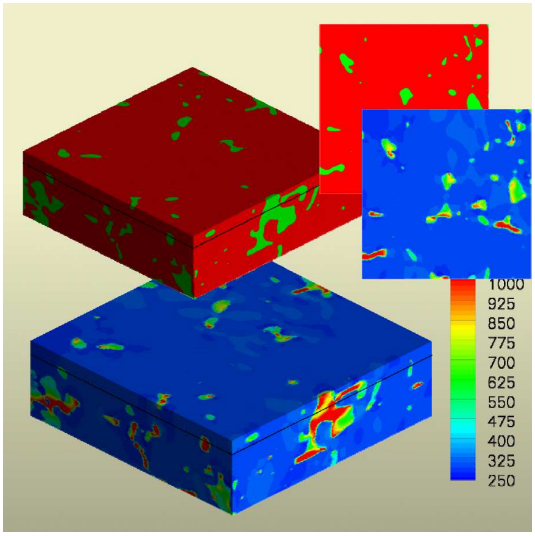
University of Duisburg-Essen

11th. GAMM-Seminar on Microstructures

Program



UNIVERSITÄT DUISBURG ESSEN

January 20-21, 2012

Organizers:
J. Schröder, P. Neff, D. Balzani

Welcome

to the

11th GAMM-Seminar on Microstructures

Dear participant,

we are glad to welcome you at the 11th GAMM-Seminar on Microstructures at the University of Duisburg-Essen.
After the fifth GAMM Seminar on Microstructures in January 2006 we meet in Essen again 6 years later. With its 11th Seminar our conference is becoming nearly a tradition. Still, we have had more applicants for presentations than available time slots. This shows that the topic of our meeting is still of ongoing interest.
We wish us all a pleasant stay with productive discussions and presentations of high scientific impact.

The Organizers

Jörg Schröder
Patrizio Neff
Daniel Balzani

Miscellaneous

Objectives of the Seminar

The seminar will focus on various aspects of microstructures in solid mechanics, material science and applied mathematics:

- theoretical and computational modelling of materials with evolving microstructures (plasticity, damage, phase transitions, electro-magneto-mechanics, thin walled structures, films, dislocations, ...),
- experimental results on the formation and evolution of microstructure (lamination, phase transformation, ...),
- mathematical analysis, variational formulation, asymptotic analysis, homogenization and relaxation methods, non-convex problems,
- multiscale methods and other computational tools for the determination of effective properties of micro-heterogeneous materials.

The seminar is intended to give the opportunity to discuss and compare different approaches to the above areas as well as to stimulate and create perspectives for future research. It provides a platform for the interaction among young and established researchers in solid mechanics, mathematics and material science.

Organizers

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Local Organizing Team

Dominik Brands, Joachim Bluhm
Institute of Mechanics, University Duisburg-Essen
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45117 Essen, Germany

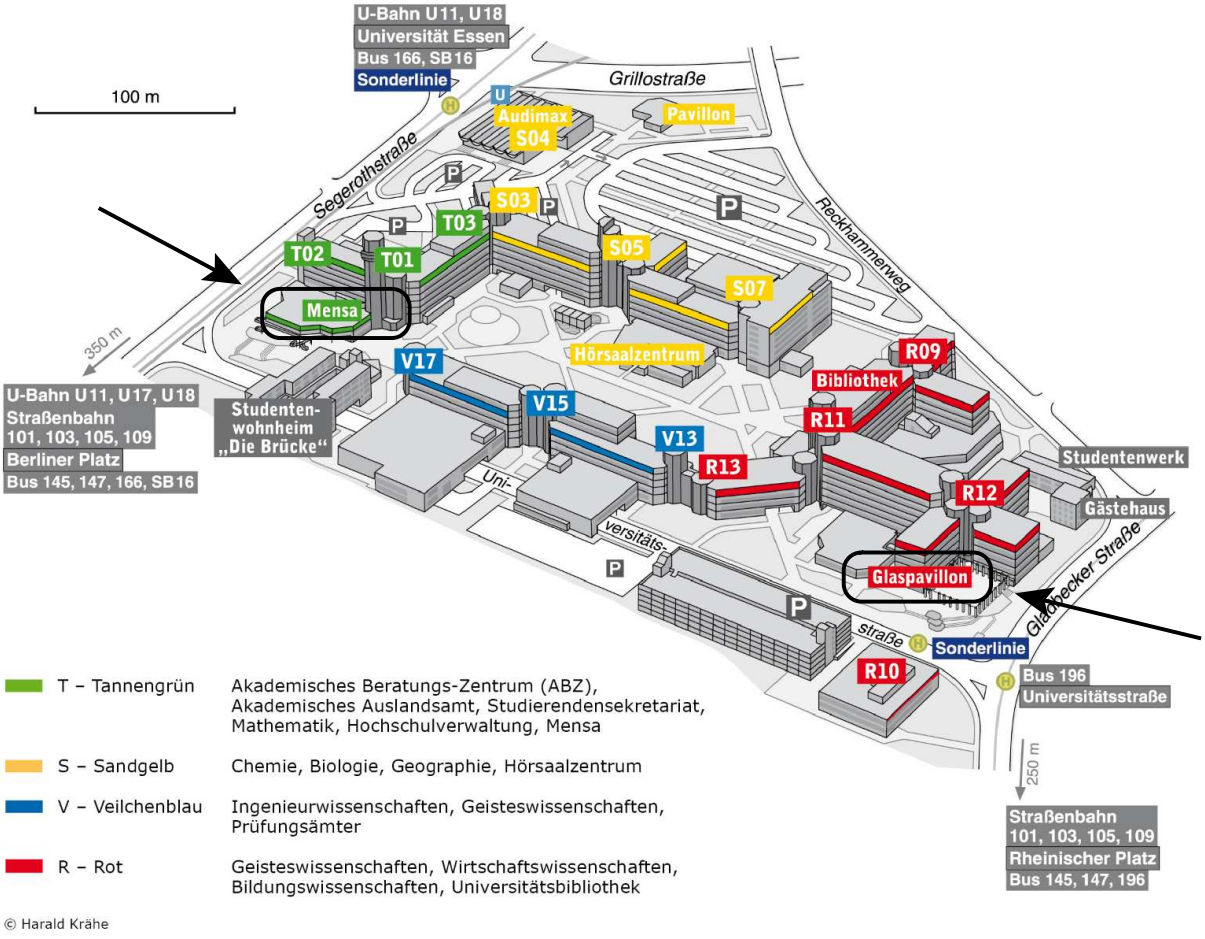
Venue

The seminar is to be held in the

"Glaspavillon der Universität Duisburg-Essen" (R12 S00 H12),
Universitätsstraße 12, 45141 Essen

in the "red-building" area at the Campus Essen of the University of Duisburg-Essen, see map of Campus Essen below. The Essen Campus is located centrally in the city. within 20 minutes walking distance from the central railway station. Essen, an important city in the Rhine/Ruhr region, is connected through an extensive road transport network to all cities in Germany and Europe and is easily accessible from all directions by railroad and air. For detailed travel information, please refer to the route description at
`http://www.uni-due.de/de/universitaet/orientierung.php`.

Map of Campus Essen



Local Transportation

Public local traffic is provided by the “Verkehrsverbund Rhein-Ruhr”,
`http://www.vrr.de/de/index.html`

Accomodation

For accommodation we recommend three hotels in the centre of Essen. For more information please visit the seminar homepage. The participants are responsible for making their reservations.

