceptable computing time. However, the reliability strongly depends on number of records used in teaching procedures. The main objective of the project is to compare quality of results returned by procedure of inverse analysis based on variously taught metamodels. Capabilities of metamodels as direct problem models in inverse analyses of material tests was explored in [2]. Testing of the approaches based on various techniques (ANN, Kriging) and evaluation their applicability depending on the type and the complexity of the material model is a complex task. Therefore, the objective of the present work was to support selection and training of the metamodel for a particular application, eg. flow stress or phase transformation model. A dedicated computer system, which supports the comparison of selected metamodels, was proposed. This system allows import of different metamodels and their application in the inverse procedure automatically. The computer system was designed as multiuser and multi-access application on the basis of the Client-Server architecture, where server side consists only of database engine and its procedures. The database is composed of several tables, which join together information about material experiments, models and metamodels. Such solution influences directly functionality of Graphical User Interface (GUI) allowing users to define their projects through selection of the type of experimental data with measurements originated from thermo-mechanical testing devices e.g. from Gleeble simulation or dilatometer. System is designed on the basis of the reflection mechanism in the .NET platform. This platform allows dynamic extension of new functionalities to the system. In consequence, the system has flexible construction, which enables easy implementation of new modules in the form of external libraries (plugins). These programs, implemented as dynamic linked libraries (dlls), can have very wide range of applications – they may be responsible for parsing of input and output files, analysis of experimental data, filtering and, finally, metamodelling. The plugins, accordingly to the current requirements, can be used from the database or implemented by a user, which allows further extension of the system functionality. This solution allows to add new module of reading measurement data, new filter, as well as new metamodel. All plugins are integrated in the form of complex optimization loop facilitating performance of the inverse analysis with different algorithms, different values of their parameters and different data sets.

**Acknowledgments:** Financial assistance of the NCN, project N N508 629 740, is acknowledged.

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It was shown in [1] that accuracy of the inverse analysis with metamodel is close to that obtained from the conventional inverse approach with FE used as a direct problem model. Very good agreement between the two solutions was obtained for a large number of different materials, see for example presented in Fig. 1 comparison of the flow stress models for low alloyed steel identified using these two approaches. The computing times for the metamodel are few orders of magnitude shorter than for the FE code. On the other hand, selection of the best metamodel for a particular application is a complex task [2].

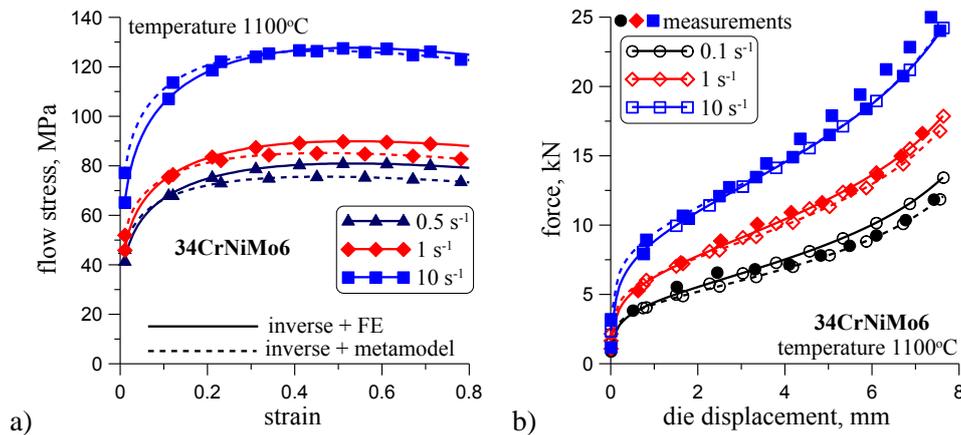


Fig. 1. Flow stress calculated by inverse with FE and with metamodel (a) and comparison of compression force measured (full symbols) and calculated by the FE model with flow stress determined by the inverse technique with the metamodel (solid line) and FE (dotted lines) (b).

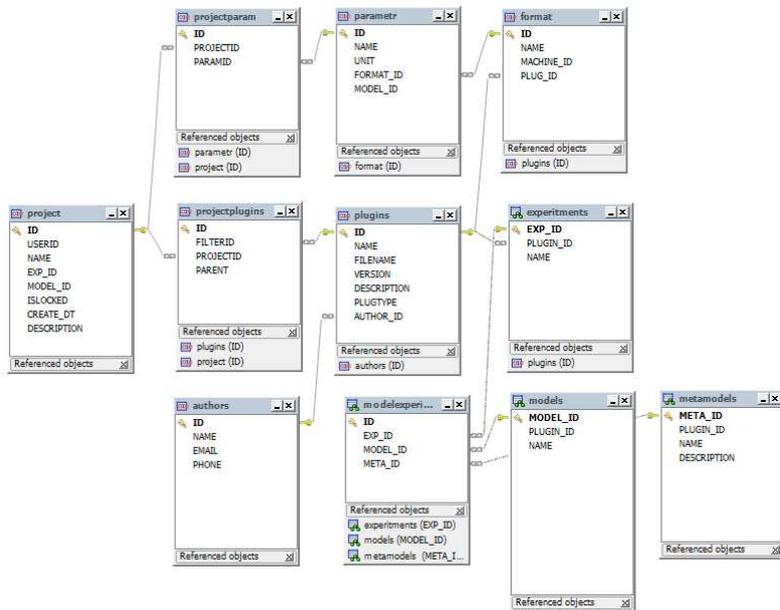


Fig.2. Figure 3. Database diagram of the proposed computer system

To enable efficient selection and training of the metamodel and fast data processing, a computer system was developed. It was designed as multiuser and multi-access application on the basis of the Client-Server architecture, where server side consists only of database engine and its procedures. The database is composed of several tables, as it is shown in Fig. 2. The most important elements only are shown in this figure. Results of tests performed for a variety of materials, metamodels and training procedures are presented in the paper.



## Session 9

# Phase transitions, twinning, and shape memory effects



## A mesoscopic thermomechanically-coupled model for thin-film shape-memory alloys by dimension reduction and scale transition

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Shape-memory alloys (SMAs) are well-known for their extraordinary response to mechanical and thermal loads—this being due to diffusionless solid-to-solid phase transitions—and the effects can be described on different scales of view, from macro through the so-called meso to microscopic scale. As the aforementioned phase transition stems from mere crystallographic lattice changes, the sizes of SMA components can be significantly reduced without affecting their functionality, exposing major power-weight ratio. SMA thin films are widely used as microactuators in different micro-electro-mechanical devices.

A *thermo-mechanically coupled* model for SMA evolution on the *mesoscopic scale* has been proposed only very recently by Benešová and Roubíček [2]. We develop [1] an analogous model in the *thin-film setting* in two steps. To our best knowledge this seems to be the first mathematically rigorous model of a thin film SMA taking into account thermodynamical effects.

Within the framework of generalized standard solids, first, we constitutively define the *bulk* Gibbs free energy and the dissipation potentials describing a *micro-scale* regime. Then we perform a *dimension reduction* procedure when limiting the thickness of the specimen to zero, obtaining thus a *microscopic thin-film* model for SMAs. Due to the considered interfacial-energy term in the Gibbs free energy, the deformation of the film is described also by an *additional Cosserat vector*—accounting for the deformation of the cross section—in accord with the results of Bhattacharya and James [3].

As a second step, we upscale the view by a *scale transition* from micro to meso-scale when neglecting interfacial-energy terms and pinning effect. Consequently, a *mesoscopic thin-film* model emerges described in terms of parameterized measures, more precisely, a gradient Young measure related to the in-plane deformation and a Young measure associated to the Cosserat vector. Although we loose the boundedness of the microstructure width, all the important features related to the interplay between microstructure formation, dissipation and heat conduction in the specimen remain included.

This work may be regarded as a continuation of the work put forth on the ICMM2 conference [4].

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## Quantitative elastoplastic phase field model for hydride blister formation in zirconium alloys

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A hydride blister refers to a volume of 100% solid hydrides, or very high density of solid hydrides formed in zirconium alloys during service. In service, these metals are susceptible to a slow corrosion process that leads to a gradual pickup of hydrogen from environment. If a temperature gradient exists in metals, hydride blisters may form preferentially near the cooler part of the metals, such as the surface of metals. Because of the brittleness of these hydrides, the original strength of the alloys can be reduced by orders of magnitude, and fracture through these hydrides may occur, which can result in catastrophic failure of the structures. Historically, the damages caused by hydride blisters had cost billions of dollars to repair. In this work, we need to develop a new free energy functional of the system that is temperature dependent as well as quantitative. Phase field models in literature can seldom simulate microstructure evolutions quantitatively. This is due to the fact that the free energy functional of the system at non-equilibrium state and many parameters of the system must be accurately known. By definition, the system is not at the equilibrium state at the beginning of the simulation. To construct the free energy functional, we started from the phase diagram of Zr-H system, and developed a double-well free energy functional that has two minima, (1) at terminal solid solubility (TSS) of H in Zr and (2) at the equilibrium concentration of H in Zr hydride. This new functional is a function of temperature and it is quantitative. This functional was tested at dilute solution limit and it reproduced the correct and quantitative formulation based on thermodynamic theory. Then, both finite element method and finite difference method were being applied to simulate single hydride growth by using the developed free energy functional. Preliminary results of such simulations are very encouraging.

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## A constitutive model for phase transitions in Si incorporating nonlinear elastic behavior at finite strain.

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If subjected to pressure or contact loading conditions, Silicon (Si) undergoes a series of stress-driven phase transitions. During release of the applied loading, further phase transitions take place. Evidence of up to 11 different crystalline phases of Si can be found in literature [3]. When ranked by the accompanying transformation strain, the first and most important is the semiconductor-to-metal (SM) transition ( $\alpha$ -Si  $\rightarrow$   $\beta$ -Si), occurring at approx.  $p_\beta = 11.6$  GPa hydrostatic pressure and leading to a change in volume of about 20.4%. From comparison of indentation to diamond-anvil-cell experiments, it is known that the transition pressure strongly depends on the stress triaxiality. Upon rapid unloading, a metal-to-amorphous (MA) transition takes place and the  $\beta$ -Si phase continuously transforms into amorphous Si (a-Si). Most models available in the literature do not adequately reproduce this behavior.

A phenomenological, thermomechanical constitutive model published by the authors in 2012 [2] and presented in a modified version at [1], captures the SM and MA phase transitions and was successfully applied to the simulation of nanoindentation. All previous modeling efforts - including our own - were focused on an adequate description of the transformation behavior. The elastic response of the material has hardly received any attention. Comparing the bulk modulus of Si ( $K = 100$  GPa) to the transition pressure  $p_\beta$ , it becomes evident that the material experiences well over 10% *elastic* strain prior to the onset of phase transition. To appropriately capture the elastic response in axisymmetric simulations we implemented an isotropic non-linear elastic law based on the universal binding energy relation [5]. However, as pointed out in [4], neglecting the crystallographic effects in (3D) simulations of Si indentation may be inappropriate. Hence, an elastic law incorporating the full cubic symmetry of Si single crystals [6] has been included into the constitutive model for phase transitions.

Finite element simulations of nanoindentation in Si illustrate the effect of the different elastic behaviors on the size of the transformation zone as well as the influence of elastic anisotropy on the residual stress distribution.

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# Effective Thermo-elastic and Plastic Flow Properties of 3-D Fe-Mn-C Steel Microstructure Simulated by the Phase-field Method via Homogenization Techniques

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A multi-scale approach, based on either the asymptotic homogenization method, suitable for heterogeneous materials with periodic microstructures, or virtual tests [1], is applied here to predict the effective thermo-elastic and plastic flow properties of 3D steel microstructures, calculated by phase-field simulations. The multiphase-field model allows the calculation of the microstructure evolution in multicomponent and multiphase materials undergoing solid state phase transformations including linear elasticity [2]. Thermodynamic properties of the individual phases are taken from thermodynamic databases. The austenite to ferrite phase transformation during cooling of a Fe-0.17wt%Mn-0.023wt%C steel disc has been calculated. The impact of different nucleation schemes on the transformation kinetics is determined for representative volumes. Temperature and concentration dependent thermo-elastic properties are evaluated for each phase [3]. In order to predict effective mechanical properties, geometrical information about the individual grains and their orientations are transferred to the homogenization tool [4]. Effective cubic Young and shear modules and Poisson coefficients are predicted for different ferrite volume fractions. A dilatometer curve is also derived as function of the temperature. It takes into account the combined effects of the thermal expansion and the volume expansion of the grains during phase transformation. By virtual testing, the evolution of the plastic flow curves with the ferrite volume fraction is also predicted. Finally, the influence of the size and shape of the RVE on the effective thermo-elastic and flow properties is discussed.

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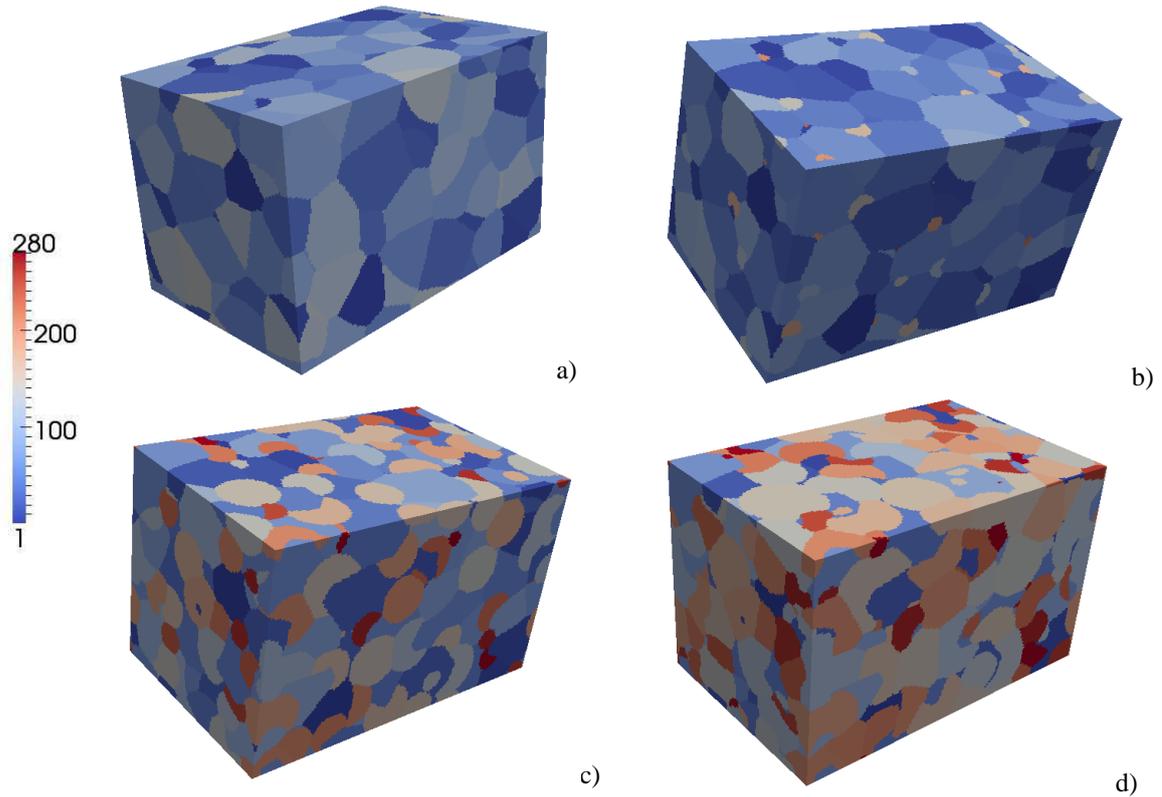


Figure 1: Sequence of simulated steel microstructures: Austenitic grains are blue and ferritic ones are red: a)  $t=0$  s,  $T=1000^{\circ}\text{C}$ ,  $f_{\text{fer}}=0\%$ ; b)  $t=40$  s,  $T=849.9^{\circ}\text{C}$ ,  $f_{\text{fer}}=2.78\%$ ; c)  $t=46$  s,  $T=832.7^{\circ}\text{C}$ ,  $f_{\text{fer}}=42.14\%$ ; d)  $t=50$  s,  $T=822.1^{\circ}\text{C}$ ,  $f_{\text{fer}}=80.3\%$ .

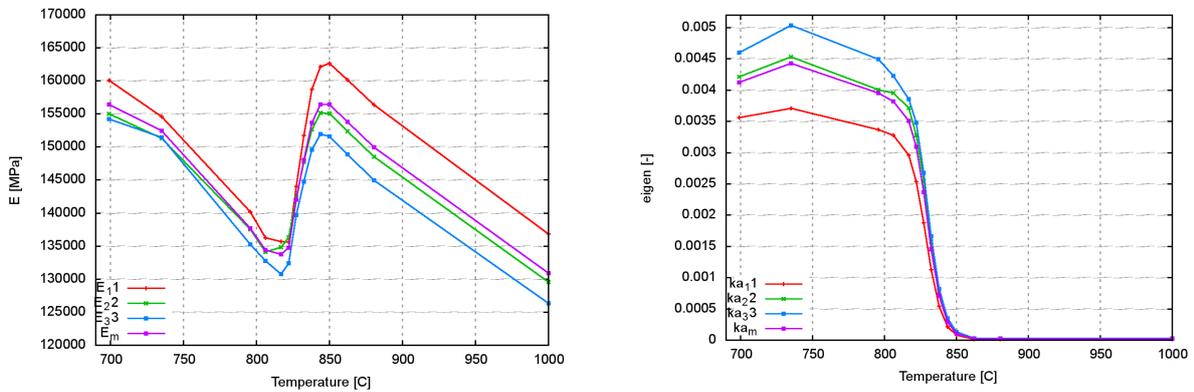


Figure 2: Effective Young moduli (left) and the generalized eigenstrains of the polycrystal as function of the temperature.

## Microscale Modeling of Multiple and Higher Order Deformation Twinning

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Deformation twinning [3] is a deformation mechanism displayed by most of the crystalline materials, such as Ti, Mg, and TWIP steels [7, 8]. It has a strong impact on the microstructure and the texture, due to grain refinement and an accompanying lattice reorientation. A reliable prediction of the material response requires the understanding of the underlying physics of the microstructural evolution. The higher order twinning phenomena and multiple twin system activation of hcp material (Ti) are modeled on the grain scale by the minimum elastic strain energy approach. As a starting point, the convex elastic strain energy ( $w_{\text{parent}}$ ) of a single crystal is mapped to the potential first order twins ( $w_{\text{tw}1}, w_{\text{tw}2}, \dots, w_{\text{tw}n}$ ) by the isomorphy condition [2] between parent and twinned material [5, 6]. The overall strain energy is composed as  $w_{\text{min}} = \min(w_{\text{parent}}, w_{\text{tw}1}, w_{\text{tw}2}, \dots, w_{\text{tw}n})$  following Ball and James [1]. The result is a non-convex strain energy. Two different transformations, one for the crystal orientation and another for a simple shear deformation, are introduced corresponding to each twin operation. These enable us to elucidate the multiple twin system activation. The non-convex elastic strain energy has to be updated depending on the activated twin variant to incorporate higher order twinning. However, the minimum elastic strain energy approach faces its limitation because of the invariance of the elastic strain energy for conjugate compound twins [4]. An introduced projection criterion can successfully identify the preferred twinning mode. Once the activated twin configuration is recognized, the successive update mechanism allows for the modeling of higher order twinning at each material point. For simplicity, a deformation controlled test is performed on a single crystal. The model can predict the compression twin  $\{11\bar{2}2\}$  of hcp (Ti) material along with a rarely observed compression twin  $\{11\bar{2}4\}$ . It also successfully predicts the tension twin  $\{10\bar{1}2\}$  of Ti.

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## Finite strain model of shape memory polymers

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Development of a finite strain model of shape memory polymers (SMP) as well as its identification and validation will be presented. The main feature of the considered polymers is thermally-induced change of material response from the rubbery one at high temperatures to a glassy-one at low temperatures, the glass transition temperature  $T_g$  being the characteristic value separating two regimes [4]. Such behavior enables a variety of applications.

A lot of work has been done to characterize and develop the possible application of SMP, however constitutive modelling of these materials is not yet at mature stage and only a few models exist. In general two types of approaches to model SMP can be distinguished: phase transition approach and thermoviscoelastic approach, cf. [1]. Our model is of the first type.

At a given temperature  $T$ , SMP is assumed to be composed of two phases: rubbery one and glassy one. The volume fraction of each phase is postulated as a function of temperature. Constitutive relations are formulated separately for each phase and the resulting behavior of the material depends on the actual material composition. At this stage simple Voigt-type averaging scheme is used, i.e. each phase is supposed to share the same deformation gradient being equal to the macroscopic one. For the rubbery phase the hyperelastic Aruda-Boyce eight-chain model is assumed, while the glassy phase is assumed to be hyperelastic-viscoplastic. The formulated model uses the concepts outlined in [2], however the description of viscoplastic deformations of glassy phase is modified in line with the 1D 'power law-type' proposal of [3].

The model will be validated with use of experiments performed for polyurethane SMP including dynamical mechanical analysis (DMA), uniaxial tension tests at different temperatures and strain rates, as well as cyclic loading-unloading tension tests. First results indicate that  $T_g$  for this material is 292°K, while material properties vary between  $T_g \pm 30^\circ\text{K}$ . This observation has been used to estimate the relation between the temperature and the volume fraction of the phases. Using this relation preliminary identification of material parameters has been performed on the basis of uniaxial loading-unloading tension tests performed at room temperature and three strain rates.

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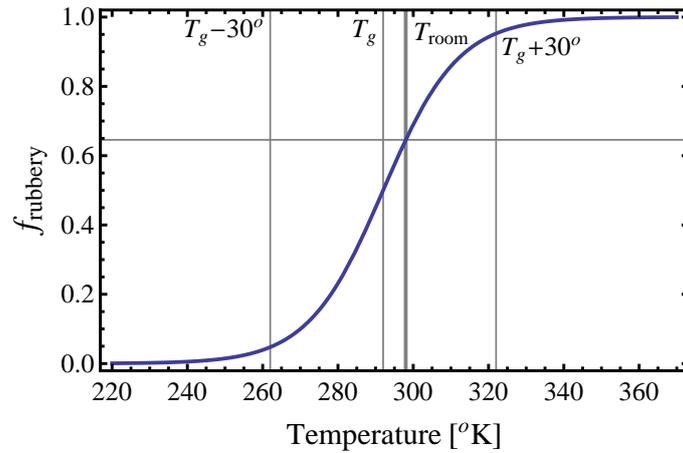


Figure 1: Assumed dependence of volume fraction of rubbery phase  $f_{rubbery}$  ( $f_{glassy} = 1 - f_{rubbery}$ ) on temperature: glass transition temperature  $T_g = 292^\circ\text{K}$ , room temperature  $T_{room} = 298^\circ\text{K}$ . Estimated volume fraction of rubbery phase at  $T_{room}$ ,  $f_{rubbery}(T_{room}) \cong 0.65$ .

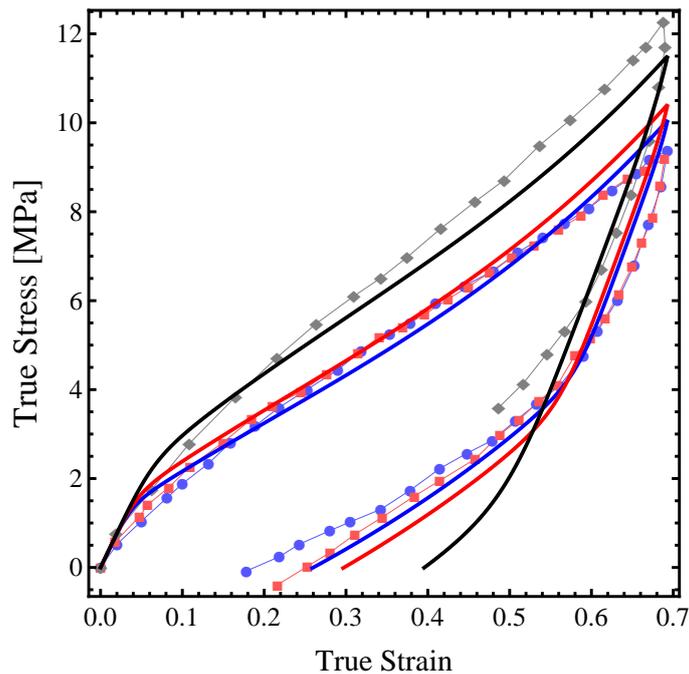


Figure 2: Uniaxial loading-unloading tension tests at room temperature with three extension rates ( $\dot{u}/L_o$ ) [1/s]: 0.005 - blue, 0.01 - red, 0.05 - black; experiment - lines with markers, modelling - continuous lines. It was observed that the process can be treated as a isothermal one for the applied strain rates.

Session 10

# Granular materials and particle systems



## Particle size effect in highly-filled particulate composites: multiscale damage modelling with a “Morphological Approach”

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This work is devoted to the mechanical behaviour of highly-filled particulate composites such as propellant-like materials. Composed of an elastomeric matrix and an important volume fraction of reactive particles (more than 60%), the behaviour of these materials needs to be well-known in order to avoid possible explosion. Its complex morphology and its strongly non-linear behaviour (large strains undergone by the matrix, grain/matrix interfacial damage,...) led to the progressive development of a multiscale method in order to estimate homogenized response and to get the local mechanical fields. This technique, the “Morphological Approach” (M.A.), is based on an explicit geometric representation of the microstructure and a direct solving without any prior linearization of local non-linear constitutive laws.

In order to evaluate the predictive capacities of the M.A. regarding particle size effect and interaction between particles, a study was performed considering an isotropic linear elastic behaviour for the constituents. Particle size plays an important role in damage chronology: debonding occurs preferentially on large particles before occurring on smaller ones [1]. Debonding phenomenology is also influenced by matrix volume fraction: the lower it is (important particle volume fraction), the earlier the first debonding occurs [2].

After a presentation of theoretical elements about the M.A. formulated in linear elasticity with interface debonding [3], results of calculations on simple periodic cells will be first exposed. The same type of evaluation is performed on random monomodal microstructures. A more complex random bimodal microstructure is also considered: it allows the access to two different sizes of particles into the same volume. The simulated effects (particle size effect and interaction between particles) are consistent with results of the literature [2].

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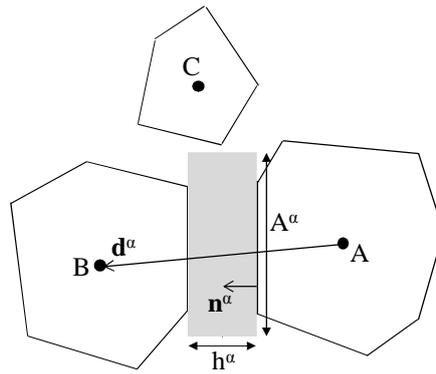


Fig. 1. Microstructure schematization: morphological parameters

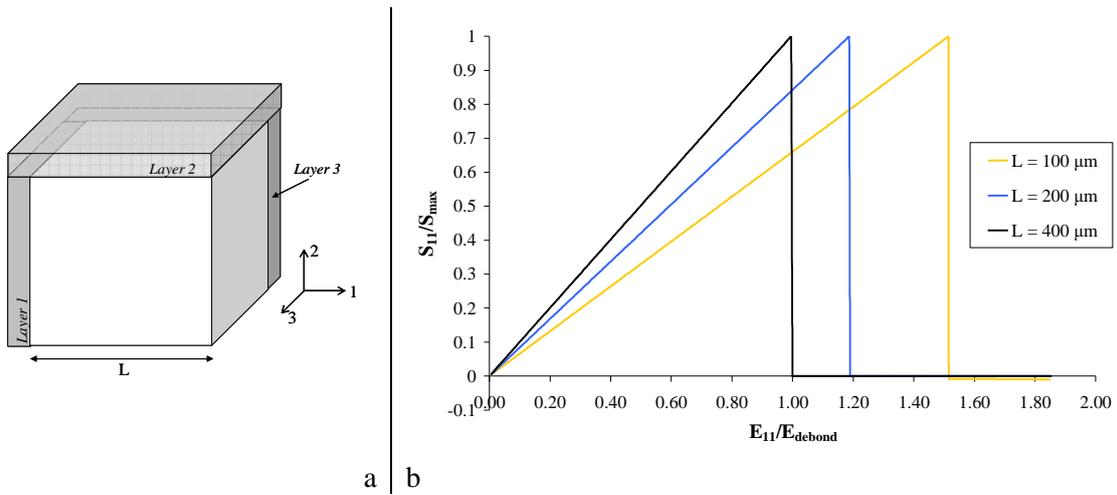


Fig. 2. Periodic cell (a) and particle size effect on a periodic cell (b - matrix volume fraction  $c = 25\%$ )

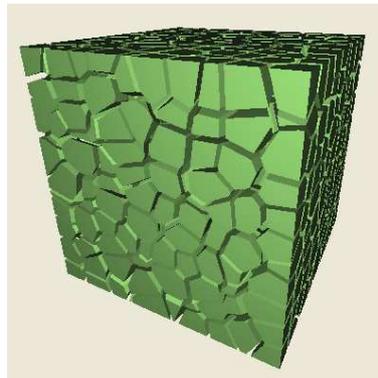


Fig. 3. Random monomodal numerically generated microstructure (matrix volume fraction  $c = 40\%$ )

## **Influence of parameter evaluation on failure mode in discrete element models of rock materials**

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Numerical programs employing the discrete element method (DEM) have achieved a status of a standard analysis tool in geomechanics. However, it seems that there is a lack of full understanding of many micromechanical mechanisms which are inherent in the DEM and influence macroscopic behaviour of DEM models. In the DEM, a material is represented by an assembly of particles interacting among one another with contact forces. Interparticle interaction models can be based on different types of contact laws incorporating different physical effects such as elasticity, viscosity, damage and friction. Constitutive models for rocks must also take into account cohesive interaction between particles. Even using a simple model such as the linear elastic perfectly brittle model employed in the present work, a complex behaviour at the macroscopic scale can be obtained. Depending on the set of local parameters a more brittle or more ductile macroscopic behaviour can be obtained.

Numerical studies of effect of parameter evaluation on a failure mode in discrete element models of rock materials have been performed. These studies consisted in simulation of the uniaxial compression test using a cylindrical specimen with particle size distributions characterized by high degree of heterogeneity. Two different approaches to evaluation of micromechanical constitutive parameters have been compared. In the first approach, the contact stiffness and strength parameters depend on the local particle size, while in the second approach, global uniform contact parameters are assumed for all the contacting pairs in function of average geometric measures characterizing the particle assembly.

Significant differences in the failure pattern have been observed. The uniform constitutive parameters result in localized brittle-like fractures, while a distributed damage typical for a ductile failure is obtained for the model with local size-dependent parameters. The difference in the failure patterns predicted for the two models can be explained analysing influence of heterogeneity of material properties on deformation behaviour.

The investigated discrete element models have been implemented in the discrete element program DEMPack [1]. Detailed results of numerical studies have been published in Ref. [2].

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## Experimental study of dense bi-disperse granular flow through a pipe with a ninety degree bend

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The flow of dense granular materials is important in several industrial applications, particularly for their transport. While most granular material in industrial applications consists of irregular particles, fundamental understanding of the flow of regularly shaped particles is still lacking. The behavior of granular matter is unlike that of a single phase material. Depending on the energy, the grains exhibit solid-like (e.g. a sand pile) [1], liquid-like (e.g. poured from a silo) [2] or a gas-like behavior (e.g. when strongly agitated) [3]. Theoretical studies based on kinetic theory for gas-like [4] and soil mechanics for slow plastic flows for solid-like behavior [5] have been proposed. However, there has been comparatively little work on liquid-like behavior of granular materials. In this work we study the flow a dense granular material comprising of steel balls through a pipe through experiments. In particular, we focus our study on the effect of flow rates of bi-disperse mixtures of spherical steel balls.

The experimental setup used in this study consists of an L-shaped acrylic pipe of circular cross section. The long section of the pipe is 2 m in length and the short section is 50 cm long. The inner diameter of the pipe is 5 cm. Large steel balls of 1/4 inch diameter are mixed with two different sizes of steel balls (1/8 inch and 1/16 inch) to obtain two bi-disperse mixtures. The long section of the pipe is kept close to vertical and the pipe is filled with steel balls just past the elbow. The time taken to empty the tube is measured by analyzing video recordings of the flow. The mass flow rate is normalized with respect to the flow rate of a freely falling column of same height.

The mass and number flow rates of the mixture of 1/4 inch and 1/8 inch steel balls and the mixture of 1/4 inch and 1/16 inch steel balls are found to increase with increasing mass-ratios of the smaller balls (as shown in Fig. 1 and Fig. 2). On the other hand, the packing fraction of the mixture of 1/4 inch and 1/8 inch steel balls decreases with increasing mass-ratios of the smaller balls whereas the packing fraction of the mixture of 1/4 inch and 1/16 inch steel balls is found to increase with increasing mass-ratios of the smaller balls. The presence of the 1/16 inch steel balls which are larger than the interstitial voids of the tetrahedral structure frustrates the formation of close packed regions and this decreases packing fraction with increase in mass fraction of the smaller balls. This results in a larger flow rate at larger mass fractions of the smaller balls. When the smaller balls are smaller than the interstitial voids, they do not break the packing, and the packing fraction increases with mass fraction of small balls. In this case, there is a nominal increase in flowrate (Figure 2). Finally, we present the dependence of the mass flow rate of the mixture as a function of the orientation of the pipe (Fig. 3). The mass flow rate is found to increase when the angle of the inlet to the elbow increased with respect to the vertical. However, the mass flow rate decrease for large orientation angles due to back pressure of balls in the short arm of the pipe.

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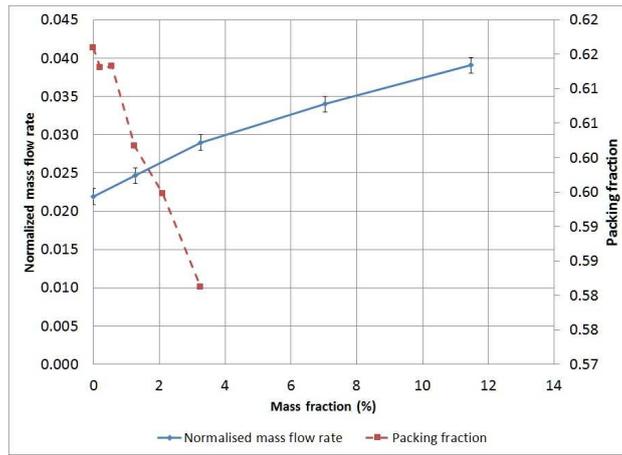


Figure 1: Flow rate and packing fractions of different mass fractions of bi-disperse mixtures with 1/8 inch balls

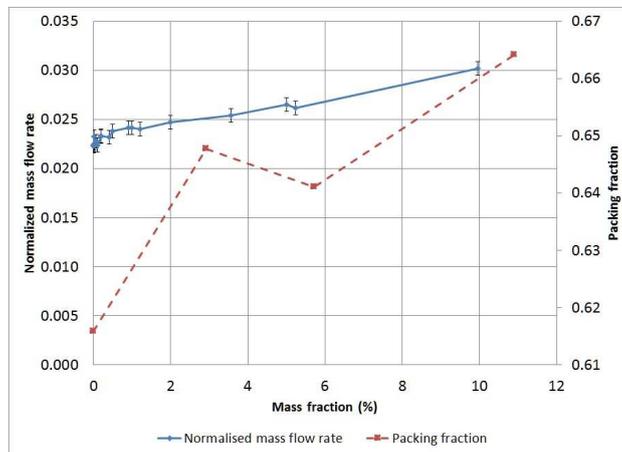


Figure 2: Flow rate and packing fractions of different mass fractions of bi-disperse mixtures with 1/16 inch balls

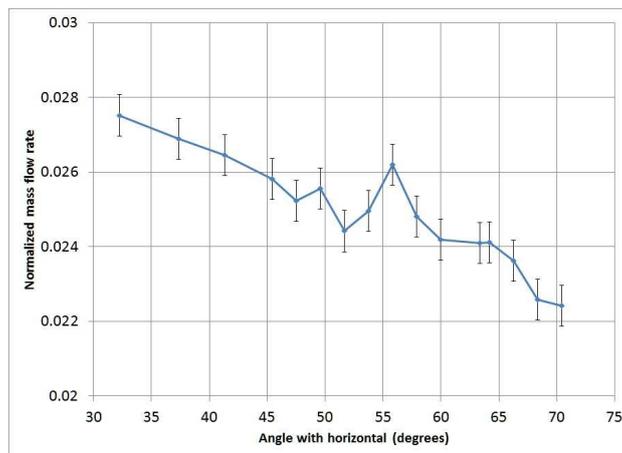


Figure 3: Orientation of the long section from the vertical versus the mass flow rate for bi-disperse mixtures with 1/16 inch balls

## **Effect of particle size distribution on the energy dissipation and mechanical response of packings of spheres under compressive loading**

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Many industries are involved nowadays in transporting, storing and processing materials in granular form. These include agriculture and food industry which rely on conveying and handling grains, seeds and their products, pharmaceutical and cosmetics industries handling pills and powders and building industry dealing with mineral and chemical powders. The majority of particle packings involved in industrial processes is composed of particles of a broad range of sizes that determines geometric and mechanical properties of packings.

The three-dimensional discrete element simulations have been carried out for monodisperse and polydisperse frictional assemblies of spheres to study the influence of degree of particle size heterogeneity on mechanical response of block shaped specimen under uniaxial compression. The simplified non-linear Hertz-Mindlin contact model was applied in simulations conducted using the EDEM software. The normal and random particle size distribution with standard deviation of particle mean diameter ( $SD$ ) ranging from 0% to 80% was applied.

The detailed analyses of fabric and microstructure of particulate assemblies included the void fraction, number of contacts and forces in contacts between particles while macroscopic study included the effective elastic modulus, pressure ratio and Poisson's ratio. The understanding of complex behavior of granular matter still remains a challenge *inter alia* due to the dissipative nature of forces acting on interacting particles. Thus additionally the analysis of distribution of energy in the normal and tangential direction in contact points as well as energy dissipation in polydisperse mixtures was carried out.

The linear increase in solid fraction was observed for standard deviation of particle mean diameter increasing up to 50% in assemblies of spheres with normally distributed diameters. Further increase in particle size heterogeneity decreased total volume of solids in system due to increase in space between large granules unfilled by smaller particles. In the case of sphere packings with random particle size distribution decrease in solid fraction with particle size heterogeneity increasing was observed in the whole range of variability of  $SD$  value. Increase in degree of disorder of granules and participation of small particles in mixtures at higher standard deviations decreased averaged coordination number by 20% in systems composed of spheres. The random distribution of particle diameter resulted in much wider distribution of number of contacts per particle as compared to the packing with normal particle size distribution. The stiffness of samples increased with compressive loads increasing, however no clear effect of particle size polydispersity on the effective elastic modulus of mixtures was found. Discrete element method predicted higher friction angles in packings of random particle diameter distribution as compared to the one with normal particle size distribution. No influence of type of particle size distribution on energy dissipation in assemblies of spheres was observed.

## Numerical modeling of stresses in composites manufactured by powder metallurgy

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Powder metallurgy technology is one of the main method of manufacture process of advanced composite materials. During the sintering process, which is the most important stage of the powder metallurgy, loose powder is converted into a solid material due to temperature (close to the melting point) and pressure (additional). In the case of sintered composite with minimal porosity in the cohesive bonds of powder grains occur concentration of residual microstresses, mainly induced by the difference in thermal expansion of the two interacting phases during the cooling stage. The complex state of tensile and compressive stresses leads to the formation of microcracks and the progressive degradation of the material.

One of the efficient and appropriate tool to determine the powder metallurgy stress of composite material is numerical modeling. The manufacture process of composite material can be efficiently modeled by the discrete element method, which is a natural approach of modeling of particulate and granular systems. Discrete element method allows to model the interactions of powder particles in places subject to the highest stresses concentration.

This paper presents numerical modeling of two-phase material stress during and after the powder metallurgy process. The original thermo-viscoelastic model of discrete elements have been performed to model the sintering and cooling stages presented in [1]. Numerical simulations were carried out on the example of the NiAl-Al<sub>2</sub>O<sub>3</sub> composite. As part of this study microscopic stress generated both in cohesive connection between the powder particles and in the same particles was determined. The knowledge of the microscopic material parameters, such as the residual stress or the radius of particle contact area, provided the data of macroscopic stress by application of averaging methods based on the concept of the representative volume element (RVE). The obtained results confirmed correct and efficient performance of the proposed numerical model.

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## A model of high-strain-rate metal viscoplasticity with application to powder shock compression

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The shock wave loading of metals involves rapid changes in pressure and temperature and strain rates greater than  $\sim 10^5 \text{ s}^{-1}$ . A challenge encountered in modeling shock wave plasticity is accounting for flow processes and structure evolution within the shock front on a physical basis. Conventional models of metal viscoplasticity are based on thermally-activated obstacle bypassing and dislocation glide, which is the controlling mechanism for applied stresses up to the mechanical threshold (equivalently, for strain rates up to  $\sim 10^4 \text{ s}^{-1}$ ). However, the stresses generated under shock wave loading tend to exceed this threshold and dislocations are subject to phonon damping and relativistic effects during their high-speed motion. To address the need for refined descriptions of high-rate flow processes, we have developed a rate-dependent constitutive model that is based on the generation and migration of dislocation line segments under dynamic loading. The model distinguishes the mobile and immobile populations of dislocations and accounts for microstructure evolution in terms of dislocation nucleation, multiplication, annihilation, and immobilization. The model has been exercised in simulations of steady shock waves in a set of fcc pure metals (Cu, Ni, and Al) and a precipitate-hardened alloy (Al 6061-T6) and is in agreement with experimentally measured velocity profiles and dynamic stress-strain curves.

The constitutive model has also been implemented in an Eulerian finite element code to study the shock wave loading of micron-scale Ni+Al powder mixtures at the particle length scale. The deformation and mixing of several Ni+Al powder configurations are investigated, as constituent mass mixing is the rate-limiting step of ultra-fast chemical reactions in these material systems. It is shown that the viscoplastic model provides improved accuracy in predicted particle flow morphology when compared to a rate-independent strength relation that is typically used in shock calculations. Finally, the simulations reveal particle velocity fluctuations among the phases when the powders are re-compressed by reflection waves. The fluctuations stem from the spatial heterogeneity of the fully dense aggregate and may be responsible for driving fragmentation processes that enable ultra-fast reactions on a sub-microsecond time scale.

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## Session 11

# Strain gradient and nonclassical approaches



## Gradient Materials Mechanics

by

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An update of Gradient Materials Mechanics is given. The interaction of "bulk" and "surface" internal lengths, as well as effects of stochasticity and multiphysics couplings are discussed.

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## Micromechanical Simulation of the Hall-Petch Effect with a Crystal Gradient Plasticity Theory including a Grain Boundary Yield Criterion

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A strain gradient crystal plasticity theory is presented that accounts for the resistance of grain boundaries against plastic flow based on an interface yield condition. This theory incorporates a numerically efficient treatment by the gradient of an equivalent plastic strain [1]. Starting from the variational setting, the field equations and thermodynamically consistent bulk and grain boundary flow rules are subsequently derived. Emphasis is put on a mechanical interpretation and understanding of the derived grain boundary equations. In addition, the Finite Element implementation is discussed. The mechanical behavior of a three-dimensional periodic grain cluster is illustrated, especially the simulated dislocation and back stress fields as well as the grain boundary yield behavior are highlighted. The prediction of the macroscopic yield strength is compared to the experimentally identified Hall-Petch relation. The formulation may be used to realize computationally affordable backstress terms in three dimensional simulations of dislocation continuum theories (e.g. Hochrainer et al. [2]).

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## Strain Gradient Plasticity Modeling including a Grain Boundary Yield Criterion and Application to Size Effects in Micro-Tensile Test Experiments

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The resistance of grain boundaries against plastic flow influences the mechanical response [1] and plays an important role in the size effects observed in the plastic deformation of micro-specimens. A strain gradient plasticity theory for single-crystals is presented that accounts for the resistance of grain boundaries against plastic flow by incorporating an interface yield condition. The previously presented numerically efficient treatment by the gradient of an equivalent plastic strain in [2] is supplemented by this yield condition. Emphasis is put on a mechanical interpretation and understanding of the derived grain boundary equations. In addition, the 3D Finite Element implementation is discussed with application to experimental data of tensile tests on micro-wires with several grains in the cross-section [3]. It is shown that the experimentally observed size effects, especially the size-dependent yield strength in the mechanical response, can be reproduced reasonably by fitting the set of parameters of the model at hand.

**Keywords:** Strain Gradient Plasticity, Grain Boundaries, Size Effects

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## From bicrystals to spherical inclusions: analytical derivation of the stress fields in presence of plastic strain gradients

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In the present contribution, the issue of an infinite bicrystal with planar boundary undergoing plastic distortion jumps at the interface in addition to possible variations along the normal to the interface is first considered. Explicit analytical solution of the stress field is derived in the context of small strains and linear heterogeneous elasticity accounting for full elastic anisotropy in each crystal. Restricting the analysis to isotropic homogeneous elasticity, it is shown that the stress field of the classic Eshelby-Kröner spherical inclusion problem can be retrieved by applying an appropriate superposition method starting from the preceding bicrystal stress solutions. The methodology is explained for interior and exterior points (i.e., inside and outside the inclusion). Such superposition method provides a convenient geometrical interpretation of Eshelby-Kröner results.

Besides, this method makes it also possible to handle spherical inclusion (or grain) problems with spatially non-uniform plastic strain in the inclusion. In particular, it is suited to handle easily intra-crystalline polynomial plastic strains with even exponents or any plastic strain that can be written as a power series representation with even exponents like  $\cos x$ ,  $\cosh x$ ,  $\sin x / x$ ,  $\sinh x / x$ . The analytical expression of the interior stress tensor for the problem of a plastic strain in the inclusion that varies as a power law with a general even exponent is given. Internal stresses and stored energy are also derived analytically for the problem of a plastic strain in the inclusion that varies as  $\sinh(r/l) / (r/l)$  ( $r$  being the polar distance to the inclusion centre and  $l$  a characteristic length), chosen to describe realistically the accumulated plastic strain gradients within grains. Remarkably, a tanh-shape is found for the evolution of the stored energy as a function of  $l/a$  in log-log scale, resulting in very similar size effects as those derived from micromorphic based continuum models as recently developed in [1].

**Acknowledgments** This work was supported by the French State through the National Research Agency (ANR) under the project PHIRCILE (ANR 2010 JCJC 0914 01) and the program “Investment in the future” (LabEx DAMAS referenced as ANR-11-LABX-0008-01).

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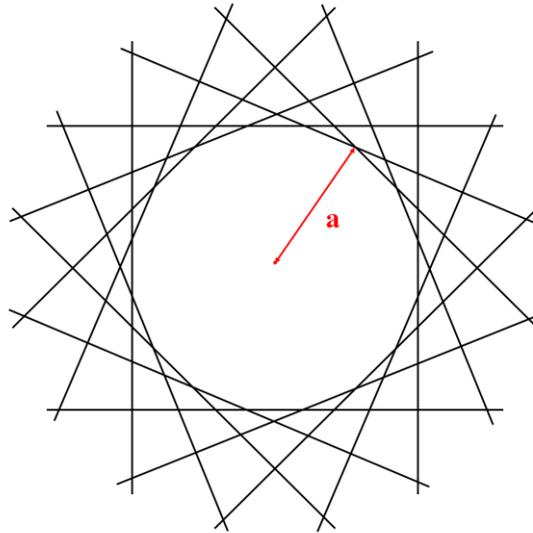
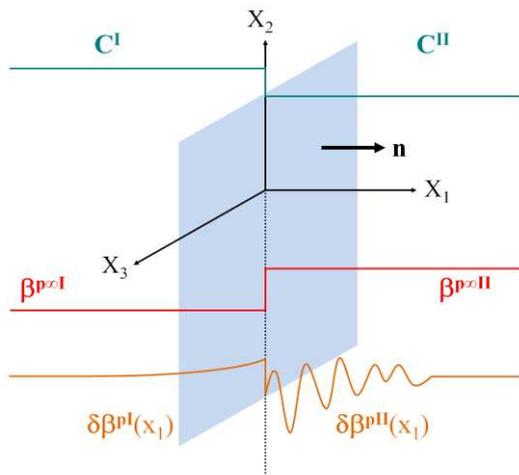


Figure 1: Infinite bicrystal with planar boundary undergoing jump of plastic distortions at the interface plus possible variations along the normal to the interface.

