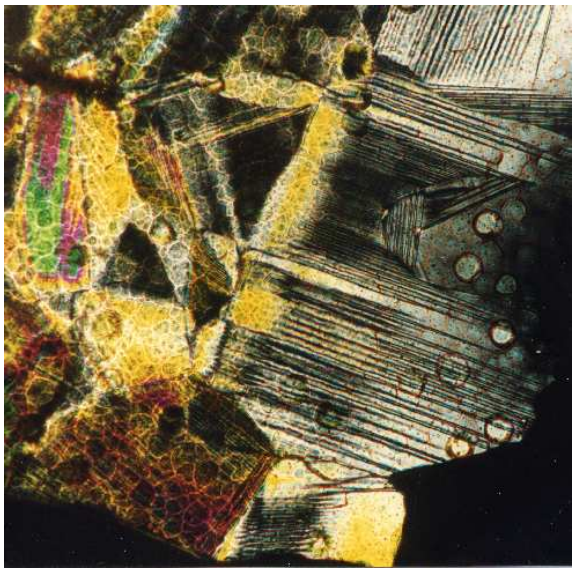
FIFTH GAMM-SEMINAR ON MICROSTRUCTURES

Program and Abstracts



Polycrystalline BaTiO3*

January 13 – 14, 2006
University Duisburg-Essen
Essen, Germany

*) The picture shows an optical image of polycrystalline BaTiO3, thinned for measurement in a transmission electron microscope. The colors arise from the thickness interference. Strong gradients of polarization render the domain walls visible.

Courtesy of H. Gorzawski, D.C. Lupascu
Department of Materials and Geo-Sciences
Darmstadt University of Technology

FIFTH GAMM-SEMINAR ON MICROSTRUCTURES

Organizers

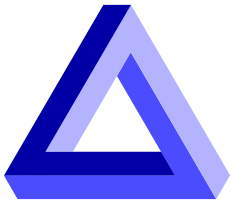
J. Schröder **J. Bluhm** **K. Hackl** **S. Conti**

Local Organizers

J. Schröder **J. Bluhm** **O. Hilgert** **A. Schwarz**

January 13 – 14, 2006
University Duisburg-Essen
Essen, Germany

The Institute of Mechanics



**and the organizers
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FIFTH GAMM-SEMINAR ON MICROSTRUCTURES

GENERAL INFORMATION

January 13 – 14, 2006
University Duisburg-Essen
Essen, Germany

Local Organizing Commitee

Postal Address:	FIFTH GAMM-SEMINAR ON MICROSTRUCTURES
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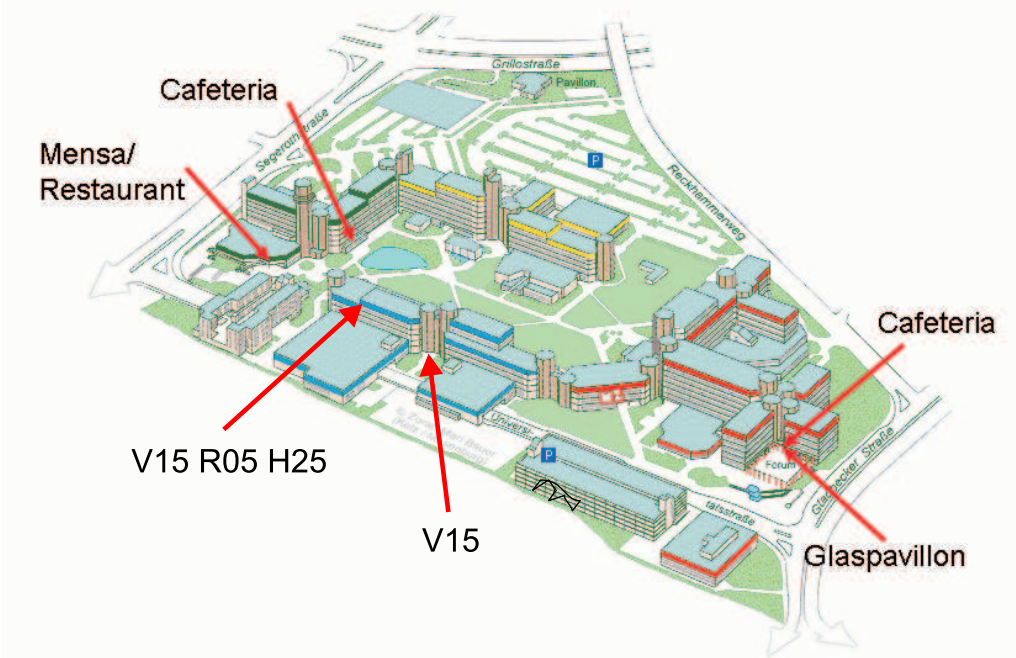
Location

The seminar is to be held in the Glaspavillon (entrance R12) of the University Duisburg-Essen, Campus Essen. The Registration and Welcome Reception as well as the Conference Dinner take place in the Room V15 R05 H25 (entrance V15).