Insurance

Participants are responsible for their own insurance. The organizers cannot be held liable for any damages, losses or accidents occurring during the journey to/from Essen or during the seminar. All guests participate at their own risk.

Language

The official language of the seminar is German or English. The presentations should be given in English; however, lectures in German are also permitted.

Presentation Duration

Each lecture is expected to last 30 minutes including discussion time.

Presentation Facilities

The lecture room will provide video beamer, overhead projector, and internet access.

Homepage of the Seminar

`http://www.uni-due.de/mechanika/gamm_micro_2012.shtml`

Lunch break

Friday, January 20th, 13:00-14:00

For your convenience we reserved a special area in the “Hauptmensa”, which is located (upstairs) in the “green-building” area at the Campus, see map of Campus.

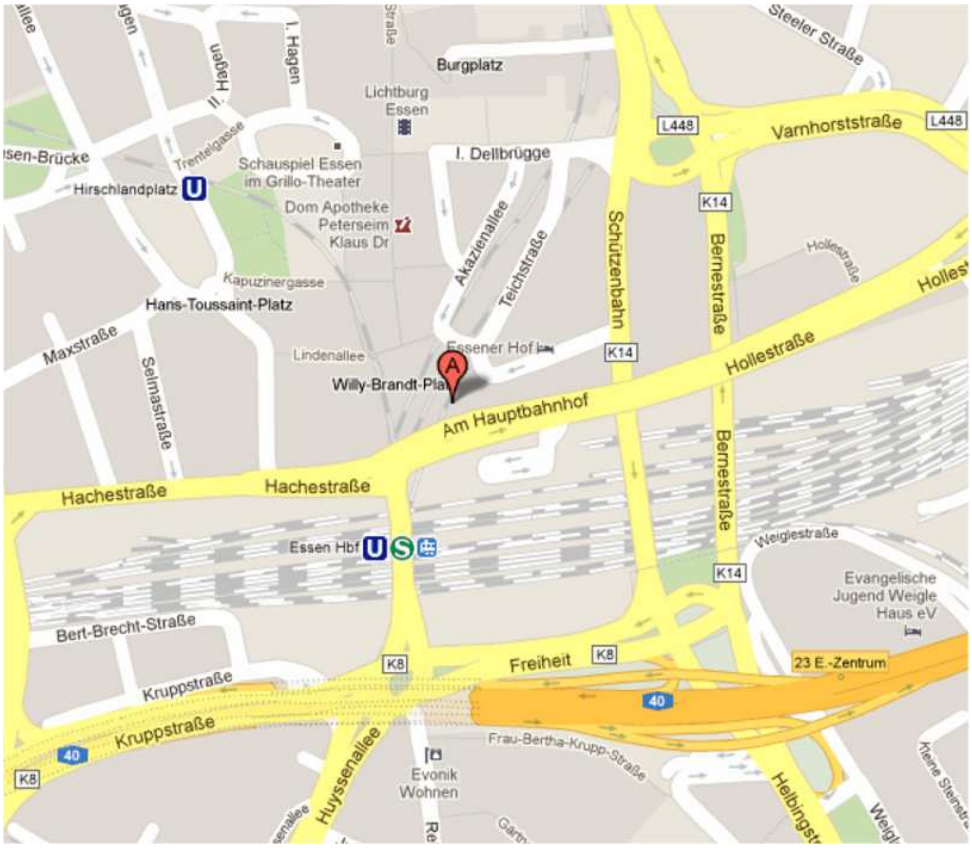
Saturday, January 21th, 13:30-14:30

A farewell lunch is arranged at the seminar venue.

Social Events

Friday, January 20th, 20:00
Conference dinner at the “Handelshof Restaurant” of the “Mövenpick Hotel Essen” in the centre of Essen.

Mövenpick Hotel Essen
Am Hauptbahnhof 2
45127 Essen
`http://www.moevenpick-hotels.com/de/pub/hotels_resorts/worldmap/essen/willkommen.cfm`



Location of “Handelshof Restaurant” (A)

“Mövenpick Hotel Essen” and “Handelshof Restaurant”

Program

Friday, January 20

Registration 8:00 – 8:25

Welcome by the Organizers 8:25 – 8:30

8:30 – 10:00, Plenary lectures, Chair: J. Schröder

M. Geers (8:30 – 9:15)
Microstructural patterning in time-dependent non-convex crystal plasticity

A. Raoult (9:15 – 10:00)
Homogenized and non-homogenized equivalent lattice models

10:00 – 11:00, Chair: P. Neff

H.D. Alber (10:00 – 10:30)
A phase field model for phase evolution in a material with three phase states

M. Kružik (10:30 – 11:00)
Domain patterns and hysteresis in phase-transforming solids: analysis and numerical simulations of a sharp interface dissipative model via phase-field approximation

Coffee break 11:00 – 11:30

11:30 – 13:00, Chair: T. Bartel

M. Sabeel Khan, K. Hackl (11:30 – 12:00)
Development of microstructure in a micropolar continuum as a consequence of energy relaxation

C. Kreisbeck, S. Conti, G. Dolzmann (12:00 – 12:30)
Relaxation of models in finite plasticity with two active slip systems

D. Pauly, P. Neff, K.-J. Witsch (12:30 – 13:00)
Poincaré meets Korn via Maxwell: On Korn's first inequality for incompatible tensor fields

Lunch break 13:00 – 14:00

14:00 - 16:00, Chair: S. Conti

B. Klusemann, B. Svendsen (14:00 – 14:30)
Application of gradient plasticity and non-convexity to the modeling and simulation of microstructure evolution

M. Redeker (14:30 – 15:00)
An adaptive two-scale model for phase transitions with evolution of equiaxed dendritic microstructures

M. Goodarzi, K. Hackl (15:00 – 15:30)
On surface energies and twinning geometry in martensite

A. Khorashadizadeh, D. Raabe (15:30 – 16:00)
Exploring the formation of different lamination configurations within the orientation space

Poster Session 16:00 – 16:30

Coffee break 16:30 – 17:00

17:00 - 18:30, Chair: G. Dolzmann

C.I. Zeppieri, L. Scardia (17:00 – 17:30)
Line-tension model as the Γ–limit of a nonlinear dislocation energy

D. Cioranescu, A. Damlamian, J. Orlik (17:30 – 18:00)
Homogenization via unfolding in periodic elasticity with contact on closed and open cracks

S. Heinz (18:00 – 18:30)
Quasiconvexity equals rank-one convexity for isotropic sets of 2×2 matrices

Meeting of GAMM activity group "Analysis of Microstructures" 18:30 – 19:30

Dinner 20:00 – 23:00

Saturday, January 21

8:45 – 9:30, Plenary lecture, Chair: P. Neff

M. Lewicka
Elasticity of prestrained structures

9:30 – 11:00, Chair: R. Müller

E. Stein, T. Gerasimov, S. Löhnert, M. Rüter (9:30 – 10:00)
Error-controlled multiscale XFEM for crack propagation at macro-scale and crack initiation at micro-scale of ceramic materials

V.A. Eremeyev, H. Altenbach (10:00 – 10:30)
On the theories of plastes and shells with microstructure