Figure 2: 2D cut of a sphere of radius  $a$  defined by the intersection of continuously superimposed tangent planes.

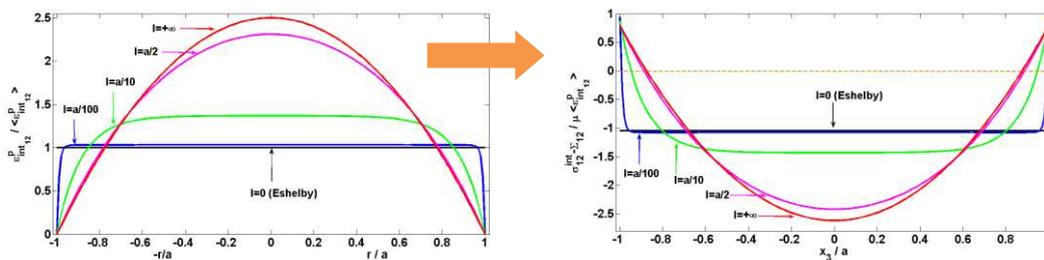


Figure 3: Distribution of the component 12 of a plastic strain in the inclusion that varies as  $\sinh(r/l) / (r/l)$  and the corresponding interior stress solution along the direction  $x_3$  for different values of the parameter  $l$ . Note that if the plastic strain components depend solely upon the distance from the inclusion centre,  $r$ , the stress solutions depend also on the angular position.

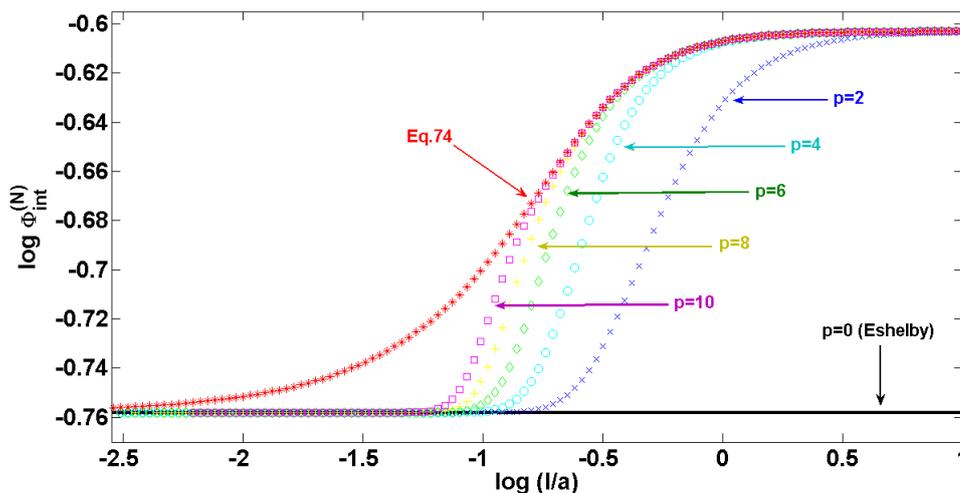


Figure 4: Evolution of the normalized elastic energy as a function of the ratio  $l/a$  in log-log scale and comparisons with polynomial solutions corresponding to Taylor developments of  $\sinh(r/l) / (r/l)$  at different orders  $p$  in the expression of the interior plastic strain.

## Strain gradient crystal plasticity enriched with vacancy diffusion controlled dislocation climb

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The physics and mechanics of metals at intermediate length scales is efficiently described through a strain gradient crystal plasticity model, which incorporates sufficient crystalline details while still being a continuum model. There is a vast amount of literature on these models, mainly aiming to capture size effects in metallic systems. At present, it remains unclear how this is affected by dislocation climb, which may be important for many miniaturized systems. The role of climb in plasticity has been addressed in several papers in a purely phenomenological manner or at the discrete dislocation level, where constitutive equations incorporate the contribution of climb. The focus of this contribution is to break through the phenomenological nature of the continuum crystal plasticity models, by coupling deformation through dislocation glide to vacancy diffusion controlled dislocation climb.

Point of departure is the thermodynamically based variational framework of Gao and Cocks [1], which links the climb of a single edge dislocation to the diffusion of vacancies. Attention is given to the governing equations and physics of the vacancy diffusion process, the driving forces acting on a dislocation to climb and the intrinsic coupling between both. The climb law is therefore diffusion-controlled. The problem is studied at the meso-scale, where pile-ups against particles can be resolved explicitly, i.e. a scale at which it is meaningful to preserve a direct coupling between the mean vacancy flux and the dislocation climb process. A rate-dependent strain gradient crystal plasticity formulation is adopted, which accounts for the net sign of the dislocation population. The dislocation problem can be described in a fully conservative manner with transport equations. Since the analysis is carried out at the meso-scale, all dislocations are assumed to be able to participate in the climbing process. The corresponding transport equations for the dislocations are updated to incorporate climb. In order to incorporate the effect of the dislocation climb on the plastic deformation tensor, the crystallographic split of the plastic velocity gradient tensor is extended for the climb kinematics associated to each slip system.

An illustrative example is shown and a qualitative comparison is made with the climb-assisted DDD glide model results presented in [2].

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## Equilibrium of Second-Gradient Fluids and Nonlinear Elastic Solids

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Recently the interest to generalized model of continuum grows with respect to development of nano-technologies and engineering of MEMS and NEMS. Nowadays it is well-known that the materials at the micro- and nanoscales may possess properties different from those of bulk materials. In particular, the capillary forces play an important role in the case of solid-fluid interaction. In the theory of capillarity there are two approaches related to the model of Young, Laplace and Gibbs with a sharp material interface endowed with surface energy and to the model of van der Waals and Korteweg with an interfacial layer, see [1, 4, 6]. In what follows we use the second approach based on the model of second gradient fluid.

Here we discuss the equilibrium conditions of a second-gradient fluid interacting with a nonlinear elastic solid under finite deformations. We also take into account the surface stresses acting at the surface of the solid according to the model of [5]. We apply the variational approach based on the energy functional  $\mathcal{E} = \mathcal{E}_b + \mathcal{E}_s + \mathcal{E}_{fl}$ , where  $\mathcal{E}_b$ ,  $\mathcal{E}_s$  and  $\mathcal{E}_{fl}$  are the energy functional of the bulk material, the elastic surface and the second-gradient fluid, respectively. Calculating the first variation of  $\mathcal{E}$  from the equation  $\delta\mathcal{E} = 0$  we derive the equilibrium equations and the natural boundary conditions. We consider various kinematic compatibility conditions at the fluid-solid interface. The most attention is paid to the natural boundary conditions at the solid-fluid interface and to the edge boundary conditions along specific curves for assumed kinematic compatibility conditions. We present both Lagrangian and Eulerian boundary-value problems for fluid-solid interaction. For recent results related with the boundary conditions of the second gradient materials, see also [2, 3].

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## The Thermodynamics of Gradient Plasticity

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The intention of this paper is to give a thermodynamical framework for the modelling of gradient effects in elastoplasticity. It is based on an approach by Ref. [1] and generalized to such gradient materials. In this case, not only higher kinematical variables are used, but also a third-order stress tensor is needed, see Ref. [2]. The theory is based on the assumption of identical thermoelastic behaviour in all elastic ranges which means that all measurable thermoelastic properties are not affected by plastic deformations. This concept has been introduced by Bertram Ref. [3] in the context of large deformations. In the present contribution, however, we limit ourselves to small deformations for the sake of simplicity and clearness.

After exploiting the assumption of identical thermoelastic behaviour, an example with a complete set of the thermomechanical constitutive equations is given, which generalizes the classical J2-theory to gradient plasticity. Then the restrictions from the second law of thermodynamics are worked out. The example still contains an arbitrary anisotropy. Finally, its reduction to the isotropic case by means of representation theory is shown. The example is formulated in a rather general matter, thus leaving enough space for specific models in particular applications. For further details see Ref. [4,5].

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## A first order strain gradient damage model for simulating quasi-brittle failure in porous elastic solids

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In order to simulate quasi-brittle failure in porous elastic solids, a continuum damage model has been developed within the framework of strain gradient elasticity. An essential ingredient of the continuum damage model is the local strain energy density for pure elastic response as a function of the void volume fraction, the local strains and the strain gradients, respectively. The model adopts Griffith's approach, widely used in linear elastic fracture mechanics, for predicting the onset and the evolution of damage due to evolving micro-cracks. The effect of these micro-cracks on the local material stiffness is taken into account by defining an effective void volume fraction  $f$ , the evolution of which starts from a given initial value  $f_0$ . Thermodynamic considerations are used to specify the evolution of the latter. The model consists of the free energy density

$$\Psi(\mathbf{E}, \mathbf{H}, f) = \frac{1}{\varrho} \frac{1}{2} \underbrace{\left[ \mathbf{E} : \mathbf{C}' : \mathbf{E} + \mathbf{H} : \mathbf{D}' : \mathbf{H} \right]}_{=W'} + \frac{1}{\varrho} \int_{f_0}^f \gamma(\bar{f}) d\bar{f} \quad (1)$$

with the macroscopic strain tensor  $\mathbf{E}$  and its first spatial gradient  $\mathbf{H}$ . The density  $\varrho$  is given by  $\varrho = (1 - f_0)\varrho^M$ , where  $\varrho^M$  stands for the density of the matrix material. A prime indicates the derivative of the quantity with respect to  $f$ . The function  $\gamma$  is interpreted as a materials characteristic which accounts heuristically for the resistance of the matrix material against micro-crack propagation. The strain energy density  $W$ , respectively the elasticity tensor  $\mathbf{C}$  and its higher order counterpart  $\mathbf{D}$  have been derived from generalised homogenisation procedure reported in [1]. Whereas  $\mathbf{C}$  depends only on  $f$  and the elasticity constants of the matrix material,  $\mathbf{D}$  hinges in addition on the internal length  $R$ . The latter is interpreted here as the mean distance between micro-voids. The second ingredient of the model is the damage potential

$$\Phi = -W' - \gamma(f) - \gamma_0 \quad (2)$$

where damage occurs if the conditions  $\Phi = 0$  and  $\dot{f} > 0$  are met.

The principal features of the model are demonstrated by means of a one-dimensional example. A suitable arc-length method was used in order to account for the expected snap-back behaviour. Key aspects are discussed using analytical results and numerical simulations. Contrary to other continuum damage models with similar objectives, the model proposed here includes the effect of the internal length parameter on the onset of damage evolution. Furthermore, it is able to account for boundary layer effects.

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Some general features of the continuum damage model are demonstrated in the following by means of a standard example with forced damage localization.

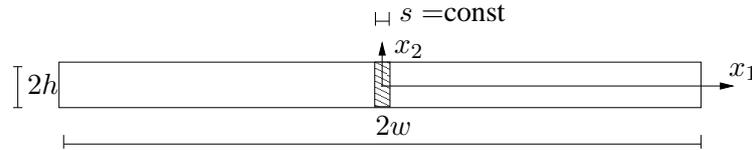


Figure 1: Geometry of the strip with a zone of reduced damage initiation resistance.

A strip of width  $2w$  and height  $2h$  is considered as sketched in Figure 1. The following displacement boundary conditions are applied

$$u_1(x_1 = -w, x_2) = -\bar{u}, \quad u_1(x_1 = w, x_2) = \bar{u}. \quad (3)$$

Furthermore,  $u_2 = u_{1,1} = u_{1,2} = u_{2,1} = u_{2,2} = 0$  are prescribed at the outer left hand side and the outer right hand side of the strip. In addition  $u_2 = u_{2,1} = u_{1,2} = u_{2,2} = 0$  is enforced at the bottom and the top of the stripe, where  $u_{i,j} := \partial u_i / \partial x_j$ . Localization of damage is enforced by reducing the resistance to damage initiation in the center part of the strip ( $x_1 \in [-s/2, s/2]$ ) while in the remaining part  $\gamma_0$  is used. As shown in Figure 2, the model predicts changes in the post-peak behaviour with increasing  $R$ . While for smaller ratios  $R/s$  the final failure is preceded by a single snap-back, the breakdown is accompanied by multiple snap-backs for higher  $R/s$  ratios. In addition,  $R$  effects significantly the slope of the load displacement curve after the initial snap-back.

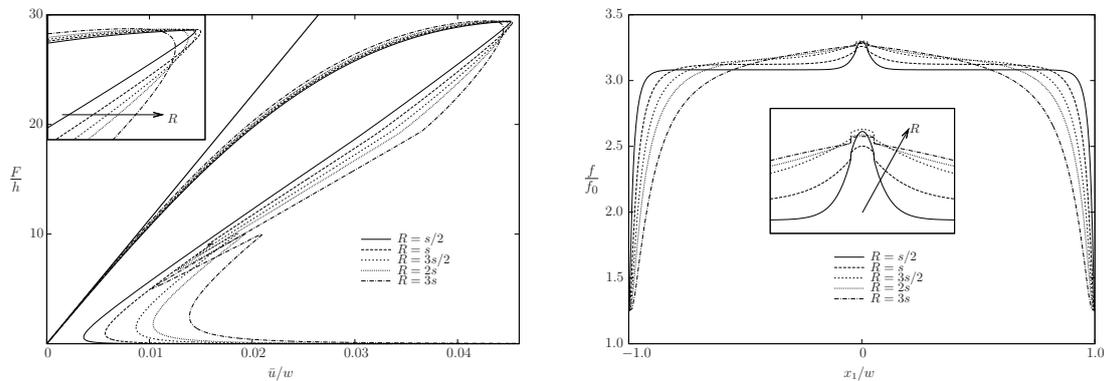


Figure 2: Load normalised by the height of the strip versus normalised displacement for different values of the internal length  $R$ . In addition, the pure elastic response for  $R = 3s$  (bold solid line) is plotted. The box in the upper left corner shows a zoom of the first snap-back (lhs). Distribution of the normalised void volume fraction  $\frac{f}{f_0}$  along the strip at maximum load for different values of the internal length  $R$  (rhs).

The regularisation capabilities of the model become apparent from the distribution of the normalised void volume fraction along the strip at maximum load which are depicted in Figure 2 (rhs). The results show the expected smoothing of the damage distribution with increasing internal length  $R$ . Furthermore, the expected boundary layer effect can be observed. The regularization capability of the model becomes also apparent by the symmetry of the obtained numerical solutions because symmetry was not enforced here a priori but it is a result of the simulations.

## **Influence of Length Scale Parameters for Nonlocal Crystal Plasticity on Localization in Polycrystalline Specimens**

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It is well known that local continuum theories are insufficient for capturing the localization process that often precedes ductile failure in polycrystalline metals. Nonlocal approaches, e.g. micromorphic or second-gradient continuum theories are capable of numerically resolving localization, but in many cases the phenomena underlying this physical process are not well understood. Consequently, the relevant physics at finer scales become smeared into a few phenomenology-inspired length scale parameters. In this work we assess the evolution of length scales characteristic of the localization of a polycrystalline specimen via numerical simulation. Moreover, we quantify the influence of length scale parameters specified at the single crystal scale on the characteristics and evolution of polycrystal localization bands. The process is demonstrated on an illustrative example problem. Using these results, we suggest that such length scale parameters are not modeling constants intrinsic to a material, rather they reflect a continually evolving interaction between the material and extrinsic characteristics of the boundary value problem.

## Generalized continua for discontinuous complex materials. A Voigt-like approach using the principle of virtual works

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The mechanical behaviour of complex materials, characterised at finer scales by the presence of heterogeneities of significant size and texture, strongly depends on their microstructural features. By lacking in material internal scale parameters, the classical continuum does not always seem appropriate to describe the macroscopic behaviour of such materials, taking into account the size, orientation and disposition of the micro heterogeneities. Attention will be focused on multi-scale approaches which aim to deduce properties and relations at a given macro-scale by bridging information at proper underlying micro-level via energy equivalence criteria. Focus will be on physically-based corpuscular-continuous models originated by the molecular models developed in 19<sup>th</sup> century to give an explanation *per causas* of elasticity. In particular, the ‘mechanistic-energetic’ approach by Voigt and Poincaré will be examined. When dealing with the paradoxes coming from the search of the exact number of elastic constants in linear elasticity, they respectively introduced moment and multi-body interactions models which allowed to by-pass the experimental discrepancies related to the so-called central-force scheme, originally adopted by Navier, Cauchy and Poisson [1–3].

Current research in solid state physics as well as in mechanics of materials shows that energy equivalent continua obtained by defining direct links with lattice systems are still among the most promising approaches in material science. Aim of this presentation is pointing out the suitability of adopting discrete-continuous Voigt-like approaches, based on generalization of the so-called Cauchy–Born rule used in crystal elasticity and classical molecular theory of elasticity, for identifying continua with additional degrees of freedom (micromorphic, multifield, etc.). These generalized continua are essentially non-local models with internal length and dispersive properties. It will be shown that, within the general framework of the principle of virtual work, the assumed generalized correspondence map relating the finite number of degrees of freedom of discrete models to the continuum kinematic fields implies the selection of the continuum equivalent to the defined discrete medium; thus providing a guidance for non-standard continuous approximation of heterogeneous media. The circumstances in which, not very differently than in the past, empirical inadequacies still call for the need of removing the local character of the classical hypothesis of lattice mechanics (central-forces or homogeneous deformations) will be also discussed. Some applications of such approaches will be finally shown with reference to masonry-like material as micropolar [4], second gradient and classical continua.

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## **Lagrangian functions for defects in three- and four-dimensional material manifolds**

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Material forces and the Eshelby tensor are quantities in the three-dimensional material space. The relation to defects has been treated often in the literature and various theories for the dynamics of defects have been proposed. The well established continuum theory of lattice defects is usually formulated in a three-dimensional material space. The defects are represented by differential geometric properties of the material manifold, e. g. the dislocation density is related to the Cartan torsion.

Moving defects lead to differential geometric quantities changing with time. This has motivated some authors to augment the three space-like coordinates in the material space by a time-like coordinate. In this way one gets a four-dimensional material space-time manifold, analogous to the four-dimensional physical space-time in the theory of relativity. A connection of a time-like material coordinate to temperature can be found in the literature on relativistic elasticity. This leads to four-dimensional formulations which include thermal variables.

These three- and four-dimensional theories involves extra field variables, e. g. the lattice vectors of a crystalline solid. These field variables need extra field equations to be determined. In a Lagrangian formulation these extra equations arise from additional Lagrangian functions which depend on the derivatives of the extra variables.

Various approaches for Lagrangian functions in three- and four-dimensional formulations will be discussed. Special attention will be drawn on the possibility of physically reasonable solutions like a homogeneous stress state.

## Continuum dislocation dynamics based on the second order alignment tensor

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The occurrence of size-effects in small scale plasticity challenged classical constitutive equations of plasticity and stimulated the development of strain gradient theories during the late 1990s through the early 2000s. However, strain gradient theories themselves were soon challenged through the discovery of scale dependent effects in macroscopically homogeneous deformations, as, e.g., in uniaxial compression tests of micro-pillars. These effects are typically ascribed to dislocation source limitation or dislocation starvation, i.e., to essentially kinematic effects on the dislocation level. The representation of such effects in continuum plasticity therefore requires a theory based on the kinematics of evolving dislocation systems. Based on a higher dimensional approach [1] we recently adopted the concept of higher order alignment tensors for a more detailed representation of the dislocation state [2] and its evolution.

In the current paper we present a continuum theory of dislocations based on the second-order alignment tensor in conjunction with the classical dislocation density tensor (Kröner-Nye-tensor) and a scalar dislocation curvature measure. The second-order dislocation density tensor is a symmetric second order tensor characterizing the orientation distribution of the dislocations in elliptic form. It is closely connected to total densities of screw and edge dislocations introduced in the literature [3]. The scalar dislocation curvature density is a conserved quantity the integral of which represents the total number of dislocations in the system. The presented evolution equations of these dislocation density measures partly parallel earlier developed theories based on screw-edge decompositions [3] but handle line length changes and segment reorientation consistently. Additionally the equations conserve the number of dislocations as is inevitable for describing effects stemming from dislocation source limitation. Small numerical examples will highlight the effects captured by the current theory.

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Session 12

## Stochastic material modelling



## Evaluation of Microstructural Fields Based on Extended Wang Tile Sets and Schur Complement Method

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In this paper we present our recent work on analysing micro-mechanical fields (e.g. stresses, strains or displacements) in materials with heterogeneous microstructure. The approach is based on method of Wang tilings [1] that uses a small set of statistical volume elements, instead of evaluating micro-mechanical fields on entire domain. The volume elements are called tiles and the fields are synthesized via stochastic tiling algorithms [2].

Wang tiling works on principle of game domino but instead of two-sided rectangular game pieces uses four-sided squared tiles gathered in sets. Tiles of one set contain complete morphological information of synthesized quantity. Synthesis of tiles is subjected to conforming edges of adjacent tiles and the result is called valid tiling.

As the fields sought are nonlocal, the adjacent surroundings must be taken into account. Hence thousands of micro-scale problems have to be solved to create so called extended Wang tile set. At this time, structured discretizations derived from raster image representation are used and solved efficiently by Moulinec-Suquet method based on the Fast Fourier Transform algorithm (FFT) [3]. However, materials with large ratios of material properties or porous materials as metallic foams, cause serious difficulty and the micro-scale problem suits better to conventional Finite Element Method.

With respect to the same finite element mesh discretization and regular distribution of nodes on edges of each tile, the solution to all admissible micro-scale problems can be obtained effectively by the Schur complement method [4], [5]. Because solutions of all admissible tilings are independent, the problem is ideal for processor farming.

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## Polynomial chaos-based methods for uncertainty quantification and reliability analysis

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Reliability analysis, lifetime prediction and modelling of structures in general need to take into account all the relevant information as well as the inherent uncertainties in the environmental conditions, loading or structural properties. Thanks to the growth of powerful computing resources and technology, recently developed procedures in the field of stochastic mechanics have become applicable to realistic engineering systems. Stochastic finite element method (SFEM) [4] is a powerful tool in computational stochastic mechanics extending the classical deterministic finite element method to the stochastic framework involving finite elements whose properties are random.

In this contribution we concentrate on the SFEM based on polynomial chaos expansion (PCE) used for approximation of the model response in the stochastic space. Fast evaluation of the PCE can be then used within Monte Carlo (MC) or Markov chain Monte Carlo (MCMC) sampling so as to quantify the uncertainty in model output, to compute the structural reliability or to update the uncertainty in model inputs based on experimental data. The efficiency of PCE application thus depends on computational requirements of the PCE construction and its consequent accuracy.

There are several methods for construction of PCE-based approximation of a model response: stochastic Galerkin method [2], stochastic collocation methods [1] and linear regression [3]. The principal differences among these methods are follows. Stochastic Galerkin method is purely deterministic, but leads to solution of large system of equation and needs an intrusive modification of the numerical model itself. Stochastic collocation method is also a deterministic method, does not require intrusive modification of a model, but uses a set of model simulations on a sparse grid constructed for a chosen level of accuracy. The computation of PCE coefficients is based on explicit formula. The linear regression is based again on a set of model simulations performed for a stochastic design of experiments, usually obtained by Latin Hypercube Sampling. The PCE coefficients are then obtained by regression of a model results at the design points, which leads to a solution of a system of equations. The aim of this paper is to compare these methods in terms of computational requirements and resulting accuracy on a simple illustrative example of a frame structure.

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## Modelling of random microstructures using Wang tilings

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This contribution presents an application of stochastic Wang tiling [5] for compression or reconstruction of disordered microstructures on the basis of given spatial statistics. A concept of Wang tiling is based on square dominoes with colored edges permitting their mutual assembly in a geometrically compatible manner. The appealing feature of Wang tilings is that they can compress and reproduce naturally looking planar patterns or three-dimensional surfaces by employing only a small number of distinct tiles [2,3]. Motivated by this observation, we further explore the potential of Wang tiles to represent long-range spatial correlations in disordered microstructures [4]. The existing approaches based on a single periodic unit cell (PUC) wrestle with the strong long-range correlations with a period of the PUC dimensions. These artifacts can be effectively controlled when utilizing small Wang tile sets [2,3], carefully designed to capture morphological trademarks of compressed media, combined with the fast stochastic Cohen-Shade-Hiller-Deussen (CSHD) tiling algorithm [1] for real-time texture generation. Although the basic features of the method are demonstrated for a two-dimensional particulate suspension, the present framework is fully extensible to generic multidimensional media.

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## Efficient methods for quantification of uncertainty in description of groundwater flow through random materials

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The prediction of groundwater flow is strongly influenced by the soil permeability generally varying within the space. Determination of the spatial distribution of the permeability is, however, unfeasible and thus the relevant uncertainties should be taken into account. One possibility is to describe the soil permeability by a random field see [4, 5]. The present contribution is devoted to propagation of these uncertainties in permeability into probabilistic description of groundwater flow. A central challenge of uncertainty propagation consists in large number of forward model evaluations required by Monte Carlo sampling of model response. With complex forward models, such as those described by partial differential equations, each single evaluation can be computationally expensive. One possible way to overcome this problem is to express the response in polynomial chaos expansion (PCE) providing a fast forward surrogate [3, 5].

In this contribution, we present a comparison of the two methods for construction PCE of groundwater flow: the stochastic collocation method [1] and the stochastic Galerkin method [2]. Their advantages and disadvantages are discussed on the basis of a numerically study performed for a groundwater flow through the embankment dam.

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## Session 13

# Damage, fatigue, reliability, and lifetime prediction



## Modeling of Damage Evolution in Porous Anisotropic Materials under Thermal Loading

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In the present, contribution a statistical model of deformation and micro-damage developed for homogeneous [1] and composite materials [2] is extended to the more general case of thermal loading. The mechanism of damage evolution in material with stochastically distributed unidirectional ellipsoidal pores is investigated on the basis of the assumption of non-homogeneity of the micro-strength. Modeling the fractured micro-volumes by a system of randomly distributed quasi-spherical micro-pores, a porous material of stochastic structure is obtained. Its damage is described as increasing porosity.

Formation of micro-damage under loading is described by a damage criterion for the micro-volume, which is given as a limit value of the intensity of average shear stresses occurring in the undamaged part of the material. The corresponding limit value of an equivalent stress from the damage criteria is considered as a random function (statistically homogeneous) of coordinates. The one-point distribution function of this limit value is given by a Weibull distribution. From the definition of the distribution function we derived the damage evolution equation. The relations for determining the effective thermo-elastic moduli of the porous transversally-isotropic material and the damage evolution equation are used as the fundamental relations. It allows us to describe the deformation, the damage and their mutual influence on the deformation properties of the material.

Deformation properties of such a material are investigated in two steps. First, the effective linear elastic properties of the porous transversally-isotropic material are determined by the method of conditional moments [3] based on stochastic equations of elasticity theory. An accidental character of the distribution of micro-pores (micro-damage) in the matrix is taken into account. Second, the non-linear deformation properties of the material are determined using the Newton-Raphson method. On the basis of a numerical solution, non-linear macro-deformation diagrams of the material with randomly distributed unidirectional ellipsoidal pores are predicted for the case of uniaxial extension and thermal loading. The influence of a material damage on the relationships between macro-stresses and macro-strains is analysed.

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## **Micromechanical modelling of a Copper-Antimony-Alloy under creep conditions**

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In many practical applications, creep damage is the limiting factor of a component's lifetime. A micromechanical model of creep induced grain boundary damage is proposed, which allows for the simulation of creep damage in a polycrystal within the framework of finite element analysis. The model considers grain boundary cavitation and sliding according to a micromechanically motivated cohesive zone model, while creep deformations of the grains are described following the slip system theory.

The kinetics of grain boundary cavitation is derived from detailed simulations of cavities nucleation, growth by grain boundary diffusion and coalescence [1]. The thickening of the grain boundaries is accounted for by smearing out the cavities as previously proposed in [2]. The model can be applied to idealised polycrystalline structures, such as a Voronoi tessellation or, like demonstrated here, to real grain structures of miniature creep specimens.

Creep data of pure Cu single crystals and a coarse-grained polycrystalline Cu-1 wt.% Sb alloy at 823 K have been used to calibrate the polycrystal model. The grain structure of the polycrystalline Cu-Sb specimens has been revealed by the EBSD method. Extensive grain boundary sliding and cavitation has been observed in the crept specimens. The cavitation model has been calibrated by direct porosity measurements. A linear grain boundary sliding model has been assumed and the viscosity constant has been adjusted to DIC data of crept specimens. Grain boundary sliding has been found to promote wedge-type damage at grain boundary triple junctions and to contribute significantly to the total creep strain. Furthermore, the assumed stress sensitivity of the models grain boundary cavity nucleation rate strongly influences the development of wedge-type damage.

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## Anisotropic ductile damage model to simulate fracture of a 2219 T87 aluminum alloy

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The cryogenic main stage of the Ariane 5 launcher contains two fuel tanks referred to as RLO2 and RLH2. These tanks supply liquid oxygen (LO2) and liquid hydrogen (LH2) to the engine. Each tank is made from 2219 T87 aluminum alloy rolled sheets which are machined and bent to form a cylinder. RLO2 and RLH2 tanks have a diameter of about 5 m and their minimum thickness is respectively 4.6 mm and 2 mm. Failure assessment of tanks containing defects is required to guaranty of the safety of launchers. These flaws are usually assumed to be semi-elliptical cracks.

The local approach to fracture is chosen to assess failure in particular for large scale plasticity. In this case this method gives more accurate predictions than the global approach. Analyses based on local approach concepts require an accurate evaluation of strain and stress fields near the crack tip. It is therefore important to take plastic anisotropy into account to model the plastic behavior of the rolled sheets. In this work this is done using a macroscopic phenomenological model developed by Bron and Besson [1]. The parameters of this model are determined by minimizing of the difference between the simulation results and the test measurements for smooth and notched tensile test samples.

The local approach to fracture is also based on the understanding of the failure micromechanisms of materials. Ductile fracture of metallic materials can be described as a three stage process. The first is void initiation at inclusions, the second is void growth and the third is void coalescence. The fracture of notched tensile samples shows low ductility and anisotropic failure by coalescence. Nucleation of defect at Al<sub>2</sub>Cu inclusions is the main damage mechanism. In this work, the proposed model for ductile fracture is based on the Gurson model [2] modified by Needleman and Tvergaard [3] which is extended to account for plastic anisotropy, nucleation and anisotropic cavity coalescence described by Thomason [4].

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## Kinetics of evolution of radiation induced micro-damage in ductile materials subjected to time-dependent stresses

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The present work constitutes an attempt to fill in the gap related to the constitutive modeling of evolution of radiation induced damage in ductile materials subjected to periodic stress states. It aims at predicting the evolution of radiation induced micro-damage in the solids subjected to mechanical loads beyond the yield stress. During irradiation, energetic particles penetrating a solid displace the lattice atoms from their original positions. Exposure to a flux of particles leads inevitably to creation of clusters of defects in the material, provided that the energy of incident particles is large enough. Collisions of particles of enhanced energy with the lattice atoms ejects the atoms from their initial position and transfers the energy to the next collisions with the neighboring atoms. These atomic interactions lead to creation of the cascade of atoms moving inside lattice and to production of radiation induced defects in the lattice. Thus, as a result of the cascade process, the pairs of interstitial atoms and vacancies (the so-called Frenkel pairs) are created. The evolution of radiation induced damage is combined with the evolution of classical mechanically induced damage within the common framework of Continuum Damage Mechanics (CDM). An additive formulation with respect to damage parameters or tensors has been used. A multiscale constitutive model comprising the evolution of radiation induced damage under mechanical loads has been formulated [1]. Two kinetic laws of damage evolution were taken into account: the Rice and Tracey model and the Gurson model [2].

Both of them address the evolution of porosity in the form of spherical or ellipsoidal voids in a different way. The Rice & Tracey model predicts the evolution of radius of spherical void as a function of triaxiality and the accumulated plastic strain. The R-T model is expressed in the form of differential equation and has therefore implicit character. Thus, in order to obtain the radius increment a differential equation has to be solved and the current radius can be updated. In order to compute the damage parameter, the volume or the surface density of voids has additionally to be known. On the other hand, the Gurson model is based on the definition of the porosity parameter. The porosity parameter can be directly recalculated to obtain the classical damage parameter in the sense of CDM. Here, a simple differential equation has also to be solved in order to obtain the porosity increment. Both R-T and Gurson kinetics may conveniently be applied to describe the evolution of radiation induced damage in the form of clusters of voids embedded in the metallic matrix.

As an application, the estimation of lifetime for coaxial target – detector configuration, subjected to combination of irradiation and mechanical loads, using experimental data taken from [3] has been carried out. New closed form analytical solutions were obtained.

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## Numerical Strategy for Calibration of Damage Models Based on Multi-objective Function

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In this contribution, it is suggested a numerical strategy to calibrate damage models dependent on two or more calibration points. The calibration strategy is assembled regarding a multi-objective function, which is based on the least square. Furthermore, in the search strategy, the gradient method is adopted where a multivariable search method is used based on BFGS strategy. In the first part of this paper, theoretical aspects of two damage models based on CDM, called as improved Lemaitre's model, and Micromechanical of defects, called as extended GTN model, are discussed. After that, the numerical strategy is also presented, taking into multi-objective function, experimental and numerical results of two independent calibration points: one of them in high stress triaxiality and another one in low stress triaxiality. Aspects related to the number of material parameters required for each constitutive model is discussed as well as the ability of convergence of the numerical method. At the end, the computer time, the value of the multi-objective function for each iteration, the agreement between the experimental and numerical reaction curves, the set of material parameters found as well as the potential ability of fracture onset for both CDM and Micromechanical models are widely discussed.

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## **Fatigue Life Prediction of Lateral Notched Round Bars Subjected to Bending-Torsion Loading**

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The main objective of this study is to predict the multiaxial fatigue life for lateral notched round bars made of 34CrNiMo6 high strength steel. In-phase bending-torsion tests for different stress amplitudes and different ratios of the normal stress to the shear stress were performed. Single torsion and single bending tests were also conducted for different stress amplitudes. In addition, the so-called beachmarking technique was used to mark the crack fronts on fracture surfaces for the different loading paths studied. Crack length at the notch surface was monitored and computer-recorded using a digital camera. Experimental fatigue lives were compared with predictions obtained using the well-known Coffin-Manson and Smith-Watson-Topper models. In order to evaluate the stress-strain field at the notch root, both the Theory of Critical Distances and the Strain Energy Density were used. Regardless of the model, a very satisfactory correlation between both experimental and predicted lives was found.

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## A novel approach simulating fatigue crack growth in long cracks

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Fatigue crack growth of long cracks is a problem usually confronted by researchers, engineers and designers when they are performing damage tolerance analysis. The quantitative relations that have been developed for predicting fatigue crack growth rate, are usually modifications of the empirical Paris' Law. In spite of the significance of plastic deformation in the crack-tip zone, Paris' Law and Linear-Elastic-Fracture-Mechanics (LEFM) approaches are used as theoretical tools to treat fatigue crack-propagation processes. Moreover the concept of Stress Intensity Factor characterizes the singular stress-strain fields ahead of the crack-tip. These approaches are not capable to describe (on a physical sound base) the dependence of fatigue crack growth rate on load ratio, thickness and geometry [1-4]. In addition existing approaches use plane stress or plane strain assumptions. These assumptions introduce errors in the determination of stress fields in the crack tip area.

In this model, crack growth is properly simulated by removing elements in front of the crack tip using finite element analysis. The crack is assumed as a notch with a small tip-radius of curvature in order to avoid the unrealistic singularity at the crack-tip. The material model adopted is described by the Chaboche's constitutive equations [5]. In the present approach, fatigue crack growth was modeled under generalized plane strain conditions in order to capture the three-dimensional stress field at the crack-tip.

The analysis aims to the construction of a map between fatigue crack growth rate for a particular load ratio, and the relevant stresses (von Mises stress, hydrostatic stress) at the crack-tip. Combining the physical principle of similarity [6], i.e. that similar crack-tip stress conditions cause the same consequences at similar systems, (namely same fatigue crack growth rate) with the map referenced above, allow us to predict the dependence of fatigue crack growth rate under various load ratios.

The methodology described here, provides the theoretical framework for enlightening critical aspect of fatigue damage.

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Session 14

# Fracture mechanics



## **DEM-Simulation of Concrete Fracture Phenomena**

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Concrete fracture phenomena are investigated in this work. It is the fracture processes and failure mechanisms which are specifically investigated rather than to reach a certain maximum load or to investigate the concrete behaviour within a range of safe working loads. Why does a crack rise just at this or that position? How do the crack positions vary from one test to another? Is it possible to identify in advance where for example micro-cracks will emerge to a global macro-crack later on? In order to go into this matter, a twodimensional numerical simulation based on the Discrete Element Method (DEM) is used for the analysis of concrete behaviour under compression load. The transmission of loading waves through the concrete body is studied. Frictional behaviour, crack initiation and damage evolution are analysed. The cracks are discrete just as in real laboratory experiments. The cracks arise due to the interaction of the concrete particle elements and without the predefinition of any crack zones or crack elements. The simulation results are compared to the ones of laboratory experiments. The ratio of longitudinal strain to lateral strain is obtained as a result of the simulation and compared to experimental results.

## **Inelastic evolution and fracture of stretched bars by means of incremental energy minimization**

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In this communication, a variational model based on a non-convex cohesive energy for predicting the post-elastic behaviour of bars made of different materials and subject to tensile loads is presented. The model, an extension of [1], considers an energy functional given by the sum of an elastic bulk energy, a dissipative inelastic cohesive energy, and a non-local gradient term. Differently than in [1], the non-local term depends on both the inelastic deformation and its gradient. The evolution is described by an incremental energy minimization problem, which is solved numerically by finite elements. At each increment of the imposed displacement, an iterative procedure of the Newton-Raphson type is adopted.

Depending on the analytical form given to the cohesive energy, a large variety of responses is predicted, with fracture as the final stage of plastic deformations. A convex cohesive energy produces a work-hardening response, with inelastic deformations almost homogeneously distributed over the bar. A concave cohesive energy may produce both hardening and softening response, with or without strain localization, as well as the overcoming of catastrophic fracture. In the case of a concave-cohesive energy, the convexity/concavity of its derivative determines two basic types of rupture mechanisms, typical of steel and concrete, respectively. In the first case the inelastic deformation concentrates on a singular surface, while in the second case it spreads over the bar, producing a gradual loss of strength without any catastrophic event.

Some simulations are performed by considering bone-shaped and notched bars made of steel and concrete. The different inelastic evolutions are presented and discussed, and connections with the shapes given to the cohesive energies are pointed out.

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## Texture analysis of polycrystals by means of an embedded strong discontinuity approach

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The paper presents a novel method to texture analysis of polycrystals at finite strains. The proposed method is based on the embedded strong discontinuity approach [1]. In sharp contrast to conventional crystal plasticity models, the shear deformation at a certain slip system is captured by a strong discontinuity (displacement jump). For each of the 12 slip systems in an FCC crystal, a Schmid-type yield function is considered, which connects the shear stresses to the tangential displacement jump, i.e., a traction-separation law is employed. In order to solve the resulting multisurface problem, the classical Karush-Kuhn-Tucker conditions are re-written as equivalent equations, cf. [2]. The predictive capabilities of the method are elaborated by means of a three-dimensional simple shear test.

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## Modelling of damage in rubber-toughened materials

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The superior ductility and toughness of rubber-toughened polymers relies on micro-scale deformation and damage mechanisms such as void growth, shear yielding and crazing, see e.g. [1–3].

A constitutive model relies on micromechanics is developed and presented here. It is based on the idea, that the formation of distributed crazes (i.e. cohesive crack-like surfaces) give rise to an overall inelastic strain in the direction of maximum principal stress. The visco-plastic model explicitly accounts for the most important micro-structural parameters such as the rubber content and the rubber particle size. The model is able to capture the inelastic behaviour in the case of changing loading-direction during deformation.

Tensile tests under different loading conditions on Acrylonitrile Butadiene Styrene (ABS), a representative of rubber-toughened polymers, are used to determine the material parameters of the constitutive model.

Numerical simulations as well as experiments are conducted on a Single Edge Notched Tensile (SENT) specimen in order to validate the model and to analyse the fracture behaviour of ABS. To analyse the suitability of the model, numerical and experimental results are compared.

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Session 15

Coupled field problems



## A Coupled Diffusion - Crystal Plasticity - Phase Field Framework to Study Grain Boundary Cavitation in Irradiated Materials

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Some of the most deleterious degradation mechanisms in high temperature polycrystalline materials are those caused by the diffusion of point defects (i.e. vacancies or interstitial atoms) through either the crystal lattice or the grain boundary regions, and by their interaction with other lattice defects such as dislocations and grain boundaries. They can lead to cavitation, local swelling, creep, hardening and embrittlement due to the formation of point defect clusters, amongst others. A detailed physical understanding of experimental observations and measurements of point defect production, diffusion, and trapping requires appropriate theoretical and modelling tools to study the complex phenomena involved.

In the present work, the coupling between vacancy diffusion and stress is first considered through a thermodynamic consistent formulation involving a pressure and concentration gradient driven vacancy diffusion mechanism coupled with single crystal plasticity to describe the behaviour of a grain. The stress-diffusion coupling is then enhanced to account for creep by self diffusion process [2] [3], the driving force being proportional to the gradient of the vacancy flux.

The coupled diffusion-crystal plasticity framework is then extended to incorporate a phase field-type order variable using a suitable non-convex free energy potential to describe the formation of stable vacancy clusters. The framework is implemented into the finite element method [1] and then used to study coalescence of vacancy clusters into stable grain boundary cavities. Such types of cavities are at the origin of the damage seen in irradiated materials. The effect of visco-plasticity at the grain level and vacancy diffusion on the growth behaviour of grain boundary cavities is investigated.

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## Strain-Tunable Functional Properties in Nanocomposite Materials

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Structural nanocomposites have been investigated for years for their mechanical properties. However many nanoparticles, being of fullerenes, organic or inorganic nature, may exhibit specific strain induced functional properties [1].

Nanoscale particles are intrinsically of discrete nature and classical field quantities such as Cauchy stress tensor and small deformation strain tensor do not have the same format in discrete systems. For small local deformations the local deformation gradient can be first computed by minimizing a least square error between the transformed reference configuration of atoms and actual configuration [2]. For large non-homogeneous deformations, deformation measures that are based on the definition of a discrete equivalent to the continuum second-order deformation gradient that accounts for non-homogeneous deformations can be formulated [3].

The configuration of the deformed state of carbon nanotube structure has been calculated using the least square method and the second-order gradient method. Atomic coordinates from these two methods are compared with the coordinates that result from the molecular optimization procedure. A significant discrepancy exists between deformed atomic positions and those calculated from the least square method. On the other hand, the second-order deformation gradient method provides very close approximation to the deformed atomic positions, Fig. 1. A similar situation is observed for an axial deformation of C60 fullerene, Fig. 2. From components of the second-order deformation gradient the non-homogeneity measure can be constructed. It unambiguously describes deformation mapping from the reference to final deformed configuration [3].

Deformation induced changes in the electronic band gap, are significantly increased by the application of the electric field while deforming the C60 buckyball. Furthermore, the electric charge of the fullerene remains constant under deformation but is markedly growing when the deformation is performed in the presence of the electric field, Fig. 3.

Absorption bands of electromagnetic radiation observed in the UV region are associated with changes of orbital occupation and for undeformed C60 fullerene exhibit two peaks at 256 nm and 308 nm, Fig. 4. The absorption spectrum changes when fullerene is deformed to the state that corresponds to non-homogeneity measure of 101. Peaks move to new positions at 288 nm and 350 nm and interestingly a new peak appears at 544 nm which corresponds to the green band in a visible range. In a similar way piezoelectric, luminescence and other physical properties can be deformation related that simultaneously provide mechanical enhancement of nanocomposites.

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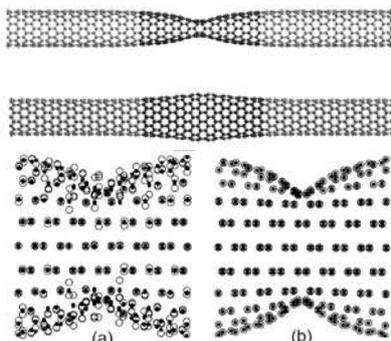


Fig. 1. Prediction of atomic positions for locally deformed carbon nanotube using (a) least square and (b) second order gradients. Solid circles are from atomistic simulation whereas open circles represent corresponding prediction.

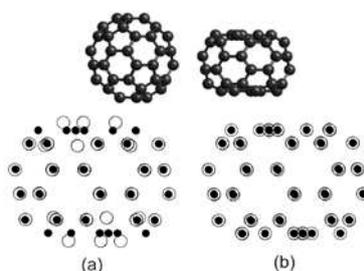


Fig. 2. Prediction of atomic positions for locally deformed C60 fullerene using (a) least square and (b) second order gradients. Solid circles are from atomistic simulation whereas open circles represent corresponding prediction.

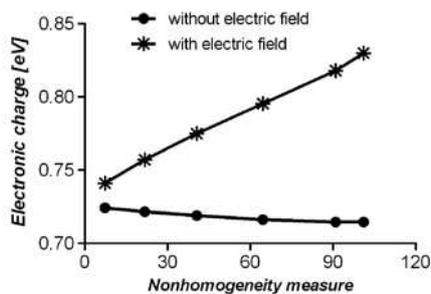


Fig. 3. Variation of C60 electronic charge with deformation.

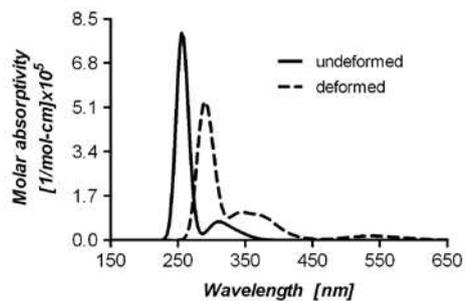


Fig. 4. Change of C60 absorptivity spectra with deformation.

## Plasticity of lithiated silicon under chemo-mechanical loading

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In the search for high-energy density materials for Li-ion batteries, silicon has emerged as a promising candidate anode material due to its ability to absorb a large number of Li atoms. However, the lithiation of silicon is accompanied by huge volumetric expansion (up to 300%) and severe structural changes. Lithiation-induced stresses may cause mechanical degradation of the electrode, resulting in capacity fading after several cycles of lithiation and delithiation. Stresses also affect the kinetics of reaction and diffusion of lithium into the Si host. Understanding the complex relationship between mechanics and chemistry in electrode materials is crucial for designing batteries with improved cycle life and reliability.

It is now well-recognized that the lithiation strain in silicon can be accommodated by plastic deformation in electrodes of small feature size. Lithiation of silicon leads to dramatic changes in its mechanical properties, from a brittle material in its pure form to an amorphous material that can sustain large inelastic deformation in the lithiated form. In particular, silicon demonstrates remarkable softening when subject to a combined chemo-mechanical loading, as compared to mechanical loading alone [3]. However, the micro-mechanisms inducing the macroscopically observed plastic deformations in amorphous silicon are not well understood.