FIFTH GAMM-SEMINAR ON MICROSTRUCTURES

PROGRAM

January 13 – 14, 2006
University Duisburg-Essen
Essen, Germany

Thursday, January 12, 2006

17:00 - 20:00 Registration and Welcome Reception
Room: V15 R05 H25

Friday, January 13, 2006

Room: Glaspavillon (entrance R12)

08:20 - 10:00 **Session 1: Variational and Relaxation Methods**

Chairman: K. Hackl

08:20 Opening

08:30 **Variational Methods in the Study of Imaging, Foams, Quantum Dots ... and More**
I. Fonseca

09:00 **Relaxation and microstructure in smectic elastomers**
J. Adams, S. Conti, A. DeSimone, M. Warner

09:30 **On the numerical relaxation of single-slip plasticity in finite strains**
C. Carstensen, S. Conti, A. Orlando

10:00 Coffee Break

Friday, January 13, 2006

Room: Glaspavillon (entrance R12)

10:30 - 12:30 **Session 2: Dislocations and Homogenization**

Chairman: S. Conti

10:30 **Homogenization of stratified thermoviscoplastic materials**
F. Murat

11:00 **Statistical and continuum thermodynamic models for continuum dislocation dynamics with application to extended crystal plasticity**
B. Svendsen

11:30 **The extended Korn's first inequality with integrable dislocation density**
P. Neff

12:00 **Regularity of solutions of the homogenized problem in plasticity**
S. Nesenenko

12:30 Lunch

Room: Glaspavillon (entrance R12)

13:30 - 15:00 **Session 3: Minimization and Evolution Problems**

Chairman: B. Svendsen

13:30 **Rate-independent evolution problems with nonconvex energies**
G. Dal Maso, A. DeSimone, M.G. Mora, M. Morini

14:00 **A Robust Adaptive Algorithm for Brittle Fracture based on Incremental Energy Minimization**
C. Miehe, E. Gürses

14:30 **Convergence of AFEM for degenerated minimisation problems**
C. Carstensen

15:00 Coffee Break

Friday, January 13, 2006

Room: Glaspavillon (entrance R12)

15:30 - 17:30 **Session 4: Ferro- and Piezoelectric Materials**

Chairman: P. Neff

15:30 **Interaction of ferroelectric domain walls with defects in Ferroelectrics**
D.C. Lupascu

16:00 **Micro-mechanical simulation of domain wall motion in ferroelectric materials**
R. Müller

16:30 **Meso-Macro-Modeling of Nonlinear Ferroelectric Ceramics**
H. Romanowski, J. Schröder, I. Kurzhöfer

17:00 **Switching effects in piezoelectric materials – a micromechanically motivated finite element approach**
A. Menzel, A. Arockiarajan

19:00 Conference Dinner
Room: V15 R05 H25

Saturday, January 14, 2006

Room: Glaspavillon (entrance R12)

08:00 - 10:30 **Session 6: Phase Transitions**

Chairman: A. DeSimone

08:00 **Configurational forces and models for martensitic transformations and grain boundary diffusion**
H.-D. Alber, P. Zhu

08:30 **Shape memory and superelastic effects of cyclic martensitic phase transformations in monocrystals – Computational and experimental results**
E. Stein, O. Zwickert

09:00 **On a thermoelastic problem with phase transition**
K. Chelminski

09:30 **Modeling of a phase transition in CuAlNi**
M. Kružík

10:00 **Prediction of energy-barriers due to nucleation in solid-to-solid phase-transitions**
T. Bartel, K. Hackl

10:30 Coffee Break

Saturday, January 14, 2006

Room: Glaspavillon (entrance R12)

11:00 - 13:00 **Session 7: Microstructure and Multiscale Problems**

Chairman: H.-D. Alber

11:00 **Multiscale problems in thin elastic bodies**
S. Müller

11:30 **Energy scaling and microstructure formation in paper crumpling**
S. Conti, F. Maggi

12:00 **Simulating the micro-structure of Hardened Cement Paste including Damage due to Frost**
M. Hain, P. Wriggers