C. Carstensen, G. Dolzmann (10:30 – 11:00)
Adaptive FEM for some nonconvex double-well minimisation problem

Coffee break 11:00 – 11:30

11:30 - 13:30, Chair: A. Menzel

J. Spahn, S. Staub, M. Kabel, R. Müller, H. Andrä (11:30 – 12:00)
A micromechanical damage model for fiber-reinforced polymer materials

S. Bargmann, H. Seddik, R. Greve (12:00 – 12:30)
Computational modeling of the influence of heterogeneous microstructure on the deformation process of polar ice

I. Münch, M. Krauß, W. Wagner (12:30 – 13:00)
Ferroelectric nano-generators for energy harvesting

S. Klinge, A. Bartels, K. Hackl, P. Steinmann (13:00 – 13:30)
Single- and multiscale aspects of modeling curing polymers

Farewell lunch 13:30 – 14:30

Presentation Abstracts

A phase field model for phase evolution in a material with three phase states

Hans-Dieter Alber

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Metallic materials often show more than two phase states with different crystal structures. These phase states correspond to different minima of the stored energy. As a model one could use the time dependent elasticity equations corresponding to such energies. However, the resulting partial differential equations form a quasilinear hyperbolic system. Little is known about the solution of such systems in higher space dimensions.
As an alternative approach we present a model, which consists of the equations of linear elasticity coupled with evolution equations for two order parameters S_1, S_2. The three phase states correspond to the values $(0,0)$, $(1,0)$ and $(1,1)$ of the pair (S_1, S_2) of order paramters. The evolution equations are chosen such that the second law of thermodynamics is satisfied and such that to every of the three possible phase transitions there exists a diffusive phase interface, which approximates a sharp interface, that is driven by the jump of the Eshelby tensor corresponding to the respective phase transition. These evolution equations are based on the hybrid phase field model [1].

References

[1] H.-D. Alber, Peicheng Zhu: *Comparison of a rapidely converging phase field model for interfaces in solids with the Allen-Cahn model.* Submitted. Preprint **2631**, Fachbereich Mathematik, Technische Universität Darmstadt (2011).

Computational modeling of the influence of heterogeneous microstructure on the deformation process of polar ice

Swantje Bargmann*, Hakime Seddik** and Ralf Greve**

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In this contribution we model the anisotropic flow in polar ice in order to gain a better understanding for the underlying microstructure and its influence on the deformation process. In particular, a continuum mechanical, anisotropic flow model, which is based on an anisotropic flow enhancement factor, the so-called CAFFE model, is applied. The polycrystalline ice is regarded as a mixture whose grains are characterized by their orientation. The approach is based on two distinct scales: the underlying microstructure influences the macroscopic material behavior and is taken into account phenomenologically. To achieve this the orientation mass density is introduced as a so called mesoscopic field. The classical flow law of Glen is extended by a scalar enhancement factor. Moreover, four different effects (local rigid body rotation, grain rotation, rotation recrystallization, grain boundary migration) influencing the evolution of the grain orientations are taken into account. A finite volume method is chosen for the discretization procedure. Numerical results simulating the ice flow in the EPICA ice core EDML, Antarctica, are presented.

References

[1] S. Bargmann, H. Seddik, R. Greve: *Computational modeling of flow-induced anisotropy of polar ice for the EDML deep-drilling site, Antarctica: the effect of rotation recrystallization and grain boundary migration*, International Journal for Numerical and Analytical Methods in Geomechanics, accepted for publication, DOI: 10.1002/nag.1034, 2011.

[2] L. Placidi, R. Greve, H. Seddik, S. Faria. *A continuum-mechanical, anisotropic flow model for polar ice, based on an anisotropic flow enhancement factor*, Cont. Mech. Thermodyn. 2009; doi: 10.1007/s00161-009-0126-0

[3] H. Seddik, R. Greve, L. Placidi, I. Hamann, O. Gagliardini. *Application of a continuum-mechanical model for the flow of anisotropic polar ice to the EDML core, Antarctica*, J. Glaciology 2008, 45(187):631-642.

Adaptive FEM for some Nonconvex Double-Well Minimisation Problem

Carsten Carstensen, Georg Dolzmann

The presentation concerns ongoing joint research on advanced and nonstandard finite element simulations in the calculus of variations. The relaxation of a commonly used model problem in the analysis of solid solid phase transitions leads to a variational problem with a quasiconvex energy density which fails to be convex. This paper presents the first convergence result for an adaptive algorithm for the computation of minimizers in finite element spaces with Courant elements and with successive loops of the form SOLVE-ESTIMATE-MARK-REFINE. The proof relies on the decomposition of the energy into a degenerate convex energy which allows convexity control in the sense of Carstensen (IMA J Numer Anal 2008) and a polyaffine energy. Convergence of the energy of the approximating deformations and strong convergence of some components of the deformation gradients is established.

On the Theories of Plates and Shells with Microstructure

Victor A. Eremeyev, Holm Altenbach

Applications of such microstructured materials as foams in thin-walled elements find wide applications in engineering. In the literature various models of materials with microstructure are suggested, see for example [1]. Various generalized 2D models of plates and shells are discussed in [2]. Here we derive 2D plate and shell equations made of material with microstructure. The following models of materials are considered:

1. Micropolar materials,
2. Micromorphic materials, and
3. Materials of second-grade.

The main goal of the lecture is to investigate how 2D equations of plates and shells inherit the generalized properties of the 3D continuum. We use the through-thickness procedure and the global form of the balances of momentum and moment of momentum to reduce the equilibrium/motion equations of the 3D continuum with microstructure to 2D equations of shell theory. For simplicity we start from the plate theory and then we generalize the results to the case of shells.

References

[1] Eringen, A.C.: *Microcontinuum Field Theory. I. Foundations and Solids*, Springer, 1999.

[2] Altenbach J., Altenbach H., Eremeyev V.A.: *On generalized Cosserat-type theories of plates and shells. A short review and bibliography*, Archive of Applied Mechanics, 80:73-92, 2010.

Microstructural patterning in time-dependent non-convex crystal plasticity

M.G.D. Geers, T. Yalcincaya and W.A.M. Brekelmans

Microstructures in materials generally originate from a non-convex free energy, whereby the evolution is controlled by the kinetics underlying the physical processes governing the patterning. Special examples thereof are microstructures in metals and dislocation microstructures in particular, which have been an interesting research topic for the materials science community for decades.
This paper analyses the intrinsic role of non-convexity in the formation and evolution of deformation microstructures, in close comparison to classical phase field approaches for microstructure evolution. Special emphasis is given on the role of kinetics that control the time-dependent evolution in a deformation microstructure. For this purpose, a non-convex rate dependent strain gradient plasticity framework is used to recover plastic slip patterning in metal crystals. The non-convexity is treated as an intrinsic property of the free energy of the material. Departing from explicit expressions for the free energy and the dissipation potential, the non-convex strain gradient crystal plasticity model is derived in a thermodynamically consistent manner, including the accompanying slip law. For the numerical solution of the problem, the displacement and the plastic slip fields are considered as primary variables. These fields are determined on a global level by solving simultaneously the linear momentum balance and the resulting slip evolution equation. The slip law differs from classical ones in the sense that it naturally includes a contribution from the non-convex free energy term, which enables patterning of the deformation field. The formulation of the computational framework is partially dual to a Ginzburg Landau type of phase field modeling approach. The essential difference resides in the fact that a strong coupling exists between the deformation and the evolution of the plastic slip, whereas in the phase field type models the governing fields are only weakly coupled. The derivations and implementations are first done in a transparent 1D setting [1], which allows for a thorough mechanistic understanding. The extension to 2D and multiple slip is presented as well, whereby the non-convexity originates from the slip system interaction.