In this work we propose a continuum model that couples diffusion, chemical reaction and large, inelastic deformations within a consistent thermodynamic framework. The model introduces a coupling between mechanical and chemical driving forces which reproduces the observed chemo-mechanical softening [1]. The model formulation and parameter identification is supported by ab-initio calculations, as well as experimental measurements on thin film electrodes. The model was implemented into a FE software, allowing us to predict the stress and electric potential in silicon electrodes subjected to cycles of lithiation and delithiation [2].

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## Thermo-mechanical modelling of the thermo shock behaviour of cellular hybrid refractories

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In steel making industry carbon containing refractory materials are often used as refractory lining of ladles, basic oxygen converter or furnaces. In all these applications the refractories are subjected to thermal shock loading arising from high thermal gradients e.g. due to the pouring of molten steel or the sudden opening of hot furnaces. Carbon containing refractories exhibit high thermal shock resistance and high slag resistance. A big problem of this materials is the oxidation of carbon accompanied by large amounts of CO<sub>2</sub> emissions. In order to eliminate this problem there is the usage of magnesia carbon bricks [1]. Further improvements are realised by open cell carbon foams filled with magnesia [2].

Modelling of the thermo shock behaviour of refractories must be done by thermo-mechanical coupling. There are two possible stress types causing failure of the materials. Permanent thermal stresses arise according to the coupling of materials which differ in the coefficient of thermal expansion (CTE). Temporary thermal stresses are caused by temperature gradients and vanish at temperature balance if the material has only been loaded elastically. The CTE of glassy carbon and magnesium oxide differ one order of magnitude. Hence, failure in the investigated cellular hybrid refractories occurs by thermal damage according to the isotropic expansion due to the pairing of the carbon foam with the magnesium oxide filling and by mechanical damage due to thermal shock loading and the resulting temperature gradients.

In the present contribution, a microstructural linear elastic model has been used with transient coupled temperature-displacement analysis in Abaqus<sup>TM</sup>. Changes in the occurring stresses by different thermo shock rates and structural variations, e.g. pore size, free pore volume and the influence of size effects have been determined in order to optimise the structural morphology of the cellular hybrid refractories. As criterion of failure the maximal occurring stresses have been chosen and compared with the fracture stresses of glassy carbon and magnesium oxide. The results of these simplified model correlates very well with the failure behaviour according to the experimentally motivated Hasselman equation [3]. The Hasselman equation describes the residual strength of brittle refractory ceramics as function of the thermo shock difference. The here mentioned model is able to characterise the damage behaviour of the cellular hybrid refractories used in this study. Even the start of damage due to crack initiation can be predicted. The effects of thermo shock rate and size effects have been modelled. Higher thermo shock rates lead to crack initiation at an early stage. In order to increase the thermo shock resistance carbon foams with small pore sizes and without free pore volume should be prepared.

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## On the Constitutive Relationships of Active Media Electromechanics

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The cardiac beating is the result of the propagation of electrical waves generated by the sequential excitation of neighboring cells, located along specialized conductive structures that provide the spreading of the electric signal into the whole heart. The excitation of a cardiac cell is induced by the variation of the electric potential across the cell membrane, related in a nonlinear manner to the transmembrane fluxes of various charged ions. The basic features of the mechanical response of biological active tissues can be sufficiently well described by hyperelastic models, disregarding in first approximation more complicated effects related to viscosity, growth and remodeling. Mathematical models of passive muscle and myocardium elasticity have been proposed, including isotropic, transversely isotropic and, more recently, orthotropic models. The interest towards the modeling of the active behavior of deformable biological tissues has been growing progressively in the last decade. In this respect, the introduction of the active stress component in the formulation encompasses the key aspects related to the description of the subcellular electrophysiological dynamics of the tissue. In order to account for the strong contraction induced by the electromechanical coupling, the behavior of cardiac tissue must be described in terms of finite deformations. The standard approach for modeling biological tissues is based on a passive response expressed in terms of hyperelastic weakly compressible or incompressible materials, combined to an active response (or active stress) formulated in an independent way, in several cases as a phenomenological description of some inelastic action. As opposed to the concept of active stress, alternative approaches rely on the concept of active strain. An alternative formulation based on the multiplicative decomposition of the deformation gradient into active part and passive part have appeared recently in the cardiac literature [2]. The formulation was based on several simplifying assumptions, which have been partially removed by other authors [1]. We propose a class of constitutive models for electro-active materials based on the multiplicative decomposition of the deformation gradient in passive and active parts, adopting a fully thermodynamical approach able to conciliate the contrasting concepts of active stress and active strain [3] and a simplified class of anisotropic electromechanical active material models, in view of numerical simulations of the behavior of muscles and heart.

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## Continuum mechanical modeling of laser-pulsed heating in polycrystals: a multi-physics problem of coupling diffusion, mechanics and thermal waves

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Pulsed laser technologies are of importance in material processing and in nondestructive testing to assess coating qualities and to detect and characterize defects and their concentration. When a pulsed laser transfers a noticeable amount of energy (tightly packed in space and time) to crystalline matter, it may happen that this transfer causes thermal and mechanical waves. Further, propagation of these waves may induce defect generation or annihilation and solid-solid phase transitions.

This contribution introduces a geometrically nonlinear, continuum thermomechanical framework for pulsed laser heating in crystalline matter: a physical process which is characterized by a non-Fourier like heat propagation, defect diffusion. The key objective of this work is to derive the highly nonlinear and strongly coupled system of governing equations describing the multi-physical behavior from fundamental balance principles. A general form for the Helmholtz energy is proposed and the resulting constitutive laws are derived from logical, thermodynamically consistent argumentation. The approach adopted to derive the governing equations is not entirely specific to laser induced heating, rather it encompasses a wide range of applications wherein heat conduction, species diffusion and finite elastic effects are coupled. The presentation is thus applicable to the generality of models for thermal and mechanical waves: an area of increasing research interest.

The constitutive relation for the heat flux follows Green and Naghdi's type III law — which includes Fourier's theory as a special case, but is much more general as the Green–Naghdi approach allows for thermal wave propagation. Conservation principles are used to determine the form of the various constitutive relations. A numerical example is presented for the fully coupled, nonlinear and transient theory.

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## Features of Contactless Excitation of Surface Acoustic Waves in Pre-stressed Thermo-elastic Layer

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In the framework of the linearized theory of thermo-elastic waves [1] the coupled dynamic problem with mixed boundary conditions of harmonic vibrations of a thermo-elastic layer, which occupies the region  $|x_1|, |x_2| \leq \infty, 0 \leq x_3 \leq h$ , is considered. The layer's surface is assumed to be free of mechanical stress, the bottom face is thermally insulated and is rigidly coupled with non-deformable base. Oscillations layer are induced by distributed in some area  $\Omega$  on its surface thermal load, determined by given temperature  $\tau e^{-i\omega t}$ . Outside of the region  $\Omega$  the surface of layer is thermally insulated. In its natural state the layer's material is orthotropic (6 mm class), with the symmetry axis oriented perpendicular to the layer's surface. The initial stress state due to both the initial homogeneous strain and the initial temperature. The solution of problem with mixed boundary conditions is reduced to the solution of the integral equation of first kind for the unknown heat flux function [2]:

$$\tau(x_1, x_2) = \frac{1}{4\pi^2} \iint_{\Omega} k(x_1 - \xi, x_2 - \eta, h) \theta(\xi, \eta) d\xi d\eta, \quad (1)$$

$$k(s, t, x_3) = \int_{\Gamma_1} \int_{\Gamma_2} K(\alpha_1, \alpha_2, x_3) e^{-i(\alpha_1 s + \alpha_2 t)} d\alpha_1 d\alpha_2. \quad (2)$$

The influence of initial stress and preheat on the surface acoustic field parameters, as well as the heat flow in the area of heat, is investigated. The possibility to compensate for the impact of initial stress on the parameters of the surface acoustic field by preheating of the layer is shown.

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## On phase decomposition and coarsening in binary and ternary solder - experimental and numerical studies

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Solder alloys provide a broad range of technical applications in automotive processing as well as in microelectromechanical systems (MEMS) and solar panels. For mechanical modelling one may distinguish between micro-mechanical models where solidification of the alloy and crystallographic details are studied and the continuum-thermodynamical approach we choose here, where the long-term evolution of the microstructure is modeled as a function of the mass concentration. This leads to the classical models of solid state phase separation and coarsening, which are the phase-field models of the Cahn-Hilliard type.

In our contribution we compare different numerical approaches to treat extended Cahn-Hilliard and Allen-Cahn phase-field models, cf. [1, 2]. In particular for the three-dimensional analysis we focus on the innovative isogeometric finite element approach and outline its considerable benefits in comparison to the other methods. The results are validated with detailed experimental studies which illustrate aging by phase decomposition and coarsening in different SAC alloys.

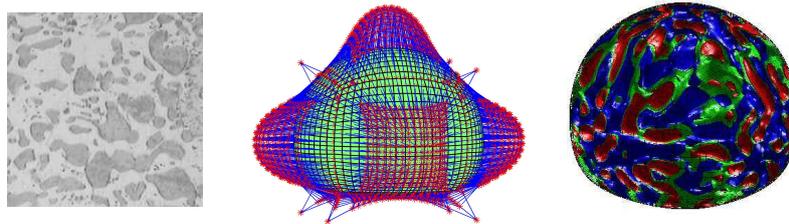


Figure 1: Phase decomposition in Sn-Pb and isogeometric simulation of a solder ball, cf. [1, 2].

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## Nonstandard Approaches to Finite Element Modelling of Piezoelectric Devices with Gyration Effects, Thermal and Acoustic Fields

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In present work the new models and numerical methods for dynamic behaviors of piezoelectric devices with rotation and temperature effects and with taking into account the acoustic media are presented.

For piezoelectric vibratory gyroscopes, working on "energy trapped" effects, we introduce the small parameter. This parameter is the ratio between rotation frequency and principal resonance frequency. For modelling the work of such piezoelectric gyroscope we use the solution expansion in series with this small parameter. In first phase we solve the eigenvalue problems and the harmonic problem close to resonance frequency. Obtained mechanical displacements are stored in the nodes of finite element mesh for utilization in the next step. In the second phase we solve the problem with axial rotation and relative displacement in the resonance frequency. These Coriolis' forces are considered as nodal body forces. Developed methods are applied in the special program modules for finite element package ANSYS. In the results the optimization calculations for investigated new effective piezoelectric vibratory gyroscopes are realized. We also apply the usual ANSYS techniques for analysis of piezoelectric gyroscopes and discuss these two approaches.

For analysis of piezoelectric transformers and smart-devices with temperature effects we consider full and loosely coupled thermopiezoelectric problems. Using additional macros for ANSYS it is possible also to solve practically important problem about dissipative initial heating of piezoelectric devices under harmonic vibration. In particular, having solved in ANSYS the harmonic piezoelectric problem by standard way one can find the displacement field. Using this field we calculate averaged dissipative function. This dissipative function is further considered as additional thermal source in heat flow problem, which is solved in ANSYS. Note, that with the dependence of the modules of a piezoelectric body on the temperature, it is possible to determine new piezoelectric moduli for the changed temperature from the oscillation period, and to solve the harmonic piezoelectric problem again, and then to solve the problem on the dissipative heating. In the upshot we receive the iterative computing process described dissipative heating.

We also present some models of piezoelectric ultrasound emitters loading on surrounding acoustic media with damping properties or loading on fluid media. We use the acoustic and hydrodynamic approaches by solving of acoustopiezoelectric problems and by using coupled ANSYS/Multiphysics and ANSYS/CFX analyses, respectively.

Then, the principal results consist in development of special finite element techniques and computer programs for analyses of piezoelectric vibratory gyroscopes, piezoelectric transformers and biomedical ultrasound devices.

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## FEA and experimental validation of an electroactive polymer actuator

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Novel electromechanical transducers based on electroactive polymers (EAPs) have gained growing attention within the last years. In particular, the use of diaphragm EAP stack actuators for valve control found several applications, [1]. In this setup a voltage is applied at an electrically conductive layer on top of the EAP foil; it induces an electric field which results in a Maxwell stress and eventually compresses the polymer film.

In order to use the advantages of this new technology in a feasible application, an EAP diaphragm actuator was tested experimentally. In addition, finite-element analyses of the coupled electro-mechanical system have been performed and validated with the experimental results. The EAP, i.e., the insulating interface between the two conductive layers consists of a hyperelastic material, a silicone. Thus, an incompressible isotropic hyperelastic material model (3-parameter Yeoh model) is employed and a circular parallel-plate capacitor has been assumed for the electrical part, [2]. By means of semi-analytically coupling the EAP structure has been optimized in terms of applied voltage and, in particular, for the biaxial prestretch of the diaphragm.

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## Effect of threading dislocation on elastic and electric properties of semipolar GaN/AlN quantum dot

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It is observed by experiment [4] that most of wurzite polar GaN quantum dots (QDs) embedded in a AlN matrix are located next to the threading dislocations (TD). It is assumed that local distortion field around dislocation influences the lattice parameters of the crystal structure and provides preferential geometric conditions for the nucleation of the QD at this site. So, on the one hand the presence of dislocations may facilitate QD growth, but on the other hand they play a highly negative role as a non-radiative recombination centres that reduce optical output, heat-up the device and reduce its operational lifetime. Except that, the presence of a long-range elastic and electric fields appearing in the proximity of a negatively charged TD [1] leads to the expectation that these fields will affect elastic, electric and finally an optoelectronic properties of the QD. Therefore, the effect of neighbouring dislocation seems to be very important for the electric properties of the semipolar QD due to the fact that semipolar growth is used to reduce a strong built-in electric field present in QD grown along polar direction. The quantification of that effects remains an open question.

To investigate that phenomena, a model of isolated, rectangular-based  $(11\bar{2}2)$  GaN/AlN QD [3] nucleated at the edge of a TD is considered. Burgers vector of a partial Frank-Schockley dislocation, common in a  $(11\bar{2}2)$  semipolar heterostructure, is assumed as:  $\frac{1}{6}\langle 20\bar{2}3 \rangle$  [2]. A boundary-value problem for piezoelectric material by was solved by use of finite element analysis and elastic, electric and optoelectronic properties (stress, strain, potential, and band edge structure) of the complex system (QD next to TD) were determined. Local elongation of the crystal structure around TD modifies intrinsic compressive stress/strain field present in the quantum dot. Axisymmetric distribution of the negative potential causes shift of the QD build-in electrostatic potential towards negative values. That causes heavy shift of the carriers opposite to the dislocation line. According to a tentative results a TD located next to a semi-polar QD increase intrinsic electric field intensity in QD therefore has negative effect on the optoelectronic properties of a dot.

**Acknowledgments** This research was supported by the projects N N519 647640 founded by the Polish Ministry of Science and Higher Education.

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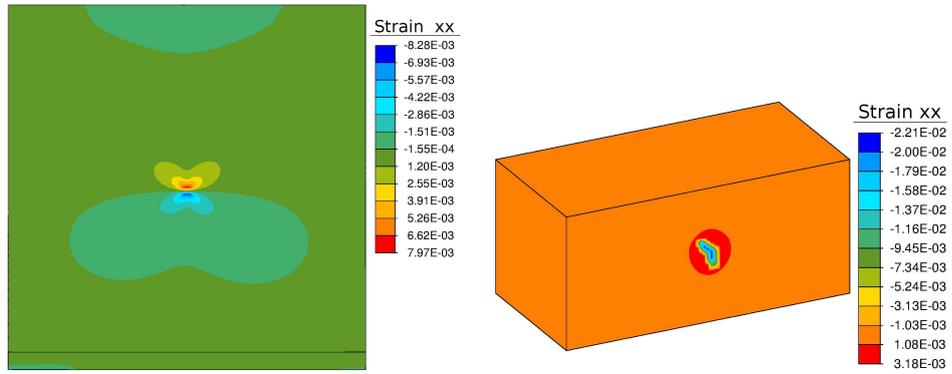


Figure 1: Strain field (xx component) around TD line and intrinsic strain in QD.

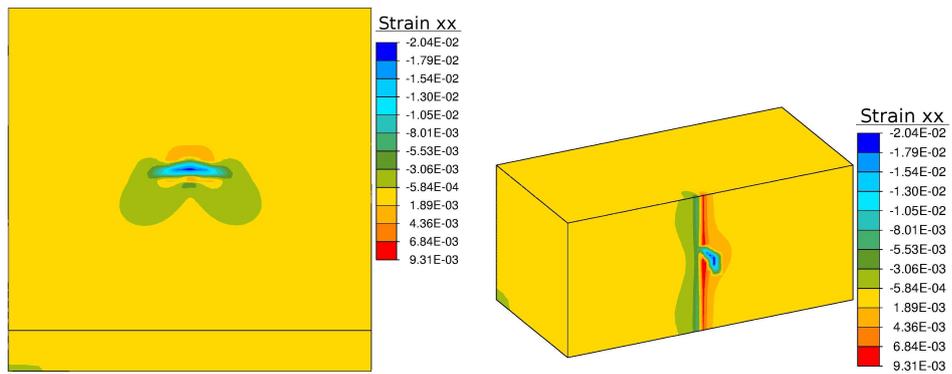


Figure 2: Strain field (xx component) of the system composed of QD grown next to TD.

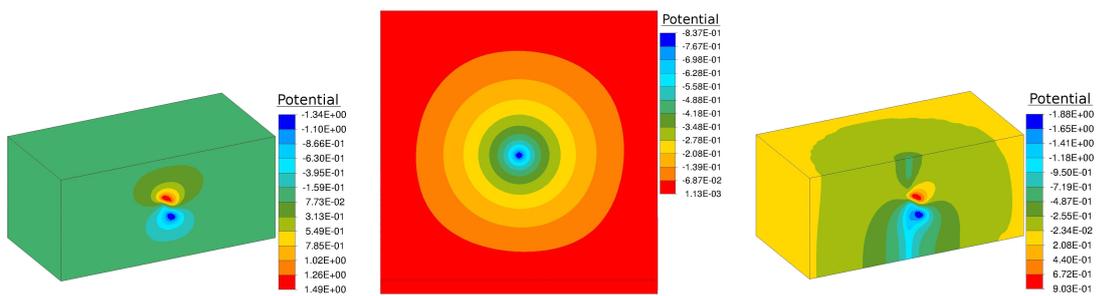


Figure 3: Electrostatic potential field in an isolated QD, around TD, and resultant potential in the sample containing QD and TD.



## Session 16

# Experimental identification and material characterization



## **Effect of the heat curing on strength development of ultra-high performance fiber reinforced concrete (UHPFRC) containing dune sand and ground brick waste**

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This work aims to investigate the strength development of ultra-high performance fiber reinforced concrete (UHPFRC) containing dune sand (SD) and ground brick waste (GWB). The variables are the addition nature (SD and GWB) in the binder and the heat curing at different temperatures (20°C and 60°C) at 7 days of curing [1]. Two temperatures 20 and 60 °C were applied to samples with intermediate levels for 8 hours in total [2-3]. In this study, a Portland cements (CEMI and CEMII), dune sand, ground waste brick, were used in the binders of UHPFRC. The GWB was replaced by the sand dune finely ground at levels of 10, 20 and 30% by weight. The results show that the obtained concretes develop a high mechanical performance with a suitable heat treatment according the cement type and fiber used. The compressive strength to 7 days of UHPFRC has increased with treatment (60 °C) compared to that obtained without 28 days curing treatment and measured at 20 °C. Also, values of compressive strength of concrete containing the sand dune are close to those obtained by the control concrete. This study has showed that the dune sand can be used in UHPRC, and that the substitution of the ground brick waste by the dune sand finely ground can provide concrete with acceptable mechanical performance.

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## Experimental investigation of discontinuous plastic flow in 304 and 316 austenitic stainless steels at liquid helium temperature (4.2K)

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FCC metals and alloys belong to the group of engineering materials massively applied at cryogenic low temperatures. These materials, in such extreme conditions, often manifest discontinuous plastic flow (DPF). DPF has been investigated experimentally by many authors (Basinski 1957, Schwarz and Mitchell 1974, Reed and Walsh 1988, Hähner and Zaiser 1997, Benallal 2006, Obst and Nyilas (1991) [1]). A physically based constitutive model of discontinuous plastic flow including the relevant thermodynamic background has been developed by Skoczeń et al. [2]. The DPF is described by the mechanism of local catastrophic failure of lattice barriers (for instance Lomer–Cottrell locks) under the stress fields related to the accumulating edge dislocations. The failure of LC locks leads to massive motion of released dislocations accompanied by stepwise increase of the strain rate. Therefore, the DPF appears in the stress-strain curve in the form of oscillations of stress against strain (the serrations). Each serration is accompanied by considerable increase of temperature, related to dissipation of plastic power and the thermodynamic instability. Single serration shows usually similar pattern: after the initial elastic process, smooth plastic flow occurs until the abrupt drop of stress. For the austenitic steel, in the next stage the relaxation takes place, after which the beginning of elastic stage is immediately observed.

The present paper is focused on the identification of parameters of the constitutive model of DPF, proposed by Skoczeń et al. Based on the own experimental data, collected during several campaigns of tensile tests carried out on stainless steel samples (304, 316) immersed in liquid helium (4.2 K), it turns out that generated slip bands move along the gauge part of the specimen (from grip to grip). Previous models did not include the observed phenomenon. Therefore, the basic idea of updated model is associated with the assumption that RVE travels together with the slip band during tensile test. It is worth pointing out, that smooth motion of slip bands occurs only for the strain range, where  $\gamma \rightarrow \alpha'$  phase transformation has not yet begun. The tests were carried out by means of experimental set up at the Cracow University of Technology. Special clip-on extensometers fixed on the specimen allow high precision measurements of strain. A film resistance cryogenic temperature sensor with fast thermal response time at 4.2 K, directly glued on the central part of the specimen, allows the temperature of the sample to be recorded during the whole test and particularly during transition of slip band across the place where the sensor is localized. Internal piezoelectric sensor, aligned with the specimen, is used to measure the force applied to the specimen.

**Acknowledgments** Grant of Polish National Science Centre 2284/B/T02/2011/40 is gratefully acknowledged.

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## Multiscale characterization and modelling of the viscoplastic behaviour of titanium at room temperature

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Room-temperature creep in titanium alloys is a key factor for several problems of structural integrity (the so-called “cold dwell effect” i.e. room-temperature creep-fatigue interactions in aircraft engine parts or subcritical crack growth in presence of residual stresses). However, the underlying mechanisms are not fully understood. The importance of this problem generally rises with the proportion of  $\alpha$  (hcp) phase. That is why this study focuses on fully  $\alpha$  commercial purity titanium. The influence of solute oxygen and hydrogen on the viscoplastic behaviour of titanium at room-temperature is investigated.

Tensile tests with strain rate jumps as well as creep and relaxation tests are performed in the rolling and transverse directions of grade 2 and grade 4 Ti plates in the as-received (1600ppm O, 5ppm H and 3200ppm O, 15ppm H, respectively) or H-charged condition (around 25ppm H). A significant plastic anisotropy appears. The yield stress and the strain-rate sensitivity rise with the O content and are higher along the transverse direction. Depending on the applied stress, room-temperature creep tends to saturate or leads to fracture. Distinctive signs of static and dynamic strain aging are observed, among which a Lüders plateau and yield points after aging in the unloaded state, small serrations at low strain rates and an incubation time before creep at low stress for the grade with the highest O content.

TEM observations of dislocation structures after 200h creep at  $0.7$  to  $0.8\sigma_{0.2}$  reveal mainly screw dislocations from prismatic and type  $\langle a \rangle$  pyramidal slip systems.

Tensile tests in longitudinal and transverse directions are also performed in a SEM after measurements of local crystal orientations by EBSD. The activation of various slip and twinning systems is monitored in real time, as well as the evolution of the Lankford coefficient, deduced from local strain field measurements by digital image correlation. Prismatic and pyramidal slip systems accommodate the largest part of the deformation, while basal slip is very limited and twinning is observed mainly in tension along the transverse direction in the Ti grade with the lowest O content.

All those data, as well as the ODF measured by EBSD are used to identify a crystal viscoplasticity model (<http://www.zset-software.com/>). The impact of oxygen and hydrogen content on the identified critical shear stresses and hardening parameters is discussed.

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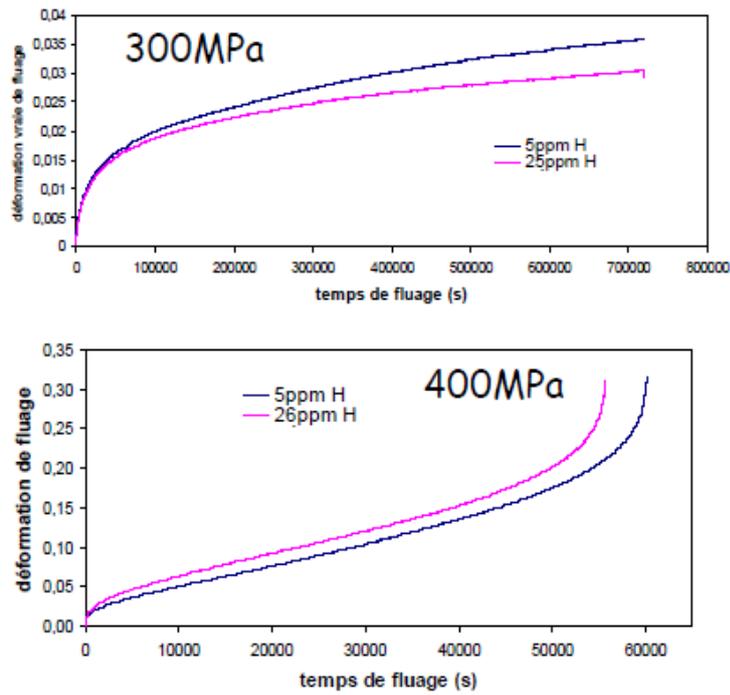


Figure 1: Influence of the H content on room-temperature creep of grade 2 titanium in the rolling direction for two stress levels

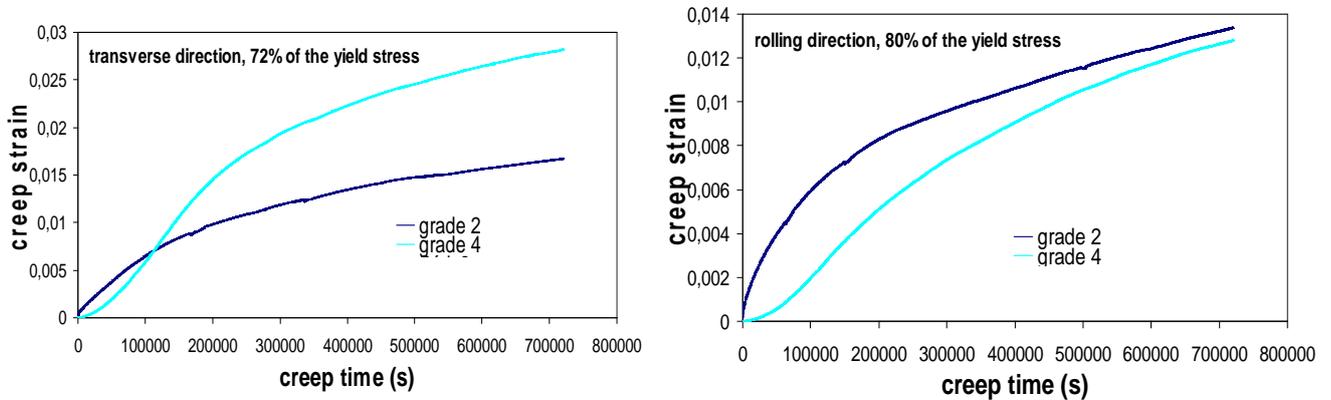


Figure 2: Influence of the O content on room-temperature creep in the longitudinal and transverse directions. Note the incubation period before creep in grade 4 Ti.

## Nanoindentation of soft polymer: Modelling and experimental investigation

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Nanoindentation technique has attracted great interest due to its ability to extract mechanical properties of materials down to the sub-micrometer scale. Therefore, recently nanoindentation has been widely used as a method to measure the nano- to micro-mechanical properties of small volume polymeric materials. Most polymers show finite elastic as well as rate-dependent properties. However, on the one hand, it is hard to characterize the finite elasticity and rate-dependent properties from nanoindentation force-displacement data by the often used Oliver & Pharr method [1]. On the other hand, surface interactions such as surface roughness [2] and adhesion [3] could contribute strong errors to the force-displacement data on the nanoscale.

It is our aim to develop a robust and reliable method of characterising the non-linear viscoelastic behaviour of polymers from rate-dependent nanoindentation tests based on inverse methods. To set up the stage, the nanoindentation experiments are performed on a series of polymer materials with different viscoelastic properties, e.g. silicone rubber, PDMS, PU and EPDM. The concept of a numerical optimisation is applied. The model parameters are determined by approximating the experimental data with the numerical model's response. Various error contributions, e. g. adhesion, surface roughness and indentation process associated factors are taken into account in order to reduce the systematic difference between the numerical model and the experimental data. The goal of our work is to quantify the influence of the polymer's viscosity and those error contributions with respect to both real experiments and numerical simulations. The results from the indentation tests are compared to results obtained in uniaxial or multiaxial tension tests and macroindentation tests appraising the guess of the model parameters.

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## Constitutive modelling and experimental study of discontinuous plastic flow in 316LN and JK2LB steels at very low temperature

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Several metals and alloys, exhibiting Face-Centered Cubic (FCC) lattice and subjected to deformation at temperature near to absolute zero feature the phenomenon of Discontinuous Plastic Flow (DPF). The DPF, reflecting the effect of Dynamic Strain Ageing (DSA), is described by the mechanism of local failure of Lomer-Cottrell (LC) locks under the stress fields surrounding pile-ups of edge dislocations [2]. During tensile straining at cryogenic temperature, each massive release and motion of dislocations is represented by a stress response defined in four stages accompanied by sudden increase of the strain rate and local rise of temperature.

The constitutive model of the DPF, well assessed for copper and copper alloys [3], has been expanded with the experimental data arising from recent campaigns of tensile tests carried out on low carbon austenitic stainless steel 316LN and high Mn-bearing stainless steel JK2LB [1] specimens immersed in liquid helium (4.2 K). Model parameters have been identified and a comparison of results is provided between the two grades, similar in a steelmaking, extrusion and drawing process as well as very comparable in terms of microstructure (inclusion, grain size, fully austenitic structure).

The unique experimental set-up developed at CERN, already highly performing with the high acquisition rate, was further developed and improved. Results presented in this paper were obtained by force measurement based on internal load cells, deformation recorded by LVDT extensometers, and temperature measured by sensor placed on the specimen inside cryostat during the test.

New accurate results, based on a large number of tests and optimized data acquisition, allow the existing DPF model to be verified and calibrated for use with high strength steels and alloys used in cryogenic environment.

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## Non-linear elastic-plastic characterization of a high strength bainitic roller bearing steel

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The mechanical behaviour of a high strength bainitic roller bearing steel was investigated through a series of uniaxial experiments. Monotonic tension, compression and torsion experiments revealed that the material showed influence of hydrostatic pressure on yielding. Furthermore, this strength differential effect remained with increasing amount of plastic strains. The associated flow rule includes plastic strain increments perpendicular to the yield surface. For a pressure sensitive yield surface such a flow rule predicts volume expansion at plastic deformation. Therefore, the density was measured on both new and deformed specimens. No change of density was detected due to the induced plastic deformations. If any volume expansion had existed during plastic deformation in the experiments, then it was less than 1/15 of the prediction of the associated flow rule. Furthermore, cyclic push-pull experiments showed that the material hardening was mostly kinematic with some component of isotropic hardening.

Also, a small but not negligible non-linear elastic behaviour was detected when investigating the cyclic uniaxial push-pull experiments. Since isotropic elastic material behaviour includes two material parameters cyclic torsion experiments were performed on thin walled pipe specimens. The goal with these experiments was to distribute the non-linear elastic behaviour between two elastic parameters. When the cyclic experiments turned out to be linear in the elastic load range and therefore well described by a constant shear modulus the shear modulus was a straight forward selection as elastic parameter. The bulk modulus was then a natural selection for the second elastic parameter.

A non-linear elastic-plastic model was derived for the material behaviour of the high strength bearing material. The model included the strength differential effect, which was modelled with a linear Drucker-Prager yield surface. The non-linear material hardening was described with the combined isotropic and kinematic Chaboche model in combination with a non-associated flow rule. Furthermore, non-linear elasticity was included; the bulk modulus was extended with a second order term that was related to the elastic dilatation and the shear modulus was constant. Expressions were derived for the influence of non-linear elasticity on the elastic-plastic hardening and the compliance tensors. The extended material model was then used to predict the elastic-plastic results from cyclic push-pull experiments with deformation control and zero mean deformation; cyclic load controlled experiments with compressive mean stress and ratchetting; cyclic torsion or shear experiments.

By changing the model parameters the effect of associated versus non-associated flow rule for the current material was illustrated. In a similar way the importance of including non-linear elastic effects were illuminated.

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## Study of the mechanical behavior of leaded copper by scratch test and nanoindentation

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The material based on copper is widely used in industry, so it is necessary to improve their antifriction behavior for use in particular bearings. Sliding bearings made of these materials for high rotational speeds do not meet the requirements for wear resistance and longevity in equipment. The addition of lead gives the material plasticity and raises its durability. This provides a material low coefficient of friction. Abrasion of hard metal has been the subject of much previous work reported in the literature, but the wear processes that occur are complex and not easy to understand [1, 2].

In this paper scratch test and nanoindentation were investigated in order to identify their mechanical behavior, and were compared with the tribological properties of a leaded copper. Scratch test, first developed to assess the adhesion of coating, gives a good idea of the practical adhesion of the deposit on the substrate, taking into account the complexity of the effect of the material microstructure, the external loading and the environmental aspects. Modern investigation techniques such as acoustic emission, in situ microscopy, and friction coefficient and penetration depth measurements are used to determine precisely the critical load and the degradation modes of the system [3, 4].

Scratch tests cannot be used to predict quantitative wear rates of materials and coatings. In order to address some of these limitations, the nanoindentation has been increasingly gaining applications in the engineering field. It is an instrumented hardness measurement method that is mainly used to study coatings. The nanoindentation process differs from macro and microhardness testing in two main ways: the load applied to the indenter is much smaller (generally a few mN) and the hardness of the material is calculated from the displacement of the indenter during loading and unloading instead of from the residual size of the indent and it is possible to measure the hardness' evolution over small areas and across coatings [5].

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## From microstructure to mechanical properties characterization of an expanded starch-based polymer

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Bio-polymer materials are currently developed as a replacement for polymers from the petrochemical industry. They are biodegradable materials created from natural ingredients, which makes them environmentally friendly, and their use as functional or structural materials, in this case, is not suspected to affect rates of commodity materials for human being since they are poor in protein.

This study focuses on materials made from starch and glycerol. A combined process of expansion and extrusion of this melt leads to cylindrical bars with an open foam microstructure. The effect of the amount of glycerol is studied in this work. SEM and optical analyses have shown that pores sizes decrease and cell wall thicknesses increase as the percentage of glycerol increases. X-Ray diffraction analysis has revealed an ability of glycerol to hinder the total destruction of the starch granules during the elaboration process.

From the mechanical point of view, the knowledge on this type of bio-based material is very poor. Mechanical property characterization has thus been performed by large deformation compression tests on pile-ups of cylindrical bars constituting a bulk foam material. This material exhibits an elastoviscoplastic behavior with a very large sensitivity to strain rate, strongly influenced by glycerol amount. Whereas it deforms according to the classical three-stage regime of deformation of foams under compression (elasticity of walls, buckling and then densification), the walls remain partially stucked to each other during unloading. This enhances the difference between tensile and compressive behavior and makes this material's constitutive behavior original compared to most kinds of porous materials. Different models are tested to reproduce this particular constitutive behavior at different strain rates: a non-linear viscoelastic model (Mooney), an elastoviscoplastic model with an elliptic criterion enabling to account for sensitivity of plasticity to hydrostatic stresses and a finite-element microstructure-based model.

## Residual stress determination based on the hole drilling method in explosively welded bimetallic composite

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Increasing requirements of operational safety and economical aspects are leading to development of universal materials such as metallic composites. The technology of explosive welding allows for producing multilayer materials that combines different mechanical properties. Main advantage of the explosive welding is ability to join materials which are very difficult or impossible to join using standard methods [1-3]. Despite many advantages and wide application of those materials in specialized mechanical systems, some of their mechanical and fatigue properties are still not well recognized. One of the important factors influencing overall properties of bimetallic material is residual stress produced during welding and heat treatment process [4, 5]. In specialized literature explosively welded bimetallics are frequently analysed in case of microstructural changes and strength under monotonic loadings [2, 6, 7]. Phenomenon of the residual stress is not investigated. Paper presents results of residual stress measurements performed on steel 355J2-titanium Grade 1 bimetallic plates before and after heat treatment. Determination of residual stress was performed using hole drilling method [8]. In order to simulate behaviour of the material consisting of two different layers, finite element method was used to modify residual stress computing process.

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Session 17

# Computational modeling of materials with microstructures



## Numerical Simulation of Microscopic Stress in Polycrystalline Materials Considering Hardening due to Irradiation

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Materials used for core internals of light water reactors are subjected to neutron irradiation and change in mechanical properties occurs. The effect of neutron irradiation on fracture behaviour should be taken in to consideration. In addition, higher local stress and strain compared to macroscopically applied stress and strain are induced in a microscopic scale due to anisotropy caused by crystal orientation. The characteristics of such local stress and strain distribution are essential to clarify the fracture behaviour of irradiated materials. In this study, the local stress distribution in austenitic stainless steel was investigated by finite element crystal plasticity analysis considering hardening due to neutron irradiation.

Finite element models of crystalline aggregate were generated and calculation of uniaxial tension was performed. The crystal orientation of each grain was determined randomly. An example of a model for the numerical simulation is shown in Fig. 1. The number of grains included in the model was 250, which was confirmed to be enough for the evaluation of the relationship between the macroscopic and microscopic stress.

In order to model the mechanical property of hardened materials due to neutron irradiation, austenitic stainless steel was cold worked and its stress-strain relationship was obtained. The cold work was introduced by rolling of plate with reduction of thickness 0, 10, 20, 40 and 50%. Stress-strain relationship for the polycrystalline aggregate was calculated by finite element simulation as shown in Fig. 1.

The material parameters involved in the theory of crystal plasticity were determined to reproduce the stress-strain curves. The comparison of stress-strain curves between experiment and numerical simulation is shown in Fig. 2.

Microscopic stress distribution at several strain levels are shown in Figs. 3 and 4 for 0% and 50% cold worked materials, respectively. Von Mises stress is shown in the figure as an example. Inhomogeneous stress distribution is observed due to crystal orientation. Based on the simulation results, the volume of elements of which von Mises stress belongs to a certain range was summed and the fraction to the entire model was calculated. The above calculation was performed for each material and for each strain levels, and they were plotted on graphs like histogram as shown in Figs. 5 and 6. It is seen from these figures that higher stress is acting locally compared to the macroscopically applied stress. The tendency is more remarkable in 50% cold worked material than 0% one. In addition, the locally high stress is observed when applied strain level is high. Such information that how much high stress are acting locally is useful for the evaluation of fracture behaviour of irradiated materials.

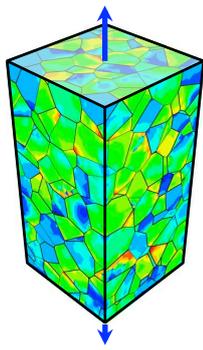


Fig. 1 An example of a model for the numerical simulation.

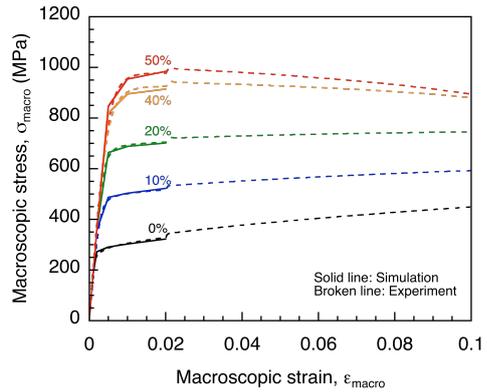


Fig. 2 Stress strain curves obtained by experiment and numerical simulation of polycrystalline model.

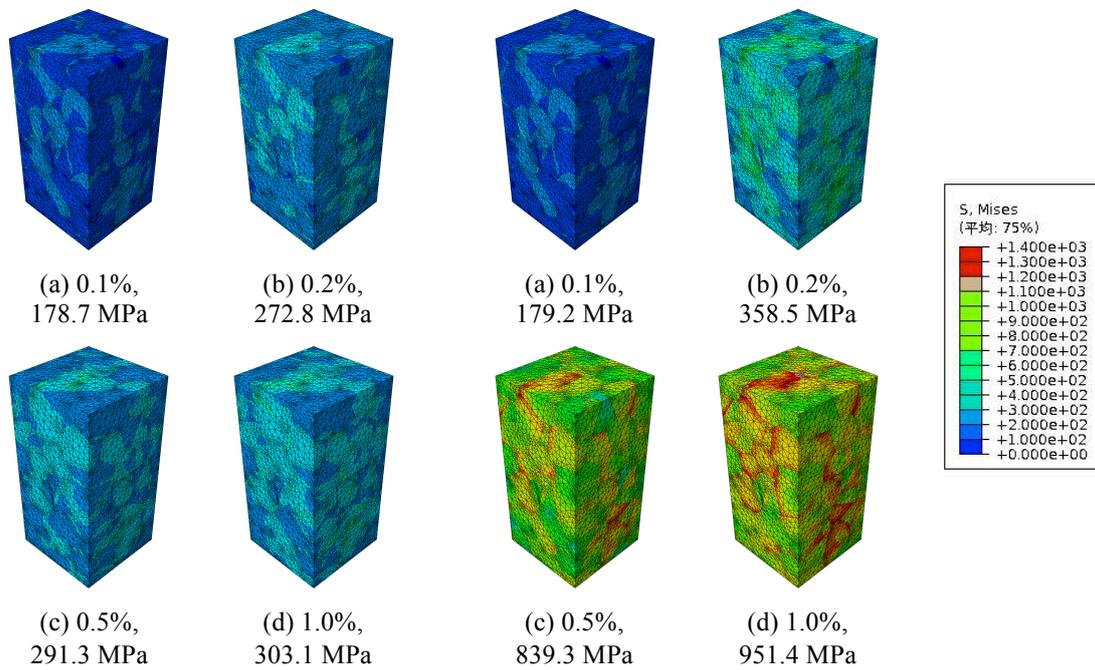


Fig. 3 Microscopic stress distribution at each strain level (0% cold work)

Fig. 4 Microscopic stress distribution at each strain level (50% cold work)

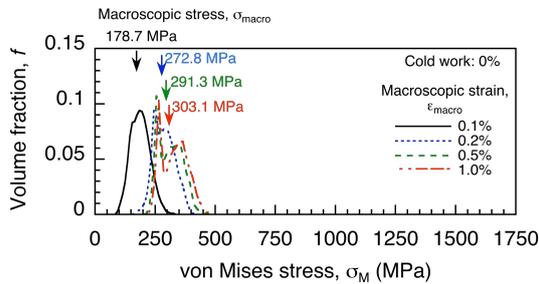


Fig. 5 Volume fraction of microscopic stress in the model (0% cold work)

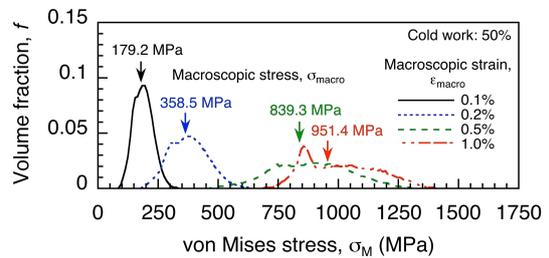


Fig. 6 Volume fraction of microscopic stress in the model (50% cold work)

## Evaluation of Ductile Fracture in Ferrite–Pearlite Steels for Drawing by the Void Model

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The ferrite–pearlite microstructure is fundamental for applications of carbon steels. Extensive studies have been conducted on the ductile fracture in ferrite–pearlite steels. These studies have demonstrated void nucleation due to the fracture of pearlite nodules and the propagation of macroscopic cracks due to the growth and coalescence of voids [1-3]. However, these previous studies are experimental; an analytical study is required to clearly understand the effect of material microstructure on ductile fracture. In our void model for the evaluation of ductile fracture [4], circular voids are assumed to nucleate [5]. In other words, voids are assumed to nucleate owing to decohesion of inclusions from a matrix. However, voids nucleate owing to the fracture of pearlite nodules in the ferrite–pearlite microstructure. Hence, it is impossible to evaluate ductile fracture in ferrite–pearlite steels using our void model in its current form.

In this study, we first improve our void model to consider the nucleation of voids due to inclusion fracture. The shape of pearlite nodules before their deformation is assumed to be circular, and their deformation is assumed to be identical to that of a ferrite matrix. When the macroscopic strain of the material attains a certain value that is dependent on its carbon content, it is assumed that pearlite nodules fracture and voids nucleate. The tangential direction of the fractured surface is assumed to be the direction of the maximum shearing stress of the material. The shape of voids is assumed to be ellipsoidal to simplify the analysis.

Second, we evaluate the ductile fracture in ferrite–pearlite steels in multi-pass drawing by using our improved void model. A ferrite–pearlite steel, which is JIS S15C and equivalent to ISO C15E4, was used. A specimen is drawn multiple times using different dies until an inner fracture defect appears in the specimen. The multi-pass drawing experiment was performed with the reduction in area and die angle specified for each die. The inner diameter of the die at which the material fractures and the material density distribution in the radial direction after drawing through the die preceding the die at which the material fractures, both calculated from the analysis, were compared with those obtained from the experiment.

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## **Kaolinite thermodynamic properties calculations using molecular dynamics simulation**

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Kaolinite is one of the most abundant clays minerals on the earth surface. It covers wide applications in engineering. The objective of this poster is the study of thermodynamics properties of kaolinite under atmospheric pressure by means of molecular dynamics calculation based on a recently developed force field (CLAYFF) [1]. The variation of structural parameters of kaolinite will be studied as function of temperature.

The variation of structural parameters will be studied kaolinite function temperature. Among our main results, the calculation of the thermal expansion, the heat capacities ( $C_v$  and  $C_p$ ) and superheating point, which is found at 1572 K [2]. The transition from solid to liquid structure has also been observed from the density profiles and radial distribution functions.

Finally, we have combined both pressure and temperature effects for the study of kaolinite. A relation has been proposed to describe solid-liquid phase and to determine the superheating point. Besides, the double effect pressure-temperature allowed us to establish a phase diagram for kaolinite which can give a precise idea on the behaviour of this clay in some specific range of temperature and pressure [3].

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## Determination of the size of an RVE for nonlinear random composites

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The representative volume element (RVE) is important to predict effective physical and mechanical of random heterogeneous materials. Several studies have been devoted to determine the size of the RVE for linear [2, 4] and nonlinear materials [1, 3, 6, 9, 10]. However, the procedures are usually based on convergence analysis associated to the stress-strain curve or on quantities related to stress and strains [7]. Defining a procedure to determine the size of an RVE for general nonlinear elastoplastic behavior with hardening remains a difficult problem.

In this paper, a new methodology to estimate the effective size of RVE for nonlinear composites is proposed. The techniques uses some features of statistical convergence analyses developed in Kanit et al., Pelissou et al. and Gitman et al. [1, 2, 6]. Realizations of 2D RVE microstructures with randomly distributed cylindrical fibers are generated. For each one, the coefficients of an empirical macroscopic law are identified. Then the statistical convergence analysis is carried out on the parameters of the macroscopic model instead of the elastic parameters as in the linear case. Two nonlinear behaviors were considered: von-Mises elasto-plastic behaviour with hardening [8] and elasto-visco-plastic behaviour with creep model using current yield Norton law [5]. Through the convergence of all identified parameters, an effective size of RVE has been determined. The size of the RVE with respect to the model parameters has been performed.