12:30 **Size Effects in Polymer Joints – A Modelling Approach**
M. Johlitz, H. Steeb, S. Diebels

13:00 Lunch

Room: Glaspavillon (entrance R12)

14:00 - 15:40 **Session 8: Modeling of Materials**

Chairman: C. Carstensen

14:00 **Modeling and simulation of magnetic shape-memory polymer composites**
S. Conti, M. Lenz, M. Rumpf

14:30 **Three-wave interaction in discrete lattices**
J. Giannoulis

15:00 **A Lamination Upper Bound to the Free Energy of Mixing of Shape Memory Alloys**
R. Heinen, K. Hackl, S. Govindjee

15:30 Closing

15:40 Meeting of the GAMM-Commitee

FIFTH GAMM-SEMINAR ON MICROSTRUCTURES

ABSTRACTS

January 13 – 14, 2006
University Duisburg-Essen
Essen, Germany

Relaxation and microstructure in smectic elastomers

J. Adams[1], S. Conti[1], A. DeSimone[2], M. Warner[3]
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Smectic A elastomers are layered materials, which have a solid-like elastic response along the layer normal and rubbery in the plane. Upon stretching parallel to the layer normal they exhibit a reversible threshold, above which the elastic modulus is drastically reduced. We model this using a Gaussian model of the elasticity, and determining its relaxation in an appropriate geometry. The minimized energy can be understood in terms of laminates corresponding to a buckling instability.

Smectic C elastomers have an additional degree of freedom, coming from the in-plane component of the director. Therefore the set of states K minimizing the elastic energy contains a one-parameter family of simple stretches. We investigate soft elasticity and its associated microstructure by determining the quasiconvex hull of the set K, and use this to propose experimental tests.

Configurational forces and models for martensitic transformations and grain boundary diffusion

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Two main types of phase transformations in solid materials can be distinguished, diffusion dominated and diffusionless transformations. The behavior of phase interfaces in materials allowing diffusionless or martensitic transformations can be studied by mathematical models, where the configurational force along the sharp phase interface acts as driving force for the evolution of the interface. A method has been developed to transform these sharp interface models into models with diffusive interface. This method suggests generalizations, which for example, lead to a model for grain boundary diffusion with diffusive interfaces.

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[3] P. Zhu; H.-D. Alber [2005], "Solutions to a Model with Nonuniformly Parabolic Terms for Phase Evolution Driven by Configurational Forces", to appear in SIAM Journal on Applied Mathematics.

Prediction of energy-barriers due to nucleation in solid-to-solid phase-transitions

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Within the framework of a micromechanical model for multiphase materials, a numerical method for the prediction of additional energy barriers due to nucleation is presented. It is a well known issue that the stress-strain-relationship of such materials reveals a stress-drop when a phase-transition is initiated. A possible physical interpretation for this phenomenon is the need to overcome an additional energetic barrier in order to form a nucleus which is large enough to enforce the growth of the new phase. The classical theory of nucleation provides formulae to determine the critical radius of the nucleus and an energy barrier respectively, where the shape of the nucleus is assumed to be a sphere. For the purpose of extending these theories by means of being applicable to solid-to-solid phase-transitions we explore the effect of an ellipsoidal inhomogeneity with specified volume and known eigenstrains within a solid matrix. Therefore, a representative volume element (RVE) is discretized spatially by finite elements and the mechanical problem is solved by a multiscale approach. An energy minimization process yields the optimal geometry of the inhomogeneity. The comparison of the total energy of the RVE with nucleus to the one without lets us draw conclusions about the critical volume of the nucleus and the energy barrier which needs to be overcome in order to initialize the phase-transition.

On the numerical relaxation of single-slip plasticity in finite strains

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The modeling of the elastoplastic behavior of single crystals with infinite latent hardening leads to a nonconvex energy density, whose minimization produces fine structures. The effective macroscopic behaviour can be characterised by means of the quasiconvex envelope of the energy density; unfortunately a closed form expression for the latter is known only in few very simplified cases. One is therefore lead to a new computational challenge, namely numerical relaxation. This is faced with huge numerical difficulties because of the minimization of a nonconvex function with clusters of local minima.

With the objective of gaining better insight in the type of microstructure that can develop, and in the type of numerical minimization algorithm that can be used for the relaxation, we study a simplified model problem in two-dimensional, geometrically nonlinear plasticity, with a single slip system and a linear hardening law. A different analysis of the relaxation of the same model was previously given in [1, 2].

First, we consider an elastically rigid problem, i.e. assume that the elastic part of the deformation is a rotation, and neglect dissipation. For this case, the quasiconvexification of the energy density can be determined in closed form [3].