References

[1] T. Yalcincaya, W.A.M. Brekelmans, M.G.D. Geers: *Deformation patterning driven by rate dependent non-convex strain gradient plasticity*, Journal of the Mechanics and Physics of Solids, 59:1-17, 2011.

On surface energies and twinning geometry in martensite

Mehdi Goodarzi, Klaus Hackl

Martensitic materials, whose characteristic laminate microstructure is the consequence of a symmetry-breaking solid-to-solid phase transformation, can be well understood within a continuum mechanical framework by investigating energetically favorable configurations of twin-compatible variants. We present a micromechanical model built upon this approach.
In this model, a specific class of laminate geometries is constructed based on coherence condition allowing for curved twin interfaces as well as three-dimensional aggregates. Then suitable ansatzes for twin interface and grain boundary energies are proposed based on scaling arguments. Afterwards we look into energy minimizing geometries within the class of morphologies we considered.
Our model successfully reproduces various empirical observations and theoretical predictions in the preceding works of Kohn, Müller, Otto, James and others. Most notably, the model is capable of reflecting the scale properties and size effects in the microstructure. It also simulates the accommodation by branching and twin refinement near the boundaries.

References

[1] R.V. Kohn, F. Otto: *Small Surface Energy*, Physica D, 107:272-289, 1997.

[2] R.V. Kohn, S. Müller: *Surface Energy and Microstructure*, Communications on Pure and Applied Mathematics, 47:405-435, 1994.

[3] K. Hackl, et al.: *Surface energies and size-effects,* Materials Science and Engineering A, 378:499-502, 2004.

Quasiconvexity equals rank-one convexity for isotropic sets of 2×2 matrices

Sebastian Heinz

We study quasiconvexity in the calculus of variations, which was introduced by Morrey [1]. Our particular interest lies in finding the quasiconvex hull for a given set K. From a solid mechanics point of view, K may represent the ensemble of deformation gradients that are favourable on the microscopic scale. Then the quasiconvex hull of K contains what is favourable on the macroscopic scale. In the planar case and under the additional assumption of material isotropy, we give an explicite characterization of the quasiconvex hull. In order to formulate our result mathematically, let K be a compact set of real 2×2 matrices that is isotropic, meaning invariant under the left and right action of the special orthogonal group. Then we prove that the quasiconvex hull of K coincides with the rank-one convex hull (and even with the lamination convex hull of order 2). In particular, there is no difference between quasiconvexity and rank-one convexity for K. This is a generalization of a result for connected sets by Conti, De Lellis, Müller and Romeo [2]. Our proof relies on the work by Faraco and Székelyhidi [3].

References

[1] Charles B. Morrey: *Quasi-convexity and the lower semicontinuity of multiple integrals*, Pacific J. Math., 2:25–53, 1952.

[2] Sergio Conti, Camillo De Lellis, Stefan Müller, Mario Romeo: *Polyconvexity equals rank-one convexity for connected isotropic sets in* $\mathbb{M}^{2\times2}$, C. R. Acad. Sci. Paris, Sér. I, 337(4):233–238, 2003.

[3] Daniel Faraco, László Székelyhidi: *Tartar's conjecture and localization of the quasiconvex hull in* $\mathbb{R}^{2\times2}$, Acta Math., 200(2):279–305, 2008.

Single- and multiscale aspects of modeling curing polymers

Sandra Klinge, Alexander Bartels, Klaus Hackl and Paul Steinmann

The curing of polymers is a complex process characterized by different phenomena such as an increasing stiffness and viscosity, volume shrinkage and isochoric material behavior. In order to simulate the mentioned process we propose a continuum mechanical model based on an assumption for free energy consisting of two parts. The first part is related to the total deformations and denoted as the equilibrium part. It has the form of a convolution integral including the influence of the time dependent material parameters. Accordingly, the equilibrium part of the free energy can be interpreted as the accumulated energy while the strain energy is rather related to the current state of deformation and thus used for the definition of the instantaneous stiffness. The second part of the free energy is related to the viscous deformations and referred to as the non-equilibrium part. This part of the model depends on the constant material parameters. The model can also be used for the simulation of polymers showing the isochoric material behavior at some stage of curing. To this end both parts of the energy are additionally split into a deviatoric and a volumetric part. Further, a multifield formulation depending on the deformations, the volume change and the hydrostatic pressure, is introduced.
As an additional aspect, the presentation considers the modeling of microheterogeneous polymers based on the application of the multiscale finite element method. This numerical homogenization approach is suitable for the modeling of heterogeneous materials with a highly oscillatory microstructure. It mainly shows one important advantage: It can be easily applied for the simulation of the material and the geometrical nonlinearity. The numerical examples presented in the course of the presentation are focused on the influence of the changeable material parameter on the stress state as well as on the influence of the material incompressibility. The multiscale concept is used for the simulation of the curing of reinforced polymers.

Application of gradient plasticity and non-convexity to the modeling and simulation of microstructure evolution

Benjamin Klusemann and Bob Svendsen

During loading of real (i.e., materially heterogeneous) metallic materials, local microscopic stress concentration activates individual microscopic defects (e.g., dislocations) in the material, resulting in a spatially heterogeneous plastic strain. During this process most metals form cellular dislocation structures, e.g. dislocation cells and dislocation walls. In general, this will take place in the material ”long” before the macroscopic activation or yield threshold is reached.
Only when a sufficient ”critical” number of such defects are activated, do they collectively breakthrough to the macroscopic level, resulting, e.g., in macroscopic yield and macroscopic stress relaxation. As is well-known, one way to model such emergent behavior in many physical systems and contexts is with the help of phase-field methods and non-convexity. Several sources of non-convexity are known in material science, e.g., dislocation-lattice interaction, glide-system interaction or large deformation. As very simple non-convex energy forms we examine polynomial-based Landau-Devonshire type forms such as that examined recently by Yalcinkaya et al.[1] and Klusemann et al.[2], as well as periodic forms such as the Frenkel form. The purpose of this work is the modeling of microstructure evolution with gradient plasticity via energetic non-convexity. To this end, a model formulation based on continuum thermodynamics and rate-variational methods is presented.

References

[1] T. Yalcinkaya, W. Brekelmans, M. Geers: *Deformation patterning driven by rate dependent non-convex strain gradient plasticity*, Journal of the Mechanics and Physics of Solids, 59:1-17, 2011.

[2] B. Klusemann, S. Bargmann, B. Svendsen: *Comparison of two formulations for the initial-boundary-value problem of a non-convex gradient inelasticity model*, Computational Materials Science, submitted for publication, 2011.

Exploring the formation of different lamination configurations within the orientation space

Anahita Khorashadizadeh, Dierk Raabe

The formation of laminated microstructures is only favorable under certain conditions. In this study we perform shear experiments on copper single crystals of different orientations to explore the formation of laminated microstructure. In our investigations the shear experiments were conducted along with the digital image correlation which made it possible to determine the exact macroscopic state of the deformed samples. The band-like microstructures have been investigated using high-resolution back scatter diffraction method. The topography of the dislocation structure within the orientation patterned areas was observed using the electron channeling contrast imaging. The study of the dislocation structure is of great importance as it gives an insight into the mechanisms of dislocation walls generation and their relation to the formation of the laminates. This work demonstrates the configuration of the laminated structure in two different copper single crystals after shear experiments.