The results show the existence of an effective size of RVE for these microstructures and the studied nonlinear behavior.

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## Phase Field modeling of microstructure evolution coupled with plastic activity

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Plastic activity is often involved during microstructure evolution. The Phase Field Method (PFM) is the most powerful method to understand microstructure evolution during phase transformations at mesoscale. In this work, a model able to describe both microstructure evolution and plastic activity is derived by coupling a phase field model with a continuum viscoplasticity model.

Several aspects of the plastic behavior have to be considered in order to achieve realistic predictions. First, plastic activity is anisotropic because it results from slip of crystal defects on crystallographic systems. Second, it is well known that, in a heterogeneous material, when the domains are small enough (below typically 1 micron) the plastic behavior of each domain depends on its size. In a continuous modeling, both effects can only be accounted for using a scale dependent crystal plasticity model.

First, we have developed a model accounting for the consequences of the second effect i.e. the confinement of plasticity during microstructure evolution. It has been achieved by coupling a Phase Field Model to an isotropic strain gradient viscoplasticity model coming from generalized continuum mechanics [1]. In a second step, the description of plasticity has been improved using a crystalline viscoplasticity-dislocations density based model. Both models have been applied to study microstructure evolution in Ni-based superalloys, more precisely, rafting during creep loading.

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## Generalized boundary conditions on representative volume elements and their use in determining the effective material properties

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The effective material behavior of a micro-structured material depends strongly on its micro-structure. For the efficient examination of the micro-macro-interaction, one needs fast and robust homogenization methods. In most cases, one relies on the representative volume element method (RVE) [2]. This method consists in selecting a material section, subjecting it to an average value of the independent variable (e.g. the strains) by appropriate boundary conditions, solving the boundary value problem and extracting the average value of the dependent variable (e.g. the stresses) from the solution. In this contribution we are concerned with the appropriate boundary conditions. We present generalized boundary conditions that involve a surface partitioning, and the prescription of an average deformation on each partition. One can show that the Hill-Mandel-condition is satisfied for arbitrary surface partitionings, and that the classical boundary conditions (homogeneous stresses, homogeneous strains and periodic boundary conditions) are contained as special cases. However, the generalization allows to specify further interesting boundary conditions with advantageous properties. Firstly, one is able to adjust the elastic stiffness of the RVE between the two extremal cases (homogeneous stresses and homogeneous strains) by a more or less fine surface partitioning. Secondly, by a stochastic surface partitioning, one is able to increase the resistance of the RVE against localization. In case of localization, an effective material behavior that is too soft is predicted. One can see this by a simple test, namely the application of a RVE to a homogeneous, softening material. In case of periodic or homogeneous stress boundary conditions, a shear band (periodic) or pop-out (homogeneous stress) will form, accompanied by a drastic deviation from the expected effective stress-strain response [1]. Due to a stochastic coupling, shear bands are diffused at the boundary. Thus, the advantages of the periodic boundary conditions of a moderate stiffness and the homogeneous strain boundary conditions of a large resistance against localization can be combined in the stochastic boundary conditions.

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## Domain Decomposition Methods For Evaluating Elastic Properties Of Random Fibre Composites

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The communication deals with the setting up of a domain decomposition framework for evaluating effective elastic properties of random heterogeneous media. We consider the context of short fibres reinforced polymer composites. Such a kind of material arouses interest of industrialists and researchers all over the world. Their extraordinary weight-to-strength ratio associated sometimes to a low cost of production, designate them as good candidates for manufacturing purposes. Numerical simulations are very useful for predicting their mechanical response., especially when the network of fibres is such as no analytical model is available. In this context, a numerical modelling is more convenient but still remains tricky. Indeed, a random generation of heterogeneities within a representative volume element (RVE) leads to a very complex geometry which is difficultly reproducible in a finite element approach.

In the present work, we generate RVEs for which all morphological parameters, namely, length, diameter, spatial position, curvature and orientation are randomly generated. A finite element mesh is built according to a grid approximation based on the model with an n-order approximate geometry [1]. This consists in combining a classical pixelisation approach with a local adaptive mesh refinement strategy in order to tremendously reduce both calculation cost and storage memory. Geometric accuracy depends on a parameter called n-order where n designates the level of refinement in powers of two.

Such a kind of concept is very reliable and efficient for evaluating effective properties of random fibre composites. In addition, this one is easily adaptable in a domain decomposition framework since mesh structures are then very regular. The principle consists in subdividing a representative pattern into several sub-domains in order to distribute the finite element resolution on several processors (see Figure 1). This strategy enables a drastic reduction of the calculation cost. Two domain decomposition methods, namely, Schur complement and FETI [2] ones, are modified in order to provide effective elastic properties in the context of the double-scale and periodic homogenization. In the present work, effective properties are evaluated with the help of both methods in the context of random fibre composites. Results highlight interesting reliability (see Figure 2) and efficiency whatever the contrast of properties and the density of fibres are.

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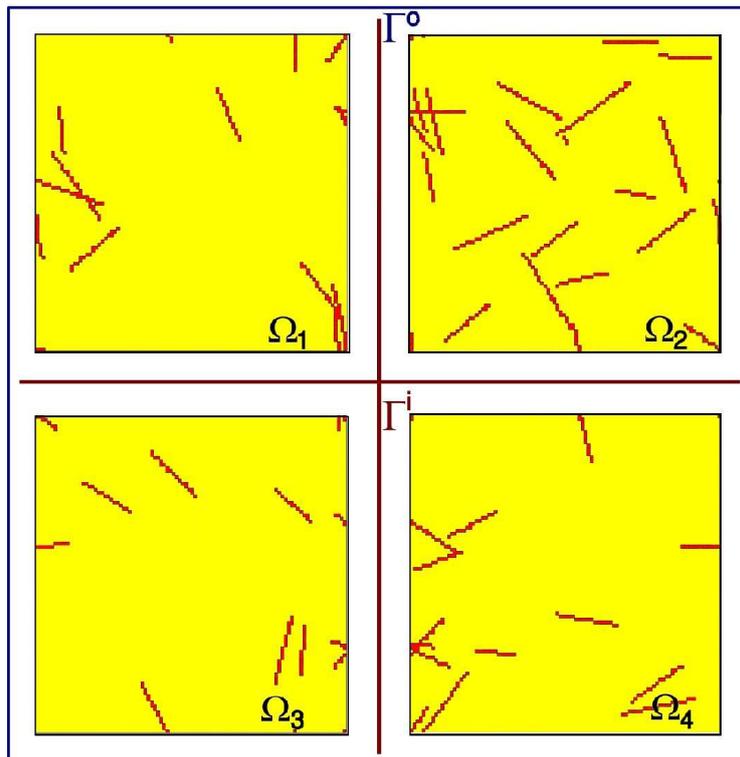


Figure 1 : 2D RVE generated with the help of the 0-order model and subdivision into 4 sub-domains.

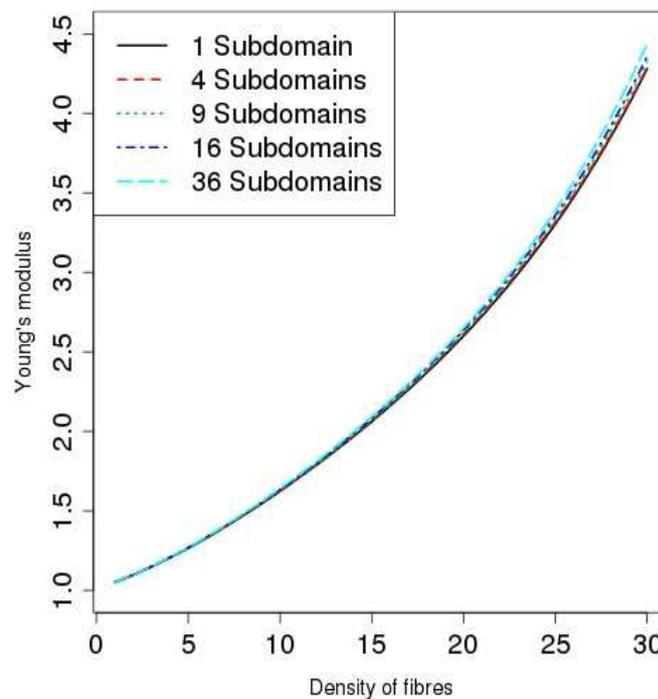


Figure 2 : Influence of the density of fibres on the effective normalized Young's modulus for a contrast of properties set at 250 and several kinds of subdivisions.

## A Random Fibre Network Model for Foetal Membranes

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Amnion, the inner layer of the foetal membrane (FM), was investigated in uniaxial and multiaxial tensile tests [1,2]. Particular features of its mechanical behaviour were observed such as the large incremental Poisson's ratio and the stiffening behaviour in multicycle experiments. We present here a random fibre network model able to rationalize the experimental observations. The model represents the collagen network of the amnion and was generated with a custom algorithm in MATLAB (MathWorks, Natick, MA) and solved with ABAQUS (Simulia, Providence, RI). Random points (crosslinks) were distributed in a 2D domain and connected to four neighbours with bilinear spring elements (crimped fibres). Fibres are modelled as simple connectors instead of beam elements, which allows simulating the whole domain in short computational time, and thus investigating the influence of model parameters, such as crosslinks density, domain size, fibres length, spring characteristics and boundary conditions.

Parameters are identified governing large transversal contraction, hysteresis, fibre reorientation and the characteristic nonlinear response observed in FM and other biological materials. Computational results are compared to observations of amnion kinematics in in-situ experiments in a multiphoton microscope.

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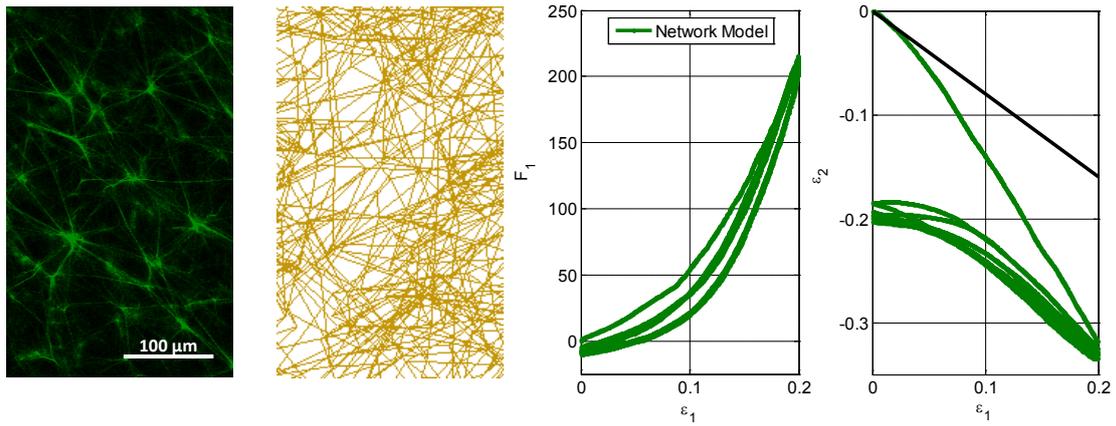


Figure 1: On the left, the collagenous microstructure of the amniotic main layer (second harmonic generation image) next to the network model. On the right, the deformation behaviour of the network shows a large partially-reversible transversal contraction. The black line represents an area preserving kinematics.

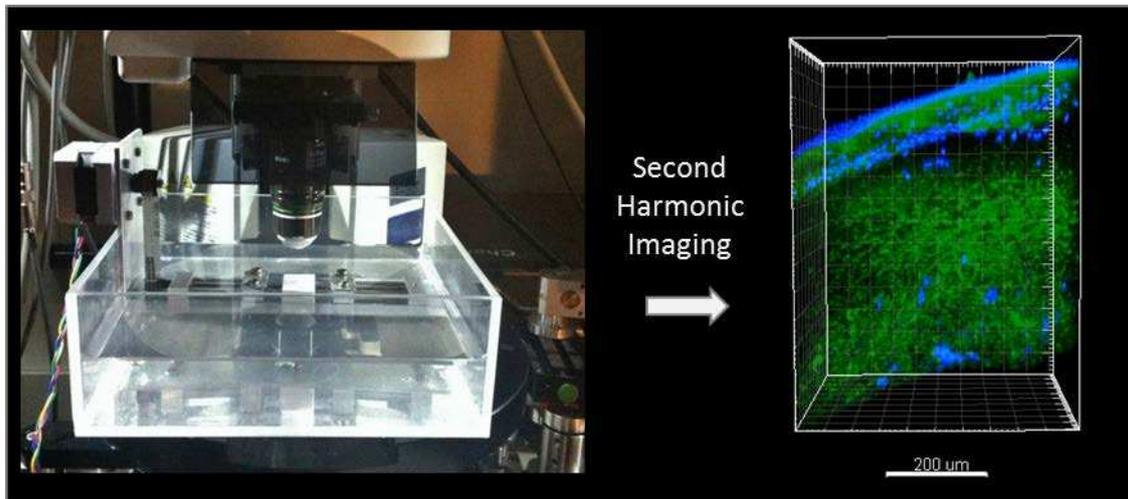


Figure 2: On the left, the in-situ stretching for second harmonic imaging of FMs. On the right, a representative 3D stack of amnion with collagen in green and nuclei in blue.

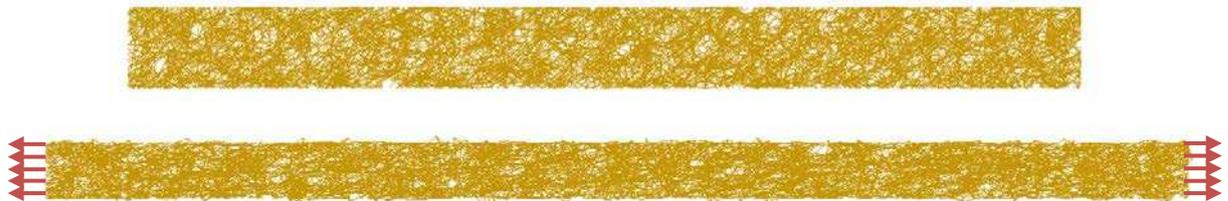


Figure 3: Network model simulation the entire domain under uniaxial tensile configuration. The network is represented at initial configuration (top) and at deformed configuration (bottom).

## Modeling of crystalline sub-micron gold with a gradient extended theory.

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The application of the gradient extended theory to the computation of a single sub-micron gold crystalline is the focus of this investigation. The research takes into account the dependence of the macroscopic behavior of a polycrystalline material from the size and morphology of the grains, the volume fraction of different phases, and the subgrain material modeling [1]. The size effect in metals is known as the Hall - Petch effect and is one of the important unresolved issues in computational material modeling. Usually, crystal plasticity models cannot predict size dependent effects. Thus, models including plastic strain gradients have been introduced in order to overcome this drawback of ordinary crystal plasticity theories. This contribution discusses the computational modeling of grain size dependence in microstructure models of crystals [2].

The numerical results of the sub-micron gold crystal modeling are presented in this presentation. Gradient theories are evaluated on the crystal level in order to simulate the influence of the grain size on the response of the singlecrystal of Au. It is assumed in the model that the grain boundaries act as barriers to plastic deformation. The 'micro-clamped' and 'micro-free' boundary conditions are applied to the grain boundary [3].

The formulation results in a boundary value problem with the displacements and the gradient hardening (internal) variables in the slip system being the unknowns, i.e. the degrees of freedom. The system of equations is highly coupled and may be solved by applying a so-called dual mixed FE algorithm [4].

The gradient hardening is included into crystal plasticity model. Numerical results for different model assumptions are presented. The gradient effect in the deformation of sub-micron gold is discussed.

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## Two level modeling of inelastic and superplastic deformation of metals

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Numerous theoretical and experimental studies show that the performance of the internal material structure determines the behavior of the material at the macro level and its performance characteristics. During intensive plastic deformation the internal structure of the material is significantly restructured: the grain and dislocation structures are changing, crystallites lattice is rotated; it is widely used to produce materials with unique properties: submicrocrystalline, nanocrystalline, textured materials and materials, which are capable of superplastic deformation. The macroscopic phenomenological theory of plasticity is poorly applicable for describing the microstructural evolution and effective properties of material. In the last 20 years the physical theories of plasticity of polycrystalline metals have been intensively developed, which explicitly consider the physical mechanisms of deformation at scales lower than the scale of the representative macrovolume (crystal plasticity).

The development of the authors' two-level model of inelastic deformation of polycrystalline metals [1] based on crystal plasticity by taking into account the characteristic mechanisms of superplastic deformation is proposed. An original variant of homogenization constitutive relations of different scale levels (differently scaled one-type characteristics) is proposed; the consistency simultaneously provides unambiguous description of macroscale geometric nonlinearity by specifying the Cauchy stress tensor derivative independent of the reference system choice. The kinetic equations for describe the grain boundary sliding, diffusion creep, fragmentation and crushing of crystallites are formulated; new crystallite rotation model is propose (with the absence of the "driving forces" of rotation and fragmentation due to the interaction of dislocation substructures). For superplastic deformation description, which is characterized by losing of local topology, and for describing the input and output from this regime the measure of local topology saving and the measure of grains equiaxing and kinetic relations for this values based on mesolevel model is included in the structure of the two-level model.

The developed model is included in the software package for solving boundary value problems with using multilevel constitutive models (in FEM-package Abaqus). Using the developed software simulated for various loading of samples from various polycrystalline metals is done. There is the good agreement between the results with experimental data.

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## Microstructural Material Modelling in Metal Forming

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One of the key factors in studying sheet metal forming processes is the material modelling. There are different aspects that influence the material behaviour in forming including one of the most challenging as the plastic anisotropy. Many researches dedicated to account for various phenomena in elastic-plastic behaviour of metals in different loading histories such as Bauschinger effect, anisotropy, strain rate sensitivity and damage. Teodosiu et al. [1] presented a microstructural based model that includes the transient work hardening behaviour due to the change of strain path. Peeters et al. [2] proposed a crystal plasticity model that shows the shape evolution of the yield surface due to the changes in the strain path. In this current work, the authors represent a microstructurally-motivated approach to account for plastic anisotropy, distortional hardening, strain rate sensitivity, Bauschinger effect and kinematic hardening in elastic-plastic behaviour of interstitial free (IF) class of steels. The necessary material parameters in the material model are identified based on the experimental results of Clausmeyer et al. [3] and Noman et al. [4]. The presented material model is applied for several loading histories to investigate its robustness and ability in prediction of material behaviour under complex loading conditions.

**Keywords:** material modelling, anisotropy, metal forming, steel

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## **Phase Field Approach for Damage Viscoplasticity and Microstructure Evolution in Ni-based superalloys**

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Creep at high temperatures involves not only dislocation motion but also microstructure evolution controlled by diffusion processes. To study creep phenomena a phase field approach incorporating damage viscoplasticity is developed in terms of thermodynamics. The free energy consists of the elastic energy and the Ginzburg-Landau free energy to take into account phase transformation and interface energies. The damage dissipation potential and the plastic dissipation potential coupled with dislocation densities are introduced to account for different creep stages. A diffusive dissipation potential is assumed as a positive definite quadratic form. Evolution equations for concentration, phase field, and internal variables can be obtained by using the minimum principle for the dissipation potentials [1, 2]. Finite element simulation of a creep test in a single crystal nickel-base superalloy LEK94 at high temperatures above 1000°C is shown to illustrate the performance of the model.

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## Subgrain martensite mechanics in multi-phase steels

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Martensite is a polycrystalline phase which is present in martensitic steels and in a number of multi-phase Advanced High Strength Steels, such as Dual Phase and low carbon TRIP steels. Its role is to improve the strength of the material, preferably without eliminating ductility.

Most modelling work related to multi-phase steels has considered martensite as a homogeneous, isotropic phase, showing little or no plasticity. Nevertheless, a number of experimental papers indicate evidence of ductile fracture behaviour of martensite under quasi-static, uniaxial loading conditions [1]. Furthermore, quite recent works (dating back to no more than 10 years ago) have shown that a martensite grain can have a well defined internal heterogeneous (crystalline) substructure [2], i.e. packets, blocks, laths. Thin layers of retained austenite may also be present between the laths [3] and are expected to influence the mechanical behaviour of martensite.

In this work, the influence of interlath retained austenite on the apparent ductility of martensitic subgrains has been investigated.

The internal heterogeneous morphology of a martensitic island is modelled using first order crystal plasticity and exploiting the well known crystallographic orientation relationships.

Laths have been modelled as BCC crystals, while retained austenite as FCC. The influence of lath morphology and phase fractions on the ductility and strength of martensite has been investigated.

It has been shown that, independently from interlath retained austenite volume fraction and the lath morphology, shearing along the lath habit plane yields high deformations: under such conditions the FCC phase acts like a greasy plane on which stiffer BCC laths can slide. The role of the orientation relationship between FCC and BCC phase is fundamental, since the same shearing mechanism is not observed to the same extent if the model does not account for the correct orientation relationship.

This may indeed explain the experimentally observed apparently ductile behaviour of martensite grains.

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## Discontinued plastic deformation effect on forest dislocations cutting

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In the process of forest dislocations cutting, dislocations on different slip planes encounter and form immobile dislocation junctions or pinning jogs which impede dislocation glide to harden the material. So cutting of forest dislocations is the main reason for plastic hardening of crystal material and it is an important part of material numerical simulation model such as the three dimensional discrete dislocation dynamics model. In classical discrete dislocation models [1, 2], the formation of jog is very difficult and some artificial rules have been used. Here, a three-dimensional discrete dislocation dynamics plasticity model including the discontinued plastic deformation of dislocation slip is introduced to simulate the process of forest dislocations cutting. The process of forest dislocations cutting is divided into two parts like the classical models [1]: firstly the crosspoint is formed for two intersecting dislocation, then the merging reaction happens between the two branches in each end of the crosspoint. The major difference is that the material points over the slip area of a dislocation move a burger's vector relative to points below the slip area when a dislocation cuts another. The intersection and merging processes can be used to simulate the annihilation of dislocation, junctions and jogs naturally. In a low energy system, a junction of two dislocations can vanish. While in high energy state, the junction is teared to form a jog owing to consideration of internal material points' deformation. Taking micrometer-scale single crystal copper including two intersecting slip planes as an example, the forest dislocations cutting process is simulated and the discontinued deformation of the crystal is obtained. The strength of junctions change with different intersection angle between two slip planes. By changing the intersection angle between the two slip planes and the amplitude of Burger's vector, the conditions for Lomer-Cottrell lock and Hirth lock formation are given.

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## Dislocation dynamics model for slip lines forming of micrometer-scale single crystal

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Experiments have found that the plastic deformation of micrometer-scale single crystal is mainly concentrated on local slip planes with discontinued slip lines on the crystal surface [1]. Discontinued deformation on the crystal surface has great effect on the behavior of material in micro-scale such as piling up of dislocations and concentration of stress. A three-dimensional discrete dislocation dynamics plasticity model is developed to simulate the process of slip lines forming on the surface of crystal. Different from the classical discrete dislocation dynamics models [2, 3], we connect the displacement of material points with dislocation slip area in a special way. When a dislocation slips a local area on one slip plane, the material points of crystal surfaces and slip planes over the slip area move a Burger's vector relative to points below the slip area. As the position of a slip plane can be affected by motion of dislocation on another slip plane, the dislocation reactions such as junction formation and junction destruction are invoked in a different way from the classic dislocation dynamics model. Superimposing the deformation of every time step for material points, the process of slip lines forming for a single crystal can be achieved. Taking micrometer-scale single crystal copper including multi-slip planes as an example, we get the discontinued deformed shape and the intermittent relation of stress and strain. A large number of slip lines form on the crystal surface by motion of the dislocations on different slip planes. The results are in good accordance with experiment of micro-pillar compression. Finally, we discuss the effect of dislocation's evolution on the deformation of single crystal.

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## Numerical Analysis of the Digital Material Representation Behavior under Plane Strain

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Several advantages of using unit cell models based on the Digital Material Representation (DMR) makes these approaches increasingly popular what can be seen in many research works connected with different engineering materials, e.g. composites, glasses, concrete, wood etc. [1-7]. The main objective of the DMR is creation of the digital representation of microstructure with its features represented explicitly to match real microstructure morphology. However, when this approach is applied, a fundamental question has to be answered: can the investigated unit cell be considered as a Representative Volume Element (RVE) [1], that will provide results that are compatible with real material behavior? Most of research works, which addresses this question are connected with heterogeneous or composite non-metallic materials. Unfortunately there is a small amount of works focused on single phase metallic microstructures [2]. That is why, the latter is the subject of the present work. Particular attention is put on the amount of grains in the digital microstructure, which can be considered as a representative volume element of the sample subjected to plastic deformation conditions. Additionally, influence of the periodic and non-periodic boundary conditions on the unit cell behavior during deformation is evaluated. Possibility of application of periodic boundary conditions on the non-periodic unit cells is also discussed. Then, the influence of different friction coefficients on obtained results is addressed. Finally, influence of FE mesh density inside grains and at the grain boundaries is highlighted. Obtained results, in the form of an equivalent strain distributions and force reaction plots, are presented and discussed within the work.

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## Numerical simulation of elastic wave diffraction

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The diffraction of time-harmonic deformation waves by rigid inclusions in an elastic medium is mostly studied by analytic methods. The efficiency of analytics depends on the separability of wave equations and on the geometric shape of inclusions. The extensive studies described by Morse and Feshbach [1], Graff [2] and others are based on the powerful integral-equation techniques applied for the analysis of many problems. For example, the problem of diffraction from a single rigid barrier in an elastic medium is analysed by Graff [2] by using the Wiener-Hopf method. Hirose and Achenbach [3] have studied the problem of the interaction of a pulse wave with a rigid circular disk. Mykhas'kiv [4] has solved the problem of the interaction of an impact wave with a rigid plane inclusion.

Diffraction of elastic waves at discontinuities resulting in the dynamic stress concentration is essential in geophysics and seismology, e.g. Compared to acoustic and electromagnetic scattering, the elasticity problem is more complicated because of the coexistence of compressional and shear waves that propagate at different speeds. For example, the well-known Talbot effect in optics is not studied in elasticity, up to the knowledge of authors. In the paper, results of numerical simulations of classical two-dimensional diffraction problems (such as one-slit and two-slit problems) as well as elastic wave propagation through a rigid grating in a homogeneous medium are presented. These results demonstrate that the self-imaging Talbot effect appears also in elastic case. Its possible application to non-destructive testing is discussed. Numerical simulations are performed by the modification of the finite-volume wave-propagation algorithm [6], which provides the stable and high-order accurate solution of wave propagation problems in inhomogeneous solids [7].

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## Grain Cluster Method for Multiscale Simulations of Steels

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The development of new steels with enhanced mechanical properties requires examining their response behavior by means of advanced numerical models that accurately account for complex microstructural characteristics. Direct numerical simulations (DNS) at the microscale, together with an appropriate averaging scheme, lead to a consistent scale transition for determining the overall behavior at the macroscopic scale. However, performing a DNS is often computationally expensive, which limits its applicability. An approximate method, which is computationally less expensive, is proposed as an alternative for computing the effective behavior at the engineering scale. The method, termed the Generalized Grain Cluster Method, relies on a set of simplifying assumptions for the distribution of the deformation field inside a grain while at the same time it minimizes the effect of discontinuities arising from the kinematical assumptions. This method, which is an alternative formulation of the Relaxed Grain Cluster Method [1], allows to study an aggregate of grains with arbitrary polyhedral shapes.

A benchmark for the proposed multiscale framework is constructed by performing a set of DNSs on polycrystalline samples composed of multiple ferritic grains. The mechanical response of the grains is computed by means of a crystal-plasticity model for BCC lattices [2–4]. Polycrystalline samples of increasing size are used to identify a representative volume element for the numerical homogenization procedure. The same set of samples is analyzed using the direct numerical simulations and the Generalized Grain Cluster Method. The macroscopic responses derived from these homogenization schemes are compared and the accuracy and numerical efficiency of the proposed method is pointed out.

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## A multiscale approach for the modeling of bainitic phase transformation in multi-variant polycrystalline low alloy steels

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In many practically relevant situations, steel shows a complex material behavior. E.g. during metal forming processes, heat treatment and mechanical loading often lead to changes within the structure of the machined component, being a result of complex processes on the microscale of the material and often leading to macroscopic stresses and strains which may cause e.g. distortion of the work-piece. For this purpose, it becomes necessary to understand and simulate these processes under consideration of physical effects like phase transformations for being able to predict the resulting material behavior.

In our work, we develop a thermodynamically consistent two-scale model for the material behavior of a low alloy steel taking elasto-viscoplasticity, heat conduction and phase transformations as well as the poly-crystalline structure into account. Here, we focus on a prototypical situation, considering only the phase transformation from austenite to bainite. In doing so, the formation of all possible bainite variants within each single crystal is taken into account. The mesoscopic configuration consists of a polycrystal which plays the role of a representative volume element (RVE). This RVE is attached to each material point of the macroscopic configuration. At the mesoscopic level, the transformation strains of the bainite variant within the grains lead via averaging to an additional component (besides elastic and visco-plastic ones) of the total macroscopic strain, expressing the macroscopic effects of volume change due to phase transformation as well as to transformation-induced plasticity (TRIP). The time dependent nature of the kinetics of bainite formation is taken into account, and the model is capable of capturing both TRIP effects, the contribution due to load-biased orientation of bainite-variants ("Magee effect") and plastic accommodation of the new phase ("Greenwood-Johnson effect"). Finally, a quantitative evaluation of both phenomena is provided for various loading paths. Basic principles and ideas for our work can be found e.g. in [1–5].

**Acknowledgments** This work is based on investigations of the collaborative research center SFB/TR TRR 30, which is kindly supported by the Deutsche Forschungsgemeinschaft (DFG).

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## A topology-reconstruction method for automated meshing of voxel-based polycrystals

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Accurate predictions of damage nucleation and propagation in polycrystalline materials require the use of representative microstructures. Single-phase polycrystals are made of grains of different size and number of neighbours, and separated by curved grain boundaries. Such microstructures can be simulated from material transformation mechanisms [1, 2], or for some materials, can be characterized experimentally [3]. In both cases, the polycrystals are generally defined on a 3D grid of *voxels*, each voxel being assigned the number of the grain it belongs to. While this is handy to describe complex microstructures, it is not suitable as such for finite element simulations, because it is overrefined and creates stepped interfaces. Therefore, developing meshing strategies is needed.

In the last few decades, methods have been proposed for surface meshing of voxel-based data, especially for biomedical applications. In principle, the result mesh can be used for 3D mesh generation. Surface meshing is divided into 3 steps: interface reconstruction, smoothing and simplification. However, interface reconstruction retains a delicate problem. The well-known marching cube algorithm enables to reconstruct an iso-value surface from a scalar field and can be used to separate two phases of a material. The method has been extended to an arbitrary number of phases (or grains of a polycrystal) [5], but it suffers from a large number of undetermined configurations.

In the present work, an alternate method is proposed for interface reconstruction, which is shown to enable proper meshing of the microstructure. The method is based on filtering of the voxel data, then a simple interface reconstruction by tracking the boundaries of the voxels. Filtering enables to avoid topology problems such as grain boundaries which locally collapse into a single point or edges connected to one vertex only. The resulting geometry is admissible for meshing, with well-identified grains, faces, edges and vertices, and topological relations between them. Such a description of the polycrystal has previously been used for meshing of Voronoi tessellations [4]. Extensions are presented for the present case of polycrystals with curved grain boundaries. Examples are provided for simulated and experimental polycrystal microstructures.

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## Impact of the geometry of inclusions at the micro-scale on the overall stochastic properties

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In this contribution, a study relating the mechanical and geometric properties of inclusions, within a representative volume element (RVE), with the overall properties and its stochastic behaviour is presented. The parameters studied include the RVE size, the dimension space of the model (2D and 3D) and inclusions features (distribution, shape, mechanical properties, etc.). These types of studies (e.g. [1] and [2]) are very important because of two main reasons. Firstly, the stochastic behaviour of the material is useful to predict the probability of failure and the characteristic values of stiffness for design purposes; secondly, as the size of the RVE increases the simulations require more degrees of freedom and, consequently, more computational resources and time, which are limited.

To conduct those analyses, a general framework that generates and simulates RVEs (on 2D and 3D) based on a commercial finite element (FEM) software ABAQUS® [3] and existing homogenization techniques (see [4]) was developed. Then, an investigation of mechanical and geometric parameters of the RVE, including the size, is performed using statistical methods. The study starts with simple models on 2D, and then more complex models are progressively used including 3D ones.

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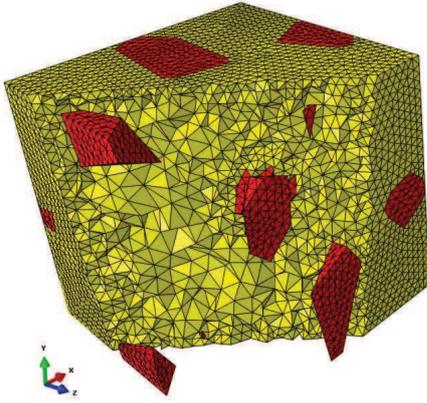


Figure 1: Microscale FEM model of a material with polyhedral inclusions

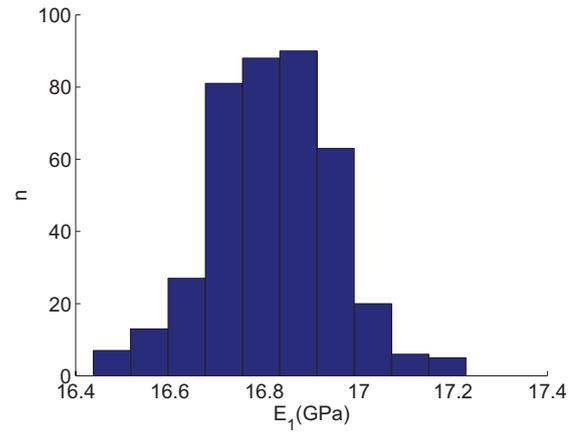


Figure 4: Histogram of the elasticity modulus  $E_1$  for a set of 2D RVEs

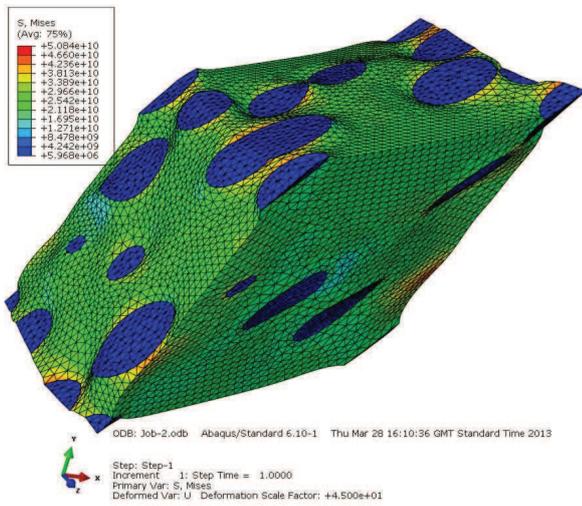


Figure 2: Deformed configuration and von Mises stress (Pa) for an RVE with spherical inclusions (periodic b.c.)

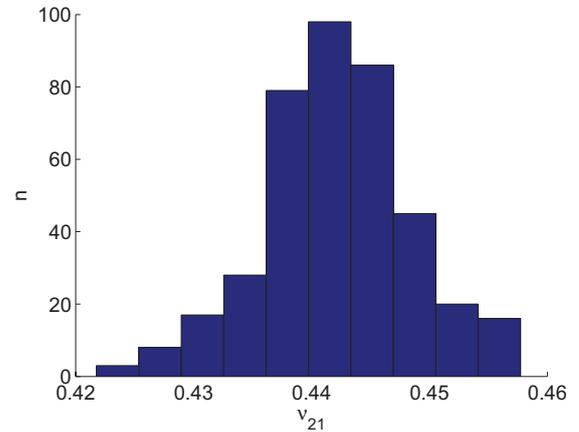


Figure 5: Histogram of the poisson ratio  $\nu_{21}$  for a set of 2D RVEs

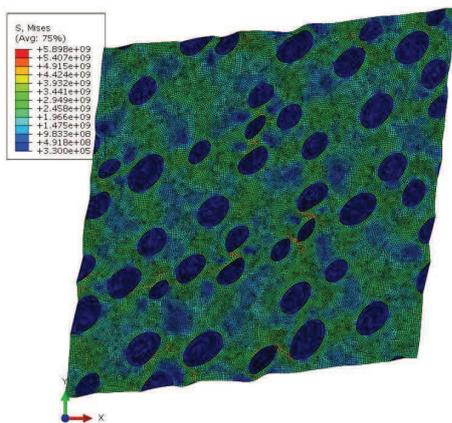


Figure 3: Deformed configuration and von Mises stress (Pa) for an RVE with disk shaped inclusions (periodic b.c.)

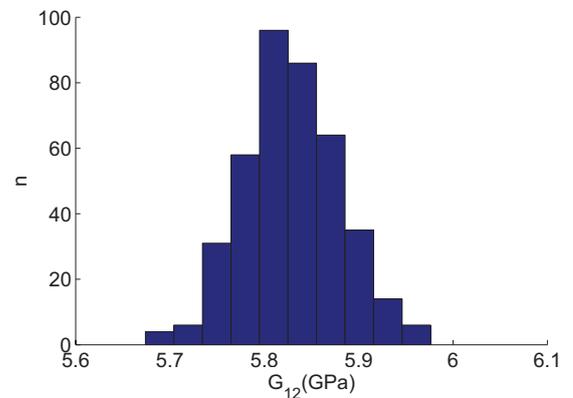


Figure 6: Histogram of the shear modulus  $G_{21}$  for a set of 2D RVEs

## Multiscale microstructure generation using Voronoi tessellations

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The mechanical properties of materials are improved by elaborating microstructures of increasing complexity. In metals, such microstructures are often “multiscale”, that is, made of geometrical features that span over several space scales. For example, bainitic steels are made of bainite “packets”, each of which is a grain with a lamellae structure. Moreover, during phase transformation, several packets can grow inside the same austenite grain. This finally makes bainitic steels a 3-scale microstructure. While numerical methods such as the finite element method are available for polycrystal plasticity simulations, there is currently no tools to generate multiscale microstructures nor appropriately mesh them.

In the last decade, Voronoi tessellations have been successfully used for (1-scale) polycrystal modelling, starting from the works of Barbe et al. [1]. A Voronoi tessellation is a partition of space into a set of convex volumes. From a material point of view, it corresponds to the process of a diffusive phase transformation where all germs nucleate at the same time and grow isotropically at the same rate. Voronoi tessellations have the advantage to be defined analytically and made of convex polyhedra, bounded by flat faces and straight edges. Robust methodologies have been provided by Quey et al. [3, 4] for good-quality meshing of large-scale Voronoi tessellations.

In the present work, a methodology is presented for the generation of multiscale microstructures using Voronoi tessellations. The method consists in applying Voronoi tessellations sequentially, at successive scales. At a given scale, each cell of the former Voronoi tessellation(s) is further divided by Voronoi tessellation. This is further enriched by introducing “lamellae tessellations”, by which a volume can be divided into parallel lamellae, as needed for bainitic steels for example. The method was first applied by Osipov et al. [2] to a 2-scale microstructure, but here is automated and generalized to microstructures with an arbitrary number of scales. We describe how to keep track of topological information between the different scales and we show how to mesh the full microstructure. The methodology enables to generate and mesh a wide range of microstructures. Applications to metals and rocks are presented.

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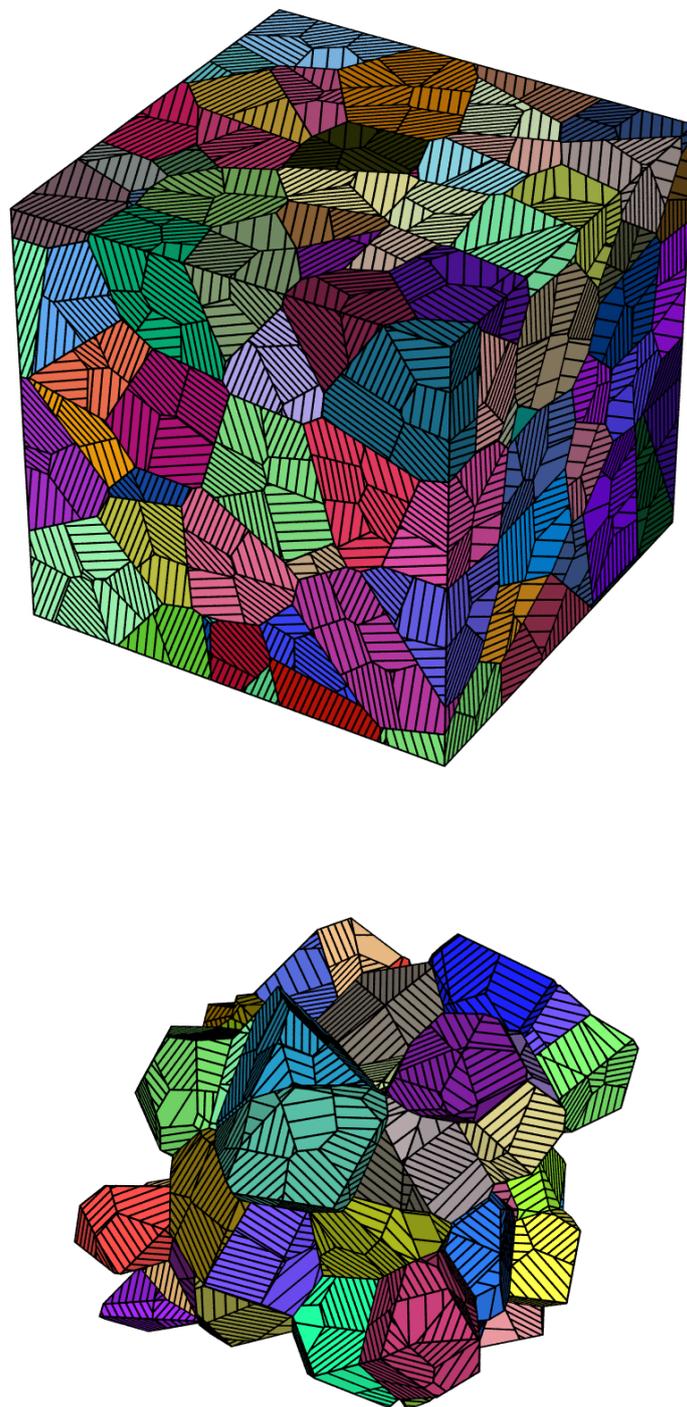


Figure 1: Modelling of a bainitic structure made of 200 austenite primary grains. Each primary grains is divided into 5 bainite packets in average and each packet has a lamellae structure. Uniform colours are assigned to the primary grains. (Top) Full microstructure. (Bottom) Inner grains.

## Dynamic and static strain aging modelling in polycrystalline alpha titanium

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Good resistance to damage and corrosion and high strength in combination with low density make titanium and its alloys are widely used in the area of aerospace, chemical industry, biomedical engineering.

The mechanical properties of titanium are generally anisotropic due to strong crystallographic texture and deformation mechanisms activated in the material to accommodate the plastic deformation. The experiments show that under certain conditions of strain rate and chemical composition, titanium demonstrates an anomalous behaviour related to microscopic strain aging phenomena. This type of spatio-temporal instability can induce strong effects on the mechanical properties and creep behaviour at room temperature.

On the macroscopic tensile stress-strain curve of titanium when the material is loaded in the transverse direction, one can observe an emergence of a stress peak followed by a smooth softening that corresponds to the static strain aging behaviour (SSA). The absence of the Lüders behaviour in the longitudinal direction seems to be related to the pronounced anisotropy of titanium in mechanical properties. The dynamic strain aging (DSA) behaviour was also observed on the macroscopic stress strain curve during the plastic deformation at lower strain rates.

On the microscopic level the phenomenon of strain aging is attributed to the pinning of mobile dislocations by solute atoms during the aging time (for the case of SSA) or during on-going plastic deformation (in the case of DSA). For commercially pure titanium it was noticed that the impurity content, mainly hydrogen and oxygen concentration, plays a crucial role in its plastic deformation. Previous studies have shown that solute oxygen and hydrogen atoms have opposite effects. Oxygen increases the yield stress of alloys by hindering the motion of screw dislocation, while hydrogen can either trigger dislocation glide and thus soften the material or can harden the alloys under some loading conditions. More profound understanding of mechanisms of deformation of polycrystalline titanium and the correlation between the hydrogen and oxygen content and the creep behaviour need to be developed.

In the present studies we aim to clarify the controlling mechanisms of the viscoplastic anisotropic behaviour of titanium in the presence of impurities. The modelling approach for strain aging initially suggested by McCormick [1, 2] is used. The internal variable called the aging time  $t_a$  is introduced in the model to simulate the effect of strain aging. Finite element simulation is then performed on the polycrystalline aggregates taking into account the effect of anisotropy of titanium.

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## Brittle failure in polycrystalline RVEs by a grain-scale cohesive boundary element formulation

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Polycrystalline materials are commonly employed in engineering structures. For modern applications a deep understanding of materials degradation is of crucial relevance. It is nowadays widely recognized that the macroscopic material properties depend on the microstructure.

The polycrystalline microstructure is characterized by the features of the grains and by the physical and chemical properties of the intergranular interfaces, that have a direct influence on the evolution of the microstructural damage. The experimental investigation of failure mechanisms in 3D polycrystals still remains a challenging task.

A viable alternative, or complement, to the experiments is *Computational Micromechanics*. The present-day availability of cheaper computational power is favoring the advancement of the subject. A popular approach for polycrystalline fracture problems consists in the use of cohesive surfaces embedded in a Finite Element (FE) representation of the microstructure, so that the evolution of microcracks stems as an outcome of the simulation, without any assumptions, see e.g. [4].

An alternative to the FEM is the Boundary Element Method (BEM). A 2D cohesive BE formulation for intergranular failure and a 3D BE formulation for polycrystalline materials homogenization have been recently proposed [1–3].

In this work, a novel 3D grain-level model for the study of polycrystalline intergranular degradation and failure is presented. The microstructures are generated as Voronoi tessellations, that mimic the main statistics of polycrystals. The formulation is based on a grain-boundary integral representation of the elastic problem for the crystals, seen as anisotropic domains with random crystallographic orientation in space. The integrity of the aggregate is restored by enforcing suitable intergranular conditions. The evolution of intergranular damage is modeled using an extrinsic irreversible mixed-mode cohesive linear law. Upon interface failure, non-linear frictional contact analysis is used, to address separation, sliding or sticking between micro-crack surfaces. An incremental-iterative algorithm is used for tracking the micro-cracking evolution. Several numerical tests have been performed and they demonstrated the capability of the formulation to track 3D micro-cracking, under either tensile or compressive loads.

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## Modeling of the metalization in integrated circuits

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One of the key factors for the rapid technological progress in our time is the development of integrated circuits - a wiring of electronic components on a single semiconductor substrate.

Growing demands on performance, reliability and durability of the modules require a deep understanding of possible damage and failure mechanisms. One main cause for damage arises from thermo-mechanical loads of the involved materials as a result of current pulses. We observe accumulation of plastic deformation (ratchetting) in the aluminum conductors, which leads to a rise of stresses in the surrounding materials. Mainly affected is the passivation layer which covers the conductors and separates them electrically from each other. These high stresses lead to crack initiation and, in consequence, to short circuits and the loss of functionality of the assembly [1].

Throughout their life, the electronic components undergo millions of load cycles, so that an experimental life cycle analysis during the development process is costly and may not be economical.

Therefore computer-based life time investigations based on the finite element method are considered. The small dimensions of the components in the range of  $\mu\text{m}$  and the large span of time scales, involving current pulses of a few milliseconds and a working time of several years, put high demands on the material model.