A more refined model is obtained by assuming the microstructure to have the form of a laminate of second order, which is supported either on rigid-plastic deformations or on purely elastic ones. In this case the relaxation can be reduced to the minimization of a function of only one variable.

Finally, we use the above results for the numerical minimization of the full energy density, including dissipation, and removing the kinematic constraint, and compare with the literature [1].

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On a thermoelastic problem with phase transition

Krzysztof Chelminski
Warsaw University of Technology
and Cardinal Wyszynski University in Warsaw

We investigate a thermoelastic initial-boundary value problem with phase transition. The particular application we have in mind is a mathematical model for the Jominy end-quench test. The system of equations describing the deformation process consists of a quasistatic momentum balance, a semilinear energy balance and a nonlinear ordinary diffrential equation for the volume fractions of perlite and martensite. We study well-posedness of the considered system, regularity of solutions and a special optimal control question.

(A joint work with Prof. Dietmar Hömberg, WIAS, Berlin)

Modeling and simulation of magnetic shape-memory polymer composites

S. Conti[1], M. Lenz[2], M. Rumpf[2]

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Ferromagnetic shape-memory materials exhibit comparably large strains in response to an applied magnetic field. For single crystals one can achieve strains of order of magnitude 10%, but in case of polycrystals the effectivity drops significantly as a consequence of the rigidity of interacting grains.

A recently-proposed alternative is that of small single crystal shape-memory particles embedded in a soft polymer matrix. This approach gives a large freedom in the material development, which includes the type of polymer, the density of particles, their shape, and their orientation. The optimization of all these microstructural parameters is still at a preliminary stage, and we aim at providing criteria based on theory and simulation.

We consider a continuous model for such a configuration describing the full range of interactions between elastic and magnetic effects. Aiming for a homogenization approach we study the affine-periodic cell problem.

We develop and use a numerical method for the study of the cell problem in two dimensions. The main ingredients are (i) the boundary element method to compute the elastic and magnetic field energies; (ii) a combinatorial component reflecting the phase transition in the individual particles (which are assumed to be single-domain); (iii) a gradient descent approach for the actual energy minimization. Simulations demonstrate the behavior of the macroscopic material properties for different possible microstructures and give suggestions for the optimization of the composite.

Energy scaling and microstructure formation in paper crumpling

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Crumpling a sheet of paper leads to the formation of complex folding patterns over several length scales. This can be understood on the basis of the interplay of a nonconvex elastic energy, which favors locally isometric deformations, and a small singular perturbation, which penalizes high curvature.

Based on three-dimensional nonlinear elasticity and by using a combination of explicit constructions and general results from differential geometry, we prove that, in agreement with previous heuristic results in the physics literature, the total energy per unit thickness of such folding patterns scales at most as the thickness of the sheet to the power 5/3. For the case of a "single fold" we also obtain a corresponding lower bound.

Rate-independent evolution problems with nonconvex energies

**Gianni Dal Maso (*), Antonio DeSimone,
Maria Giovanna Mora, Massimiliano Morini**

The purpose of the talk is to introduce some genaral tools for the study of evolution problems in the framework of Young measures. The notion of time-dependent system of generalized Young measures allows to extend to this setting the classical notions of total variation and absolute continuity in a time interval, as well as the notion of time derivative. The main results are a Helly type theorem for sequences of systems of generalized Young measures and a theorem about the existence of the time derivative in the case of absolutely continuous dependence on time. The main application of these results is the study of some rate-independent evolution problems with nonconvex energies which occur in some linerized models of plasticity with softening.

(*) The results will be presented by Gianni Dal Maso.

Variational Methods in the Study of Imaging, Foams, Quantum Dots ... and More

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Several questions in applied analysis motivated by issues in computer vision, physics, materials sciences and other areas of engineering may be treated variationally leading to higher order variational problems and to models involving lower order density measures. Their study often requires state-of-the-art techniques, new ideas, and the introduction of innovative tools in partial differential equations, geometric measure theory, and calculus of variations. In this talk it will be shown how some of these questions may be reduced to well understood first order problems, while in others the higher order plays a fundamental role.
Applications to phase transitions, to the equilibrium of foams under the action of surfactants, imaging, micromagnetics and thin films will be addressed.