Relaxation of models in finite plasticity with two active slip systems

Carolin Kreisbeck, Sergio Conti and Georg Dolzmann

Modern mathematical approaches to plasticity result in non-convex variational problems for which the standard methods of the calculus of variations are not applicable. In this contribution we investigate the macroscopic material response of a variational model in geometrically non-linear elasto-plasticity with two active slip systems, rigid elasticity, and linear self-hardening. In particular, an explicit formula for the relaxation of the underlying energy density is given, both in the two-dimensional and a related three-dimensional setting [1].
One observes that the relaxation mechanism is identical to the one derived in the regime with only one active slip system [2]. Due to the presence of a second slip systems, however, the effective material behavior is softer and the relaxed energy is finite for all volume preserving deformations. In contrast to two-slip models without hardening, where laminates of infinite order are needed to carry out the relaxation process [3], the essential tool for the treatment of the models with hardening is the construction of a first-order laminate. This allows to predict a microstructure that realizes the effective energy in the system and could be experimentally verified.
Finally, we show that the assumption of elastically rigid material behavior is justified since models with rigid elasticity can be obtained as Γ-limits of models with finite elastic energy for diverging moduli of elasticity.

References

[1] Conti, S., Dolzmann, G. and Kreisbeck, C.: *Relaxation of a model in finite plasticity with two slip systems*, in preparation.

[2] Conti, S., Dolzmann, G. and Kreisbeck, C.: *Asymptotic behavior of crystal plasticity with one slip system in the limit of rigid elasticity*, SIAM J. Math. Anal. **43** (2011), pp. 2337-2353.

[3] Albin, N., Conti, S. and Dolzmann, G.: *Infinite order laminates in a model in crystal plasticity*, Proc. Roy. Soc. Edinburgh Sect. A, **139** (2009), pp. 685-708.

Domain patterns and hysteresis in phase-transforming solids: analysis and numerical simulations of a sharp interface dissipative model via phase-field approximation

Martin Kružík

We propose a sharp-interface model which describes rate-independent hysteresis in phase-transforming solids (such as shape memory alloys) by resolving explicitly domain patterns and their dissipative evolution. We show that the governing Gibbs' energy functional is the Γ-limit of a family of regularized Gibbs' energies obtained through a phase-field approximation. This leads to convergence of the quasistatic evolutions associated with the regularized energy to the ones corresponding to the sharp interface model. Based on this convergence result, we propose a solution algorithm which allows us to perform numerical simulations of mechanical experiments for both spatially homogeneous and heterogeneous samples. This is a joint work with A. DeSimone (SISSA Trieste).

Elasticity of prestrained structures

Marta Lewicka

This talk will concern the analysis of elastic bodies which exhibit residual stress at free equilibria. Examples of such structures arise due to a range of causes: inhomogeneous growth, plastic deformation, swelling or shrinkage driven by solvent absorption. The mathematical description departs from the model of 3d non-Euclidean elastic energy, which measures the deficit of the metric induced by a deformation from a given Riemannian metric with non-zero curvature.
I will discuss different adaptations of the classical variational nonlinear elasticity theory results to the present setting taking into account the prestraining. These will include: scaling laws for thin films, dimension reduction, and atomistic to continuum derivation.

Ferroelectric nano-generators for energy harvesting

Ingo Münch, Matthias Krauß and Werner Wagner

We investigate the behavior of epitaxial sputtered ferroelectric thin films with uniform lattice orientation for the design of nano-generators to convert mechanical into electrical energy. It is important to choose an appropriate substrate which prestresses the ferroelectric material by slightly different crystal lattice parameters to enforce energy conversion. Further, the $\mathrm{BaTiO_3}$ film needs to be structured and assembled via top electrodes. At least, a base allows for mechanical loading.

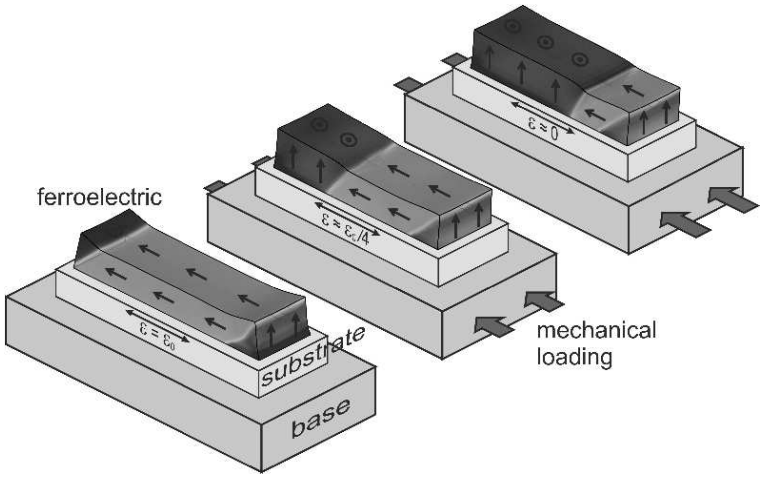

Figure 1: Domain evolution for epitaxial strain ε_0 and uniaxial loading of base.

Due to mechanical cycle load there is need for an electrical circuit to transform single-phase alternating current into co-current flow. Our numerical formulation bases on an electro-mechanical phase-field model with polarization as state variable. The complex boundary conditions are considered within the finite element formulation. The systems accounts for mechanical prestress via substrate elements. As the electrical circuit influences the efficiency of the energy harvesting process characteristics of electrodes, capacitors and diodes are incorporated. Naturally, the generators exhibit a favorable working point.

References

[1] 1. Münch, I., Krauß, M., Landis, C.M., Huber, J.E.: *Domain engineered ferroelectric energy harvesters on a substrate*, Journal of Applied Physics, 109(10), 104106, 2011.

Poincaré meets Korn via Maxwell: On Korn's First Inequality for Incompatible Tensor Fields

Dirk Pauly, Patrizio Neff and Karl-Josef Witsch

We prove a Korn-type inequality in $\mathsf{H}(\mathrm{Curl},\Omega)$ for tensor fields T defined on a bounded N-dimensional domain Ω with Lipschitz boundary. For gradient tensor fields $T=\nabla v$ the estimate reduces to a generalized version of Korn's first inequality, whereas for skew-symmetric tensor fields $T=\mathrm{skew}\,T$ Poincare's inequality is recovered.
Applications are, among others, gradient plasticity theory, micromorphic models and dislocation theory.