This study presents simulation results of a three dimensional model regarding an aluminum conductor sputtered on a silicon substrate and surrounded by a passivation layer. The conductor is loaded by a cyclic heat flow. The problem is solved utilizing the Abaqus/Standard solver. The passivation layer and the silicon substrate are supposed to behave elastically. The material behavior of the conductor is defined by a user subroutine implemented in Fortran. The subroutine bases on DAMASK [2], a phenomenological anisotropic visco-plastic material model, which takes into account the microstructure and the grain orientation. This model was extended in order to address heat flow and thermal expansion.

Simulation results are presented, which reveal the development of the stresses in the conductor and the passivation layer caused by structural changes in the aluminum. Moreover, a possible method for a lifetime prediction with regard to the large span of time scales is outlined.

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## Numerical and experimental investigation of closed-cell foams, focusing on failure

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Polymer foams combine a low density and high weight-specific stiffness. Therefore they are the ideal sandwich-core material for many lightweight constructions. Typical applications can be found in the automotive and aerospace industry as well as in sport equipment. Their mechanical properties depend mainly on the cellular microstructure and the material data of the matrix material.

The current paper focuses on the rigid foam ROHACELL<sup>®</sup> IG-series (industrial grade) produced by Evonik Röhm GmbH, Germany [1]. It is a closed-cell foam based on polymethacrylimide (PMI) chemistry with a homogeneous and isotropic cell structure.

In contrast to many other approaches, the presented work combines experimental investigations and numerical simulations and provides a holistic viewpoint of the mechanical behaviour of the foam. In the experimental part standard tests like e.g. uniaxial compression, uniaxial tension, torsion, superimposed loadings, and advanced multi-axial tests, like biaxial and hydrostatic compression were conducted [3]. The geometrical data describing the microstructure were obtained from image analysis. Among others the cell size, the curvature of the cell walls, and edges and the material concentration of the material in the edges were measured.

In the numerical part a finite element (FE) model on the basis of a tetrakaidecahedron was implemented, and the effective material behaviour was analysed with the concept of numerical homogenisation [2]. In doing so, the FE model was adapted to the results of the image analysis by considering several imperfections in the cell geometry. The elastic material properties were calculated, and geometrical non-linear stress-strain curves were generated. With suitable failure concepts on the microstructure, the effective failure behaviour can be described, and the comparison to the extensive experimental data yields information about the quality of the models.

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## Modelling Sound Waves in Rigid Porous Media Using Regular and Random Periodic Representations of Microstructure

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Sound propagation in a porous material with rigid frame and open porosity can be very effectively modelled with the Johnson-Allard model [1] which uses the Helmholtz equation for time-harmonic acoustics. This model uses several macroscopic parameters (globally characterizing the geometry of porous material), namely: the porosity and tortuosity, the viscous permeability and its thermal analogue, and two characteristic lengths – the viscous and thermal one. These parameters can be in fact measured experimentally, or they can be calculated from the microstructure [2–4]; inverse identification of these parameters is also possible [5].

The microstructural approach is based on the Multiscale Asymptotic Method, which leads to two uncoupled micro-scale Boundary-Value Problems (BVPs) [3,4], namely: a harmonic, viscous, incompressible flow, and a harmonic thermal flow. A scaled Laplace problem should also be solved in order to calculate some of the parameters. All BVPs must be solved using the same periodic cell representative for the microstructure. The present work discusses this approach and advocates the usage of randomly-generated, periodic representative volume elements (RVEs). To illustrate this the acoustic absorption for freely packed assemblies of spherules (each 5.9 mm in diameter) is measured and compared with the result calculated from the microstructural analysis using periodic RVEs generated using some regular sphere packings [2, 3] (SC – simple cubic, BCC – body-centered cubic, and FCC – face-centered cubic) adjusted to match the actual porosity of 42%. The discrepancies, although not very big, suggest that better microstructural representations are necessary. It seems reasonable that those can be achieved by using some random packing assemblies. A comparatively simple method of generation periodic yet random assemblies of spheres is proposed. The method is suitable for constructing RVEs for real sound insulating foams with spherical pores. Such random periodic RVE is generated for a foam of porosity 70% for which the acoustic impedance and absorption is calculated from microstructure.

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## Possibility of the Nanostructured Metals Creation by Severe Plastic Deformation at High Strain Rate

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The severe plastic deformation methods (ECAP, high-pressure torsion e.t.c.) can be usually used for fabrication of ultrafine grained metals [1], not the nano-crystalline one. Furthermore, the created structures often do not possess a thermal stability and the grain sizes can increase up to 10 times for some week or month. There are natural reasons for this behavior because of limitation of the defects density in the material and excess volume energy leading to the recrystallization processes. Such effects make the fabricated materials unusable for the technical applications. In spite of this, the new methods for nanostructured materials fabrication are appearing. One of them is based on the severe plastic deformation at high strain rates and it is called the dynamic channel angular pressing (DCAP) [2]. Material characterizations of the samples fabricated by this method demonstrate the presence of nanocrystalline grains in the material, which makes it substantially more stable than the analogous materials fabricated at the low strain rates [1].

In this report we present the simulation results for the DCAP processes, where we demonstrate the effects of macroscopic and microscopic shear localization. Also we demonstrate a shock wave contribution to the defect structure formation in the material at the DCAP process. The main result of this simulation is the demonstration of possibility of the nanostructure formation at the intersection region of the shear bands. This mechanism was partially verified in the friction experiments, where similar effects were detected by the experimental way [3]. For modeling of the dislocation kinetics and dynamics we use the original models [4,5]. To find the macroscopic deformation we solved a continuum mechanics equations using the finite-difference 2D code CRS.

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## Finite element simulation of contact problems for materials with heterogeneities, surface effects and defects

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Under contact interactions in such tribomechanical systems as frictionless bearings, gear transmissions, "wheel-rail" system, etc., different defects can appear and mechanical properties of materials in the near-surface layers can vary as a result of high pressures, temperatures, plastic strains and contact fatigue. The indicated factors determine the interest to the investigation of the elastic and coupled contact problems for media with heterogeneities and defects. For the analysis of actual tribomechanical systems, especially taking into account heterogeneity, plasticity, temperature fields and defects, it is necessary to use direct numerical approaches such as finite element method which appeared to be the most effective one.

In the present work the set of contact problems for elastic and coupled-field materials with inhomogeneous properties, cracks and dislocations was considered. For solving these problems the finite element techniques and specialized software for finite element package ANSYS were used. The stages of solving the contact problems with inhomogeneous properties include such processes as development of the finite element model for homogeneous bodies with concentration around supposed contact zone, finite element modifications by redefinition of their material properties according to the law of heterogeneity, creation of the finite element contact pairs and numerical solution of nonlinear contact finite element problems [1, 2].

For deformable bodies with dislocations the considered technique is complemented by the modeling of multiplex edge dislocations with Burgers vectors, construction of finite element mesh with dislocations and account for additional nodal forces caused by dislocations.

In order to model the singularities of the stresses in the vicinity of the crack tip and to insure necessary asymptotic of the displacements field it is required to condense the mesh of finite elements in the vicinity of the crack vertex and to displace middle nodes of quadratic finite elements surrounding the crack vertex for a quarter towards the vertex.

It was shown that for taking into account the surface effects for nanosized bodies the finite element software ANSYS could be also used with additional introduction of surface membrane elements in the computation models.

As an important example the mathematical and computer models of contact interaction between rigid and deformable indenters and structurally inhomogeneous bodies with antifriction multilayered nanostructured covering were developed and analyzed.

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## **New Algorithms for Modelling High Homologous Temperature Plastic Deformation**

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A set of new algorithms are proposed to model the motion of dislocations under both thermal activation and mechanical loading. The mechanical and thermal effects are incorporated by the assumption that dislocation glide occurs on time scales much smaller than all other events controlling dislocation motion.

In the mechanical part, dislocation slip is treated in a quasi-static manner, meaning the whole configuration transforms from one equilibrium state to another when the external load changes. This is achieved by minimizing the total elastic strain energy, which captures long range effects. Short range effects, such as nucleation, annihilation, escape from obstacles and boundaries, are treated as discrete events altering the energy state of the body. This quasi-static method allows decoupling of dislocation sliding time scales from events occurring on larger time scales.

In the thermal part, all thermal activation is treated as stochastic events that depend on the temperature and residence time of dislocation at its current equilibrium position. The activation energy is formulated in terms of obstacle strength and mean obstacle spacing which characterize the different strengthening mechanisms. We present several examples comparing our new quasi-static method with full dynamics simulations under mechanical loading.

## Energy balances within metallic polycrystals: numerical and experimental perspective

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Polycrystalline metallic materials are made of an aggregate of grains more or less well oriented, with respect to the loading axis, for plastic gliding. Under mechanical loading, this leads to a heterogeneous deformation at the microstructure scale. This local plasticity triggers a heterogeneous thermal dissipation caused by mechanical irreversibility, while a certain proportion of plastic work remain latent in the material and is associated with microstructural changes [1]. Thus, the analysis of plasticity micro-mechanisms through energy balance is an alternative view which focuses on one hand, on the energy related to its intrinsic constituents (dislocation, defects) and on the other hand on the bulk and local sign of plasticity flow.

Some original experimental works enabling the simultaneous determination of infrared and visible fields, in the same area, at this scale have already been realized in house on a A316L stainless steel under monotonic tensile loading [2]. In addition, some complementary experimental data-treatments have been proposed to recover a fully coupled thermomechanical data-set, i.e. simultaneous surface displacement and thermal fields, at the grain scale of the polycrystalline aggregate [3,4]. Strain fields are obtained thanks to Digital Image Correlation performed on images of the deforming sample covered with a speckle pattern while temperature ones are obtained by Infrared Thermography. Data are analysed grain to grain through a projection on the crystallographic texture provided by EBSD analysis [4]. The spatial resolution of the kinematic fields as well as temperature ones are higher than mean grain size, i.e. 118  $\mu\text{m}$ . It allows a multiscale study and more particularly, an intra-granular one on some specific bigger grains. Finally strain and thermal resolution are 0.1% and 3mK respectively [3]. The objective of this paper is to deal with mean and local experimental energy balance as well as to confront and confirm results with numerical crystal plasticity based simulations. A 3D polycrystalline aggregate model, with extended grains along the out-of-plane axis has been generated from EBSD data and experimental displacement and temperature have been applied on boundaries. A numerical energy balance is done and the partition between the different energy storage mechanisms is analysed. Such numerical/experimental dialogue allows a better understanding of micro-plasticity mechanisms leading to observable variation of temperature.

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## Modelling interphase effects on large deformation behaviour of thermoplastic polymer-clay nanocomposites

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Clay-based nanocomposites promise to offer cost effective solutions for mechanical property improvement of thermoplastic polymers. However, the reinforcing efficiency of clay nanofillers depends on their distribution within the polymer matrix. Quasi-solid state processing of thermoplastic nanocomposites near their glass transition offers promising means for their morphology modification and end-use property improvement. However, this requires a careful optimisation of processing parameters such as deformation, deformation rate and temperature. Advanced material modelling can assist experiments in finding the most optimum processing conditions for polymer nanocomposites.

Modelling of large, temperature- and rate-dependent nonlinear deformations typical for quasi-solid state processing of thermoplastic nanocomposites is quite complex and it is still in its infancy. Thus only few papers addressed this industrially important problem [1,2]. However, they did not consider the effect of interphase region around nanofillers, which is believed to affect the nanocomposite response. The interphase region softer than the surrounding matrix is modelled here, as suggested by available experiments and data from the literature. The extent of the interphase is assumed to be governed by the length of surfactant chains (i.e. nanofiller surface modifiers), while its mechanical behaviour is described through the relevant modification of polymer matrix viscosity. A three-component nanocomposite model was proposed here to capture initially agglomerated morphologies. Advanced morphology reconstruction tools were used to generate relevant representative volume elements (RVEs), and combined with constitutive models for the polymer matrix, interphase and galleries, to track the morphology evolution during deformation. Additionally, a nonlinear Finite Element (FE)-based computational homogenisation was used to predict the macroscopic nanocomposite response.

Our predictions show that the interphase with the viscosity smaller from that of the surrounding matrix leads to the nanocomposite softening within the entire deformation range up to strains of  $\sim 2$ , at strain rates  $\sim 1s^{-1}$ . Thus, smaller forming stresses would be required to process nanocomposites with softer interphase. Softer interphase increases slippage of adjacent nanofillers for the agglomerated morphologies, and hence can improve dispersion of nanofillers. In both cases (i.e. with and without soft interphase), the nanofillers undergo significant reorientation within the nanocomposite during deformation.

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## Modelling of biodegradable thermoplastics and their nanocomposites during melt processing

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Poly lactide is a thermoplastic, biodegradable polymer that is derivable from renewable resources and thus it is attractive for packaging industry. However, its mechanical preoperties can be improved to make it stiffer and decrease its gas permeability by incorporation of stiff, high-aspect ratio and cost-effective clay nanofillers [1]. However, mechanical and physical properties of those materials depend strongly on their underlying morphology (e.g. clay distribution and orientation), which is affected by forming processes (e.g. film blowing) and their parameters (temperature, rate of deformation, mangnitude of deformation). Hence, optimisation of those process parameters is necessary to achieve desirable morphologies and end-use properties. Therefore, in our project we seek to investigate and optimise the relationship between processing, morphology and end-use properties of poly lactide-clay nanocomposites using experimental and modelling means to facilitate their commercial exploitation.

The main objective of the modelling part of our project is to develop experimentally-validated advanced material model, which can assist property optimisation of those nanocomposites. Then, we aim at using that model to capture morphology evolution and predict their macroscopic response during processing. This requires development/implementation of a constitutive model for the polymer matrix in the processing regime, governed by large, nonlinear, rate and temperature-dependent deformations. Additionally, nanocomposite morphology must be reconstructed, and combined with the polymer constitutive model, to predict nanocomposite deformations through a nonlinear numerical homogenization method.

This particular contribution is about the constitutive modelling of polymer (poly lactide) matrix in extensional flows typical of film blowing processes. For that purpose we implemented a simple phenomenological, single-mode model of Leonov [2] into Matlab. The model has only three parameters to fit to experimental data: the shear modulus  $G$ , the time constant  $\tau$  and the bulk modulus  $K$ . Those parameters were fitted into results of extensional viscosity obtained in our laboratory at  $T=168^{\circ}\text{C}$  and the strain rate  $1\text{s}^{-1}$ . Then, we compared our predictions with the experimental results at other strain rates of  $0.1\text{s}^{-1}$  and  $10\text{s}^{-1}$ . As expected, the polymer did perform reasonably well for lower strain rates, and it underestimated the viscosity at the highest investigated strain rate. This has set limits for its use in simulations of poly lactide-clay nanocomposites.

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## **Experimental verification of phase composition obtained for computational modelling of phase transformations based on displacive mechanism in low alloy steels after quenching or austempering**

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This paper presents results of computational calculations of T0 curve for low alloy steels obtained in MatCalc and mucg83 software, which were used to calculate phase compositions of several steels after different heat treatments. Paper evaluates models used in both programs, comparing the results with experimental data. Possible reasons for differences between results obtained in different software as well as differences between experimental and calculated results were discussed.

Performed heat treatments consisted of austempering and of oil quenching. Austempering of the samples resulted in carbide-free nanobainitic microstructure containing bainitic ferrite, retained austenite and martensite. Lack of carbides provides good verification of the models as it provides measurement of average supersaturation of carbon in the retained austenite and in the bainitic ferrite phases.

Phase composition of the samples and carbon concentrations were measured using Rietveld refinement of the XRD profiles. Calculated phase compositions were compared with results obtained using conversion electron Mössbauer spectroscopy (CEMS) method.

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## Elastic and electric properties of a semi-polar $(11\bar{2}2)$ GaN/AlN quantum dots

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In an effort to reduce the strong built-in electric field that is present in wurtzite heterostructures, Quantum Dots (QDs) orientated in a direction other than the polar direction have recently become a topic of intensive research. Alternative growth directions induce different QD geometries that in turn induce different stress/strain states and a reduced electric field intensity in the dot and its vicinity. The reduced intensity of the internal electric field in the case of semi-polar orientated nanostructures may allow for higher internal quantum efficiency of optoelectronic devices based on a semi-polar heterostructure. One candidate for this is the  $(11\bar{2}2)$ -orientation.

A study with Transmission Electron Microscopy (TEM) of a  $(11\bar{2}2)$ -orientated GaN/AlN heterostructure grown by plasma-assisted molecular beam epitaxy revealed three main QD geometries within the same sample [1]. Two of the QD geometries featured in the sample are described by rectangular- and trapezoidal-based truncated pyramids and lie in nominal- $(11\bar{2}2)$  plane. The third main geometry is described by a kite-based truncated pyramid whose base lies in the  $(10\bar{1}1)$  plane, *ie.*, it is slightly inclined with respect to the nominal growth direction. This variation in QD geometry is probably due to local deviations of the growth plane from the nominal orientation that is caused by threading dislocations. The average size of the QDs at their base was around 25 nm.

In this work, finite element (FE) analysis was used to solve the boundary-value problem for a piezoelectric material and investigate the residual elastic and electric fields for three isolated semi-polar QDs based on the main geometries described above. The numerical results show that, in comparison with polar QDs the general character of elastic relaxation does not change much [2], though the basal in-plane compression and tension perpendicular to the basal plane are only slightly modified by the different geometry. The distribution of the electrostatic dipole potential is largely orientation dependent. In polar QDs the positive and negative regions are localised around the top and bottom facets of the dot respectively and in semi-polar QDs the localisation of the dipole continues to manifest itself along the  $c$ -direction. The intensity of electric field in semi-polar QDs is reduced by an increased physical separation of the potential peaks as well as by a reduction of its peak-to-peak intensity. From the classical bulk band-edge structure, modified by the piezoelectric field, an estimation of the emission spectra and carrier localisation is obtained.

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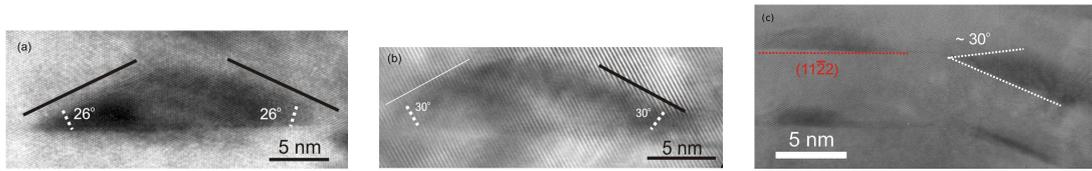


Figure 1: TEM images of a semi-polar  $(11\bar{2}2)$  and  $(10\bar{1}1)$  QDs.

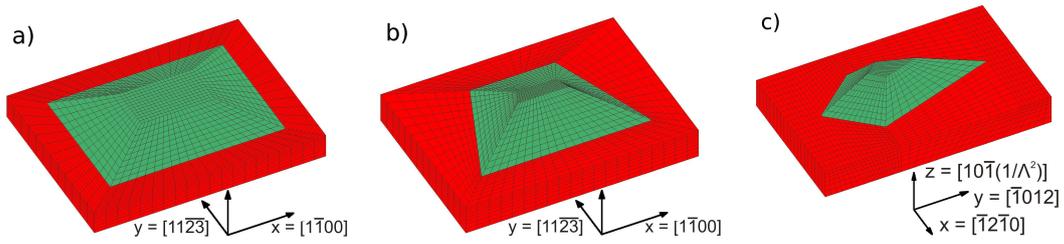


Figure 2: FE mesh of a semi-polar QDs: a) rectangular, b) trapezoidal, and c) inclined.

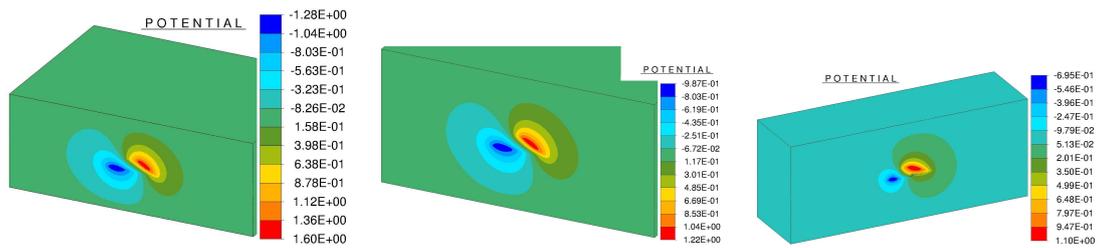


Figure 3: Electrostatic potential field in a semi-polar QDs: a) rectangular, b) trapezoidal, and c) inclined.

## Rate effects on predicted TRIP and product phase elastoviscoplastic properties for austenite-to-ferrite transformation

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When combined to an external mechanical loading, phase transformations in steels can result in plastic strain, called TRIP, even though the applied stress is small compared to the yield stresses of the constituting phases. This phenomenon can be interpreted from the elastoplastic interactions that occur locally between a diffusively growing particles and a parent matrix and which preferentially develop in the load direction. This model mechanism provides a first-order agreement on TRIP, as shown by the analytical Leblond model [3] or by numerical simulations [2, 4], for displacive as well as diffusive transformations and for simple or non-proportional biaxial loadings.

However, in most experimental and modelling analyses, viscous strains are neglected. This assumption can be valid only for low-temperature diffusive transformations or martensitic transformations. On the other hand, it has been shown that, in the case of isothermal austenite-to-pearlite transformation of a 100Cr6 steel occurring at a temperature of about 700 °C [5], both phases show high strain-rate sensitivity. In such cases, accounting for viscosity can lead to major changes in the prediction of TRIP, by a factor of 2. This is unfortunate since TRIP is supposed to be plastic strain only. Thus, accounting for viscosity in modelling appears necessary, but still is an open problem.

In this study, accounting for viscosity is addressed from a numerical modelling viewpoint. On the one hand, the contribution from viscosity to TRIP is quantified for different strain-rate sensitivities of the parent and child phases. On the other hand, the effect of the (arbitrarily-set) phase transformation duration in the simulations is characterized. This is carried out using different numerical models [1, 5]: phases are considered either as homogeneous (no crystallography) or as crystalline and the studied system is constituted of either a single nucleus (parent-to-child particle interactions only) or randomly set nuclei (parent-to-child *and* particle-to-particle interactions). Different kinds of rate effects are observed, some of which significantly depend on the configuration of modelling.

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## A Coupled Finite Element Polycrystal Texture model of the Accumulative Roll Bonding Process

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Accumulative Roll Bonding (ARB) [1] has attracted considerable interest as a process for producing metal sheets with ultrafine-grained microstructure [2]. The high mechanical strength exhibited by these sheets shows potential for applications in the automotive industry. To date, most research work has been focussed on experimental investigations of the properties of ARB sheets, and their relation to process parameters. By contrast, very few numerical investigations can be found in the literature, especially those that focus on the description of the microstructure and texture that is fundamental to the enhanced properties of such sheets.

In this work, we formulate a simulation framework that allows us to investigate both the ARB process and the texture evolution during the process. Our framework embeds the well-known visco-plastic self-consistent (VPSC) model in a finite element realization [3] of the ARB process. This coupling is achieved through a user material subroutine for Abaqus/Explicit. Furthermore, to ensure efficient computations and reduced computation times, we implement a multilevel parallelization of the user material subroutine. This is achieved by decomposing the computation domain using message passing interface (MPI) and subsequently parallelizing the material response in each domain on multiple threads using openMP. Additionally, we implement a piecewise linear stress updating scheme which allows to avoid the relatively time-consuming VPSC calculation if the material response is close to or purely elastic.

The accumulative nature of the roll bonding process is realized by mapping the hardening parameters and the texture after a roll-bonding pass, to the initial configuration of the next pass. This approximation allows us to account for the state of the polycrystalline sheet after each pass, whilst keeping the number of elements and the expected computation time to a minimum.

Preliminary simulations show that our simulation framework produces a graded microstructure for single-pass rolling, as is expected from experiments. Furthermore, computation times can be reduced by up to 30% with the thread-based parallelization in comparison to simulations that only exploit domain decomposition techniques. We attribute this to the dynamic scheduling of openMP threads, which allows for better load balancing.

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## Residual stress prediction in deep drawn cup using crystal plasticity finite element method

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High manganese TWIP steels have superior mechanical properties and excellent strength to weight ratio, making them ideal for the development of lightweight vehicles. Achieved high strength and ductility rely on the optimization of the stacking fault energy, which governs mechanical twinning as the primary deformation mechanism in addition to dislocation glide and TRIP. However, abrupt fracture may be encountered in these steels under severe forming conditions, with complex and yet poorly known fracture mechanisms. In order to understand failure in severe forming conditions, the residual stress state plays an important role. This study focuses on the behaviour of TWIP steels subjected to deep drawing at room temperature and crystal plasticity based modeling in TWIP-aided sheet steel grade (X60Mn22,  $\sigma_{0.2} > 1000$  MPa) for residual stress state prediction.

A dislocation density based constitutive model for face-centered cubic metals incorporating twinning, validated based on a comprehensive and experimental dataset for twinning induced plasticity (TWIP) steels, is used in the current work. Two scale transition schemes namely; Relaxed Grain Cluster (RGC) and a classical Taylor Homogenization are tested. The constitutive law applied at the grain level, relies on the evolution of dislocation density based description of work hardening and also latent hardening due to presence of twins. For validation of the numerical findings, high angular resolution EBSD (HR-EBSD) is used for the measurement of residual stress and strain maps.

**Keywords:** Deep drawing, TWIP Steels, Twinning, CPFEM, Residual stress, HR-EBSD



Session 18

Atomistic and ab-initio modelling



## Kinetics of structural transformations in nano-structured intermetallics: atomistic simulations

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Kinetics of vacancy-mediated atomic ordering processes in nano-layered  $L1_0$  and triple-defect B2 ordered intermetallics was the subject of extensive atomistic simulations. The two groups of systems differ substantially in their vacancy thermodynamics: very low and very high vacancy concentration is observed in  $L1_0$  and triple-defect B2 intermetallics, respectively. Special attention was focused on the analysis of an effect of free surfaces on superstructure stability and defect concentration in the examined materials.

Simulation of “order-order” kinetics in [001]-oriented FePt nanolayers initially perfectly ordered in the c-variant  $L1_0$  and modelled with two-body interactions revealed a tendency for superstructure transformation from c-variant (monoatomic planes parallel to the (001) free surface) to a- and b-variants (monoatomic planes perpendicular to the (001) free surface) [1]. Remarkably, the  $L1_0$  c-variant  $\rightarrow$  a(b)-variant transformation was experimentally observed in FePt epitaxially deposited multilayers [2].

The triple-defect NiAl was modelled with an Ising-type Hamiltonian and the temperature-dependent equilibrium concentration of vacancies was determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations [3]. The system was then simulated for “order-order” kinetics by kinetic Monte Carlo (KMC) implemented with the temperature-dependent equilibrium vacancy concentration determined by SGCMC. The procedure was comparatively applied to bulk and nano-layered B2 AB systems. The simulated “order-order” kinetics showed two stages: (i) extremely fast generation of triple defects – i.e. creation of A-antisite defects and related shift of almost all B-vacancies to A-sublattice; the process, which, however, did not lead the system to thermodynamic equilibrium, (ii) extremely slow continuation of the process towards thermodynamic equilibrium. It was shown that the slow rate of the stage (ii) was due to extremely low efficiency of disordering jumps of A-atoms, which were reversed with very high probability resulting from numerous vacancies residing on A-sublattice. It is claimed that only the stage (ii) of “order-order” kinetics is observed experimentally as (surprising) low rate of “order-order” kinetics in bulk NiAl. In nano-layers, an additional effect of vacancy segregation on free surfaces and its influence on ordering kinetics was modelled.

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## **A comparative study for attenuation measurements of Rayleigh waves in acoustic microscopy**

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Attenuation of surface acoustic waves (SAWs) occurs when a wave loses some of its energy while propagating through a fluid or solid medium. The sources of dissipation may be the result of the losses within either the medium or its boundaries, which may be due to a combination of reflection refraction, diffraction and scattering.

The attenuation coefficient of SAWs on a liquid/solid structure is characteristic of the material bulk elastic properties as well as the surface state of substrate, topographic variations, grain size and distribution. Thus, SAW attenuation is a sensitive means of surface characterization. Therefore, the scanning acoustic microscopy technique, based on the emission and reflection of ultrasonic waves, would be a very useful and promising tool for attenuation investigations.

In this work, we use three different methods for attenuation coefficient measurements at 225 MHz via the determination of the output signal,  $V$ , received by the transducer as function of sample defocus,  $z$ . We apply our calculations to dioxide of silicon ( $\text{SiO}_2$ ) which's very used in the industry of the microelectronics where it serves as a layer of passivation, an oxide gate for transistor MOSFET or still as an anti-reflection layer.

Finally we compare our results to those given by J. Kushibiki & al. The obtained values are in good agreement with published data by the same technique.

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## **Analyzing Multiaxial Inelastic Yield and Flow in Nanocrystalline Metals using Molecular Dynamics Simulations**

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The objective of this research is to computationally quantify the influence of multiaxial stress states on the elasto-plastic deformation behavior of nanocrystalline metals using molecular dynamics simulations. In the present work, we express the inelastic yield transition in terms of an avalanche in stress-driven defect migration events. We resolve this avalanche from the atomic dynamics under non-equilibrium deformation using a novel method based on ensemble thermometry. The deformation response of a Cu ensemble of 5 nm mean grain size was computed at a temperature of 10K under both stress-controlled as well as strain-controlled biaxial loading. Our results suggest that initial yield in nanocrystalline Cu at the grain size considered is weakly anisotropic and shows tension-compression strength asymmetry. Additionally, we observed that the inelastic strain evolves in a direction normal to the von Mises yield surface at large strains when the flow is well-developed, but not in the regime of initial yield.

## Coarse-graining Dislocation-mediated Plasticity: Equilibrium Behavior of Dislocations and their Influence on Elastic Response

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In the macroscopic modeling of the elasto-plastic response of materials, constitutive equations are used. Dislocation motion as the underlying mechanism of plastic deformation is generally incorporated in the constitutive equations in a phenomenological way. Today's technological demands require more reliability and predictability, in particular for modeling the behaviour of microsystems. However, the currently used constitutive equations are not accurate enough at small scales and moreover lack a rigorous coupling to the microscale plastic events. Therefore, new models of metal plasticity, based on microscopic descriptions, are called for.

In this study, the effective material properties of metal at a coarse level are calculated from the description of the system at a fine scale using methods from equilibrium statistical physics. The fine-scale description consists of discrete, straight and parallel dislocations that interact via the isotropic, elastic continuum in which they are embedded. The coarse-scale level of interest is the continuous dislocation distribution and the corresponding elastic field. The coarse-scale quantities of particular interest are the effective stiffness and the pair correlation of dislocations. The latter is studied intensively, as it plays a crucial role in the closure of the BBGKY hierarchy that describes the dynamics of dislocation density profiles [4-8].

Explicit expressions were derived for the pair correlation and the effective stiffness. This yields the following conclusions. Firstly, the obtained pair correlation implies that, without loading, statistically stored dislocations will arrange in pairs of oppositely charged dislocations, which is energetically the most favorable state. A comparison of the interaction energy and the thermal energy of dislocations indeed shows that the behavior of dislocations is mainly governed by energy minimization, rather than entropy maximization.

Secondly, the effective stiffness under small externally applied loads was found to be equal to the microscopic stiffness, and hence it is not influenced by the presence of strong dislocation pairs. This is in line with the currently used constitutive models.

Current efforts concentrate on extending these results to systems subjected to finite loads.

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## Quantum effect on thermally activated glide of dislocations

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Crystal plasticity involves the motion of dislocations under stress. So far, atomistic simulations of this process have predicted Peierls stresses, the stress needed to overcome the crystal resistance in the absence of thermal fluctuations, of more than twice the experimental values, a discrepancy best-known in body-centred cubic crystals. We show [1] that a large contribution arises from the crystal zero-point vibrations, which ease dislocation motion below typically half the Debye temperature. Using Wigner's quantum transition state theory in atomistic models of crystals, we found a large decrease of the kink-pair formation enthalpy due to the quantization of the crystal vibrational modes. Consequently, the flow stress predicted by Orowan's law is strongly reduced when compared with its classical approximation and in much closer agreement with experiments. This work advocates that quantum mechanics should be accounted for in simulations of materials and not only at very low temperatures or in light-atom systems.

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## Atomistic study of microscopic plastic deformation process in $\beta$ -Sn

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The  $\beta$ -Sn crystal structure is a tetragonal distortion of the diamond crystal structure with two atoms per primitive cell. Owing to such a complex tetragonal crystal structure, active slip systems in  $\beta$ -Sn have not been fully clarified yet, although some tensile tests and microscopic observations of  $\beta$ -Sn single crystals have been conducted [1]. It is becoming increasingly important to clarify microscopic plastic deformation processes in  $\beta$ -Sn because of the need for strength analyses of Sn-based lead-free solder joints. The size of solder joints has been decreasing and reaching less than 100  $\mu\text{m}$  [2]. Such small solder joints contain few or only one crystal grain, which means that phenomenological constitutive models cannot be used to analyze their strength, and hence, crystal properties of  $\beta$ -Sn must be considered. To precisely analyze plastic deformation in microscale lead-free solder joints, the knowledge of active slip systems in  $\beta$ -Sn is of great importance.

As a first step towards understanding active slip systems in  $\beta$ -Sn, we herein analyze ideal shear deformation of  $\beta$ -Sn perfect crystal using first-principles density functional theory (DFT), and investigate the ideal shear strength [3] and generalized stacking fault (GSF) energy surfaces of 15 nonequivalent slip systems in  $\beta$ -Sn. It is found that  $(101)[\bar{1}01]$  has the lowest ideal shear strength among the 15 slip systems. The ideal shear strength of the 15 slip systems and Schmid's law indicate that, depending on crystal orientation, uniaxial tension activates seven nonequivalent groups of slip systems in  $\beta$ -Sn. It is also found from GSF energy calculations that the slip path of  $(110)[\bar{1}11]/2$ ,  $(101)[010]$ ,  $(101)[11\bar{1}]/2$ ,  $(121)[\bar{1}01]$ , and  $(121)[1\bar{1}1]/2$  deviates from the straight line path. The results indicate that perfect dislocations on these five slip systems dissociate into partial dislocations as in cubic and hexagonal crystals.

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## Atomistic Simulation of Crystal Change and Carbon Diffusion in Nano-sized Wiredrawing of Pearlitic Steel

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Wiredrawing is one of efficient material processing techniques for metals such as copper, aluminum and iron-steel, etc. It is known that unique and characteristic stress field occurs inside hollow die of wiredrawing and it makes the drawn wire stronger with smaller specified diameter. Pearlitic steel is recognized as one of the most reliable and strong wire materials for industrial use. However, microstructure of pearlite phase is quite complicated, where nano-sized lamellae-structured cementite crystals (iron-carbide, Fe<sub>3</sub>C) are contained. Carbon atoms should diffuse from cementite to ferrite across their boundary and may be pinned during wiredrawing process, as well as during heating treatment. But, the detailed atomistic mechanism of carbon diffusion caused by plasticity process is not sufficiently clarified yet.

At first, we study the nano-sized wiredrawing process of pure iron by using molecular dynamics (MD) simulation model [1]. A simple many-body potential of FS-type is adopted. In drawing simulation of two-dimensional arrangement of an  $\alpha$ -iron crystal with 7 nm diameter and 7 degrees die-semi-angle, conditions of [100], [010], or [001] drawing direction are compared as for atomic stress and strain distribution. In full three-dimension model, crystalline rotation is detected by using atomic-SSF (static structural factor) analysis. Phase transformation from bcc (ferrite) to fcc (austenite) is observed inside drawing die where the hydrostatic stress is enormous. It is also investigated by MD simulation that a pre-existing atomic-sized void (defect) changes its shape and interacts with plastic defects (dislocations) during wiredrawing. It is understood that these all are caused by a strong and unique stress field inside drawing die, which are naturally composed of the combination of tensile, compressive and shear components.

Three-dimensional models of pearlitic steel, where a cementite layer occupies one half or one thirds in the cross-section of wire, are simulated by using a Johnson-type pairwise potential for Fe-C system [2]. In this nano-sized pearlitic steel model, behavior of carbon diffusion is clearly captured. Since, in our pearlitic steel model, bcc->fcc phase transformation occurs certainly in ferrite layer during drawing, carbon diffusion seems to be enhanced. As our computational challenge, we also investigate the efficiency of the speeding-up GPGPU technique for longer-time MD simulation of carbon diffusion around ferrite-cementite interface.

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## Defects Interactions between Dislocations and Grain Boundaries by Molecular Dynamics Simulations

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Yielding of ductile materials can be fundamentally realized by transfer of dislocation across a grain boundary (GB), or by incorporation between the residual GB dislocation and the dislocations nucleated in the near-field of GB due to applied stress [1]. These phenomena are determined by the crystallographic orientation and the multiaxial stress state around GB. In the present research, a boundary interaction criterion of  $L$ - or  $L'$ -value has been newly proposed, which considers both contributions of the geometric relationship between two grains and a GB, and the stress state applied to the representative volume element containing them [2]. The dynamic transfer and incorporation of the nucleated dislocations to GB plane under uniaxial compression (refer Fig. 1(a)) and also under indentation by a spherical rigid punch (refer Fig. 1(b) and [3,4]) were then examined using molecular dynamics simulations. Two kinds of  $\langle 110 \rangle$  symmetric tilt grain boundaries of  $\Sigma 3A$  (boundary plane of  $(1\bar{1}1)$ ) and  $\Sigma 3B$  (boundary plane of  $(1\bar{1}2)$ ) of copper were atomistically modeled normal to the applied stress. The individual reaction process between the dislocations nucleated in grains and GB was, in detail, resolved and discussed in combination with the preferential slip systems across GB. The case of  $\Sigma 3B$  with the easier slip transfer is identical to the proposed interaction criterion, meanwhile an incorporation of the displacement shift complete (DSC) dislocation migrated on  $\Sigma 3A$  boundary plane was observed, which was possibly given by the dissociation of  $(a/2)[01\bar{1}]_A \rightarrow \{(a/6)[1\bar{1}\bar{2}] + (a/6)[21\bar{1}]\}_{DSC} + (a/2)[\bar{1}10]_{res}$  where  $a$  is lattice constant. It makes the defect interaction complicate, which leads the larger critical stress necessary for slip transfer across  $\Sigma 3A$  GB.

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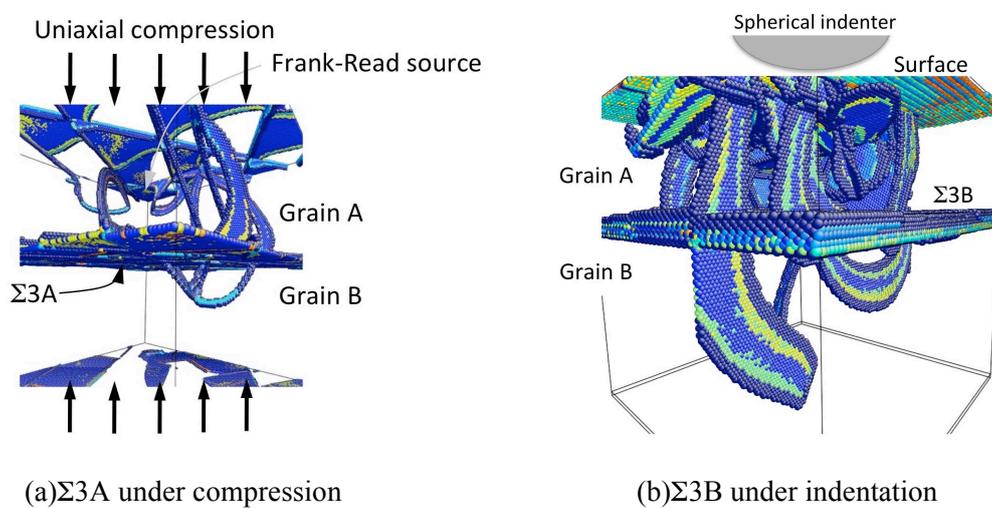


Fig.1 MD simulations of dislocation-GB interactions.

## A molecular static/molecular dynamics study of crack-void interaction in $\alpha$ -Iron

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The fracture properties of materials are strongly influenced by second-phase inclusions. In atomic scale, the voids can be treated as a type of the second-phase inclusions which can change the behavior of the crack growth in complex manners depending on their different distributions around the crack tip [1-3].

In this work, a study on crack-void interaction in bcc  $\alpha$ -iron by using the molecular static (MS) and the molecular dynamics (MD) simulations with an EAM potential [4] is presented. Three distributions of void are considered: (i) void positioned at varying distance normal to the crack tip, (ii) void inserted at varying distance in front of the crack tip along the crack path, and (iii) void placed at varying distance in the emission direction of the dislocations after the dislocation nucleation around the crack tip. The following parameters are investigated: (1) crack-void configurations; (2) strain rates; and (3) temperatures. Depending on different configurations, elastic shielding or anti-shielding is observed as a function of the temperature and strain rate. The increase of the temperature results in the decrease of the dislocation nucleation stress. Comparing with the un-voided crack growth, the simulated results show that the crack-void interaction slows down the crack growth.

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## Self-consistent pseudopotential theory of electronic structure using real-space piecewise basis states

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The champion of numerical methods in quantum many-body theory are self-consistent mean-field methods that are used as an approximate solution to the initial many-body problem. For non-relativistic systems, the basic requirement is to have good resolution of the energy-wavefunction eigenpairs that arise from diagonalisation of Schrödinger's equation. To that end, real-space grid-based wavefunction methods play a key rôle in our understanding of the nature of materials. Applying grid-based methods to the many-body problem pose a number of challenges in applied mathematics and theoretical physics. These are for instance related to the choice of basis functions, the representation of the grid, the approximations required to obtain self-consistency, and the number of eigenspectrum problems that need to be solved in the process of obtaining a self-consistent field. A general approach to the quantum many-body problem that is variational and basis orientated is reviewed with an application to atomic-scale electronic structure. The key-stone of the scheme is the use of local piecewise basis sets composed of polynomials to represent the wavefunction. The strictly local nature of the basis allows variable resolution of the problem in real space; for example, with grid and/or polynomial-order adaptivity via goal-based error estimates. It is shown that this scheme constitutes a flexible framework that allows for systematic improvement and resolution of the wanted eigenpairs to high accuracy that is essential for progress in real space descriptions of self-consistent mean-field quantum many-body problems.

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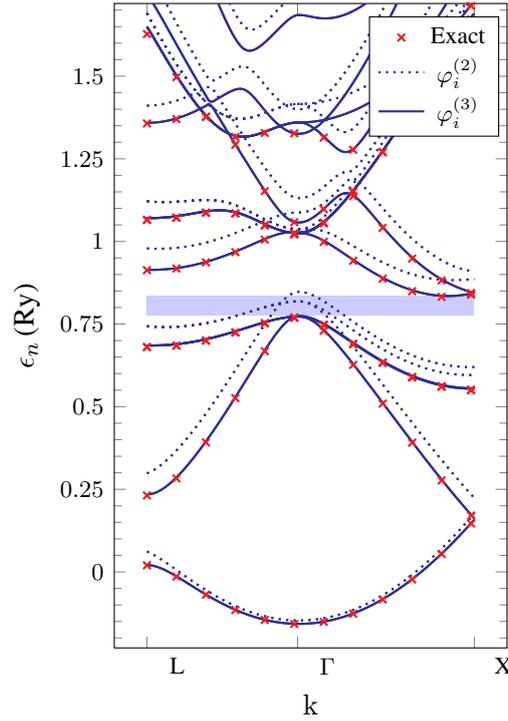


Figure 1: Self-consistent band structure of silicon. Computations were performed on a real space grid with finite basis functions  $\varphi_i^{(p)}$  and polynomial order  $p \in 2, 3$ . Convergence to the exact solution is systematic and variational with respect to the eigenenergies  $\epsilon_n$ .

**Integral form of Schrödinger's equation** A non-relativistic Lagrangian  $L = -\Delta + U(x)$  is supposed with a periodic potential  $U$  and leads to Schrödinger's time-independent equation:  $L\psi(x, k) = \epsilon\psi(x, k)$ . For any real vector  $k$  there exist a countable number of solutions of Bloch's form:

$$\psi(x, k) = e^{i k \cdot x} u(x, k), \quad (1)$$

where  $u \in \mathbb{C}$  is a cyclic function. Substituting Bloch's form of the wavefunction into Schrödinger's equation and evaluating the Lagrangian

$$e^{-i k \cdot x} [L e^{i k \cdot x} u(x)] = \epsilon u(x),$$

gives the kernel

$$-\Delta u(x) - 2i k \cdot \nabla u(x) + (U(x) + k^2 - \epsilon)u(x) = 0,$$

where  $k^2 = \|k\|^2$  is the square of the Frobenius norm of the reciprocal vector  $k$ . By taking the left-hand inner product with a test function  $v^* \in \mathbb{C}$  and integrating over all space (by parts where necessary) the bilinear integral formulation of Schrödinger's equation follows:

$$\int_{\Omega} \nabla v^*(x) \nabla u(x) d\Omega - \int_{\Gamma} v^*(x) \cdot \hat{n} \nabla u(x) d\Gamma + \int_{\Omega} v^*(x) [-2i k \cdot \nabla u(x) + (U(x) + k^2 - \epsilon)u(x)] d\Omega = 0.$$

The integral form of Schrödinger's equation is solved on a real space grid with discretised subspaces of the general form  $U_h = \{u \in U : u|_K \in P(K), K \in \mathbb{T}_h\}$ , that is defined on physical decompositions  $\mathbb{T}_h$  of  $\Omega$ . Here,  $P(K)$  denotes a suitable space of polynomial functions defined on the cell  $K \in \mathbb{T}_h$ .

## Atomistic calculations of dislocation core structures in MgSiO<sub>3</sub> perovskite

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MgSiO<sub>3</sub> perovskite is the most abundant mineral of the Earth's lower mantle (i.e. between 700 and 2900 km depth) and accounts for half of Earth's mass. At lower mantle pressures (25-135 GPa) MgSiO<sub>3</sub> crystallises in a distorted (orthorhombic) perovskite structure (described in the following using the *Pbnm* space group). In this structure, SiO<sub>6</sub> octahedra are tilted with tilt angles increasing with increasing pressure. Since it is very difficult to perform deformation experiments under the extreme P, T conditions of the lower mantle, little is known about plastic deformation of MgSiO<sub>3</sub> perovskite and its slip systems are still a matter of debate. To overcome this difficulty, we model dislocation core structures in this mineral taking into account the influence of pressure. In this study, we focus on dislocation core structures of dislocations with [100] and [010] Burgers vectors (which derive from <110> Burgers vectors of the underlying pseudo-cubic structure).

Atomistic calculations are performed using pair-wise potentials as implemented in the LAMMPS code. The choice of potentials was initially validated by comparing generalized stacking fault (GSF) energies to similar calculations performed with the density functional theory (DFT). The core structures of screw dislocations are calculated using two independent methods. The first one is based on Peierls-Nabarro-Galerkin simulations involving GSF as an input. Direct calculations have also been performed using cluster approach.

It turns out that screw dislocations with [100] Burgers vector are characterised by a core mostly spread in the (010) plane. The core exhibits two edge-sharing octahedra in a configuration very similar to that modelled in SrTiO<sub>3</sub> cubic perovskite. The structure of [010] screw dislocations is more complex with dissociation into fractional dislocations instead of well-defined partial dislocations. Nevertheless, we will show that the two core structures can be considered as planar core. As a consequence, both dislocations exhibit high Peierls stresses, especially for gliding in (001) plane. It is worth noticing that we found using either Peierls-Nabarro model or classical atomistic calculations that the Peierls potentials for these dislocations are non-symmetric. This illustrates the effect of orthorhombic distortions on lattice friction in perovskite materials.