Three-wave interaction in discrete lattices

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We consider the interaction of three pulses in a multidimensional monoatomic lattice $\mathbb{Z}^d$, $d \in \mathbb{N}$. The scalar displacement $x_\gamma \in \mathbb{R}$ of each atom $\gamma \in \mathbb{Z}^d$ is described by Newtons equations of motion

$$\ddot{x}_\gamma = \sum_{\alpha \in \mathbb{Z}^d} V'_\alpha(x_{\gamma+\alpha} - x_\gamma) - W'(x_\gamma), \tag{1}$$

where V_α is a general pairwise-interaction potential between atoms at a mutual distance $\alpha \in \mathbb{Z}^d$ and W is a general external potential. We model the pulses as macroscopic (small-)amplitude modulations of three plane-wave solutions to the linearization of (1)

$$x_\gamma(t) = \varepsilon \sum_{j=1}^{3} A_j(\varepsilon t, \varepsilon\gamma) \mathrm{e}^{\mathrm{i}(\omega_j t + \vartheta_j \cdot \gamma)} + \text{complex conjugate} + \mathcal{O}(\varepsilon^2),$$

with $0 < \varepsilon \ll 1$, which are in resonance: $\omega_1 + \omega_2 + \omega_3 = 0$ and $\vartheta_1 + \vartheta_2 + \vartheta_3 = 0$. In this case, we formally derive as a macroscopic limit a system of three nonlinearly coupled equations *(three-wave-interaction equations)*, which describe the macroscopic evolution of the amplitudes A_j, $j = 1, 2, 3$. Our main objective is the mathematically rigorous justification of the validity of this macroscopic limit.

Simulating the micro-structure of Hardened Cement Paste including Damage due to Frost

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In this contribution, a multi–scale model for hardened cement paste is introduced. Based on a three–dimensional computer–tomography at the micrometer length scale, a finite element model is developed with different constitutive equations for the three parts unhydrated residual clinker, pores and hydrated products. For the hydrated products, a visco–plastic material model of PERZYNA-type including damage is applied.
The constitutive equations at the micro–scale contain parameters, which cannot be obtained through experimental testings. Therefore, one has to solve an inverse problem which yields the identification of these properties. For computational efficiency and robustness, a combination of the stochastic genetic algorithm and the deterministic LEVENBERG-MARQUARDT method is used.

Effective elastic material properties are obtained using homogenization techniques. Here, representative volume elements (RVEs) with an edge length of $64\mu m$ and accordingly 64^3 finite elements are used. Based on the finite element solution, the volume averages of the stress and the strain can be evaluated. Subsequently, the effective elastic material properties are calculated using a least-square approach. For a reliable analysis, the homogenization procedure is performed for a sufficient number of RVEs. The obtained probability densities for the effective properties are close to a GAUSSian distribution. Furthermore, they correspond very well to accompanying experimental results.

Due to frost, the moisture inside the abovementioned microstructure freezes. This increase of volume is applied at the micro–model and leads to damage which yields an inelastic material behavior. For different moistures and temperatures, a correlation between these properties and the inelastic material behavior will be obtained. In order to describe those inelastic phenomena at the macro–scale, an effective material model similar to the hydrated part at the micro–scale is chosen. However, the constitutive parameters on the macro–scale depend on the moisture and the temperature. Numerical examples will show that the developed approach reproduces the material behavior realistically.

Keywords: hardened cement paste, microstructure, parameter identification, homogenization, damage due to frost

A Lamination Upper Bound to the Free Energy of Mixing of Shape Memory Alloys

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Modeling of the energetic behavior of materials showing martensitic phase transformations usually leads to non-convex energy formulations. In most models based on quasi-convex analysis, the Reuß lower bound, which neglects the compatibility constraint for the deformation fluctuations, is used as an estimate for the so-called energy of mixing.

We derive an upper bound that is on the one hand based on the *lamination mixture formula*, which gives an estimate of the free energy of two-variant materials and is extended to the n-variant case in our work. On the other hand, we rely on experimentally well established assumptions about the type of microstructure that forms in such alloys. More precisely, we restrict the set of admissible microstructures to the subset of second order laminated microstructres consisting in austenite and twinned martensites. We further refine our upper bound by taking into account the notion of twin-compatibility.

For the physically relevant examples of 13- and 7-variant Cu-Al-Ni shape memory alloys, striking congruence is shown in the comparison of the Reuß lower and our new upper bound.