Homogenization via unfolding in periodic elasticity with contact on closed and open cracks

D. Cioranescu, A. Damlamian, J. Orlik

In this paper, we consider the elasticity problem in a heterogeneous domain with $\varepsilon-$periodic micro-structure, $\varepsilon << 1$, including a multiple micro-contact between the structural components. The structural components are a simply connected matrix domain with open cracks, or inclusions, completely surounded by cracks, which do not connect the boundary. The contact is described by the Signorini and Treska-friction contact conditions. In the case, when inclusions are compleately surounded by cracks, they can have rigid displacements. In this case, in order to obtain the preliminary estimates for the solution in the ε-domain, the known Korn's inequality should be modified for these inclusion domaines, first in the fixed context and then for the ε-dependent periodic case. Additionally, for all states of the contact (inclusions can freely move, or are locked / sticked to the interface with the matrix, or the frictional traction is achieved on the inclusion-matrix interface and the inclusions can slide in the tangential to the interface direction) the uniform in ε estimates for the solution in the ε-domain is obtained.
An asymptotic analysis for the non-linear functionals over the growing as $\frac{1}{\varepsilon}$ interface is based on the application of the periodic unfolding strategy ([1],[2]) for sequences of jumps in the solution on the oscillating interface, implying their two-scale convergence. Furthermore, this implies the weak convergence of the nonlinear continuous convex functions applied to these interface jumps.

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Homogenized and non homogenized equivalent lattice models

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We will discuss results that were recently obtained in collaboration with Hervé Le Dret (Part 1) or with Nicolas Meunier and Olivier Pantz (Part 2). In both cases, we aim at deriving an equivalent continuum model for a lattice by letting the rest length go to 0.
Hexagonal lattices are examples of complex lattices (their nodes cannot be generated by the translation of two vectors). We follow a classical description by separating nodes in two groups. For pair interactions between adjacent nodes, we are able to prove convergence towards a Min problem whose stored energy density is a homogenized energy ([1]). This density is obtained in three steps: first, we write the discrete lattice energy under an integral form that uses a piecewise affine deformation associated with nodes 1 and a piecewise constant increment that allows to take nodes 2 into account, second we minimize the local energy with respect to the increment (thus obtaining an expression close to Cauchy-Born formulas), third we homogenize over an infinite number of multiples of the unit parallelogram. Let us mention that some arguments are reminiscent of [2] and that related results can be found in [3].
Another topic we are interested in is a proper way of dealing with an energy accounting for changes in angles (for instance, when pairs of bars interact through a spring). For a square lattice whose all pairs of bars interact, we show ([4]) that for compatible local energies the limit stored energy density can be obtained by a mere quasiconvexification formula and that Cauchy-Born rule holds true.

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An Adaptive Two-Scale Model for Phase Transitions with Evolution of Equiaxed Dendritic Microstructures

Magnus Redeker

We develop a fast and accurate adaptive algorithm that numerically solves a two-scale model describing a phase transition of a binary mixture with the evolution of equiaxed dendritic microstructures.

The two-scale model consists of a macroscopic heat equation and a family of microscopic cell problems that model the phase transition of a binary mixture. Both scales are coupled; the macroscopic temperature influences the evolution of the microstructure and the microscopic fields enter to the macroscopic heat equation via averaged coefficients. Adaptivity exploits the fact that the evolving microstructure depends in a continuous way on the macroscopic temperature field; we use the same microscopic data for macroscopic nodes with similar temperature evolutions. We define a metric that compares temperature evolutions and invent adaptive strategies to select active macroscopic nodes. Microscopic cell problems are solved for active nodes only; microscopic data in inactive nodes is approximated from microscopic data of active nodes with similar temperature evolution. The set of active nodes is updated online: it is coarsened until all active nodes have different temperature evolutions and it is refined until every inactive node has at least one active node with a similar temperature evolution.

We present numerical examples which show that the adaptive method is almost as accurate as the direct solution of the two-scale model while being computationally much more efficient.

A micromechanical damage model for fiber-reinforced polymer materials

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Fiber-reinforced polymers exhibit a complex micro structure and thus their mechanical behavior depends on the local fiber orientation distribution, the fiber volume fraction, the geometrical structure of the fibers and as well as on the mechanical properties of the fibers and the polymer matrix itself. Furthermore, failure and progressive damage of fiber-reinforced materials occur as the result of a variety of complex microstructural damage mechanisms such as fiber breakage, fiber pull-out or matrix cracking. In order to predict the macroscopic response of the material in a proper way, one has to consider these microstructural effects, see e.g. [1].
In the work at hand, a micromechanical continuum damage model (CDM) is developed which firstly predicts progressive matrix damage and secondly indicates the fiber pull-out due to localization effects in the surroundings of inclusions. In the framework of a multi-scale approach the model can further be used to detect critical microscopic points under uncritical cyclic loading conditions applied on the macro scale. This yields a progressive macroscopic reduction of stiffness and thus a reduction of the durability. Instead of relying on deterministic failure criteria on the composite level, the model is applied on discrete phases and thus only assumptions for the single constituents have to be made. In order to discretize the microstructure, a robust meshing ansatz is used, which in particular is suitable for generating meshes from 3D computer tomography images, see [2]. On the statistical volume elements the so-called μFE-simulations are carried out by the software FeelMath (Finite Elements for elastic Materials and Homogenization), which has been developed at Fraunhofer ITWM.

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Development of microstructure in a micropolar continuum as a consequence of energy relaxation

Muhammad Sabeel Khan, Klaus Hackl

A rate-independent inelastic material model for a micropolar continuum is presented. The energy of the material is enriched with an interaction potential taking into account the intergranular kinematics at the continuum scale. As a result the total engergy becomes non-convex, thus giving rise to microstructure development. To guarantee the existence of minimizers an exact quasi-convex envelope of the corresponding energy functional is derived. As a result microstructure occurs in both the displacment and microrotation field. The corresponding relaxed energy is then used for finding the minimizers of the two field minimization problem corresponding to a micropolar continuum. Finite element formulation and numerical simulations are presented. Analytical and numerical results are discussed.

Error-controlled multiscale XFEM for crack propagation at macro-scale and crack initiation at micro-scale of ceramic materials

Erwin Stein, Tymofiy Gerasimov, Stefan Löhnert and Marcus Rüter

The eXtended Finite Element Method (XFEM) a substantial generalization of FEM within the concept of partition of unity methods (PUM) using fixed, usually regular meshes has been proven to be an extremely powerful tool for crack simulations, especially, while modeling and computing complex systems with micro- and macro-structural features.
The problem we are interested in contains the three topics: the crack propagation on a macro-scale, the initiation of cracks on a micro-scale and their coalescence, resulting in the appearance of new macrocracks, and finally - and most importantly - the micro-/macro- scale processes interaction. The direction of a growing macrocrack which triggers microcrack nucleation and coalescence, is affected, in turn, by changing material response due to microcracks.
In this talk we first give an idea of error-controlled crack propagation modeling and show that adaptive mesh refinements, which are guided by explicitly computed local error indicators, provide more accurate values of stress intensity factors and crack propagation angle, than those computed without refinements. Furthermore, the direct error estimation for the J-integral, serving as a criterion for crack propagation, will be explained and presented.
Modeling of microcrack nucleation and coalescence is realized within the framework of Continuum Damage Mechanics (CDM), in particular in terms of a non-local damage model using the enhanced gradient formulation. Error estimation for this problem is our ongoing research.
Finally, the transition between the two scales will be tackled in terms of the multiscale projection method (Löhnert, Belytschko, 2007), the idea of which will be explained. The notion of a model error, which aims at optimizing the shape and size of a fine scale domain, will be discussed.