## From Orowan to Prismatic loop during bypass of impenetrable obstacles by edge dislocations in magnesium

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Assuming dislocations as the main provider of plasticity in crystalline solids, one possible path to increase the material's strength is to alter the dislocation motion by introducing obstacles. The nature of the obstacles introduced in the materials to decrease the dislocation mobility can be of different nature: from nanovoid to incoherent particles. From a mechanical point of view, if one assumes an ideally plastic matrix reinforced by perfectly rigid particles, it has been demonstrated that in the absence of stress relief mechanisms (plastic relaxation), large stresses are built in the neighborhood of the particles in addition to the long-range stresses. Analyzed using dislocation physics, gliding dislocations can bypass perfectly rigid particles by leaving Orowan loops around the particles. Such a bypassing mechanism leads to linear work-hardening. However, parabolic work-hardening can be predicted when stress relief mechanisms are taken into account in the modeling.

The aim of this work is to study numerically the interaction between an edge dislocation and an impenetrable particle to reveal the dynamics of a dislocation bypassing mechanism. To this end, we simulated by molecular statics the process of dislocation bypassing impenetrable particles in model magnesium crystal in the framework of the (modified)-embedded atom method.

It was found that for the particle size considered in this study, the particle has to be encircled by a minimum of one Orowan loop before a stress relief mechanism can be activated. Once a second edge dislocation interacts with the particle, a series of cross-slip manoeuvres that transform the former Orowan loop and the bypassing dislocation into prismatic loops were identified. Furthermore, a comparison with continuum prediction of the bypassing stress was performed as a function of the dislocation length and particle size.

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## Atomistic Modelling of Thermo-Elastic Properties for Graphene Monolayer Using Energy-Based Approach

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The atomistic statics approach is used for computation of elastic moduli for graphene monolayer. The initial configuration of graphene crystal is defining to satisfy the density of potential energy minimization condition, and the form of graphene specimen is chosen to be in agreement with symmetrical properties of crystal lattice. The implied deformational gradient transforms the initial graphene sheet into the actual configuration. The full potential energy of the deformed graphene monolayer divided on its area is calculated. Quadratic items of its Taylor series in terms of deformational parameters are assumed to be equal to the elastic potential in the general non-symmetric form. Energy minimization procedure guarantees that linear items of series are equal to zero. This trick allows finding the graphene lattice elastic moduli. It is shown that graphene lattice, which is combined with two simple sub-lattices, could not be homogeneously deformed under the prescribed affine deformation. For supporting minimum of potential energy density for graphene monolayer in the deformed configuration, it is necessary to impose a vector of relative shift between sub-lattices depending on the deformational parameters. The components of sub-lattices relative shift vector are considered as additional degrees of freedom for graphene crystal. The elastic moduli of graphene lattice are obtained to be symmetric and not depending on the specimen size. Using Mie interatomic potential allows getting different values of Poisson coefficient (from 0.2 up to 0.5) under varying of Mie power exponents.

For the aim of crystal temperature control the computational-statistical approach to studying thermo-mechanical properties for finite sized crystals is presented. The approach is based on combination of the high-performance computational techniques and statistical analysis of the crystal response on external thermo-mechanical actions for specimens with statistically small amount of atoms (i.e. for nanoparticles). The heat motion of atoms is modelled in the statics approach by including independent degrees of freedom for atoms connected with their oscillations. The amplitude  $A$  of the oscillations is considered as a variable of the state, but the frequency distribution among the atoms is supposed to be constant and considered as a material function to be identified. These oscillations are simulated by applying the random displacements with amplitude  $A$  under uniform distribution of directions for such perturbations in space. Each obtained perturbed configuration of crystal is frozen for calculating its potential energy density. Equilibrium thermo-mechanical parameters have been computing by averaging of huge amount of different realizations of the perturbed crystal configurations. The dependence of graphene crystal lattice parameter on heat perturbations amplitude is calculated and the graphene thermal expansion coefficient is obtained for wide interval of  $A$ . The dependences of graphene lattice elastic moduli on temperature are also obtained.

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## Molecular Dynamics simulations on the bcc $\rightarrow$ fcc phase transition of Cu precipitates in $\alpha$ -Fe

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The mechanical behaviour of steels is strongly related to their underlying nano structures which evolve during processing or thermal treatment. In copper-alloyed  $\alpha$ -iron, Cu precipitates form within the iron matrix, especially when operated at temperatures above 300°C, yielding a change of the material's mechanical properties, i. e. an increased flow stress and a ductility reduction. Pure copper, appearing in nature in fcc structure, takes bcc structure if embedded as precipitates with radii smaller than approximately 2 nm into an  $\alpha$ -Fe matrix. During thermal ageing, the growing Cu precipitates undergo a structural bcc  $\rightarrow$  9R  $\rightarrow$  3R  $\rightarrow$  fcc phase transition [1, 2] in order to achieve their natural lattice structure.

Molecular Dynamics simulations are performed in order to analyse the structural transition in detail applying the IMD code [3]. Cu atoms placed onto bcc lattice sites in  $\alpha$ -Fe are annealed at different temperatures followed by a relaxation. During heat treatment, the Cu atoms displace their positions towards an energetically favourable position due to the applied EAM potential [4]. However, the surrounding  $\alpha$ -Fe forces the precipitates to remain in bcc structure. As this force decreases in the centre of the precipitates with increasing radius, a structural change is facilitated. Slight deviations start at a precipitate size of  $r > 4$  lattice constants of  $\alpha$ -Fe. A transition to the 9R structure is observed. Further growing precipitates show a loss of the 9R structure due to an increase of fcc regions. The computationally found precipitate sizes of the different structural characteristics (bcc, 9R, 3R and fcc) are in good agreement with experimentally observed Cu precipitates [1, 2]. Structural transitions are found to nucleate in the precipitate's centre while the surface is still forced to remain bcc, especially in the case of small precipitates. We will investigate Cu precipitates with radii up to 32 nm (112 lattice constants). Furthermore, the effect of the coherency loss of the Cu precipitates on the critical resolved shear stress of an edge dislocation will be analysed.

Prospectively, the detailed analysis of this transition on the atomistic length scale by means of Molecular Dynamics simulations is important with respect to sequential multiscale coupling with Phase Field Methods and Dislocation Dynamics which are able to simulate particle growth, particle coarsening and the interaction of dislocations with large obstacle fields, respectively.

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## Displacive phase transformations in iron: Nucleation, kinetics and morphology

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An extensive, systematic molecular dynamics (MD) study is performed for analysing the nucleation, kinetics and morphology characteristics of thermally-induced, displacive phase transformations from face-centered cubic (fcc) to body-centered cubic (bcc) iron. At the atomic level these transformation characteristics are influenced by a number of factors, including (i) the appearance of free surfaces, (ii) the initial presence of fcc-bcc grain boundaries, (iii) the existence of point defects (i.e., atomic vacancies) near a grain boundary, (iv) the initial thermal velocities of the atoms, and (v) the specific interatomic potential used. Other MD studies that capture the overall transformation behaviour of iron well have often underestimated or ignored the influence by these factors on the transformation response, with the risk of putting the accuracy, generality and physical explanation of the MD results on loose grounds.

The present research illustrates the relative contribution of each of the above factors by means of a detailed comparison study for three different interatomic potentials. The accuracy of the interatomic potentials is established by validating for the fcc and bcc phases the calculated elastic moduli, cohesive energy, vacancy formation energy and interfacial energy against experimental and ab initio data reported in the literature. The importance of calibrating material data of *both* the stable bcc phase and the metastable fcc phase - instead of the stable bcc phase only - is demonstrated. The numerical results call for general caution when interpreting phenomena that start close to instability points and therefore are sensitive to small disturbances; a large spread in the overall transformation time is found under different initial thermal velocities, interfacial lattice incoherence, boundary conditions (free vs. periodic), and interatomic potentials, where for completely transformed atomic systems the discrepancy between the maximum and minimum transformation time appears to be more than a factor of 150. Also, the morphology of the bcc product phase is remarkably sensitive to the type of boundary conditions and the choice of interatomic potential, while the influence by both the set of initial thermal velocities and the interfacial lattice incoherence only becomes apparent for specific atomic samples that transform relatively slowly. The presence of fcc-bcc grain boundaries increases the spatial heterogeneity of transformation events, with the appearance of an increasing number of vacancies at the grain boundary giving rise to a larger overall transformation time.

More information on this research can be found in Ref. [1]

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## FE2AT: Finite Element Informed Atomistic Simulations

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Atomistic simulations have, in recent years, established themselves as an important tool in helping and advancing our understanding of nanoscale materials and properties. Methods such as first principles calculations and atomistic simulations offer greater physical insight into material properties and phenomena that are either expensive and difficult, or even impossible, to measure experimentally.

Classical atomistic simulations that use empirical interatomic potentials, also referred to as molecular simulations, are gaining increasing popularity due to their ability to treat larger systems (in the order of millions or billions of atoms) in comparison to ab-initio simulations that are usually limited to system sizes of a few hundred atoms.

Most molecular simulations are, nonetheless, still restricted to simple geometries and homogeneous loading conditions. Additionally, a significant amount of computational time is spent on calculating the elastic response of the material, while the focus of such studies is usually on the mechanisms of plastic deformation and failure.

In this work, we present a simple but versatile approach called FE2AT to use finite element (FE) calculations to provide appropriate initial and boundary conditions for atomistic simulations [1]. The role of the relatively inexpensive FE computation is to solve for the anisotropic elastic response of a continuum sample subjected to arbitrary loading conditions. The elastic displacements obtained from the FE computation are then mapped onto the atomistic configuration, by interpolating between the nodal displacements of the corresponding finite element.

FE2AT thus allows us to forgo large parts of the elastic deformation in atomistic simulations, leading to a significant reduction in computation times. Additionally, the method can also be used for cases with complex geometries to provide non-homogeneous initial and boundary conditions. The nicety of this method is that the FE computation does not need to perfectly represent the atomistic situation; it merely needs to provide starting configurations which are close to the minimal energy structure. The so generated FE informed atomistic configuration can then be used for subsequent molecular (static or dynamic) simulations as well as other simulation methods like Monte Carlo, accelerated MD or diffusive MD etc.

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## ***Ab initio* studies of heteropolar SiC/GaN junctions**

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In this work, we present *ab initio* studies of 4H-SiC/wz-GaN, 3C-SiC(111)/wz-GaN, and 3C-SiC(111)/zb-GaN(111) junctions in the framework of the density functional theory. We have calculated the atomistic details of the interfaces, their formation enthalpies, valence band offsets (VBO's), induced interface charges, and electric fields at the interfaces. The theoretical studies of the similar interfaces have been reported previously for some cubic structures [1-2]. In the present calculations, we employed the supercells with up to 136 atoms, and performed precise calculations employing the SIESTA code.

The present studies shed light on the physics of heteropolar SiC/nitride junctions and provide microscopic knowledge of interface morphology together with theoretical predictions of important parameters of the junctions. They constitute also the basis for reliable modeling of important phenomena in these junctions such as the charge and spin transport across the interface and the thermal boundary resistance effect.

In heteropolar SiC/nitride systems, the abrupt interfaces contain 'oversaturated' or 'undersaturated' tetrahedral bonds with more than 2 or less than 2 electrons per bond, respectively. This bond heteropolarity leads to a macroscopically charged interface that is typically energetically unstable and undergoes various reconstructions to roughly restore charge neutrality. For example, the simplest atomic reconstructions leading to the neutral interfaces are those with one mixed layer (e.g., N/C or Ga/Si). We consider various possible interface reconstructions and determine the energetically most stable ones. Further, we calculate the valence band discontinuities (VBOs) for interfaces of different morphologies and find out that the VBOs lie in the range of 0.4 – 1.4 eV depending on the atomistic details of the reconstruction. Depending on the orientation and chemical composition of the interface, the SiC/GaN heterostructures can be of the type I or II. Generally, the theoretically calculated values of VBOs compare reasonably well with available experimental data [3-4].

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## Elastic Properties of Covalently Functionalized Carbon Nanotubes and Graphene Layers

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Recently functionalized carbon nanotubes (CNTs) and graphene layers (GLs) attract a lot of research activity, mostly because of their potential applications in nanotechnology, such as novel composites and/or functional materials for future electronics. New composites made by adding CNTs or graphene flakes to various materials, such as polymers or metals, are expected to enhance their mechanical strength, electrical and thermal conductivity, and chemical stability.

We have studied the effects of covalent functionalization of single wall carbon nanotubes (CNT) and graphene layers, focusing in this presentation on elastic properties of functionalized systems. We consider simple organic molecules  $-NH$ ,  $-NH_2$ ,  $-CH_2$ ,  $-CH_3$ ,  $-OH$  attached to CNTs' and graphene's surfaces at various densities. As prototypes of CNTs, we consider (9,0) nominally metallic, and (10,0) and (11,0) semiconducting tubes. The studies are based on the first principles calculations in the framework of density functional theory, employing the SIESTA code. They give us physical insight into structural, mechanical, electronic, and electrical properties of the functionalized CNTs and graphene layers. For all studied structures, we have determined the changes in the local and global geometry, binding energy, heat of formation, elastic moduli (Young's, Shear, and Bulk, as well as Poisson's ratios), electronic structure and resulting band gaps and effective masses, as a function of the density of the adsorbed molecules. Some very preliminary results are to find in Ref. [1].

It turns out that elastic moduli of functionalized systems diminish with increasing concentration of adsorbents. The strongest effect is observed for CNTs functionalized with  $-CH_2$  radical, where the Young's modulus of the functionalized system is by 30% smaller than in the pristine CNTs. Shear modulus and Bulk modulus exhibit similar behavior. The weakest reduction of bulk moduli is observed for  $-NH$ , being roughly equal to 15%. In spite of this reduction in the magnitude of elastic moduli, stable functionalized CNTs and graphene monolayers are strong enough to constitute enforcement in the composite materials.

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## Nanoparticles elasticity: surface and size effect

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The variation in the bulk modulus of semiconductor nanoparticles has been studied within first-principles electronic-structure calculations using the local density approximation (LDA) for the exchange correlation. In a first study on semi-conducting nanoparticles [1], an enhancement was observed in the bulk modulus as the size of the nanoparticle decreased. The origin of this enhancement has been discussed. The description of the surface was notably mentioned as a possible explanation but could not be widely investigated at that time. The present investigations particularly focus on the theoretical description of the surface, and the independence of the analysis towards the boundary conditions applied.

Nanocrystals are constructed by taking a central atom. Atoms were added keeping bulk-like coordination and symmetry. The truncation condition used to terminate the cluster is to consider all atoms within a sphere of a desired radius. The surface atoms of the nanocrystal would have dangling bonds as a result of truncation. In order to make the comparison meaningful with experiment where passivants, usually organic molecules, are used to saturate the dangling bonds, we use hydrogen or pseudohydrogen for this purpose.

The structural and electronic properties are calculated using a plane-wave pseudopotential implementation of density-functional theory (DFT) within VASP [2-3]. Projected augmented wave potentials are used. The nanocrystal is simulated as a periodic unit cell with a vacuum between neighboring clusters of at least 10Å thick. Complete optimization of the internal coordinates is carried out to minimize the energy of the structure. The structure obtained is considered as the equilibrium structure at that size for which the bulk modulus is computed. Expansions and contractions about the equilibrium geometry are carried out in order to compute the bulk modulus. Total energies of the expanded/contracted structure are computed for the structures in which the outermost atoms are kept fixed while those in the interior are optimized to minimize the total energy. The total energies at different volumes were fit to the Murnaghan equation of state [4]. The volume of the nanocrystal is here defined by that of the convex hull [5] formed by the outermost atoms making the structure.

These ab initio simulations provide a fairly comprehensive look at the various factors considered: surface effect, size, anisotropy.

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Session 19

## Interfacial Mechanics



## Geometrically nonlinear higher-gradient elasticity with energetic boundaries

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The objective of this contribution is to formulate a geometrically nonlinear theory of higher-gradient elasticity accounting for boundary (surface and curve) energies. Surfaces and curves can significantly influence the overall response of a solid body. Such influences are becoming increasingly important when modelling the response of structures at the nanoscale. The behaviour of the boundaries is well described by continuum theories that endow the surface and curve with their own energetic structures. Such theories often allow the boundary energy density to depend only on the superficial boundary deformation gradient. From a physical point of view though, it seems necessary to define the boundary deformation gradient as the evaluation of the deformation gradient at the boundary rather than its projection. This controversial issue is carefully studied and several conclusions are extracted from the rigorous mathematical framework presented.

In this presentation the internal energy density of the bulk is a function of the deformation gradient and its first and second derivatives. The internal energy density of the surface is, consequently, a function of the deformation gradient at the surface and its first derivative. The internal energy density of a curve is, consequently, a function of the deformation gradient at the curve.

It is shown that in order to have a surface energy depending on the total (surface) deformation gradient, the bulk energy needs to be a function of at least the first derivative of the deformation gradient. Furthermore, in order to have a curve energy depending on the total (curve) deformation gradient, the bulk energy needs to be a function of at least the second derivative of the deformation gradient. Clearly, the theory of elasticity of Gurtin and Murdoch is intrinsically limited since it is associated with the classical (first-order) continuum theory of elasticity in the bulk. In this sense this contribution shall be also understood as a higher-gradient surface elasticity theory (see [1] for further details.)

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## Two Models of Three-dimensional Thin Interphases with Variable Conductivity and Their Fulfillment of The Reciprocal Theorem

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Interphases appear in heterogeneous media in a variety of forms. Often the treatment of a thin interphase as a separate phase in a multiphase solid is not convenient in analytical or numerical solutions of those systems. Thus, approximate models of a thin interphase that make possible to obtain a solution for the fields in the media adjacent to it, without the need of determining the fields within the interphase itself, become a necessity in many cases. The question then arises whether a global property which was present in the original heterogeneous medium will continue to prevail after an approximate representation of the thin interphase has been introduced in the system. A global property, known to have important consequences on the behavior of the heterogeneous solid, is the "reciprocity" relation between a pair of two different solutions, as stated by the reciprocal theorem. Since the formulation of an approximate model for the thin interphase involves several assumptions, the fulfillment of the reciprocal theorem in the original system does not necessarily imply its fulfillment in the transformed system in which an approximate model of the thin interphase has been introduced. The preservation of the reciprocity relation by the approximate model, if proved, would be considered to be an important consistency quality of the model. In this study [1] we consider steady thermal conduction phenomena, and generalize the two approximate models of a thin interphase of [2,3,4] to the case of thin interphases with a variable conductivity. The fulfillment of the reciprocity property in the presence of those models is studied in the context of their developed generalized version herein and it is proved that both models fulfill the reciprocal theorem.

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## Inspection of free energy functions in gradient crystal plasticity

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The dislocation density tensor computed as the rotational part of plastic distortion is regarded as a new constitutive variable in crystal plasticity. Energy can be stored by accumulation of dislocations with the same sign. The dependence of the free energy function on the dislocation density tensor is explored starting from a quadratic Ansatz already proposed in the literature. An alternative rank one potential is also presented providing new expressions for the double stress tensor conjugate to the dislocation density tensor in the work of internal forces. It can be shown that the balance equation for the double stress tensor combined with a generalized Schmid law leads to the existence of size-dependent kinematic hardening [1,2,3]. Interfaces like grain boundaries or between plastic and elastic phases play an essential rôle in the analysis due to the additional boundary and interface conditions arising in the model. Logarithmic dependencies are then envisaged based on considerations from the statistical theory of dislocations [4] and from the Read and Shockley analysis of low angle grain boundaries. The relevance of the presented free energy potentials is evaluated from the analytical solutions to the periodic two-phase laminate problem under shear where one layer is a single crystal material undergoing single slip while the second one remains elastic. The presented solutions provide the profiles of plastic slip in the plastic phase and the scaling law for the kinematic hardening as a function of the unit cell thickness [5,6].

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## Thermomechanics of solids with generic imperfect coherent interfaces

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Interfaces within a solid can play a significant role in the overall response of a body and their influence increases as the scale of the problem decreases. Furthermore their thermomechanical properties can differ significantly from those of the surrounding bulk. Imperfect interfaces at which the bulk fields possess discontinuities are of particular interest, e.g. in the work of Özdemir et al. [1] who describe an imperfect interface using a cohesive zone formulation. The current contribution presents the computational aspects of modelling thermomechanical solids with generic imperfect coherent interfaces. The interface is termed generic imperfect in the sense that it allows for the jump of the temperature as well as the normal heat flux across the interface, including Kapitza and highly conductive (HC) interfaces as special cases [2]. In order to describe such effects, a fully energetic formulation of interfaces, an extension of the interface elasticity theory [3], is used, see [4] for details. The interface is assumed to be energetic in the sense that it possesses its own energy, entropy, constitutive relations, and dissipation. Assuming thermo-hyperelasticity, the dissipation inequality on the interface is fulfilled using two sufficient conditions [4], i.e.

$$\bar{\Theta}^{-1} - \{\{\Theta^{-1}\}\} = -\bar{s} \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \quad \text{and} \quad \llbracket \Theta \rrbracket = -\bar{r} \{\{\mathbf{Q}\}\} \cdot \bar{\mathbf{N}},$$

where  $\Theta$  and  $\bar{\Theta}$  denote the temperatures in the bulk and on the interface. The jump and average of a quantity  $\{\bullet\}$  is denoted as  $\llbracket \bullet \rrbracket$  and  $\{\{\bullet\}\}$ , respectively. The heat flux is given by  $\mathbf{Q}$  and the interface unit normal by  $\bar{\mathbf{N}}$ . The constants  $\bar{s} \geq 0$  and  $\bar{r} \geq 0$  represent the thermal sensitivity and resistance of the interface. Setting both coefficients to zero renders a HC interface and assuming a continuous normal heat flux across the interface and  $\bar{r} \neq 0$  yields a Kapitza interface. If the first condition is trivially satisfied by  $\bar{\Theta}^{-1} = \{\{\Theta^{-1}\}\}$  and  $\bar{s} = 0$ , the generic imperfect interface is termed semi-dissipative otherwise fully-dissipative. For the fully-dissipative model, the interface temperature is considered as an independent degree of freedom in the current contribution.

Consistent linearisations of the nonlinear governing equations are provided. Key features of generic imperfect coherent energetic interfaces are then elucidated via a series of three-dimensional numerical examples. In particular, it is clearly shown that a jump in the heat flux across the interface is possible even in the absence of a heat flux along the interface.

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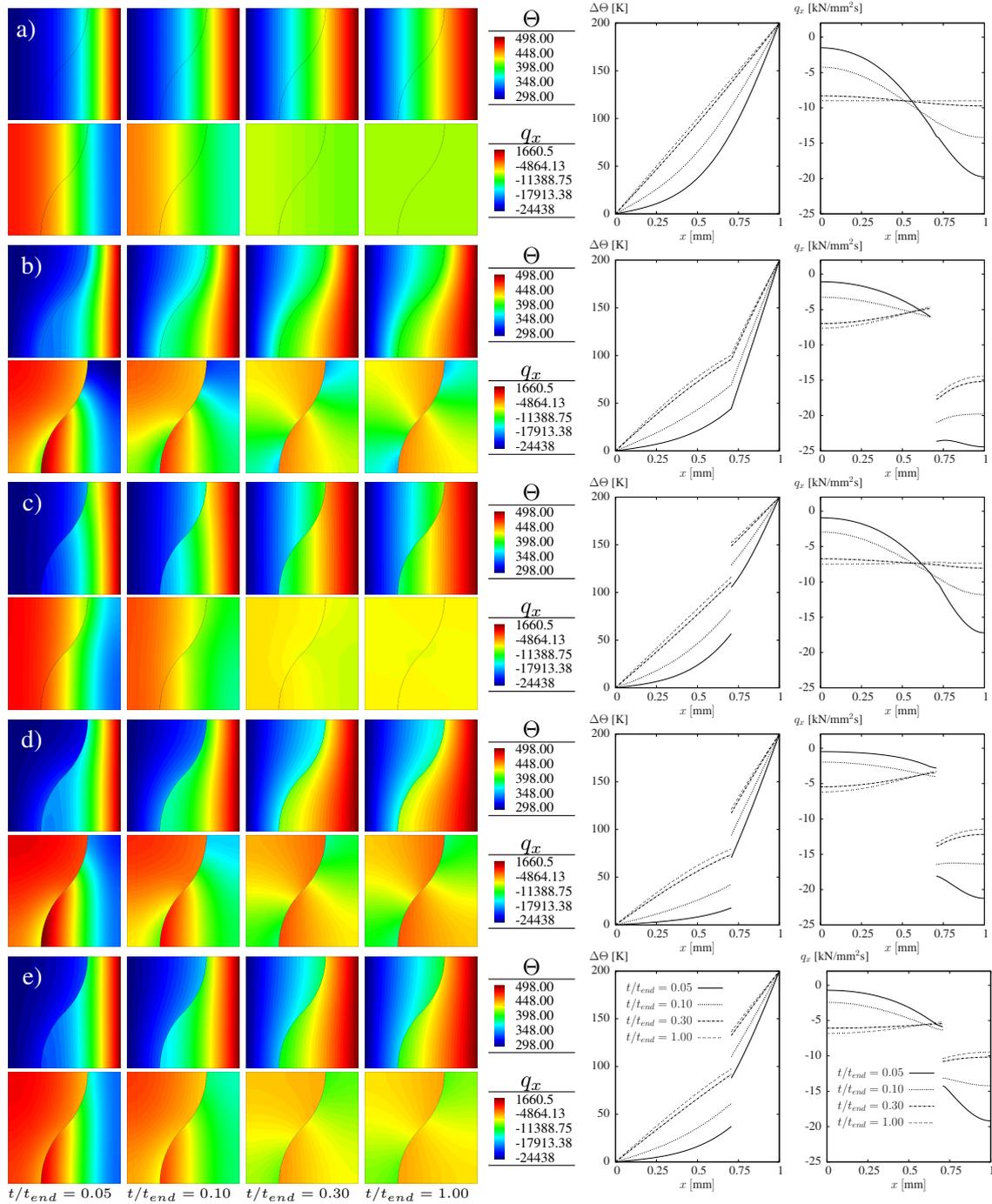


Figure 1: Thermal response of a strip with a) no interface, b) a HC interface, c) a *Kapitza* interface, d) a semi-dissipative generic imperfect interface, e) a fully-dissipative generic imperfect interface at times  $t$  with  $t_{end} = 0.1s$ . The temperature on the left (298K) and right edge (498K) of the strip is prescribed, homogeneous Neumann boundary conditions are applied to the remaining boundary. The graphs belong to upper edge of the strip, where the position  $x = 0mm$  is the left upper corner and  $x = 1mm$  the right upper one. The bulk conductivity is set to  $k = 45.0 N/sK$ , the heat capacity to  $c_F = 3.588N/[mm^2K]$ . The interface is endowed with a conductivity  $\bar{k}/k = 100mm$ . All examples are computed using the fully-dissipative generic imperfect interface model by variation of  $\bar{s}$  and  $\bar{r}$  only.

## Continuum dislocation transport in two-phase materials

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In the past years much attention has been given to the incorporation of dislocations in crystal plasticity models, as they are the carriers of plastic deformation. Several higher-order crystal plasticity models have been developed to properly capture phenomena such as dislocation pile-up and dislocation patterning in poly-crystalline metals. Here a formulation is considered based on a statistical-mechanics description of the transport of dislocations in [1]. The governing equations, however, are derived from a deterministic perspective for a more transparent analysis and understanding of the framework. Previous work pointed out that all dislocation interactions have a significant contribution to the internal stress [2]. Therefore, the continuum expression for the dislocation interactions is derived from all dislocation interactions, as opposed to only (gradients of) GNDs, where positive and negative dislocations are arranged in an idealised configuration.

In order to study the effect of the transport of dislocations on the behaviour of metals with complex microstructures, a simplified two-phase laminate material is considered [3]. The material contains a soft and a hard phase, c.f. Dual Phase steel, and contains one slip system. Parameters such as the dislocation content, grain size, volume fraction and the resistance to plastic deformation of the hard phase are varied to investigate their effect on the overall material response. A shear deformation is applied and the result of the continuum dislocation transport model is compared to classical averaging techniques, e.g. Taylor and Sachs methods.

The continuum model of dislocation transport is capable of simulating the effect of the various changes in the simplified microstructure, thereby showing that the classical averaging methods have shortcomings, e.g. to predict size effects. The transport of and interaction between dislocations are important factors to consider in accurately predicting material and size effects in poly-crystalline metals.

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## **Investigation of the effect of adsorption layers and surface roughness on the final bond strength in multi layer roll bonded metallic material compounds**

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Roll bonding is one of the most used production technologies for metallic materials compounds. Due to a process similar to pressure welding commercially up to 5 layers will be welded at one forming step. Beside surface treatment and annealing steps the main parts of this technology are the processes of roll bonding and further rolling of the layered structures [1].

On the one hand differences in mechanical and thermal properties of the alloys used for each layer are the reason for several technological problems [1, 2]. On the other hand small tolerances are expected concerning variations in layer thickness, bond strength and the maximum allowed residual stresses.

From industrial experience and laboratory trials the influence of adsorption layers and surface roughness is known. A general theoretical investigation of their influence on optimum process conditions are still missing.

In the given presentation a multi - scale bond strength model is presented, which is based on film theory of adhesion, contact and fracture mechanics as well as thermodynamically considerations concerning surface tension and the effect of adsorption layers on it. The used equations are an extension of the model presented in [1], [3].

Based on a coupled computation of bonding process and bond strength development parameter identification is performed concerning the dependence of the final bond strength on initial material state and process conditions.

Several aspects of the bond strength model were evaluated in laboratory trials. A comparison of theoretical and experimental results is given.

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## Surface Roughness Effect on Static, Dynamic and Mechanical Properties of Polymers at Interfaces

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Cohesively bonded polymer-solid interfaces play an important role in coatings and composite materials, applications of which include renewable energy production structures, sandwich panels used in automobiles and food packaging. These interfaces are generally characterized by substrate roughness scale of few nanometers to several micrometers that leads to strengthening of polymer-solid bonding either by increase in the effective contact area (quantified as roughness factor:  $RF = \text{Area}_{\text{rough}}/\text{Area}_{\text{planar}}$ ) or by mechanical interlocking of polymer between surface undulations. While polymer conformation is essentially independent in the case of micrometer sized roughness patterns [1], it is expected to be strongly influenced in the nanometer limit, when the roughness scale becomes comparable to the characteristic dimension of polymer (determined via, e.g. radius of gyration,  $R_g$ ). Very little is known at present regarding the role of relative dimensions of polymer chains with respect to surface undulations in effecting the static, dynamic and mechanical properties of the polymers at interface. Such information can be used in substrate surface engineering for improving bonding without changing the interface chemistry. To understand the elementary mechanisms of adhesion, we have performed molecular dynamics (MD) simulations to access this information. Coating systems are realized by confining the polymer between a planar substrate and a rough substrate of varying roughness scale. Periodic boundary conditions are used along directions parallel to the substrate. To quantify the role of roughness, the undulation features are varied in comparison to the average  $R_g$  of the polymer. The coating systems are subjected to different loading modes while monitoring their stress-strain behavior and the work of separation. As obtained by static and dynamic properties of the polymer close to the interface, we find that confinement is caused by roughness features with dimensions of the order of  $R_g$ . At these dimensions, mechanical interlocking appears to play a role in improving polymer bonding in place of increase in the effective contact area. Furthermore, confinement also shows the ability to switch the mode of failure from adhesive to cohesive type [2].

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## A model of gradient crystal plasticity at finite deformations accounting for themomechanical surfaces and grain boundaries

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The response of crystalline materials to applied loading can be approximated using continuum models. The kinematic description of the plastic deformation is obtained from the assumption that plastic flow arises due to slip on the individual slip systems that constitute the crystal structure. Constitutive relations are then used to describe the evolution of the resistance to slip. Continuum models are well developed for polycrystalline materials where, due to the large number of grains, the role of the grain boundaries can be ignored (see e.g. [4] among others).

Classical continuum descriptions lack a length scale. Thus, they are unable to capture the scale-dependent response that crystalline materials exhibit when the size of the continuum domain and the grain size are of similar order. Gradient plasticity theories overcome this limitation by including higher gradients of measures of the plastic deformation, and thereby introducing a length scale. In addition, the gradient theories allow additional microscopic boundary conditions to be specified. They do not however automatically account for grain boundaries and surfaces.

The objective of this presentation is to attempt to account for the presence of both grain boundaries and surfaces within the gradient theory of plasticity proposed by Gurtin [1]. The work is thus an extension of the infinitesimal theory presented in [2] to the finite strain regime.

The influence of the grain boundary and the surface is modelled by endowing these lower-dimensional structures with their own energetic and dissipative structures. This is done by extending the surface elasticity theory of Gurtin [3].

A series of numerical examples, implemented using the finite element method, will serve to elucidate the key features of the theory.

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## Rate Sensitive Continuum Damage Models and Mesh Dependence in Finite Element Analyses

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The experiences from the orthogonal machining simulations, cf. [1], show that the Johnson Cook dynamic failure model appears to exhibit a significant element size dependence. Such pathological mesh dependence is a direct consequence of the use of damage models unless some type of regularization is introduced. The current contribution investigates the extent of possible pathological mesh dependence, and a comparison of the resulting behavior in the case of the Johnson Cook (JC) plasticity model combined with two types of damage evolutions. Both the plasticity and the damage models considered in the formulation are rate dependent and the damage evolutions for both models are defined as a post-processing of the effective stress response. The results show that both damage models, with a realistic representation of the pearlite material properties, exhibit a similar extent of mesh dependence and that viscous regularization effects do not suffice in the current investigation.

As a remedy for the observed mesh sensitivity, it is proposed to use a continuum-damage approach for the modeling of continuous deformation behavior up to the critical point along the stress-strain curve where discontinuous bifurcation occurs. Whenever a critical stress-strain state has been diagnosed, a Cohesive Zone (CZ) is established to allow for objective fracture energy release as the stress is degraded in the CZ. The formulation is made in a completely general kinematical context thus allowing for large deformations, central in machining applications. To characterize the homogenized continuous/discontinuous macro-behavior, a discontinuous enhancement of XFEM-type is proposed at a sub-scale based on homogenization theory. It appears that the associated local momentum balance is manifested by the condition for traction continuity across the discontinuity surface. Thereby, the formulation generically contains e.g. the classical condition for diagnosing discontinuous bifurcation. In the corresponding FE-application, localized CZ damage is kinematically realized as an element embedded discontinuity, which is introduced elementwise, thereby facilitating the model implementation in standard FE-packages. Both pre-peak continuum behavior and post-peak CZ behavior are modeled using the concept of (visco)-plasticity coupled to damage, representing distributed and localized damage evolutions by separate constitutive modeling considerations, respectively. To arrive at a computationally attractive formulation, both the pre- and post-peak damage evolutions are defined as a post-processing of the effective stress response. In the considered numerical examples of typical shear and tensile deformation the new continuous/discontinuous ductile fracture modeling exhibits no significant element size dependence.

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Session 20

Biomechanics



## Mechanical behaviour of human fetal membrane in different experimental configurations

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The fetal membrane (FM) surrounds and protects the developing fetus during pregnancy. Recently renewed interest for the mechanical behavior of fetal membranes is related to the problem of iatrogenic preterm rupture, limiting the effectiveness and applicability of minimally invasive fetal surgery.

Separation of the constitutive layers, amnion and chorion, of the FM is an event occurring prior to failure. In a previous study [1], we have shown that separation is caused by a difference in the layer specific Poisson's effect. A corresponding phenomenological constitutive model has been formulated, which is able to reproduce the exceptionally high incremental Poisson's ratio (up to 8) and the large biaxial stiffness of the amnion layer.

Model equations for amnion and chorion were implemented in a finite element (FE) code in order to obtain a realistic two layer FE model of the human FM. The underlying constitutive model and its implementation will be presented and the simulation results will be discussed with reference to experimental results and the microstructure of human fetal membranes.

The FE model is applied to investigate the mechanical response of FM in different experimental test procedures such as uniaxial tension, inflation and puncture testing. In particular, the latter was widely-used to test membranous biological tissues, but, if applied to FM, discrepancies were observed when compared with other testing configurations [2,3].

The influence of parameters, such as interaction at the interface between amnion and chorion, clamping and contact conditions, and thickness of the layers are analyzed in numerical simulations and discussed with respect to observations of deformation and rupture behavior in puncture test.

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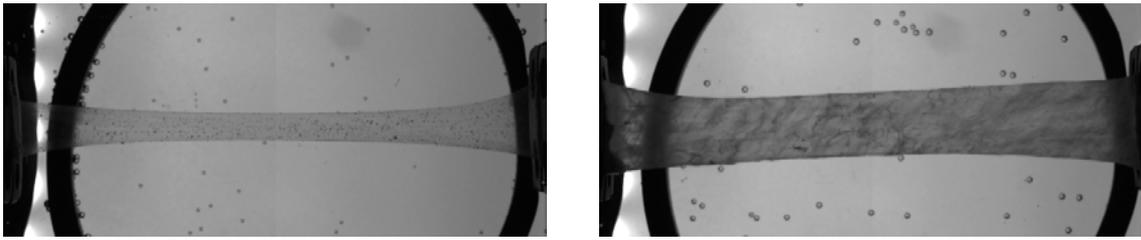


Figure 1: Images of an amnion (left) and chorion (right) sample during a tension test at the same level of longitudinal deformation. The images indicate the pronounced difference in the layer specific Poisson's effect.

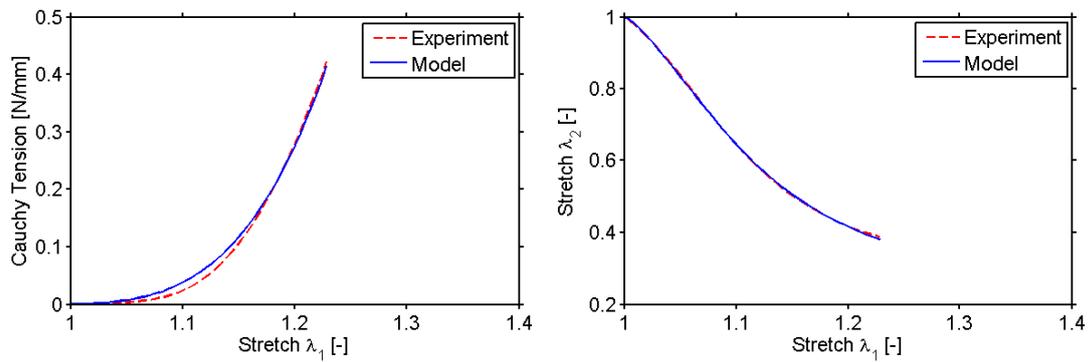


Figure 2: Optimization results of the formulated phenomenological constitutive model for averaged amnion response. (left) tension-stretch and (right) kinematic response.

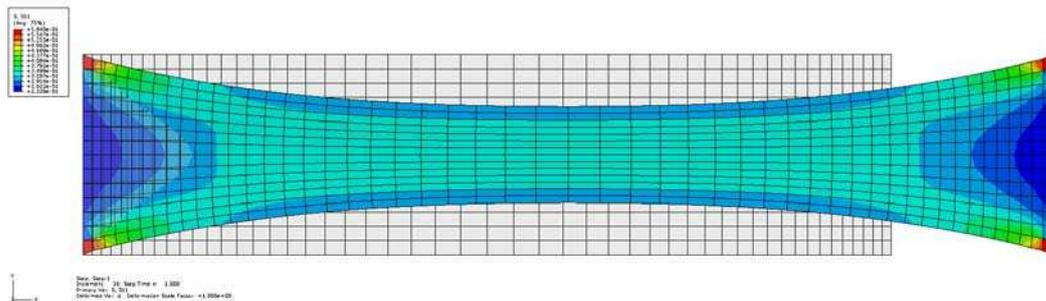


Figure 2: Simulation of a tension tests on an amnion sample with the implemented constitutive model.

## Hyperelastic modelling of the anterior cruciate ligament and patellar tendon

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The anterior cruciate ligament (ACL) is the most frequently injured knee ligament, and is one of the structures most commonly injured in sport [5]. Due to the fact that it does not heal naturally, the standard treatment for a ruptured ACL is surgical reconstruction [4], to which there are several approaches, the most common being patellar tendon (PT) and hamstring tendon autograft. There is currently no consensus with respect to the choice between these two grafts [4], however, the PT is the most commonly used [1]. In this poster, we mathematically model the ACL and PT in order to compare their mechanical properties within the same framework.

Ligaments and tendons have an extremely hierarchical structure [3]. Their main subunit is the fascicle, which is made of fibrils arranged in a crimped pattern (see Figure 1). The diameter of fascicles is typically in the range of 50-300  $\mu\text{m}$  and that of fibrils is 50-500 nm [3]. Further subunits in the hierarchy can be observed; in order of decreasing diameter they are: sub-fibrils (10-20 nm), microfibrils ( $\sim 3.5$  nm) and tropocollagen ( $\sim 1.5$  nm) [3], however, the mechanics on these lengthscales will not be considered here. We shall instead focus on the fascicular structure of the ACL and PT. We utilise a strain energy function proposed by Holzapfel *et al.* [2], which was proposed for the modelling of arteries but is equally applicable to tendons and ligaments, to show that the differing alignments of the fascicles within the ACL and PT have a significant effect on their stress-strain curves (see Figure 2).

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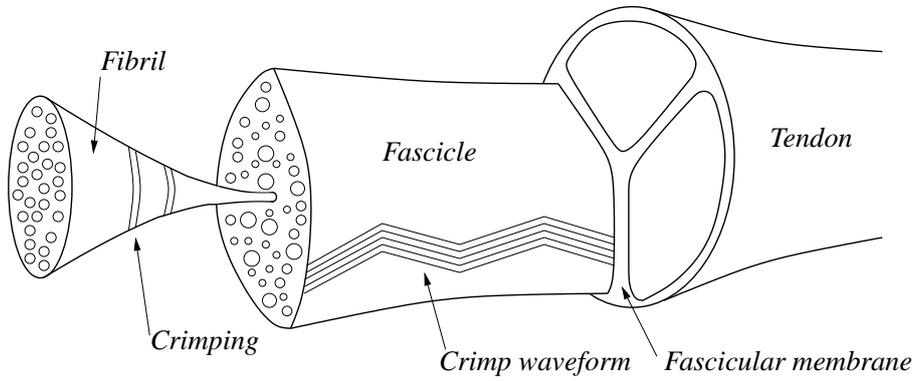


Figure 1: Tendon hierarchy (adapted from Kastelic *et al.* [3])

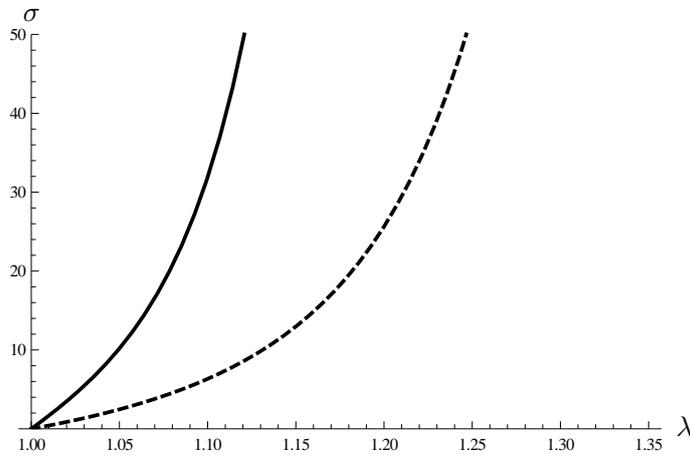


Figure 2: The effect of fibre alignment on the engineering stress  $\sigma$  as a function of the stretch  $\lambda$ . Solid line represents ligament/tendon with fibres perfectly aligned with its axis, dashed line represents ligament/tendon with fibres arranged helically making an angle of  $\pi/5$  with its axis.

## Failure Modeling of Human Femur

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A patient specific femoral bone fracture model is developed. Using Quantitative Computed Tomography (QCT) medical imaging technique the bone is scanned for its geometry as well as its spatial density distribution. Conventional techniques can convert the density data into stiffness and strength based on empirical definitions which yield isotropic properties for the bone. Models based on plastic deformation only can be fitted to bending experiments, but will subsequently lead to erroneous results in torsion loading. A shear type ductile failure is obtained and not the typical helical shape of brittle failure. Furthermore the conventional QCT technique results in the so-called Partial Volume Effect (PVE) which has a significant influence on the prediction of the initial fracture location. To counteract this effect a cortical shell is defined at the surface of the femoral neck with assumed properties based on the cortex. It is shown that it is essential to include these improvements in the model in order to improve the prediction of crack initiation and the final fracture pattern. Fracture of the bone is modeled using the finite element (FE) method and a smeared crack approach which make it possible to carry out a full femur fracture simulation efficiently. In this approach the crack is modeled in the framework of continuum mechanics. In the FE model the existence of the crack deteriorates the stiffness of the damaged element in a certain direction defined by the crack orientation. The failure and plasticity definitions are improved by including element size correction factors on parameters obtained by experiments. The model is implemented in a commercial FE software and validated by torsion experiments carried out on actual cadaveric femurs with metastatic lesions. A good correspondence of the fracture location and pattern as well as the load carrying capacity is obtained.

## Multiscale modeling of spider silk fiber mechanics

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Spider silk has attracted the attention of many scientists due to its combination of high strength, ductility, and toughness. Spider dragline silk fiber is a composite material largely composed of two structural proteins called crystalline and amorphous phase. The crystalline region consists of short polyalanine segments that form  $\beta$ -sheet nanocrystals, which provide stiffness, whereas the amorphous phase is formed from glycine-rich segments, which provides extensibility of the fibers. However, there remains a lot to learn regarding mechanical properties of each of these components of spider dragline silk fiber.

We present an overview of the mechanical properties of spider silks, and introduce a finite element model to study silk structure and material properties of each component in silk. For the continuum approximation of spider silk fiber, we obtained geometrical as well as material parameters from all atom simulations. Here, we focus on the finite element modeling of elastoplastic and viscoelastic behavior of the crystalline and the amorphous phases, respectively. This bottom-up computational approach helps to reveal the nanoscopic determinants for spider silk's macroscopic mechanical behavior. The ultimate goal of studying the properties of this amazing material is to find ways to design an artificial material with similar properties.

**Keywords:** Spider silk, finite element modeling, fiber model

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Session 21

Composite materials



## Formulation and physicochemical characterization of ultra-high performance fiber concrete based of sand dunes (UHPFC)

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Progress in the field of manufacturing of cement, adjuvant and the incorporation of other components (fibers and fines) in the composition of concrete with reduced diameter of the aggregates to assure maximum compactness material gave birth to a new generation of concrete (UHPC, fiber-reinforced concrete ultra-high performance). These concretes are more resistant and more compact and confer good durability compared to other types of concrete.

Generally fines used in the composition of UHPC is silica fume, the rarity of this material and its availability in all regions of Algeria has imposed on us to do our study on the possibility of using other types of fine such as electrostatic dust recovered during the production of clinker and sand dunes of Oued Souf (southern region of Algeria) rich in silica.

The addition of metallic fibers best tensile strength ensures ductile behavior of UHPC. The thermal treatment is an important factor to improve the characteristics of UHPC, so the determination of the best method of treatment in water or saturated air, the right temperature and time are the best part of this study.

In order to improve the mechanical properties of concrete, we are interested in the development of UHPC based on local raw materials and cheap (composed 42.5 Cement, Sand washed, Silica Sand Oued Souf, metallic fibers and an adjuvant type-reducer superplasticizer Tempo12 of SIKA). Obtaining a compact skeleton with high mechanical properties. The composition of UHPC is deferent of SCC by their strong cement content, these ultra-fine, his low W/C ratio and sensitivity to mixing.