Size Effects in Polymer Joints – A Modelling Approach

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In recent years experimental investigations have shown that polymers form interphases in contact with substrates like metal sheets or glass plates. These interphases influence the mechanical stiffness of the bound significantly in form of a size effect. Physically, these effects are not understood in detail on the micro-scale. Phenomenologically, it is assumed that the stiffness change is affected by a change in the cross linking density, the glass temperature, the chemical composition of the polymer film near substrates and by internal stresses, c.f. Bockenheimer [1] and Krüger [2]. The above described phenomena motivate the developing of a phenomenological extended continuum model which is able to capture the above mentioned size effects with respect to finite deformations. Our approach is based on a scalar-valued order parameter which takes the microscopic behavior of the interphases into account. In contrast to kinematically extended continua the presented approach allows for stiff and for weak boundary layers, therefore size effects "smaller is stiffer" and "smaller is weaker" are possible. From the general point of view, the applied theory fits into the general framework of extended continuum theories, c.f. Capriz [4], Capriz et al. [5] and Svendsen [6].

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Modeling of a phase transition in CuAlNi

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The talk will concentrate on convergence analysis of an evolutionary model describing a phase transition in shape memory alloys. Computational examples of a a stress-induced austenite-martensite transformation in CuAlNi will be shown.

REFERENCES

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Interaction of ferroelectric domain walls with defects in Ferroelectrics

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Macroscopic material behavior of single crystalline as well as polycrystalline ferroelectric materials highly depends on the microstructural features encountered in the particular compound. The description of dislocation motion in metals is a highly developed field and most features of metal plasticity have been described by sufficiently correct microscopic models and appropriate homogenization procedures. In ferroelectrics the task of establishing a consistent set of material laws is still in its early development. Dislocations being linear defects may interact with point defects or with other dislocations. Ferroelectric domain walls are planar defects and typically interact with point defects or grain boundaries while the domain system as a whole generally maintains its more or less ordered substructure within a grain of a ceramic microstructure. This presentation focuses on possible scenarios of interaction of domain walls with defects of different origin fro the experimental point of view and is intended to inspire theoretical work in this field. Examples reach from simple single crystalline uniaxial materials with very low mechanical coupling, single crystals with multiaxial domain systems and high electromechanical coupling to the highly complex features of ceramic ferroelectric material changes during fatigue where a consistently increasing interaction strength of the domain system with defects in encountered.

Switching effects in piezoelectric materials – a micromechanically motivated finite element approach

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Ferroelectric and piezoelectric materials are commonly made of ceramics and widely used for the design of smart materials and intelligent systems as for instance transducers and actuators. Nonlinear response of these engineering materials is experimentally observed under high electromechanical loading. This effect mainly stems from phase transitions which result in spontaneous polarisation and lattice distortion – so-called spontaneous strains. Various micromechanical as well as phenomenological and thermodynamically consistent formulations for the modelling of piezoelectric materials and domain switching have been proposed in the literature; see for instance [2, 3, 5, 6] and references cited therein.

In this contribution, a micromechanically motivated approach is elaborated wherein an electromechanical energy-based switching criterion as advocated by Hwang and McMeeking [4] is adopted. The onset of domain switching is thereby not only initiated by means of the energy criterion itself but additionally combined with a probabilistic model in order to phenomenologically capture intergranular effects; see for instance Arockiarajan et al. [1]. First numerical examples presented in this study address coupled electromechanical loading conditions whereby a rather simple but robust staggered iteration algorithm is applied. Standard volume averaging techniques finally enable the computation of representative hysteresis and butterfly curves which turn out to be in good agreement with experimental data.

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A Robust Adaptive Algorithm for Brittle Fracture based on Incremental Energy Minimization

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The lecture considers a variational formulation of brittle fracture in solids and proposes a numerical implementation by a distinct finite element method. The starting point is a variational setting of fracture mechanics as conceptually oulined by Francfort and Marigo [1998] that recasts a monotonic quasistatic fracture process into a sequence of incremental energy minimization problems. The proposed numerical implementation exploits this variational structure. It introduces discretized crack patterns with material–force–driven incremental crack–segment releases. These releases of crack segments constitute a sequence of positive definite subproblems with successively decreasing overall stiffness, providing an extremely robust algorithmic setting in the postcritical range. The formulation is embedded into an accompanying crack–pattern reorientation procedure with material–force–based indicators. We demonstrate the performance of the proposed algorithmic setting by means of representative numerical simulations.