Line-tension model as the Γ-limit of a nonlinear dislocation energy

Caterina Ida Zeppieri, Lucia Scardia

The motion of dislocations is regarded as the main cause of plastic deformations, therefore a large literature is focused on the problem of deriving plasticity models from more fundamental dislocation models. The starting point of our derivation is a semi-discrete dislocation model. The main novelty of our approach is that we consider a *nonlinear* dislocation energy, whereas most mathematical and engineering models are based on quadratic energies. Our choice of a nonlinear stress-strain relation guarantees that the dislocation strain energy is well defined also in the vicinity of the dislocations, eliminating the need of introducing a fictitious cut-off radius that is typical of the linear theories. The Γ-limit of our nonlinear dislocation energy as the length of the Burgers vector tends to zero is a strain-gradient model for plasticity and has the same form as the limit energy obtained by starting from a quadratic dislocation energy. Our result, however, is obtained by starting from a more reliable physical model.

Poster Abstracts

Asymptotics for elastic fibers in contact

Zoufine Bare, Julia Orlik

In this work a 3-D uni-lateral contact elasticity problem for a thin fiber with a rigid foundation is studied. We approximate the contact condition by a linear Robin-boundary-condition (by meaning of the penalized and linearized non-penetration and friction conditions, [1]). The Robin parameters are scaled differently in the longitudinal and cross-sectional directions. The dimension of the problem is reduced by a standard ([2], [3]) formal asymptotic approach with an additional expansion suggested to fulfill the contact conditions. The 3-D contact conditions result into 1-D Robin-boundary-conditions for corresponding 1-D PDEs. The Robin-coefficients of the 1-D problem depend on the ones from the 3-D statement, on the cross-section of the fiber and on the solution of auxiliary problems in the boundary layer. The error is estimated and the theoretical results are illustrated by a numerical comparison of the solutions to the contact problems for 3-D and 1-D beams for validation.

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A Virtual Laboratory to Derive Mechanical Properties

M. Diehl, P. Eisenlohr, F. Roters, and. D. Raabe

The mechanical performance of alloys is based on the kinetics and interactions of lattice defects at the nano- and microscale. Most high strength steels gain their excellent stress–strain profiles from effects that are related to the interaction of different phases, solutes, athermal phase transformations, dislocation kinetics, mechanical twinning, precipitates, and microbands. Crystal plasticity (CP) methods allow the description of the interactions that may occur in such compounds, based on adequate constitutive descriptions of the kinetics that reflect the underlying physics. Usually, the underlying constitutive laws to capture the evolution and structure–property relations associated with certain defects represent homogenized approaches themselves, as they are formulated as mean field approximations. A key feature of advanced constitutive models is the use of internal variables that reflect defect populations that are accessible to an experiment and to a history-dependent treatment of materials mechanics.
The simulation of the homogenized macroscopic mechanical behavior of such complex ensembles, which often go through more than one homogenization assumption is often done on a volume element (VE) with a structure representative for the material (RVE). Usually, periodic boundary conditions (PBCs) are enforced on the RVE. While the most commonly used Finite Element Method (FEM) is flexible and widely accepted, it has several disadvantages: unfavorable scaling for large problems, the necessity of meshing, and the inability to capture high spatial gradients. An alternative for (R)VEs with PBCs are spectral methods. They enable the high resolution necessary to capture the details of a complex microstructure.
We will show the capabilities of a spectral method [1] on the example of a dual phase steel using a CP based material model [2]. As the input data for the simulation is directly derived from real microstructures, the simulation results can be easily compared to experimental data. The computation of the macroscopic mechanical response is used as a “virtual laboratory” to substitute mechanical tests in deriving parameters for the component scale simulation of sheet metal forming.

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Structural simulation of composites with morphological anisotropy based on the NTFA

Felix Fritzen and Thomas Böhlke

Most engineering materials have a specific heterogeneous microstructure. The topology of the microstructure is an important influence factor for the macroscopic material response and is, hence, subject of many investigations. While the prediction of the linear properties is well understood, physical non-linearities cannot be treated following the same conceptual line. In order to overcome this short-coming Michel and Suquet [1] developed a computational method for the estimation of the non-linear behavior of isotropic two-dimensional materials by extending the concept of the Transformation Field Analysis introduced by Dvorak [2] through introduction of non-uniform inelastic modes. The methodology has been adapted to the Finite Element Method in [3] with success. In this contribution the ability of the method to capture the inelastic response of metal matrix composites with anisotropic particle morphologies is investigated. The elastic particles serve as a reinforcement of the ductile elasto-plastic metallic matrix material. The macroscopic constitutive anisotropy of the heterogeneous material is examined in terms of the effective stress response and the load partitioning between the matrix and the reinforcement and a good accuracy of the predicted load partioning is found by comparison with numerical full-field computations [4]. A structural application of the homogenized material model using isotropic and anisotropic particle morphologies is presented. The differences in the structural response induced by the particle morphology are exemplified.

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Time-continuous evolution of microstructures in finite plasticity

C. Günther, D. M. Kochmann, K. Hackl

We investigate the initiation and evolution of material microstructures in finite single-slip crystal plasticity, which are not inherent to the material but occur as a result of deformation. An interesting feature of such microstructures is, that they tend to form similar spatial patterns, hinting at a universal underlying mechanism. For purely elastic materials this mechanism has been identified as minimization of global energy. For non-quasiconvex potentials the minimizers are not anymore continuous deformation fields, but small-scale fluctuations related to probability distributions of deformation gradients, so-called Young-measures, which can be calculated via relaxed potentials.[1,2]
We briefly review the variational framework which allows to extend these concepts to inelastic materials. Central to this framework will be a Lagrange functional consisting of the sum of elastic power and dissipation due to change of the internal state of the material. Modifying this approach for the treatment of laminate microstructures in finite crystal plasticity, we present explicit time-evolution equations for volume fractions and internal variables and outline a numerical scheme by means of which the microstructure evolution can be computed. Numerical results will confirm the effective applicability of the numerical procedure.

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DFG-Forschergruppe 797, Subproject P5 “Regularizations and relaxations of time-continuous problems in plasticity”

Alexander Mielke and Sebastian Heinz

The theory of finite-strain elastoplasticity has been developed quite rapidly during the last decade. The major impulses for this were twofold: on the one hand, the discovery that time-incremental problems can be formulated as minimization problems and, on the other hand, the recent developments in the field of microstructures generated by infimizing sequences of functionals. In mathematical theory, the formation of microstructure is mostly treated via global minimization for static problems. In contrast to that, our aim is to derive models for the evolution of microstructure under slowly varying loads.

This project is devoted to the study of temporal evolution models for plasticity and for systems with microstructure in general. Using spatial regularization via higher gradients and temporal regularization via viscosity, we first want to derive mathematical models that allow for an existence theory of solutions without microstructure. The temporal regularization will lead to time-continuous solutions and thus avoid the problems occuring through global minimization. Starting from these solutions, we then generalize the recently developed energetic formulation for rate-independend processes.

As a prelimenary step, this program will be studied via simplified model problems, for which existence, uniqueness and convergence of numerical schemes can be proven and tested. Finally, the more difficult case of geometrically exact finite-strain elastoplasticity will be attacked.