During a thermal treatment at high temperature, the UHPC containing a certain percentage of fibers reaches maximum compressive stresses acting on the fibers as microcracking induced by high thermal gradients and mineralogical changes (104.34 MPa for compressive strength and 20.22 MPa for flexural strength).

Based on our results we can say that the compressive strength and flexural strength increased by introducing the fiber and using a thermal treatment.

**Keywords** : Sand of dunes, ultra-high performance fibers concrete (UHPFC), thermal treatment, mechanical properties.

## A Dynamic Theory for Laminated Thermoelastic Composites

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A higher order continuum model (CM) suitable for predicting the steady state and transient dynamic response of periodic laminated thermoelastic composites is developed. This study is an extension of the authors' earlier work [1] for elastic composites, by including the interactions between the thermal and mechanical effects in the context of generalized thermoelasticity. The formulation of CM is based on a higher order plate theory for anisotropic thermoelastic plates developed in Ref. [2]. This plate theory has an important property: it contains, as field variables, not only generalized variables (GV) representing the weighted averages of displacements, stresses, temperatures and fluxes, but also face variables (FV) defined on the faces of the plate. The CM developed in this study for periodic layered composites may be viewed as a mixture theory with higher order microstructure. Its formulation involves the use of the following steps: writing the equations of the above mentioned plate theory for each lamina; expressing the interface conditions in terms of FV's of the plate theory; applying smoothing operations to the field variables, which appear in the equations of the composite body.

The novelty of the proposed CM and its contribution to existing literature lie along the following lines: the lamina material is assumed to be triclinic with no material symmetry; the number of laminae in the unit cell of periodic layered composite is arbitrary; the orders of the theory and continuity conditions in the model are kept arbitrary; it accommodates all kind of deformation modes in the composite; dynamical and thermal effects are included in the formulation. The CM also contains inherently the Floquet wave conditions for the waves propagating in periodic layered composites. This property of the model enables it to predict correctly the filtering behavior of layered composites for the waves normal to layering.

The assessment of the CM, for isothermal case, is performed by comparing its prediction with the exact for the spectra of harmonic waves propagating in two-phase periodic composites. This spectral comparison criterion for the assessment may be justified on the basis that a dynamic model is described completely by its spectrum. It is found that the match between the exact and the approximate dispersion curves is good. Further assessments for thermoelastic composites will constitute the next stage of our study.

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**CM model for a periodic layered composite with two alternating laminae**

The CM model is based on a refined dynamic theory for triclinic anisotropic plates. The equations governing the linear dynamic thermoelastic behavior of the plate are:

equations of motion:  $\partial_j \tau_{ji} + b_i = \rho \ddot{u}_i$  ; constitutive equations:  $\tau_{ij} = C_{ijmn} \partial_m u_n - \beta_{ij} \theta$

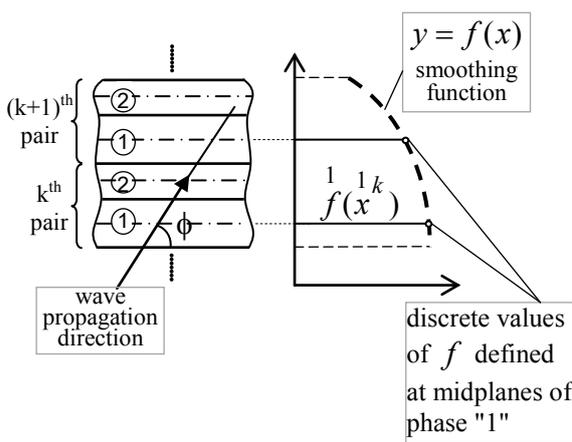
energy equation:  $-\partial_i q_i + r = c_v \dot{\theta} + T_0 \beta_{ij} \partial_i \dot{u}_j$ ; modified Fourier's law:  $\tau \dot{q}_i + q_i = -k_{ij} \partial_j \theta$

where  $\tau_{ij}$ : stresses,  $b_i$ : body forces,  $\rho$  : mass density  $u_i$ : displacements,  $C_{ijkl}$ : elastic coefficients,  $\beta_{ij}$ : thermal coefficients related to thermal expansion coefficients  $\alpha_{ij}$  by  $\beta_{ij} = C_{ijkl} \alpha_{kl}$  ,  $\theta$ : temperature deviation from reference temperature,  $q_i$ : heat flux,  $r$ : rate of heat generation per unit volume,  $c_v$  : specific heat per unit volume at constant deformation,  $T_0$ : absolute temperature of the reference configuration,  $\tau$ : retardation time for heat flux and  $k_{ij}$  : coefficients of heat conduction. To develop  $m^{th}$  order theory for thermoelastic plates, the operator  $L_n = 1/2h \times \int_{-h}^h (\bullet) \phi_n dx$  ( $n = 0 \dots m$ ) is applied to the equations given above, which yields the weighted integrated equations  $(\mathbf{M}_i^n, \mathbf{C}_{ij}^n, \mathbf{E}^n, \mathbf{T}_i^n, \mathbf{Z}_i^\mp, \mathbf{P}^\mp) = 0$  ( $n = 0 \dots m$ ) in symbolic form. The last two equations,  $(\mathbf{Z}_i^\mp, \mathbf{P}^\mp) = 0$ , describes the constitutive equations for FVs. In the development of the theory a set of distribution functions  $\phi_n(x)$  is chosen, where  $x$  is the distance measured along the midplane of the plate.

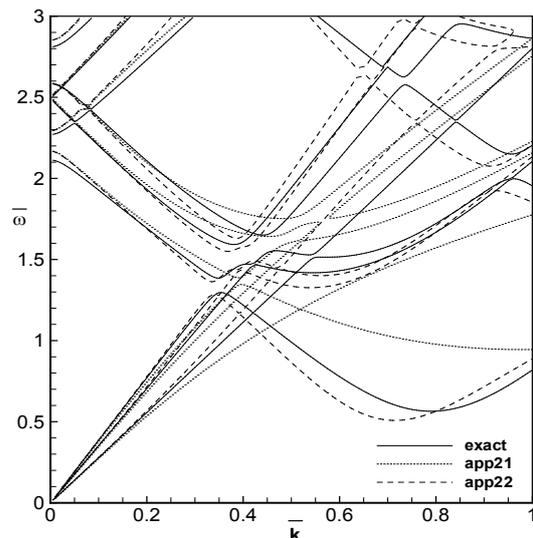
For establishing CM, a smoothing operation (SO) is employed to the discrete formulation, where field variables  $f(x^k)$  defined discretely at midplanes of laminae of each  $\alpha$  phase. After SO, discrete values are interpolated by a continuous function of  $x$ ,  $f(x)$  (see Fig. 1). The equations of CM obtained through SO take the form

$$(\mathbf{M}_i^\alpha, \mathbf{C}_{ij}^\alpha, \mathbf{E}^\alpha, \mathbf{T}_i^\alpha, \mathbf{Z}_i^\mp, \mathbf{P}^\mp) = 0 \quad (\alpha = 1, 2 ; n = 0 \dots m)$$

The CM is assessed by using the spectra of harmonic plane waves propagating in fiber reinforced layered composites with ply angles  $\theta = \mp 30^\circ$ . The dispersion curves are compared with the exact in Fig.2 for oblique waves with inclined propagating direction (see Fig.1) of  $\phi = 75^\circ$ .



**Fig.1** Layered composite and smoothing operation



**Fig.2** Comparison of spectra

## **Vibration Analysis of Cracked Laminated Glass Beam with Bolted Joint**

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In this study, in order to determine the load transfer behavior in the bolted joint connection, dynamic analyses of different laminated glass beams including two surface cracks are considered. For this purpose, both three different plastic interlayers (i.e., three types of PVB) and three different glass-lamina thicknesses are taken into account.

First, vibration tests are performed to present free vibration characteristics of the laminated glass beams under clamped-free boundary conditions. Experimental dynamic analyses consist of six parts: (I) Vibration analysis with no-crack and no-hole with a bolted joint, (II) Vibration analysis with a surface crack and no-hole with a bolted joint, (III) Vibration analysis with two surface cracks and no-hole with a bolted joint, (IV) Vibration analysis with no-crack and a hole with a bolted joint, (V) Vibration analysis with a surface crack and a hole with a bolted joint, (VI) Vibration analysis with two surface cracks and a hole with a bolted joint. For these experimental steps, an impact hammer with a force transducer is used to excite the uncracked or cracked composite beams through the selected points. After the excitation, the responses are obtained by an accelerometer. The vibration measurements are completed using a microprocessor-based data acquisition system and nCode GlyphWorks software.

Second, regarding to the reference [1], numerical prediction of resonant frequencies for the modal responses of the laminated glass beams is investigated by using general purpose finite element code MARC.

At last, effects of the plastic interlayer, thickness of the glass-lamina, surface crack size (i.e., length and depth) and location on the vibration characteristics/structural performances examined both experimentally and numerically. Numerical predictions of the finite element model proposed are good agreement with the experimental evaluations.

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## Stiffness of damaged micro-truss structures

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Micro-truss sandwich structures are well-known representatives of light-weight structures which combine high stiffness and strength with low density. These hybrid materials are able to fill gaps in the material properties space. The truss core structures are dominantly loaded in tension-compression therefore they are superior to the foam core structures which are dominantly loaded in bending [1,2]. However this superiority is sustained only for the perfect shaped core. The damaged trusses become loaded also in bending therefore their mechanical properties degrade down to the properties of the foam core structures. An evolution of stiffness degradation with the core damage is investigated using experiments, FEM and mechanical model.

The experiments are performed with the pyramidal core micro-truss structure made of aluminium alloy. The test specimens are loaded in compression to reach certain level of damage measured by the new core height after unloading [3]. Degradation of stiffness is measured by compression of the damaged core specimens. The experiments are performed for different temperatures (RT to 550°C).

The FEM model represents one unit cell of the pyramidal core consists of two sheets and four trusses. Structural parts are modelled by the shell elements (sheets) and the beam elements (trusses). The material properties are taken from the tensile tests. The mesh density and the nodes connections are set to fit the experimental observations. The FEM simulations reproduce the load-unload-reload pattern from the experiments.

Simple mechanical model for the damaged core stiffness evolution was developed. This model is based on calculation of stiffness of bended/buckled elasto-plastic beams under compressive loading. Using the arc approximation of the bended beam shape, it provides closed analytical solution for the problem of damaged core stiffness.

Presented study shows good agreement between the experimental observations and the theoretical predictions given by FEM and mechanical model. Stiffness of the micro-truss core structure degrades rapidly so it reaches stiffness of foam core at damage level about 10%.

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Fig. 1: a) Compression experiments of the pyramidal truss core structures. b) Finite element representation of the unit cell of pyramidal core. (Shell and beam profiles are rendered by Abaqus.)

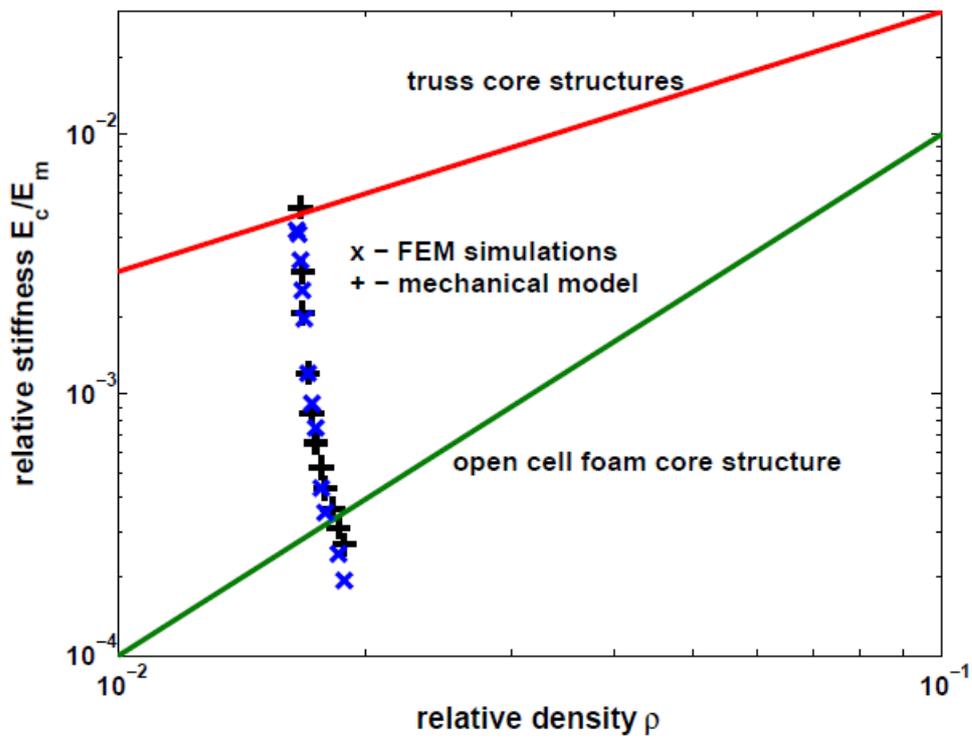


Fig. 2: Comparison of the degradation of damaged truss core stiffness modelled by FEM and developed mechanical model. Plot shows rapid stiffness decrease towards the cell foam structures. ( $E_c$  – core stiffness,  $E_m$  – material stiffness)

## **A gradient-enhanced scalar continuum damage model for fibre-reinforced materials at large strains**

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A non-local gradient-based damage formulation within a geometrically non-linear setting is presented. The elastic constitutive response at local material point level is governed by a hyperelastic strain energy which is additively composed by an isotropic matrix and an anisotropic fibre-reinforced material, respectively. The inelastic constitutive response is governed by a scalar  $1 - d$ -type damage formulation, where only the anisotropic elastic part is assumed to be affected by the damage. The local free energy function is enhanced by a gradient-term. This term essentially contains the referential gradient of the non-local damage variable which, itself, is introduced as a further independent variable. In order to guarantee the equivalence between the local and non-local damage variable, a penalisation term is incorporated within the free energy function. Based on the principle of minimum total potential energy, a coupled system of Euler-Lagrange equations (balance of linear momentum and balance of (non-)local damage) is obtained which has to be solved in weak form. The resulting coupled highly non-linear system of equations is symmetric and can conveniently be solved by a standard incremental-iterative Newton-Raphson-type solution scheme. Several three-dimensional displacement- and force-driven boundary value problems—partially motivated by biomechanical problems—highlight the mesh-objective characteristics and constitutive properties of the model and illustratively underline the capabilities of the formulation proposed.

## Multiscale modelling of the long term behaviour of textile reinforced composites

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The design process of novel hybrid structures made of textile reinforced composites with thermoplastic matrices requires an integrated simulation of the deformation behaviour as well as the prediction of effective properties which can be applied in a macroscopic structural analysis. Especially, knowledge on the macroscopically nonlinear material behaviour of the composite is needed for consistent lightweight design.

In this contribution a particular composite – with a polypropylene (PP) matrix and rovings consisting of PP and glass filaments as textile reinforcement – is analysed experimentally and numerically, paying special attention to long term phenomena such as creep and relaxation. The behaviour under compressive loading and large time periods is of particular interest in lightweight engineering when parts are assembled e.g. with bolts or screwed joints. For the PP, a viscoplastic material model based on an overstress formulation [1] has to be used to model its short term and long term behaviour. Focussing on time intervals larger than  $10^3$  seconds, this viscoplastic model can be reduced to a linear viscoelastic material model.

Due to the fact that the reinforcement structure is made of rovings which consist of glass filaments and PP matrix material at the microscopic scale, a viscoelastic homogenisation procedure is used to obtain a viscoelastic, homogeneous equivalent medium at the mesoscopic scale. The approach is based on HILL's principle, the equivalence of the stored stress power and it takes advantage of the elastic-viscoelastic correspondance principle in combination with a LAPLACE-CARSON transformation [2].

In order to use these material models for the PP matrix and the roving in a numerical simulation of the composite, it is necessary to create a proper geometric model of the reinforcement structure at the mesoscopic scale. Therefore, two strategies are followed. The first one uses individual pictures of a computer tomographic scan (CT scan) to obtain the dimensions of the rovings and the layers of the composite. An idealized mesoscopic representative volume element is build by means of these values. The second strategy uses directly the information of the full CT scan and proper segmentation algorithms to create a more realistic model of the reinforcement structure. Long term creep and relaxation simulations are carried out and both approaches are compared to experimental data.

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## A numerical model for prediction of the uncertainties in long fibre reinforced thermoplastics

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Long fibre reinforced composite materials with thermoplastic matrix are a new class of composite material suitable especially for industrial scale applications. They combine the advantages of short fibre reinforced plastics and infinite fibre reinforced materials. Due to the limited fibre length, LFT materials may be processed by many standard technologies for thermoplastic materials. In comparison to short fibre reinforced materials, the increased fibre length results in superior properties. However, for the numerical analysis of components in the industrial design process, LFT material suffer from their disordered irregular microstructure which causes a distinct uncertainty in the macroscopic material and thus the structural response of components consisting thereof.

The present study is concerned with the development of a numerical method for prediction of the uncertainty in the effective material properties of structures and components consisting of LFT materials. Based on a micromechanical analysis of the single fibre problem using the standard rules of mixture, a stochastic model for LFT materials is proposed. In this model, the local fibre orientation distribution and the local relative density are considered as stochastic variables with prescribed probability distributions. The probability distributions may be different at different positions within the structural component due to different process parameters such as flow direction and flow distance at individual positions. By a repeated determination of the material properties for predefined sets of the random variables in conjunction with the individual probability of occurrence for the analysed cases in the (hyper)-space of the random variables, the probability distributions for the macroscopic material properties are obtained as a function of the microstructural uncertainties. The space of the random variables is discretized for this purpose in order to limit the number of necessary computations for individual sets of the stochastic variables.

The results of the probabilistic homogenization procedure can be employed as input for a stochastic finite element analysis on structural level in order to assess the uncertainties in the structural response of the respective component.

**Acknowledgments** This work has been financially supported by the Deutsche Forschungsgemeinschaft (DFG) under Grant No. HO1852/6-2.

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## Multi-scale 3D Image Based Modelling of Woven Composite

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Detailed thermal and mechanical finite element analyses of woven composites are computationally challenging due to their heterogeneous nature and geometrical complexity. Due to that researchers have been developing models based on idealisations of the composite microstructure. Most of the time, these idealisations lead to inaccurate and invalid results. However, the fast and rapid growth in computer science and image processing technologies has resulted in a new technique of modelling complex material such as woven composites. In this technique, which is called image based modelling technique, a detailed 3-D model of a material is created from high resolution images, mainly tomographic images of the material microstructure. This conversion of images involves two main steps. Firstly, image processing or image segmentation where the different phases of the material are separated by setting a suitable threshold to the grey scale of the raw images[1]. The second step involves the generation of the finite element mesh. This technique has been used successfully to model different types of composites[2-3].

In this study, image based modelling technique has been used to create two finite element three-dimensional models at different length scales. The first model was generated from SEM micrograph of the carbon tow cross section whereas the second model was derived from high resolution x-ray tomographic images of the composite. These models were used to evaluate the thermal and mechanical properties of a 2-D twill weave carbon/carbon composite. The modelling results were in excellent agreement with the experimental results

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## Elastoplastic behaviour of interpenetrating phase composites: Combining mechanics of cellular solids with mean-field theory

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Interpenetrating phase composites (IPCs) are a class of composites in which both the matrix and reinforcing phases form a continuous intertwined three-dimensional network. The continuity of the reinforcing phase has been envisioned to yield unique thermomechanical properties when compared to their discontinuous counterparts such as the fiber/particulate reinforced composites [1]. The majority of literature on IPCs focuses on elastic response or fracture toughness. However, the role of reinforcing phase connectivity in determining the overall mechanical behaviour has not been fully understood. The existing literature attempts to explain the strength of an IPC in terms of (i) direct strengthening due to load partitioning as a result of interphase constraints and (ii) indirect strengthening in the matrix caused by dislocations interacting with the reinforcing phase and with other dislocations (e.g. see [3]). Indirect and direct strengthening are hard to distinguish experimentally. Using polymer infiltrated nanoporous gold (np-Au) composites, in which indirect strengthening is believed to be absent, we show that the open-cell foam nature of the reinforcing phase in its stand-alone configuration will alter the load partitioning in an IPC when compared to a discontinuously reinforced composite, leading to a greater direct strengthening.

In this study, we compare micromechanical tests with incremental mean-field calculations and full-scale finite element simulations on polymer-infiltrated and uninfiltrated np-Au. Uniaxial compression simulations have been carried out using both real np-Au structure (reconstructed by nanotomography [2]) and regular unit cell-based IPCs, see Fig.2 (electronic version only). We have also compared the strength of Al-foam based composites from Periasamy et al. [4] in a similar manner. These observations suggest that the elastoplastic response of IPCs is a combination of the behaviour of the reinforcing phase treated as an open-cell foam and the composite behaviour given by the classical self-consistent theory.

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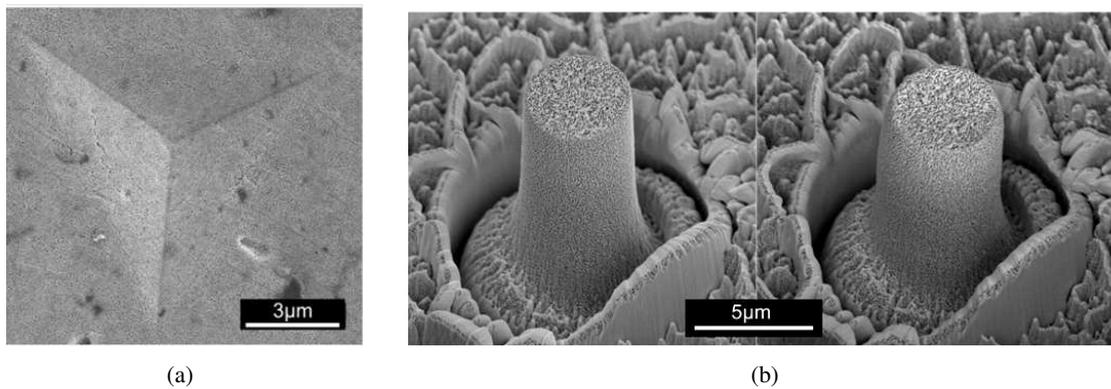


Figure 1: (a) A Berkovich indentation in the surface of np-Au showing the deformed region under the nanoindenter. (b) Undeformed (left figure) and deformed (right figure) geometries of np-Au/epoxy resin nanocomposite micropillars tested in compression.

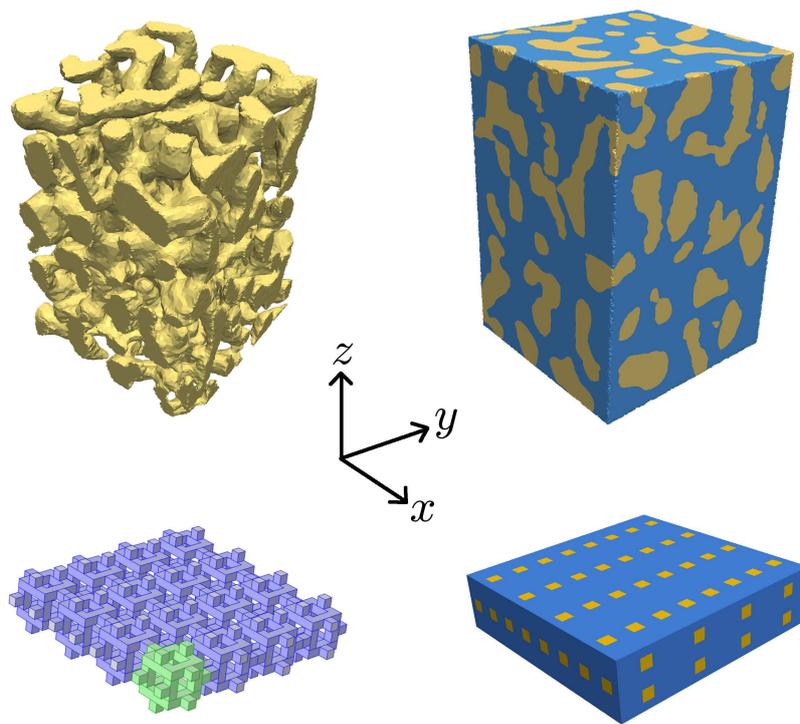


Figure 2: Visualization of a section of the reconstructed np-Au structure ( $500 \text{ nm} \times 500 \text{ nm} \times 750 \text{ nm}$ ) from nanotomography (top left) and the corresponding composite (top right) and an array of  $4 \times 4 \times 1$  Gibson and Ashby type unit cells (bottom left) and the corresponding composite. One unit cell is shown highlighted in the unit cell array.

Session 22

Aeronautic materials



## On Some Analytical Methods for Calculating of Cusped Prismatic Shells and Beams

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Cusped plates and beams, on the one hand, are very important details from the practical point of view, such plates and beams are often encountered in spatial structures with partly fixed edges, e.g., stadium ceilings, aircraft wings, submarine wings etc., in machine-tool design, as in cutting-machines, planning-machines, in astronautics, turbines, and in many other areas of engineering (e.g., dams); on the other hand, their theoretical analysis and calculation are mathematically connected with the study of very difficult problems for degenerate partial differential equations which are not covered by the general theory for degenerate partial differential equations (see, e.g., [1]). Some satisfactory results are achieved in this direction in the case of Lipschitz domains but in the case of non-Lipschitz domains there are a lot of open problems. To investigate such open problems are the main part of the the present talk. To this end there are used function-analytic, approximate and special methods (suitable to problems peculiarities). As results, boundary value problems in the zero approximation for I.Vekuas hierarchical models (for hierarchical models see, e.g., [1-2]) of cusped plates and beams in case of 3-D non-Lipschitz domains is investigated. Mathematically the above problems lead to the investigation of systems of second order partial differential equations with variable coefficients (in particular, with order degeneration). For such systems the issues of existence and uniqueness of the solutions of the corresponding boundary value problems are studied, in the suitable spaces.

**Acknowledgments** The present work was supported by the Shota Rustaveli National Science Foundation within the framework of the project DI/13/5-106/12.

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## **Biaxial Deformation Behaviour of AZ31 Magnesium Alloy: Crystal-Plasticity-Based Prediction and Experimental Validation**

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Motivated by the growing demand for light weight materials, research on magnesium and its alloys has been getting more attention. Magnesium is the lightest metal in use for the production of structural components in the automotive and aircraft industry. Despite the high strength-to-weight ratio, the application of wrought magnesium (i.e. sheets and extruded profiles) for light weight structures is limited. This limitation for the structural application of magnesium sheets is correlated with its pronounced anisotropy, the tension-compression asymmetry, its comparably poor formability as well as its low fracture strain, especially at room temperature. These characteristics are directly related to the microstructure of the material: its texture and the active deformation mechanisms. Understanding of this interplay is essential for the development of constitutive laws aiming e.g. on sheet metal forming processes.

Plastic deformation of the commercial magnesium sheet alloy AZ31 under monotonic loadings has been investigated by means of mechanical tests and numerical simulations. Additionally to the commonly used uniaxial test two complementary mechanical tests have been performed: a biaxial test using cruciform specimens and a hydraulic bulge test. Both tests lead to consistent results and evidence the differential strain hardening character of the considered material. A polycrystalline aggregate has been generated from measured texture data. Simulations using the visco-plastic self-consistent (VPSC) scheme indicate the primary role of pyramidal slip in equibiaxial tension. Contours of equal plastic work have been generated using a methodology based on probing the aggregate in space of principal strains. The contours were compared with respective tests. Hardening parameters have been fitted in order to capture initial yield and evolution of iso-work contours. Limitations of the numerical framework's predictive capability as well as directions for parameter identification of phenomenological yield surfaces are formulated.

## Numerical Study Of Closure Models Applied To Turbine Blade Film Cooling

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Accurate prediction of turbine blade heat transfer, so crucial to the efficient design of blade cooling schemes, still remains important work in the turbo machinery area. The main cause for the lack of agreement with experimental data in such predictions is usually cited to be the turbulence modelling. This is due to a complex flow phenomenon which is encountered in turbine passage and to the interaction of the injection with the aerodynamic curved surface flow around the blades. Stagnation flow heat transfer, heat transfer in the presence of steep pressure gradients both favorable and adverse, free stream turbulence, high Mach number, blowing rate ratio and three-dimensional effects are only some of the items in a long list of phenomena present in these passages.

The experimental flow field and heat transfer measurements are available for the flat plate at many axial locations for fixed inlet Mach number, Reynolds number, inlet turbulence intensity as well as the inlet boundary layer thickness. By far the most popular turbulence models utilized today for flow and heat transfer calculations are the high and low Reynolds number two-equations eddy viscosity models. The  $k-\epsilon/k-\omega$  are the most used models. These models often offer a good balance between complexity and accuracy.

The ability to predict transition to turbulence which is often present on turbine blades and the ability to integrate to the walls are other reasons for their widely using.

In this paper, numerical simulations have been performed using the FLUENT software which is an explicit multigrid finite volume solver, with a  $k-\epsilon$ , RSM and SST (shear stress transport) turbulence models. The SST model encompasses both the  $k-\omega$  model (Wilcox, 1988) activated in the near-wall region and the standard  $k-\epsilon$  model (Jones and Launder, 1973) activated in the outer wake region and in the free shear layers. The single row of jets into cross compressible flow interaction is investigated. The jet-to-cross-stream velocity ratio is 0,6 and the Mach number is 0,8. Components of mean and turbulent velocities and the mean temperature are compared with experimental results at upstream and downstream locations in the (x,y) plane injection. The velocity is non dimensionalized with the cross-stream velocity, while the temperature is represented by the non dimensional local temperature in film.

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## Modelling of grain refinement using a three-scale crystal plasticity model

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For advanced materials nowadays used in automotive and aeronautic industry, such as metal-matrix composites or metals and alloys of high specific strength, novel techniques of metal forming are often used. These processes are usually characterized by multiple (e.g. ECAP, cf. [1]) or continuous (e.g. KOBO [2]) strain path changes enhancing material ductility and leading to substantial grain refinement in polycrystalline materials.

Predictive modelling of grain refinement phenomena on complex strain paths is still at an early stage. There exist energy minimization approaches that are applied to model microstructure evolution in single crystals and phenomenological approaches providing the evolution of selected microstructural parameters on the macroscopic level, cf. [5]. This work is devoted to development of a micromechanical model of grain refinement formulated within the crystal plasticity framework.

Three scales are considered in the model. It is assumed that a single crystallite within the polycrystalline representative volume element (RVE) is initially subdivided into several subdomains with the orientations slightly mis-oriented with respect to the nominal orientation of the crystallite. A viscoplastic model of crystal plasticity model is adopted for each subdomain deforming by slip and twinning [3]. As a scale transition rule between the domains and the crystallites, a visco-plastic self-consistent scheme (VPSC) is used [4], while the classical Taylor model is used as an averaging scheme between the crystallite level and the macroscopic level. During plastic deformation, e.g. on a complex non-proportional strain path, an evolving mis-orientation of each subdomain is determined with respect to a specially defined mean orientation of the multiple subdomains forming the corresponding single crystallite. This mis-orientation is then assumed to be an indicator of grain refinement that depends on the strain path, initial grain orientation, and the related activity of different deformation modes. It is also expected that the model should deliver better texture predictions than the available two-scale models.

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## Fatigue life modelling of high temperature nickel base superalloy in isothermal and non isothermal conditions

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Lifetime prediction of turbine blades is of great interest for engine manufacturers in order to enhance the engine performances or to optimize the inspection intervals. To perform accurate lifetime estimations, the first step of the approach is to propose a constitutive model able to simulate properly the mechanical behavior of the representative volume element [1]. In a second step, it is necessary to consider fatigue and creep interaction under complex anisothermal loadings. The originality of this work ensues from the rich available experimental database which demonstrates the high capability of the proposed model to reproduce a very large set of experimental data (both isothermal and anisothermal conditions) and, then, the sturdiness of the model for lifetime assessment.

A stress based continuous damage prediction model developed in the Continuum Damage Mechanics framework is proposed [2]. Two damage variables are introduced in this creep-fatigue interaction model.  $D_c$  is related to creep and  $D_f$  to fatigue damage. Creep relation generalises Kachanov-Rabotnov's equation. Using a reduced stress and a Taira's [3] type equivalent temperature procedure, the non linear fatigue model derived from the one proposed by Chaboche et al. [2] can be used to compute complex anisothermal cycles. The writing of the equations and the integration procedure of the fatigue model in anisothermal conditions will be tackled in this presentation. Although the damage relations are defined for the general anisotropic multiaxial case, only the [001] crystallographic direction will be considered here.

The experimental database includes more than one thousand fatigue and creep tests performed from 20°C up to 1150°C. Many different fatigue tests are available with various stress or strain ratios, various signal forms and various frequencies from 0,05Hz to 100Hz.

The way to achieve properly the calibration of such a model, in isothermal conditions, will be discussed and illustrated with some results. Once the model is fully calibrated, it becomes possible to predict the lifetime of the representative volume element, over the whole temperature range [20°C-1200°C], for complex anisothermal thermomechanical tests which are more representative of turbine blade service conditions.

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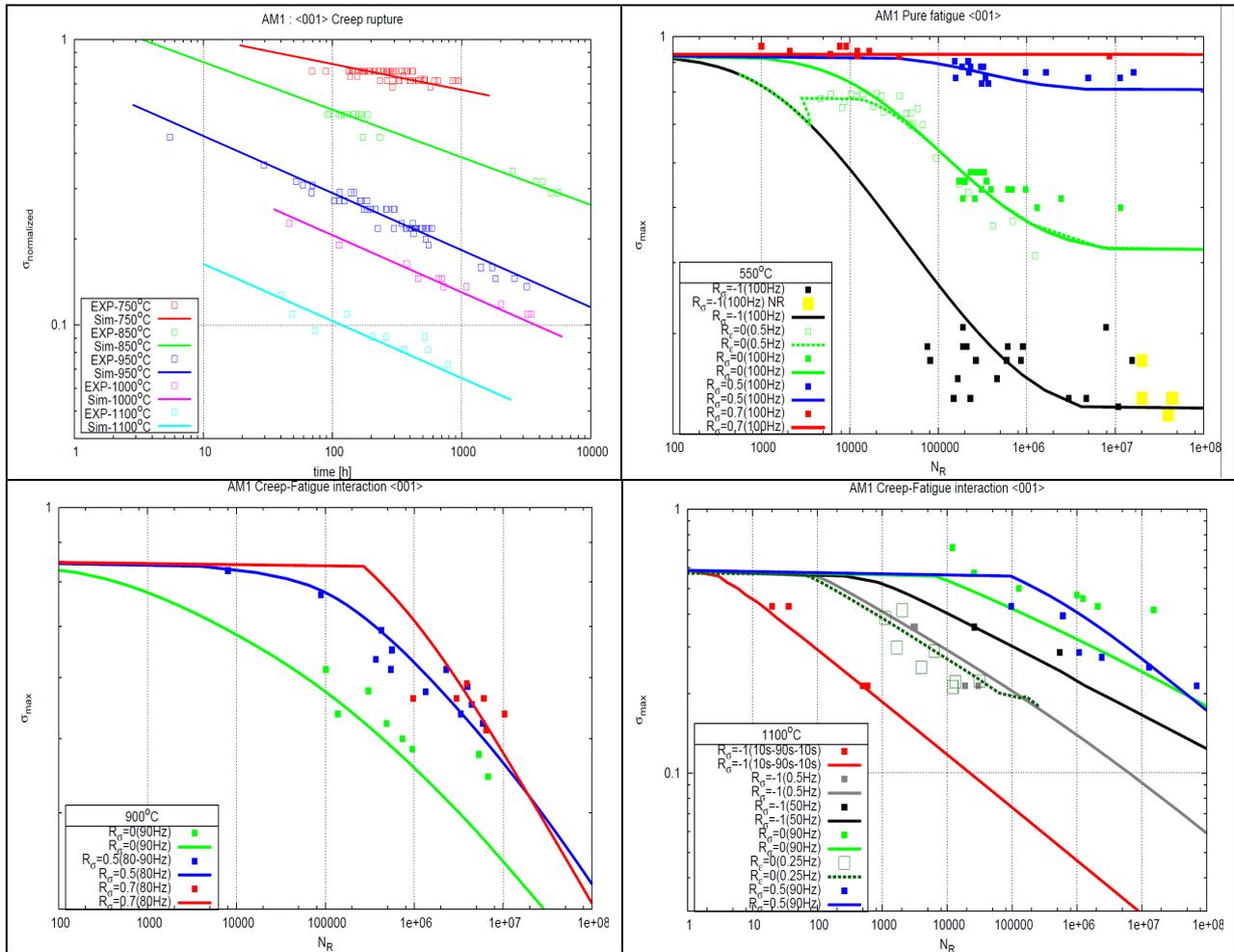


Figure 1.- Comparison between experimental results and simulations for various temperature in isothermal conditions.

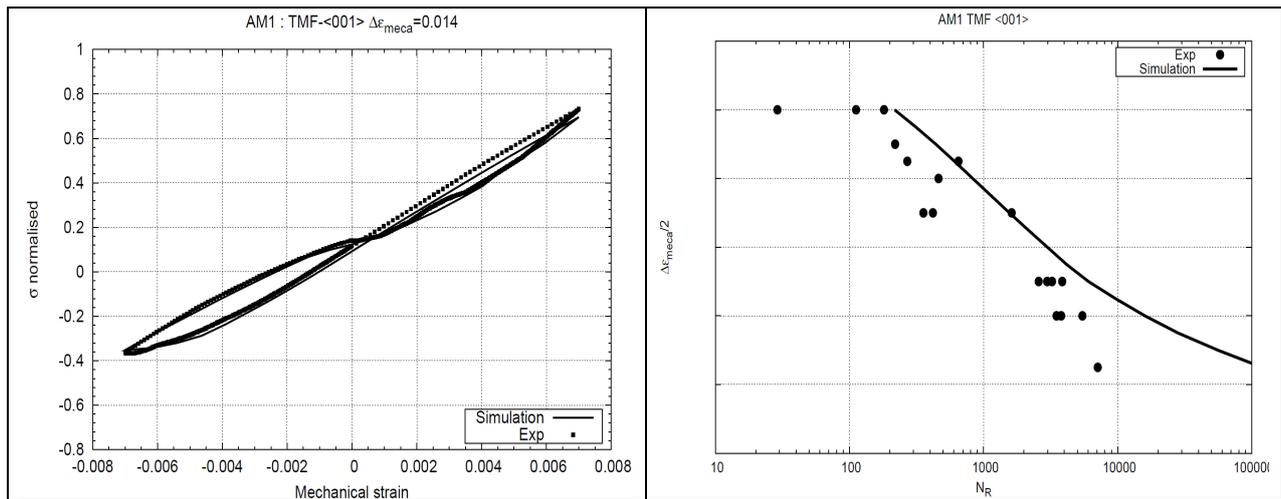


Figure 2.- Comparison between experimental results and simulations for complex anisothermal thermomechanical tests performed over the whole temperature range [20°C-1200°C].  
On the left: Constitutive behaviour. On the right: Lifetime predictions.

## The Compressive Strength of Ceramic Open-Cell Foams with the Variability of Cell Sizes

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New aeronautic materials are obtained by liquid metal infiltration into a ceramic foam, called a preform. Ceramic preforms are produced by a new method of manufacturing of porous ceramics foams known as gelcasting. Porous ceramics fabricated by this method is characterized by a continuous network of spherical cells interconnected by circular windows. The open porosity due to the presence of windows creates good hydro-dynamical properties for liquid metals infiltration. For better understanding mechanical properties of such composites a numerical model of ceramic foam is needed, see e. g. ref. [1-4].

Geometry of ceramic foams can be generated in two steps. First, the coordinates of the center point of the spherical bubbles and its diameter are produced by PYTHON scripts. The diameters of spherical bubbles were estimated from microtomography and scanning electron microscopy images. On the other hand, the coordinates of the center points are determined in such a way that the bubbles have to intersect with each other. Finally, the intersecting bubbles are subtracted from the bulk block of any shape. Using this information, numerical foam model was proposed (Fig. 1) and good agreement between numerical model and real foam structure from microtomography was obtained.

In this work we present a numerical model of real foam of alumina with different cell sizes and discuss its mechanical properties using several examples. The numerical simulations of uniaxial compression test have been performed. The bottom surface of the sample was full constrained and the top surface of this sample was moved parallel to the z- axis. The force was resulted from the final step of displacement in simulation. As a result the compressive strength of the investigated foams with porosities changing from 60 to 95 % were determined.

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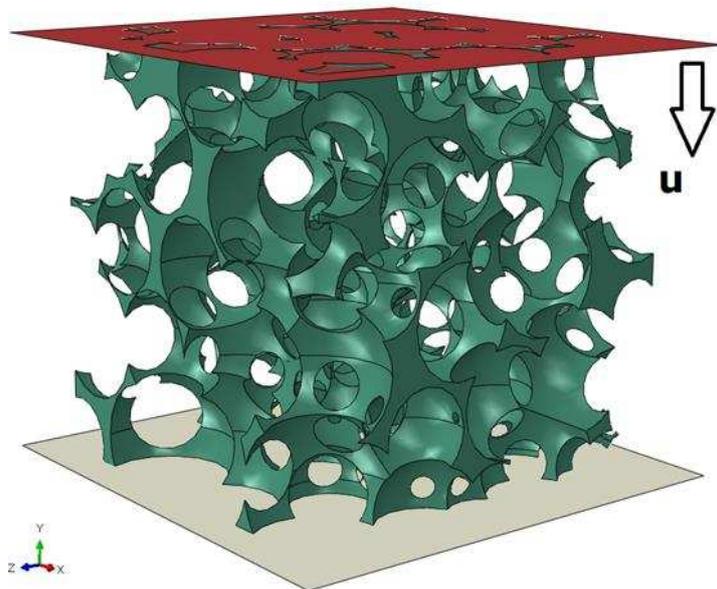


Fig.1. Example of numerical foam structure used in numerical simulations of the compression tests with 90 % porosity.

## A Classical Finite Element Beam for Free Vibration Analysis of a Model of Composite Light Aircrafts

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In the present work, the finite element method is adopted for modal analysis of a model of a light aircrafts in composite Timoshenko beams. We are interest in this study to flexural - torsion coupling due to the fiber orientation of the laminate composite materials. The plane is modeled by spatial beam elements, where the fuselage is a long beam of isotropic constant section, wings and empennage (horizontal and vertical) are modeled by of composite Timoshenko beams elements (bending-torsion coupling).

The Lagrange Principle is adopted to determine the mass and stiffness matrices elementary, where the coupling terms are presented in the last. After assembling in global mass and global stiffness matrices all elements of the structure (fuselage, wings and empennage) and the introduction of the boundary conditions, we use a numerical method to determine the natural frequencies and associated modes. The results obtained are compared with other methods for cantilever Timoshenko beams reported by other authors [1] and other analytical methods (dynamic stiffness method).

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## Fatigue damage modelling in layered material system

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The modelling of the low cycle fatigue of layered materials based on the continuum mechanics is presented. The fatigue damage model takes into account the mechanical part of load under constant service temperature. The considered material is consisting of homogeneous layers of various reinforcement fraction and consequently various material properties of each layer. The modified Tamura-Tomota-Ozawa rule of mixture, (TTO) [1] is applied to determine the material properties of each layer. It is assumed that the fatigue damage of metal matrix composites is strongly influenced by the inelastic deformation in metallic matrix. Hence, this feature is taken into account in the constitutive equations of LCF damage model. The combined linear isotropic/kinematic hardening model is adopted. The scalar damage parameter associated with the plastic energy dissipation is used to describe cyclic material degradation under mechanical loading. This energy based approach is a common technique in cyclic damage calculation since Inglis presented the report [2] on the relation between hysteresis energy and fatigue behaviour. Since then many studies of the energy methods and several failure criteria based on strain energy were made. It has been shown that an energy-based damage parameter can unify the damage caused by different types of loading such as thermal cycling, creep, and fatigue. Mean stress and multiaxial loads can be also incorporated into the energy-based multiaxial fatigue damage models based on strain energy. The fatigue damage model presented in this paper is applied to fatigue damage analysis of cooling channel of thruster used in space shuttles and rockets. It is assumed that the delamination of layers would not be possible. The cooling channel is subjected simultaneously to the thermal and mechanical loading. The mechanical cyclic loading is considered at constant maximum high temperature, 700<sup>o</sup>K. The data given by Andrews and Armstrong [3] are used in comparison of the fatigue damage process under mechanical cyclic loading and under the constant high temperature (700<sup>o</sup>K) for the material of CuAg3Zr0.5 used currently in thruster and the new layered material of Al<sub>2</sub>O<sub>3</sub>-Cu.

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Session 23

Poster session



# Wear behaviour 3D AFM roughness of sintered nanomaterials produced by hot isostatic pressing (HIP)

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**Keywords:** Powder, Characterization, Wear resistance, Wear, Surfaces, Surface states, Roughness,

## Abstract

We propose an experimental study of the surface to dry and analysis of the evolution parameters roughness. The simplified model was proposed to predict the metrological parameters in the contact area of the deformed surface. The model is based on the analysis of the topography 3D of the deformed surface.

The hot isostatic pressing (HIP) is the only process that will develop fully dense samples, From Fe,Cr,Mo,Ni,Ti,W powder. This sample is hot pressed at 1500°C under 150Mpa of argon pressure. Moreover, the grain size of the consolidated samples was analyzed by SEM, ABSD and optical microscopy.

Study aims to characterize the topography of sintered materials obtained by wear tests. Therefore it is interesting initially in the evolution of wear for the loads applied and to characterize the different roughness emerging from 3D AFM observations.

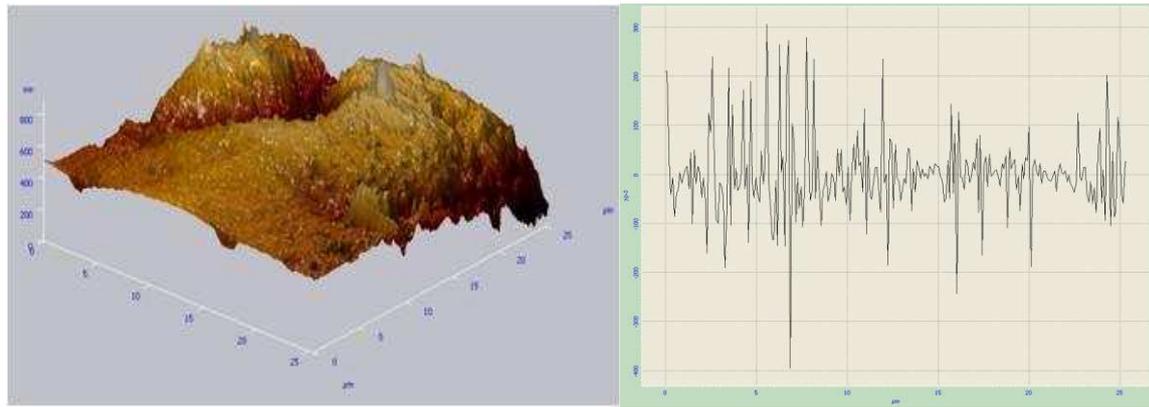
Experimental and theoretical research on the topography changes during dry contact deformation was carried out in [1], [2], [3] and [4], providing results that demonstrate the persistent nature of roughness asperities even under high loading when bulk plastic deformation appears. Most theoretical investigations of the problem have been based on a simplified model neglecting the statistical distribution of asperities on the real surface, [5]. In [6] used test and 3D measurement of surface topography in order to investigate its frictional behaviour. The mechanism of contact of a rigid plane with a rough surface in the presence of a lubricant is different than in the case of dry contact.

The topography of the samples was measured both in initial undeformed and in the deformed state after removal of the load. In these states, however, a change of the shape of the samples when compared to the initial state was observed. Thus, prior to the determination of roughness parameters of the deformed surfaces, their curvature was removed using a filtration procedure.