Micro-mechanical simulation of domain wall motion in ferroelectric materials

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Ferroelectric materials are frequently used in sensor and actuator applications. The long term use in cyclic loading is however limited by the so called 'electric fatigue' effect, see [1]. Under this terminology various micro-mechanical phenomena are summarized. On the macroscopic level a reduction of the mechanical output for a cyclic electric excitation is observed. One of the suspected micro-mechanical mechanisms is the hindering and blocking of domain wall motion within the material. Possible sources of these blocking phenomena are (point) defects in the material. These defects interact with the domain wall (inhomogeneity) and the applied external fields, see [2]. The characterization of these (point) defects is however an experimentally difficult task.
In the presentation the concept of configurational (or material) forces will be used to indentify the energy changes associated with domain wall motion and with defect motion. In the the model system of gadolinum molybdate domain wall motion is experimentally well documented. The numerical simulation is intended to provide a qualitative understanding of the interaction of defects and domain walls for a model system of gadolinium molybdate. The calculation of the driving forces requires the solution of the coupled electro-mechanical field equations. These equations have to take remanent polarisation and remanent strain into account.
A kinetic law based on experimental observations for gadolinum molybdate is used. Simulations for different defect situations show the possible blocking scenarios of 180° domain walls. The numerical results are compared with the experimental observation, which are availible for the chosen model system.

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Homogenization of stratified thermoviscoplastic materials

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In this lecture I will report on joint work with Nicolas Charalambakis. We study the homogenization of the following system of partial differential equations

$$\rho^\varepsilon(x)\frac{\partial v^\varepsilon}{\partial t} - \frac{\partial}{\partial x}\left(\mu^\varepsilon(x,\theta^\varepsilon)\frac{\partial v^\varepsilon}{\partial x}\right) = f,$$

$$c^\varepsilon(x,\theta^\varepsilon)\frac{\partial \theta^\varepsilon}{\partial t} = \mu^\varepsilon(x,\theta^\varepsilon)\left(\frac{\partial v^\varepsilon}{\partial x}\right)^2,$$

posed in $a < x < b$, $0 < t < T$, completed by boundary conditions on v^ε and by initial conditions on v^ε and θ^ε. The unknowns are the velocity v^ε and the temperature θ^ε, while the coefficients ρ^ε, μ^ε and c^ε are data which are assumed to satisfy

$$0 < c_1 \le \mu^\varepsilon(x,s) \le c_2, \quad 0 < c_3 \le c^\varepsilon(x,s) \le c_4, \quad 0 < c_5 \le \rho^\varepsilon(x) \le c_6,$$

$$-c_7 \le \frac{\partial \mu^\varepsilon}{\partial s}(x,s) \le 0, \quad |c^\varepsilon(x,s) - c^\varepsilon(x,s')| \le \omega(|s-s'|).$$

This sequence of one dimensional systems is a model for the homogenization of non-homogeneous, stratified, thermoviscoplastic materials exhibiting thermal softening and temperature dependent rate of plastic work converted into heat.

Under the above hypotheses we prove that this system is stable by homogenization. More precisely one can extract a subsequence ε' for which the velocity $v^{\varepsilon'}$ and the temperature $\theta^{\varepsilon'}$ converge to some homogenized velocity v^0 and some homogenized temperature θ^0 which solve a system similar to the system solved by v^ε and θ^ε, for data ρ^0, μ^0 and c^0 which satisfy hypotheses similar to the hypotheses satisfied by ρ^ε, μ^ε and c^ε. These homogenized data ρ^0, μ^0 and c^0 are given by some explicit (even if sophisticated) formulas. In particular, the homogenized heat coefficient c^0 in general depends on the temperature even if the heterogeneous heat coefficients c^ε do not depend on it.

The extended Korn's first inequality with integrable dislocation density.

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I show a Korn-type inequality with nonconstant coefficients. More precisely let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and let $\Gamma \subset \partial\Omega$ be a part of the boundary with nonvanishing 2-dimensional Hausdorff measure. Define $H^{1,2}_{\circ}(\Omega,\Gamma) := \{\phi \in H^1(\Omega) \mid \phi_{|\Gamma} = 0\}$ and let $F_p \in L^\infty(\Omega, GL(3,\mathbb{R}))$ be given with $\det F_p(x) \geq \mu^+ > 0$. Moreover suppose that $\operatorname{Curl} F_p \in L^1(\Omega, \mathbb{M}^{3\times 3})$ and that F_p is a symmetric matrix. Then

$$\begin{aligned} \exists\, c^+ > 0 \quad & \forall\, \phi \in H^{1,2}_{\circ}(\Omega,\Gamma) : \\ & \|\nabla\phi \cdot F_p^{-1}(x) + F_p^{-T}(x) \cdot \nabla\phi^T\|^2_{L^2(\Omega)} \geq c^+ \, \|\phi\|^2_{H^1(\Omega)} \,. \end{aligned}$$

This result extends earlier results. In [1] it was assumed that F_p is continuously differentiable as well as its curl and in [2] it is assumed that F_p is continuous. In both cases however, no assumption of symmetry for F_p were needed. The new result shows that continuity of F_p is not really necessary. In the future one should be able to remove also the symmetry assumption on F_p. In [2] a counterexample has been given showing that $F_p \in L^\infty(\Omega)$ alone is not sufficient. In this sense, the new result is nearly optimal apart for the symmetry of F_p.