The essential differences in surface topography of samples loaded in dry condition are confirmed in the analysis of roughness parameter evolution. The following 3D parameters were considered:

In the unloaded state, flattened asperities can be observed on the deformed surface Fig 1.a. The real contact area corresponding to the maximal load attained in the surface compression experiment can be identified from measurement of the deformed roughness after unloading.

The identification of the real contact area was carried out using a special algorithm based on single profile analysis. The single, randomly selected profiles, i.e., their coordinate's  $x_i$ ,  $z_i$ , were extracted from the measured topography of the deformed surface. It should be noted that the profiles obtained in this way have a common reference level Fig 1.b. The selected profiles also have the same direction, which, in the case of anisotropic surfaces (turning, grinding) should be perpendicular to the direction of the movement of the machining tool.



(a)

(b)

Figure 1. a)- measurement 3D of surface topography in order to investigate its frictional behaviour. b) Profile corresponding to real area

The proposed model was applied to analyze a wear of four kinds of rough surfaces. The predicted values were compared with experimental results Table 1.

Max	Min	Peak-to-peak, Ry	Ten point height, Rz
577,339 nm	430,073 nm	147,266 nm	506,714 nm
Average	Average Roughness, Ra	Root-mean-square, Rq	Dispersion
510,674 nm	28,7048 nm	511,831	34,3946 nm
Surface skewness, Rsk	Coefficient of kurtosis, Rka	Entropy	Redundance
-0,157453	-0,696865	7,88768	-0,0936811
-0,157453	-0,696865	7,88768	-0,0936811

Table1. Roughness parameters of the deformed surfaces of the samples figure 1.a

The wear and surface roughness based on the parameters of dry friction tests were measured. This study suggested the optimal parameters of chemical composition, and analysis of the effects of alloying elements on surface roughness and wear in the process dry friction tests.

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## **Finite element analysis of the mechanical behaviour of the different cemented hip femoral prostheses**

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The designs of cemented hip femoral stems have an influence on both the quality of the metal–bone cement contact and the failure rate of the cement mantle. Finite element stress technique has been used to optimize both design and material selection in load-bearing components in artificial hip joints based on the static load analysis, by selecting the peak load during the patient activity. In this study, two stem shapes (CeraVer Osteal and Charnley stems) for total hip arthroplasty (THA) were modelled. Static behaviour of these designed stem shapes were analyzed using commercial finite element analysis code ABAQUS. Linear elastic analysis is adapted; Von Mises stress, normal stress and shear stress are the criterions that are of concern. Results show that, the stresses distribution in the femoral arthroplasty components depends on the material and design of the stem. In addition, the cement-bone and cement-stem interfaces seem to be crucial for the success of the hip replacement, hip prosthesis with Charnley stem induces the more stresses on the interfaces cement.

**Keywords:** Biomechanics, THA, Bone cement, Finite element, Interface, Stress

## **Effect of the Human activities on the mechanical behavior of the total hip arthroplasty**

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The PMMA is the unique material used currently for fixing prosthesis in bone in cemented arthroplasty. Mechanical properties of bone cements are of key importance for a successful surgery and further use of the joint as well as its behavior during complex load which appears during patient's activity. In addition, the distributions of the mechanical properties of the cement-bone and cement-metal interfaces affected by the non-homogeneous distributions. Forces applied to the implant due to human activities generate dynamic stresses varying in time and resulting in the fatigue failure of implant material. In this study, the three-dimensional finite element method is used to analyze the distribution stresses on the hip prosthesis components (stem, cement mantle and bone). Dynamic analyses were performed under normal walking, up stairs, down stairs, standing up, and sitting down loads.

**Keywords:** Biomechanics, prosthesis, Cement mantle, Finite element, Dynamic, Stress

## Hardening Laws in Multilevel Crystal Plasticity Models and Its Influence on the Macro Effects of Complex Cyclic Loading and Damage Accumulation

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Changes in the physical and mechanical properties of the specimen during deformation in complex cyclic path is a consequence of a substantial restructuring of the micro- and mesostructure of the material, mainly - due to a significant evolution of the dislocation (wider - defective) material structure. Describing such processes is impossible without studying and establishing appropriate mathematical models that explicitly take into account the physical root causes of the microstructure evolution of the material under large deformations and can be applicable to the description of damage accumulation and fracture processes. The foregoing explains the considerable attention in crystal plasticity, which is paid to the modification of hardening laws.

The goal is to study the effects produced by polycrystalline material under proportional and non-proportional cyclic loading (and the transition from one to another type of loading) as a consequence of changes occurring at the dislocation structure in the process of loading, and attempt to modify the hardening laws so that they can be transparently physically describe these changes and effects. In particular, there is attempt to justify and describe the known experimental effects, such as the dependence of additional cyclic hardening of the disproportionality of loading, cyclic softening the transition from non-proportional to proportional loading, transverse hardening, which manifests after proportional loading in one direction is followed by proportional loading in the other direction.

We received both general and particular form of hardening laws of mono- and polycrystalline allows describing the formation and destruction of dislocation barriers, the annihilation of dislocations as well as additional hardening, resulting from the interaction of intragranular and grain boundary dislocations. Hardening is divided into "non-oriented" and "oriented". The first type describes the hardening regardless of the direction of deformation (under this definition, processes such as the formation of the intersection of dislocations, plaits, braids, dislocation barriers), and a hardening increases the critical shear stress at once on many slip systems (or even all at once). The second type is related to the accumulation of elastic energy to "pursed dislocations" (at different barrier) and this energy may be (fully or partially) released at the change the direction of deformation. The analysis of the possible mechanisms of interaction between carriers and the plastic deformation of the crystal lattice defects is executed; hardening laws that discovers a good agreement with experimental data are proposed. We also introduce the parameters characterizing the accumulation of damage and formulate fracture criterion using methodology of multilevel modeling.

**Acknowledgments** This work was supported by RFBR (grants №12-08-33082-mol\_a\_ved, №12-01-31094-mol\_a, №13-01-00242-a, №13-01-96005-r\_ural\_a), the President Grants №MK-3989.2012.1, №MK-390.2013.1, Federal Target Program "Scientific and scientific-pedagogical personnel of innovative Russia in 2009 - 2013 years" (activity 1.2.2, Agreement 14.B37.21.0382).

## Biophysical examination of the skin and subcutaneous tissues

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The fundamental role of human skin is to protect the body from invasion by external factors. The skin could prevent biological and chemical invasions of the body, which include circulating cells of the innate immune system. Furthermore, protection from physical invasions—such as mechanical force and thermo injuries—are also important to maintain the homeostasis of the human body. Skin consists of 3 layers, which include the epidermis, dermis, and subcutaneous tissue. Skin covers most of the body's surface, except for some "holes such as oral cavity". Thus, the physical barrier that skin provides is crucial to protect the human musculoskeletal system and internal organs. The physical properties of skin have been measured using several devices [1]. In this study, the authors measured the mechanical properties of the skin by dynamic indentation. This study noted that the measurement of these mechanical properties by indentation is not well correlated with that by suction [2]. Furthermore, they also reported the aging-associated alteration of mechanical properties of the skin [3]. The Cutemeter™ has been used to measure the viscoelasticity of skin. Additionally, we have recently established a novel method to measure the viscoelasticity of skin using a rheometer (AR instrument, AR 550).

Using this method, skin is treated as a complex of different materials. The skin surface at the bottom of an appendage is immobilized so that deformity is only obtained by the external force generated from the upper probe. From the results shown in Figure 6, viscoelasticity of skin (and subcutaneous tissues) was estimated to be approximately 30 kPa. This data was not influenced by muscle contraction, thus indicating that the origin of the physical properties of skin could be the fascia [4].

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## **A nanoscale simulation study of the structural and elastic properties of spherocobaltite (CoCO<sub>3</sub>)**

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The study of structural and mechanical properties of carbonate rock is an interesting subject in engineering and their different applications. The results presented in this study were simulated by atomistic simulation based on energy minimization technique [1]. We have using an interatomic interactions potential to describe the crystal structure of spherocobaltite. Spherocobaltite is a cobalt carbonate with formula the CoCO<sub>3</sub>. It crystallizes in the rhombohedral lattice system [2].

At first, I will focus on the structural properties of spherocobaltite mineral. The elastic properties have been calculated, including the elastic constants, bulk modulus, shear modulus, the S- and P-wave velocities. The second part of this presentation, the pressure effect will be studied on the structural and elastic properties of CoCO<sub>3</sub> under high-pressure from 0 MPa to 500 MPa.

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## Damping effect observed in the internal friction behavior of a single crystal alloy Al – (20%at.Ag)

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The aim of this study is to highlight the origin of damping effect observed in internal friction behavior on aluminum single crystal alloy Al - (20% at. Ag).

After quench these alloys exhibit generally a precipitation hardening represented by the following sequences:

$\alpha$  (Supersaturated Solid Solution)  $\rightarrow$  GP (Guinier-Preston zones)  $\rightarrow \gamma'$   $\rightarrow \gamma$  (Ag<sub>2</sub>Al).

Where  $\gamma'$  are the precipitates metastable and  $\gamma$  are the precipitates stable of intermetallic phase  $\xi$  (Ag<sub>2</sub>Al)

The closely relation between the relaxation effects observed in this alloy and its structural transformations is evidenced in this work.

So ; tests are performed, using the Isothermal Mechanical Spectroscopy technique (IMS), at various stabilized temperature levels on a sample quenched after homogenization for two (2) hours at 828 K

The specimen have been progressively heated to 530 K and then cooled down to room temperature. During heating the annealing temperature ( $T_{ANN.}$ ) is equal to the temperature of measurement ( $T_{MEAS.}$ ) and during cooling after annealing  $T_{MEAS.}$  is lower than  $T_{ANN.}$

The obtained results reveal the existence of two (2) independent peaks we call respectively: P<sub>Z</sub> and P. The first corresponds to a thermally activated effect and the second to a not thermally activated effect.

The P<sub>Z</sub> peak was identified to a Zener relaxation peak. Its origin being due to the reorientation, under constraint, of the pairs of aluminum atoms. This peak is reproducible and does not depend on the annealing temperature. This phenomenon is explained by a mechanism based on local reversible transformation under the applied stress.

The P peak, located at 10<sup>-3</sup> Hz, appears in the temperature range : 404 K - 449 K. It correspond to the precipitation of the semi-coherent  $\gamma'$  metastable phase.

**Keywords:** Isothermal Mechanical Spectroscopy, Relaxation peak, Single crystal, Phases, Alloy, Temperature, Precipitation.

## Prediction of the geometry during a bending test on a pipe

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The objective of this study is to predict the geometry of a pipe during a cold forming process and to reduce scrap. The material is an austenitic stainless steel, AISI 321 without strain-induced martensitic transformation during the process. In order to predict elastic recovery with the maximum of accuracy, a macroscopic elasto-viscoplastic model based on theory developed by Lemaitre and Chaboche in 1985 [1] is implemented in the software Abaqus. A three-point bending test on pipe was designed and installed in a classical tensile test machine to measure and analyse elastic recovery phenomenon. [2, 3]

To determine model coefficients for the studied material, two mechanical tests were used: uniaxial tensile tests and torsion tests in order to characterise the material in different directions. Different strain rates, relaxation phases and several cycles, provided a large amount of data and gave a good knowledge of the material behaviour. After this step of characterisation, model coefficients were identified using the software SiDoLo. [4]

A 3D finite element model was set up with the software Abaqus to simulate the three-point bending test. The model was developed into a subroutine UMAT. Comparisons of simulation with experimental tests were done to verify the relevance of the chosen model and its ability to predict the final geometry.

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## Prediction of the Failure Locus of Fiber Reinforced Composites under Combined Transverse Compression and Axial Tension through Computational Micromechanics

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A computational model based on the finite element method is presented for the estimation of strength of a fiber-reinforced lamina subjected to a combination of the transverse compression and axial tension. Composite specimens subjected to this kind of biaxial loading may fail according to two distinct mechanisms. Tensile deformation along the fibers leads to fiber fracture while compressive deformation perpendicular to the fibers results in inter-fiber fracture by the localization of the matrix plastic strain along shear bands and the fiber/matrix decohesion. The use of a regular unit cell that includes a small number of the damageable planes makes it possible to find a solution to this problem.

The most important feature of the presented approach is that failure behavior of unidirectional composite is affected by fracture properties of the constituent materials and interface. Another important feature of the proposed micromechanics model is the incorporation of an interaction between transverse and longitudinal loading. A complex damage mechanism including fiber breakage, fiber/matrix debonding and matrix plastic deformation is reproduced in the proposed model by using appropriate constitutive equations.

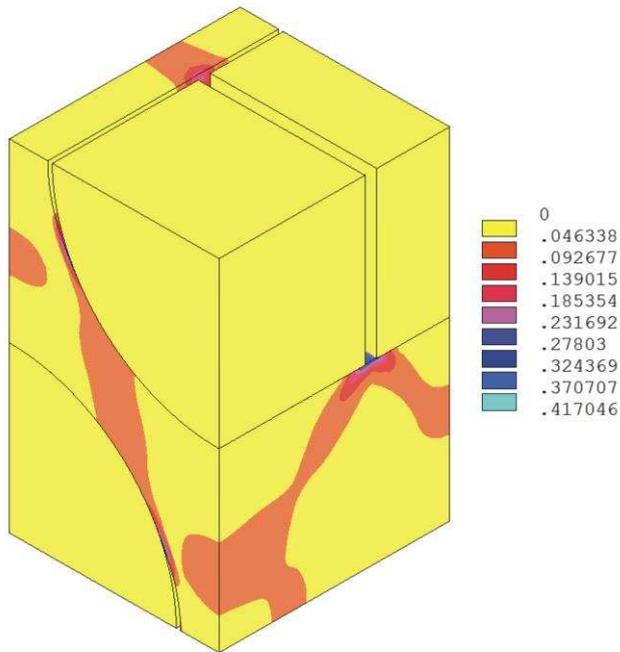
The pressure dependent, elasto-plastic behavior of matrix was simulated by the Drucker–Prager yield criterion [1]. The fiber fracture and the fiber/matrix debonding were controlled by the cohesive zone model [2]. Numerical simulations of mechanical response of the glass/epoxy lamina for thirteen biaxial loading ratios are used to obtain the failure locus. Subsequently, the model prediction is verified against an analytical solution [3] and experimental data [4]. It was found that the numerical calculations agree better with experimental results than analytical predictions. For more details on the proposed computational model, see Ref. [5].

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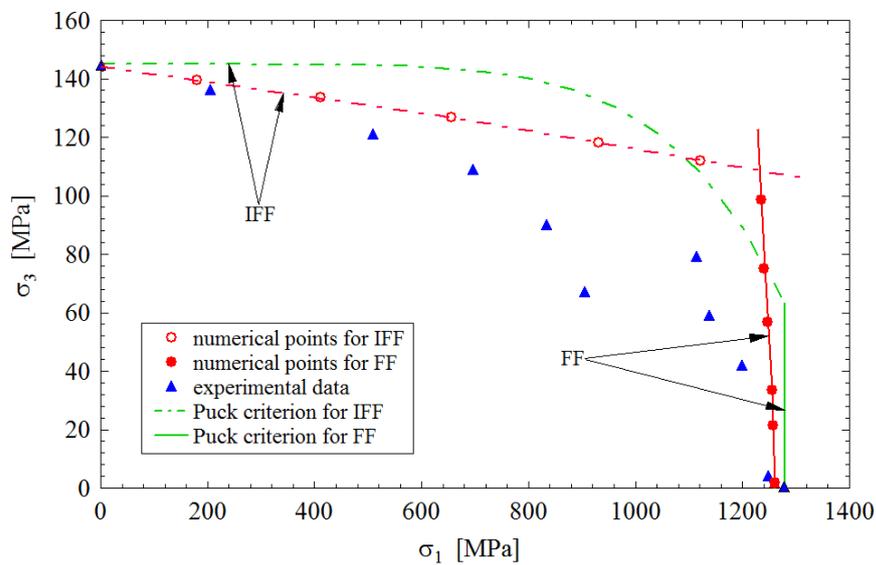
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## Additional figures



**Fig. 1.** Contour plot of the equivalent plastic strain in the glass/epoxy composite subjected to biaxial loading for  $\kappa = 2$ .



**Fig. 2.** Failure locus of the glass/epoxy composite subjected to combined transverse compression and axial tension. Experimental data from [4].

## Nanomaterials and Nanomechanics

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A continuum nanomechanics framework is outlined for modeling elasticity, plasticity, and diffusion in nanomaterials. It is based on distinguishing between “bulk” and “surface” regions which are viewed as independently evolving but mutually interacting continuum phases. Size effects on elastic and hardening moduli, as well as inverse Hall-Petch, and abnormal diffusion behavior are efficiently interpreted. Size dependent nanoscale instabilities and pattern formation in micro/nano pillars are also discussed.

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## **Elastoplastic finit element analysis for porous metals**

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Powder forming involves fabrication of a preform by conventional press-and-sinter processing, followed by various forming processes, citing as examples, rolling, compaction, forging, extrusion, among others, of the porous preform into a final shape through substantial densification. This work makes a finite element analysis for porous metals. The finite element model was applied to simulating the case of cold compaction of nanocrystalline copper under uniaxial compression conditions in order investigate the densification behavior. The model was simulated using explicit integration method as applied to the evolution variation of the relative density and the dislocation density of the compact. Finite element analysis program used was Abaqus. Finite element calculations were compared with literature experimental data. The agreements between finite element model and literature results for densification of nanocrystalline copper were good.

**Keywords:** copper, finit element, nanocrystalline, powder forming.

## Evolution of stored and dissipated energies in metallic materials under cyclic loading: application to a medium carbon steel

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In-service loading conditions usually generate complex cyclic stress states. As such, the choice of an appropriate multiaxial fatigue criterion plays a crucial role in obtaining correct fatigue predictions. In the case of high cycle fatigue, the observation of the stabilized behavior is generally required to build either stress-based criteria [4] or energy-based criteria [2, 3]. The different energy-based approaches can be classified according to the kind of energy which is assumed to drive the fatigue process. Indeed, the total strain energy is not entirely dissipated into heat since a fraction is stored in the material. While the link between fatigue damage and dissipated energy remains unclear [1], the interest for stored energy approaches is motivated by the correlation that exists between stored energy and fatigue damage accumulation [6]. More specifically, energy storage and fatigue damage are both related to the behavior of dislocations. Energy storage corresponds to an increase of the free energy associated with the multiplication of defects (e.g. dislocations, vacancies) while fatigue damage often results from the evolution of the dislocation substructure [5]. Consequently, constitutive laws must include a correct description of the energy balance to obtain robust estimations of the fatigue life under multiaxial loading conditions from energetic approaches.

In the present work, a polycrystalline plasticity model is developed to study the evolution of the energy balance in a medium carbon steel (0,35%C) which is submitted to a uniaxial cyclic loading. The proposed model, which is based on FFT homogenization techniques, is developed within a crystal plasticity framework. Material parameters are identified from an experimental dataset including cyclic stress-strain curves and estimations of the energy balance at a macroscopic scale. An alternative definition of the internal variables associated with isotropic hardening is proposed to reproduce the diminution of the average stored energy per cycle which is experimentally observed with an increasing number of applied cycles. From the results of the model, it is observed that both the stored energy and dissipated energy fields are strongly scattered. The dispersion is mostly explained by the crystallographic orientation distribution and the two-phased microstructure.

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## Material Modelling and Lifetime Prediction of Ni-base Gas Turbine Blades under TMF Conditions

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Under cyclic thermomechanical loading conditions, various effects such as strain accumulation, creep damage, ageing, fatigue etc. may occur in the material of a gas turbine blade. Depending on the loading conditions, all these effects contribute to reduce the lifetime of the component.

Subject of the present work is the development of a material model to describe the mechanical effects mentioned above, as well as the development of a lifetime model able to discriminate the different damage mechanisms.

Starting point for constitutive modelling is the well known viscoplastic Chaboche-model [1], which provides descriptions of isotropic and kinematic hardening, as well as dynamic and static recovery. The works of Ohno/Wang [2], Kachanov [3] and Kindrachuk [4] are utilized to modify and extend this basic model, respectively concerning strain accumulation, creep and strain induced ageing.

Moreover, an alternative formulation of the model has been elaborated, replacing the occurring Norton functions by hyperbolic sine functions in order to obtain a model which accounts for thermally activated processes and incorporates explicitly temperature dependent parameters. The developed lifetime model consists of three modular parts concerning fatigue, creep and oxidation. These parts are basing on lifetime models after Christ [5], Danzer [6] and Miller/McDowell [7] and are modified by Heitmann's [8] parameter  $Z_D$  as an approximation of the  $\Delta J$ -integral. Also, some advantage concerning the creep part of the model has been achieved by the appliance of Kachanov's work [3] at the estimation of creep rupture time.

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## Research of a Transient Response of Complex Beam with Granular Core

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This paper presents research results concerning how does the stiffness and damping characteristics of a complex structure, made of two spring steel cantilevers, with granular material encapsulated in a chamber between them, are tuned by the underpressure within the elastomer sleeve (Fig. 1). The length of the complex beam was 0,72 m and the cross section  $0,048 \times 0,040$  m. The ABS (acrylonitrile butadiene styrene), roller shaped granules were  $\phi 2,7 \times 3$  mm size. When loose grains, which are encapsulated in an elastomer chamber (Fig. 1), are subjected to underpressure controlled by the vacuum pump, the jamming mechanism among the granules is intensified [1]. Loose grains transform into a rigid, viscoplastic body [1, 2]. The intensified global dissipative properties allow for original strategies of semi-active damping of vibrations. The presented results were obtained for the optimized parameters and construction of the beam.

Experimental results were performed to obtain the transient time-history response of the structure for the free vibrations, of the clamped-free configuration. The influence of the underpressure on the response of the system and its properties, were extensively studied. The detailed discussion on the displacement, damping ratio and the frequency of vibrations is provided.

In Fig. 2 the displacement amplitude for the bottom point of the beam is presented for the excitation of 0,03 m. By examining the free-decay time traces of the displacement, one may find that the granular damping in the jammed state is significant, when compared to the compliant state for  $p = 0$  MPa. The displacement plots cannot be approximated by a simple exponential decay damping curve, typical for viscoelastic systems, or curves typical for dry friction. At particular stages of vibration different dissipating mechanism dominate over others.

The proposed model with Rayleigh damping equivalent allows describing the dynamic response of the beam damped with the granular structure subjected to an internal underpressure [1]. The author finds good agreement between experimental results and numerical modelling. Detailed discussion related to the experimental results, concerning the frequency and amplitude of vibrations of a continuous granular beam system is provided.

The presented solution for damping can lead to further improvements of available damping systems and increase number of applications utilizing properties of granular materials, which gives a chance of manufacturing a low-cost, efficient damping systems.

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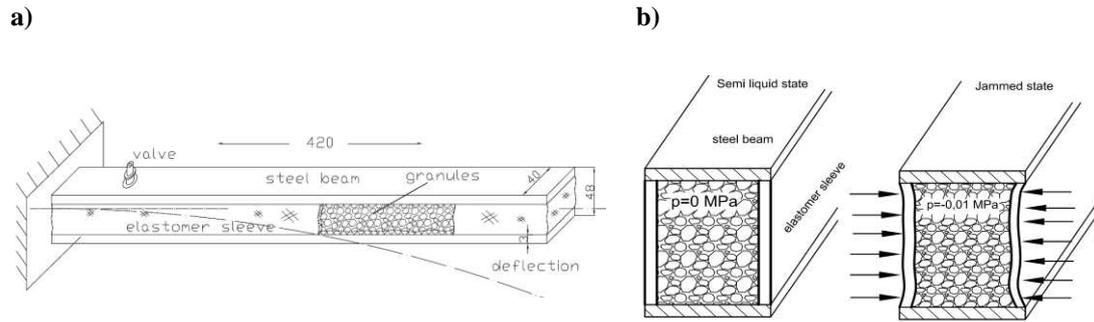


Fig. 1. a) Construction of the complex beam b) behavior of the granular structure with no underpressure and some underpressure applied - cross section view.

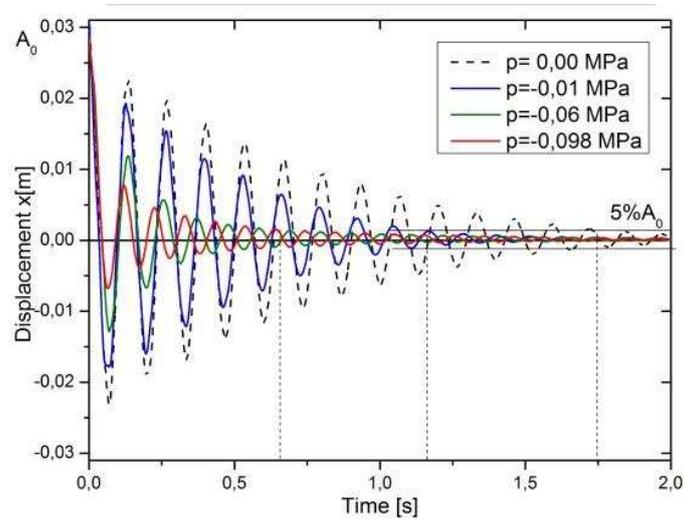


Fig. 2. Time history of amplitude of the displacement of the beam's tip

## Modelling Parameter-Property Relationships of Relaxation Measurements for Parameter Recognition Problems

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In material science and material engineering, there are tasks, when definite quantitative information to be of interest for a user must be extracted from the measurements of material properties, which correlate with the desired information in some way. Such tasks are very urgent for solving various materials evaluation tasks, such quality control, non-destructive testing, materials characterization, etc., where specific performance and service parameters have been determined from the measurements of the properties.

The mentioned information extraction can be formulated as *parameter recognition* task, which, in mathematical context, is an inverse problem with well known complexities of solution due to the fact that measurement data sets are inevitably inaccurate, corrupted by noise, discretely sampled and incomplete (truncated). However, the main difficulty of parameter recognition tasks in material research usually comes from a lack of knowledge about the functional or correlation relationships between the *parameter-property relationships* (PPRs). Because of complexity and large varieties of structures of modern materials, PPRs may be extremely complex and it is very difficult, if it is not impossible, to describe PPRs analytically.

Parameter recognition problems can be solved by using artificial intelligence technologies, such as artificial neural networks (ANN), which have already shown promising results in comparison with more traditional approaches. However, limited possibilities to obtain accurate comprehensive data for neural network training are an obstructive key factor in the development of ANN-based parameter recognition methodologies.

At beginning stage, to search for optimal ANN architectures and learning strategies, we have tried to solve this problem by PPRs simulation. In this paper, a PPRs simulation model is presented developed for relaxation measurements. As it is well known, dielectric and mechanical relaxation characteristics correlate with various performance and service parameters, such as moisture content, density, content or concentration of impurities, additives, binders, etc. The dielectric and mechanical properties are also very sensitive to physical, chemical and other structural changes in materials (polymerization, aging, damage accumulation, etc.).

The developed PPRs model simulates the exponential multi-effect actions on the relaxation/retardation spectrum and allows to simulate PPRs in 4 complexity levels, when the parameter: (i) affects the relaxation strength only, (ii) affects the relaxation strength and accelerates/decelerates the characteristic relaxation/retardation time, (iii) affects the relaxation strength, accelerates/decelerates the characteristic relaxation/retardation time and broadens/narrows the relaxation/retardation spectrum, (iv) affects the relaxation strength, accelerates/decelerates the characteristic relaxation/retardation time, broadens/narrows the relaxation/retardation spectrum and changes asymmetry of the relaxation/retardation spectrum.

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## Experimental identification of growing plate model.

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The mathematical modeling of different technological processes such as concreting, electroplating, laser deposition, thermal spraying, vapor-phase deposition, photopolymerization and other involve the description of the solid growing processes. The result of these processes is a phenomenon of growing body, that in particular may be represent from the mechanical point of view as continuous aggregating of deformable material surfaces. Key mechanical features of such bodies differ from the conventional ones due to special distribution of residual stresses that depends on the scenario of accretion. This residual stresses among all may be the reason of undesirable consequences, such as distortions of the geometric shape of the object being created, local violations of continuity, loss of stability.

In the present work we study a dynamical problem for transversally accreted plate. The theoretical model is based on Kirchhoff type hypotheses. The solution of dynamical problems for circular growing plate is obtained in the form of spectral expansion over the complete set of eigenfunction of biharmonic operator defined in unit disc.

It is shows, that the coordinate functions satisfy the initial value problem of third order with variable coefficients. We utilize analytical solution and found the relations between dynamical deflections and tensions on the adhering plies. These relations form the theoretical background for the experimental method of identification.

For this purpose a special experimental setup was assembled. A circular plate of copper foil clamped along it's contour was studied. The growing process was performed by electrolytic deposition of copper on the lateral surface of the plate. During the growing the bends and the values of it's displacement may be used for identifications. Clearly, these deflections are small, so have to use precisions measurement methods, namely holographic interferometry. After receiving the interference pattern displacement in real time, we can measure the displacement the substrate, at any time. The microstructure of adhered layers was studied also.

The relations between displacements, values of electrical current and schedule of accretion process were found experimentally.

Finally, using the program code for numerical processing of the holograms at any one time, we can reconstruct the process of deposition of plate.

**Acknowledgments:** The research was financially supported by the Russian Foundation for Basic Research (under grants Nos. 12-08-01119-a and 12-08-01260-a), by the Department of Energetics, Mechanical Engineering, Mechanics and Control Processes of the Russian Academy of Sciences (Program No. 12 OE), and by the Russian Science Support Foundation (NSh-2611.2012.1).

## A Study on Joints for Composite Material Application in High-Speed Maglev Train

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In this paper, we propose a design using sandwich composites and aluminum extrusions to fabricate lightweight hybrid car-bodies for use on a 550 km/h maglev train. When attempting to use sandwich composites and aluminum extrusions together, the bonding of the two different materials is the problem [1]. Thus, the roof of the maglev train under development has aluminum guide frames with four edges. The sandwich composites are combined with aluminum extrusions by co-curing. This arrangement would make the roof modular and allow the side-frame of the car-body and aluminum extrusions to be joined at the roof by welding. There, in order to prevent thermal deformation and chemical transition to resin, design dimensions were selected by thermal analysis. In order to improve adhesion between the sandwich composites and aluminum extrusions, the contact surfaces were made convex as in Fig. 2. This increased the area of adhesion for the high-temperature-curing adhesive film, FM73 [2]. For finishing and reinforcement, the one- or two-ply carbon prepregs were laminated onto the upper surface of the sandwich composites and aluminum extrusions. This hybrid car-body design using sandwich composites and aluminum extrusions was verified in accordance with Korean Railway Safety Law using commercial finite element analysis.

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Fig. 1 shows the co-curing of the roof composite material and extruded aluminum.

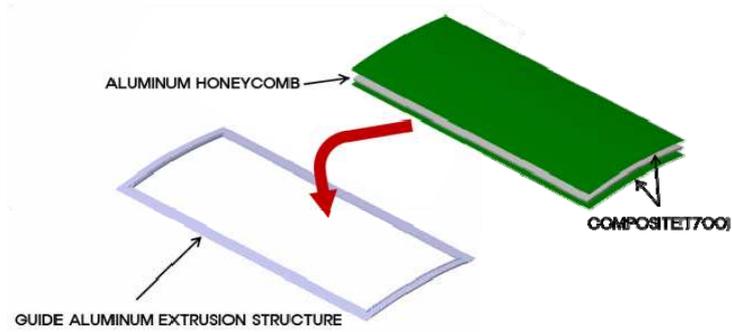


Fig. 1 Composite Roof with Guide Structure

Fig. 2 shows the method of joining the roof and side-frame.

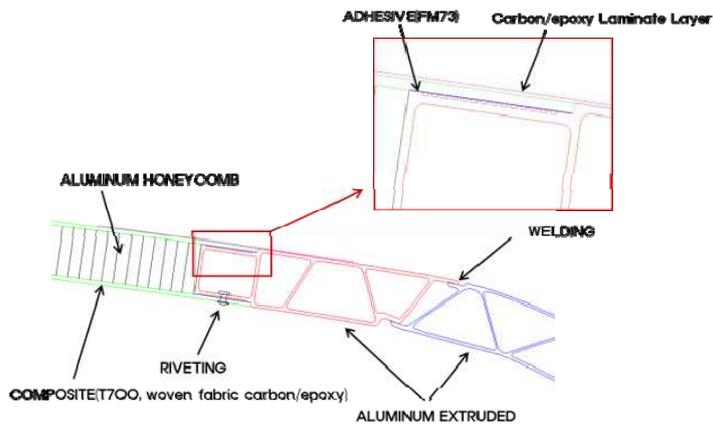


Fig. 2 Method for Joining Roof and side-frame

## The Use of 3D Method in Energy-based Models' Approximation

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This paper shows a method of approximation of the values of material constants referring to energy-based models of hyperelastic materials. The energy-based modelling, as a method of complex mechanical problem solving is based on fulfilling the conditions of the law of conservation of energy and material compressibility, which leads to a proper material description.

The validation process was based on Mooney model [1] and its subsequent modifications made by Wegner [2,3]. The abovementioned approximation was made by means of so called 3D method presented in the paper [4]. The main idea of the method is to create a graphic presentation of three, connected with each other, values describing a physical process. Later by proper projection of an obtained three-dimensional curve three planar characteristics are received. Each of them is described by an appropriate mathematical relation, which include mentioned material constants.

The chosen measure of adjustment in whole the process is the mean square error value (MSE) of the stress and strain, depending on a diagrammatic presentation, referring to the positions of the points on the theoretical curve, compared with corresponding experimental values. MSE values have been made dependent on strain values in the direction of force that caused them, taking into account transverse strains impact at the same time.

Created, using Matlab software, algorithm based on the 3D method enables finding the values of material constants determining the best adjustment of a theoretical curve to the experimental one.

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## Finite Element Analysis of Masonry Bed-Joint Damage

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The lime-based mortars were widely used in history and because of their limited strength and excessive shrinkage, their properties were often enhanced by additives in form of pozzolans. The Phoenicians added various crushed clay products, such as crushed bricks, into the mortars in order to increase their resistance to water. The technology was later extensively used in Byzantine structures and by Romans, who called the material *cocciopesto*. Interestingly, it was found that the masonry structures with mortars containing crushed brick particles exhibit a higher resistance to seismic loading [1,5].

The most common failure of masonry structures is cracking of bed joints due to excessive shear loading. In that case, the pre-compression of the joint is increasing its shear resistance. Our paper is focused on the performance of bed joints having various thicknesses and being reinforced with large-size aggregates of different properties, when subjected to pure shear or shear and compression. In particular, the attention is paid to the damage localization, utilizing the non-local formulation of anisotropic damage model [3].

The microstructure generation was implemented in MATLAB software with the use of multi-parametric toolbox for MATLAB [4]. The conforming triangular finite element mesh was then generated using ANSYS software and the plane-stress numerical simulations were carried out in the OOFEM finite element code with the object oriented architecture [6]. Finally, the results were processed in MATLAB and visualized in ParaView software [2].

The analysis results indicate that the bed joints of lower thickness exhibit higher strength. It also revealed that the presence of low quality aggregates, such as crushed bricks in the case of *cocciopesto* mortars, contributes to a distributed cracking instead of its localization into a major crack. The findings explain the good performance of many historical masonry structures.

**Acknowledgments** This work was supported by the Ministry of Culture of the Czech Republic, project No. DF11P01OVV008.

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## Iron-filled polymers for magneto-rheological elastomers: Experimental study and constitutive modelling

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In the preparation of magneto-sensitive elastomers, relatively small amount of iron particle is used as filler. Such inclusion has influence on the mechanical properties of matrices. In this work, the influence of filler particles on the stress-strain response has been investigated. First, a comprehensive experimental study is performed for iron particle-filled silicon-based elastomer where the experimental investigation is mainly probing the behavior of the filled-rubber with varied filler content. In order to quantify the dissipative behaviour of the filled-elastomer, several standard viscoelastic tests such as single-step relaxation tests, multi-step relaxation tests as well as loading-unloading tests will be performed [2]. Later, few standard test results will be presented with the application of a magnetic field. In an attempt to model the purely mechanical behaviour of the filled elastomer, several finite strain approaches that have been proposed in the literature are applied. Then, the selected model will be extended to incorporate the magnetic influence. A direct comparison of all selected constitutive relations with experimental data will be shown [1, 3].

**Acknowledgments** This work is supported by an ERC advanced investigator grant MOCOPLY.

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In this paper, we investigate the material properties of iron-filled silicon-based polymers. Such filled polymer with iron particles is utilized in preparing magneto-rheological elastomers (MREs). MREs are a class of smart materials whose mechanical properties, such as the modulus and damping ratio, can be reversibly and rapidly controlled by an external magnetic field. This is achieved via the addition of microsized magnetizable particles into the elastomers or rubber-like materials. When such a mixture is exposed to a magnetic field before curing, the field-induced interactions between particles can result in the formation of an anisotropic ordered preconfiguration such as chains or more complex three-dimensional structures. After the mixture is cured or cross-linked, these structures are locked into place. When such prepared MREs are exposed to an applied magnetic field, the field-induced dipole magnetic forces between the particles result in the field dependence of mechanical performance. The change of the modulus is usually termed an MR effect. In this contribution, we will study the experimental behaviour of iron-filled elastomer with and without the application of a magnetic field. The aim of this study is to present a comprehensive experimental results as well as modelling the data.

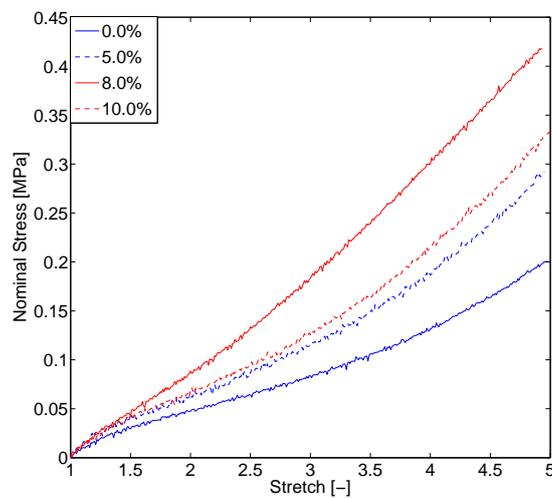


Figure 1: Experimental study : Response of iron-filled polymer in uniaxial tension tests for various percentage of iron particles.

The figure (1) demonstrates a typical stress-stretch response of a iron-filled silicon-based polymer. It shows that the amount of filler (normally expressed in percentage) enhances the stiffness of the material upto a certain level. In this contribution, we will model this data including its viscoelastic effects as well as the influence of the magnetic field.

## Strain Fields and Barrier Heights of Ge Quantum Dots Buried in Si/SiO<sub>2</sub> for Modelling Thermoelectric and Photovoltaic Devices

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The performance of thermoelectric energy conversion devices depends on the thermoelectric figure of merit ( $ZT$ ) of a material defined as  $ZT = S^2 \sigma T / \kappa$ , where  $S$ ,  $\sigma$ ,  $\kappa$ , and  $T$  are the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature, respectively. Recently, there has been increased interest in employing Ge and GeSi quantum dots for improving thermoelectric performance. This system offers an intriguing ability to independently control thermal and electronic properties of the dots, stimulating remarkable interest devoted mainly to possible thermoelectric and photoelectric applications [1,2].

We model the experimentally available structure, which consists of a silicon substrate and a thin SiO<sub>2</sub> dielectric film on top of the substrate with a high-temperature annealed spherical Ge quantum dots inside the film. The dots migrate through the thin film and become embedded into the Si substrate to a varying depth, generating the strain near the Ge/Si interface. Due to a high-temperature preparation conditions, the Si/SiO<sub>2</sub> interface is no longer flat, so that one comes to the symmetrically and asymmetrically buried Ge dots, depending on whether the right- and left-hand side buried depths are the same or different.

Our theoretical modelling of the local strain in and around the dot is performed by using standard finite-element method (FEM) techniques, and the strain is then translated into a variation of the band-gap energy using deformation potential theory. Calculation details are given elsewhere [3]. The strain calculation results are experimentally verified using Raman scattering to analyse the Ge-Ge optical phonon region, and a good correspondence between the calculations and experiment is obtained.

We present the strain distributions in and around the spherical Ge quantum dot and optimise the strain maxima with respect to the buried depth, both for symmetrically and asymmetrically buried dots. We also map the Ge/Si energy band barrier heights, which are determined using the effective mass formalism for strained Ge/Si. The resulting distributions demonstrate localized regions of increased barrier heights below the bottom of the buried dot and decreased heights on the Si side of the Si/SiO<sub>2</sub> interface. We then propose a simplified model of the free charge transport properties including the charge trapping in the confinement potential of the Ge dot

The results may be of interest for tailoring Ge and Si band gaps and modelling thermoelectric and photovoltaic devices.

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## Influence of Nanostructured Alumina Filler on the Structure and Properties of Polymer Composites

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It is known that level of interfacial adhesion polymer-filler is influenced by two primary factors: level of physical and chemical interactions polymer - a filler and structure of an interfacial layer. Therefore studying crystal and microstructures of composite materials with fine-disperse fillers is necessary for their purposeful planning and preparation.

The influence research a nanostructured active filler  $\gamma$  - and  $\alpha$  - alumina on structure and properties of polymeric composites with different types of matrixes was the purpose of the present work.

Epoxy resin ED-22, polytetrafluoroethylene (PTFE) and aromatic polyamide FENILON C-2 were used as matrixes. Nanostructured fillers - alumina with  $\gamma$ -,  $\theta$ -,  $\alpha$ - phases prepared from hydrated cellulose fibers. They were impregnated with aluminum chloride solution and were heat treated on a special regime up to differential temperatures. As a result, the highly porous (85-90 %) with the large surface (120-200 m<sup>2</sup>/g) alumina fibers with various crystal structure:  $\gamma$ ,  $\theta$ ,  $\alpha$ , consisting of oxide nanograins have been prepared.

Oxide fibers were ground in fine-particle powder and then it was filled into polymeric matrixes. Curing of epoxy composite with active filler was carried out at room temperature, and with application PTFE and FENILON C-2 - at heating to 150-300°C. Research of structure of matrixes, filler and composites was carried out by X-ray, IR - spectroscopic and electron microscopic methods.

It has been established that nanostructured filler caused change of matrix crystal structure, infrared spectra in some cases were changed too. Morphological researches of a surface and chips of composite samples have confirmed the assumption of physical and chemical interaction on border of phases: alumina nanostructured filler – a polymeric matrix. It made appreciable impact on structure and property of composite materials.

The content growth of nanomodifier in PTFE matrix caused a decrease the sizes spherulites. After mechanoactivation of PTFE powders with filler mixes more ordered small mesh structure of composite was formed.

The introduction of nanostructured filler in epoxy matrix raised its adhesive durability with a reinforcing component - a steel wire on 30 %. Deterioration of a composite with gamma-alumina and matrix PTFE went down in 150 - 200 times. The module of elasticity of samples of a composite based on FENILON C-2 with nanostructured  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> was raised in 1.5 times.

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## Occurrence of Violet Colour in Ruby: An Experimental Investigation

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Ruby is an attractive gem which generally exhibits red colour and its very best colour is called “pegiion’s blood”. Although ruby’s demand is quite high from gem and jewelry point of view, its technological applications in laser, maser, modern mechanical clock, scanning probe tips in a coordinate measuring machine, etc. further enhances its importance in the market domain. Aluminium oxide (corundum) is the basic matrix of ruby and the red colour originates due to chromium as impurity. When a small fraction of aluminium ions are replaced by chromium ions in  $\alpha$  alumina, the  $\text{Cr}^{3+}$  ion octahedrally surrounded by six  $\text{O}^{2-}$  ions results in absorption of light in yellow green region of visible light but re-emission of the light takes place at a lower energy level leading to red luminescence. Thus, the generally observed red colour in ruby arises due to a luminescence effect.

The market price of natural ruby is relatively high compared to its synthetic counterpart because of jewelry and astrological uses. It is known that natural rubies exhibit secondary hues like orange, purple, violet and pink, out of which violet is a rare occurrence. In this investigation, an effort has been made to experimentally investigate the genesis of the violet colour which is so far not yet correctly understood.

Naturally available violet ruby gemstones collected from Kalahandi area of Odisha (India) were chosen as the research specimens in this work. The stones were microstructurally characterized by XRD, SEM, TEM, SAED, EDS, optical reflectance spectra, Raman spectra and XPS to identify the genesis of violet colour. The sharp step observed in optical spectra between 410-420 nm indicating violet region of spectrum points out that either the colour origin may be due to diffuse reflectance caused by microstructural texture of crystal or owing to some impurity other than Cr occurring in the alumina matrix. From EDS and XPS studies it was observed that Ti is the only traceable impurity other than Cr in the corundum crystal. Detailed XPS analysis for core electrons and photoluminescence (PL) studies of the Kalahandi ruby conclude that the origin of violet colour in the ruby is due to Ti impurity. Further details of the investigation with a model for titanium impurity shall be discussed in the full text of the paper.

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## A mesoscopic stochastic model for micron-scale plasticity

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Plastic deformation of micron-scale single crystalline specimens is accumulated by large intermittent strain burst (dislocation avalanches) [1]. The size of these bursts is power law distributed, with a cut-off depending on the external shear stress (driving force). At a critical stress value the cut-off tends to infinity, showing analogy with continuous phase transitions. This phenomenon is often investigated numerically in a depinning framework [2–4].

In this poster we investigate the statistical properties of strain bursts with a model that uses dislocation dipoles as the elementary sources of deformation. Due to the properties of dislocations, the interaction is long-range with strong anisotropy. Contrary to previous models, due to the non-positiveness of the interaction kernel we also allow bursts in the opposite direction of the driving force. After investigating which parameters of this model influence the statistical properties of the plastic response, we highlight the differences and similarities between the results of this model and experimental measurements, 2D discrete dislocation models and other mesoscopic models. In addition, this model gives an effective method to investigate the effect of the specimen size on the size distribution of bursts and leads to an unexpected result in this respect.

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## Atomic Scale Analysis of Structural Instability in Nanostructures

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To fully understand the strength and deformation mechanisms of solid materials under load, such as dislocation nucleation, crack initiation, etc., it is ultimately essential to reveal the nature of structural instability at the atomistic level. A scheme of atomistic structural instability analysis (ASIA) proposed by Umeno et al. gives a rigorous criterion for the occurrence of instability and its deformation modes in arbitrary structures [1-3]. However, the relationship between instability modes and defect character, how instability modes are localized under external loading, and the mechanism of activation of latent instability at relatively high temperatures, have not yet been studied in detail.

To address these open questions, various structures and materials must be explored to collect more data, which will allow to better understand the mechanism of mechanical instability at the atomistic level. In this study, we perform atomistic model simulations for Au crystals subjected to external loading using the Embedded Atom Method (EAM) interatomic potential, applying the ASIA scheme to evaluate the evolution of instability modes. We first investigate crystals containing either a notch at the surface or a bore subjected to tensile loading. We discuss how deformation modes due to such structures look like, and how they evolve under increasing global strain. Furthermore, we examine samples with a rough surface, to discuss how symmetry affects the instability modes.

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## **Constitutive modeling of a polymer and its composite**

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A model for the viscoplastic behavior of a thermoplastic polymer and a micro-macro simulation of this polymer with filler particles is presented. In a first step, the development of viscoplastic constitutive equations within the theory of finite deformations is discussed with the focus on a polymeric material. A strong backflow behavior during unloading motivates the use of two terms within the flow rule. Besides hardening and viscosity functions, the model also contains a criterion to regulate the activity of the included terms. The developed model gives reasonable results in comparison to uniaxial cyclic tensile tests and a relaxation test. A second step is done by combining the developed model with a standard plasticity model to create a representative volume element with an idealized microstructure. This two-scale simulation is compared to a polymeric composite material with metallic filler particles.



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