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Regularity of solutions of the homogenized problem in plasticity

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We study regularity properties of solutions of the homogenized problem derived formally from the quasistatic initial boundary value problem which models the deformation behavior of plastic materials with a periodic microstructure. In [3] it is shown that the difference of the exact solution and the special constructed asymptotic solution tends to zero if the lengthscale of microstructure converges to zero. To complete the rigorous justification of the homogenized model it must be shown that the solution of the homogenized problem possesses more regularity than the existence theory for this problem delivers. We use the standard difference-quotient method [4], the existence theory for the quasistatic initial boundary value problem [2], [1], a specially defined operator distance [6] as well as the regularity theory for linear elasticity problem [5] to get the required result.

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Meso-Macro-Modeling of Nonlinear Ferroelectric Ceramics

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The challenge in the field of ferroelectric ceramics is the modeling of complicated interactions between electrical and mechanical properties of the material on the macro scale, caused by switching processes on the micro scale, see e.g. [1]. In this investigation we start on a meso scale, which is defined by domains represented by unit cells of equal spontaneous polarization. On this scale we present a thermodynamically consistent phenomenological model for an assumed transversely isotropic ferroelectric crystal and mainly focus on the hysteresis loops, that occur in the ferroelectric phase, within a certain range of temperature, where the material becomes spontaneously polarized, see [2] and [3]. For this (restricted) material symmetry group there is no ferroelasticity and mechanical depolarization within a mesoscopic cell, as a consequence of the fixed polarization directions. On the macro scale a remanent polarization and remanent strains, due to the reorientation of the polarization in consequence of domain wall motions, are observed, if an electric field above the so-called coercive field is applied. In order to describe the polycrystalline material behavior we use a simple homogenization procedure that is performed over a representative microstructure, which is assumed to consist of individual grains with individual domains. This simple transition procedure is based on discrete orientation distribution functions in order to approximate the different domains. The main equations of the mesoscopic boundary value problem are the balance of momentum and the Gauss law respectively. The boundary conditions on this scale are derived from a generalized macrohomogenity condition, which equates the macroscopic and the mesoscopic electro-mechanical work. The anisotropic behavior is governed by isotropic tensor functions, which satisfy automatically the symmetry relationships of the considered body and which are formulated in terms of a finite set of invariants, see [4].

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Shape memory and superelastic effects of cyclic martensitic phase transformations in monocrystals – Computational and experimental results

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The classic geometrically linear C^1-continuous thermomechanical macro model is used based on Bain´s principle and represented by a unified Lagrangian functional including phase evolution equations with mass conservation and quasi-convexification during phase transformation processes [1]. Iterative time integration of the evolution equation was programmed in C++ and implemented into the UMAT-interface of the Finite Element program Abaqus in which spatial 3D-tetrahedral elements are used [2].
A special feature is the likewise analysis of shape memory and superelastic effects of $Cu_{82}Al_{14}Ni_4$ monocrystals [2], for which reliable expermental measurements are available in [3].
Comparisons show good agreement of computed and measured data in general and the important result that the macro-analysis of shape memory effects yields upper bounds of the measured stress-strain curves with complicated "yield tooth" properties (irregular zig-zag curves).

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Statistical and continuum thermodynamic models for continuum dislocation dynamics with application to extended crystal plasticity

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Most size-dependence-based extensions to phenomenological and crystal plasticity (e.g., Svendsen, 2000, Gurtin, 2002, Svendsen, 2002, Acharya, 2004) as well as many micromechanical ones (e.g., Evers *et al.*, 2004), are based on the premise that characteristic material lengthscales mediating the interaction of microstructural and continuum processes are independent of state. More fundamental considerations show, however, that this is not the case (e.g., Groma *et al.*, 2003). Indeed, such lengthscales depend for example on the dislocation density. In the current work, continuum dislocation dynamics and statistical mechanics are used to obtain at the glide-system level a non-local model for additional kinematic-like hardening due to an inhomogeneous distribution of excess dislocations. In particular, the corresponding characteristic lengthscale depends on the total dislocation density. Applications to large-deformation crystal plasticity will be discussed.

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