On thermodynamical interpretation of the Cosserat continuum with microstructure

E. A. Ivanova

The mechanical model of a two-component medium is considered. The first component of the medium is the classical continuum and the other component is the continuum having only the rotational degrees of freedom. The presence of additional rotational degrees of freedom and additional inertia and elastic characteristics allows us to assign them the sense of the thermodynamical variables and constants [1, 2]. The mathematical description of the proposed mechanical model includes the classical formulation of coupled problem of thermoelasticity as a particular case. In the context of proposed theory we consider the original model of internal damping and give interpretation of the volume (acoustic) and shear viscosities. There exist different macroscopic and microscopic models of internal damping [3, 4]. This fact indicates that internal damping can have a different physical nature. In our opinion there exists a sort of internal damping which, as well as the heat conduction mechanism, should be considered as a result of interaction of atoms with some infinite surrounding medium. This medium can be called the vacuum, or the field, or else the "ether", the name is not important. We propose the mechanical model of the medium which is the continuum of particles having the translational and rotational degrees of freedom and interacting by the elastic moments. We consider some problems of elastic interaction of the medium with the particle being in it. As a result we show that the influence of the surrounding medium on the particle can be modelled by the damping moment proportional to the angular moment of the particle. Using of the damping moment in the model of a two-component medium allows us to describe the internal damping and the heat conduction mechanism.

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Microstructural Optimization of Dielectric Elastomer Actuators

M. Klassen, B. X. Xu and R. Müller

Dielectric elastomer actuators (DEAs) are characterized by the deformation behavior of a dielectric elastomer which is deformed through the application of an electric field. This physical phenomenon is based on the electromechanical coupling where an electric field polarizes the dielectric elastomer leading to the deformation of the material. Since dielectric elastomers are rather soft materials, the deformations are relatively large but with a low actuation force. The range of the actuation forces and deformations is comparable to natural muscles. This motivates the application of DEAs in the field of robotics where they can be applied as artificial muscles. But this is only one of the many possible application fields for this type of actuators.
In the present work the deformation performance of DEAs is studied in the context of the finite element method. For this reason a brief overview of the fundamental equations for electromechanics is given. Furthermore a modeling approach to realize a numerical implementation is also presented. In this modeling context different material models are taken into consideration to model the dielectric elastomer numerically. One of the main focuses on this study is the optimization of the compression behavior of dielectric actuators. For this purpose a sandwich structure consisting of the dielectric material between two compliant electrodes is considered. For optimization purposes microstructural inhomogeneities are inserted in the elastomer material. Numerical studies are made to analyze and compare the compression behavior of the microstructural sandwich structure. In this optimization context different material inclusions and geometries are considered.

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A two scale model for liquid phase epitaxy with elasticity

Michael Kutter

We study a two-scale model for liquid phase epitaxy with elasticity. The model has been derived via homogenization by formal asymptotic expansion in [2]. It consists of a macroscopic Navier–Stokes–System and a macroscopic convection-diffusion equation for the transport of matter in the liquid, and a microscopic problem that combines a phase-field approximation of a BCF-model, a Stokes system and an elasticity system for the growth and the elastic deformation of the solid film. For each of these problems we proved in [3] the existence and uniqueness of solutions under the assumption that the coupling data are given, sufficiently regular functions. These results are a first step in the proof of the existence of solutions to the full model via a suitable fixpoint argument, applied to the composition of appropriate solution operators, as it has been done for a corresponding model without elasticity in [1]

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Convergence rate for the approximation of effective diffusion by periodization in stochastic homogenization

Stefan Neukamm, Antoine Gloria and Felix Otto

We consider the stochastic homogenization of linear elliptic equations with random statistically homogeneous coefficients. The large scale behavior of such an equation is described by effective coefficients that are deterministic. They can be obtained by solving a *corrector problem*. Since the corrector problem has to be solved on an infinite domain, in practice, one has to make approximations. We are interested in the convergence rate to zero of the associated error.
Therefore, we study a simple situation, namely a discrete elliptic equation on the lattice $\mathbf{Z}^d$, $d \geq 2$, with random coefficients that are identically distributed and independent. We estimate the L^2-error made in the approximation of the effective coefficients by the periodization method. We show that the error decays (up to a logarithmic correction for $d = 2$) with the rate $L^{-d/2}$ where L is the size of the underlying periodicity cell. In our argument we decompose the error into two contributions that we call the random and systematic error. They monitor the fluctuation of the periodic approximation around its mean, and the effect of the periodic boundary conditions, respectively. We show that the random error is dominant, while the systematic error is of higher order. We explain that this observation can be used to setup and analyze approximation schemes that combine periodization, regularization and empirical averaging.

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TRIP steel – modelling and simulation of the interactions between phase-transformations and plasticity

R. Ostwald, T. Bartel, A. Menzel, M. Tiffe, D. Biermann, M. Lebsanft, B. Scholtes

The interactions of phase-transformations and plasticity play an important role in machining workpieces made of functionally graded materials [1]. In this work, we present an efficient model for the simulation of phase-transformations and plasticity in TRIP steel. The model is based on a micromechanically motivated and thermodynamically consistent scalar-valued material model for shape memory alloys [2], in which the evolution of volume fractions is based on laws derived from statistical physics. We adapt the model to TRIP steel and extend it to the incorporation of plasticity by an appropriate generalisation of the Helmholtz free energies of the material phases considered. Based on representative driving forces, we derive evolution equations for the individual plastic strains in each material phase [3].
Though the model allows to consider an arbitrary number of phases, we focus on the diffusionless transformation between the austenitic parent phase and a martensitic tension and compression phase in the current work. The obtained systems of evolution equations are solved in a staggered algorithm, where we additionally introduce a physically motivated plasticity inheritance law in order to account for incremental changes of plastic strains resulting from incremental changes of volume fractions.
The overall scalar-valued material model is embedded into a micro-sphere formulation in order to simulate three-dimensional boundary value problems. Numerical examples are carried our for homogeneous deformation states as well as for inhomogeneous deformations in a finite element context. It is shown that the model is capable of reflecting experimentally observed behaviour of TRIP steel.

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Finite Element Based Electronic Structure Calculations

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Many properties of condensed matter as for example electric conductivity, magnetism, mechanical response upon external excitations but also the formation of microstructures can be determined by the electronic structure of the material. The evaluation of the electronic structure represents a coupled, quantum mechanical many body problem, consisting of the positively charged atomic cores and the negatively charged, fermionic electrons. By the Hohenberg-Kohn theorem a method was established to calculate the ground state electron density through a density functional [1]. The resulting Kohn-Sham equations resemble a nonlinear, single body problem with an effective potential, accounting for the Coulomb interactions between the particles as well as for quantum mechanical effects. They can be solved within a self consistent field procedure.

We implement a real space formulation for the calculation of the electronic structure in the context of density functional theory. In a first step a finite element based solution algorithm for the Kohn-Sham equations is developed in line with [2], based upon which the electron density can be obtained in a non-periodic setting. We will present the basic elements of our implementation together with some results for the electron structure of single atoms and molecules.

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Construction of Statistically Similar RVEs for 3D Microstructures

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The improvement of the stability and the reduction of weight are important requirements in many fields of steel application, e.g. automotive engineering or aircraft construction. On that account, several advanced high strength steels (AHSSs) have been developed, which exhibit higher strength and enhanced formability compared to conventional steel types. Their microstructure strongly influences the overall material properties and should therefore be incorporated in numerical calculations. The FE^2 method, also known as direct micro-macro transition, is a suitable numerical tool for this purpose, see e. g. [1],[2]. A drawback of these direct homogenization methods is the high amount of memory and high computation time when applying them to large random microstructures. In this context, the definition of a statistically similar representative volume element (SSRVE), cf. [3], which is characterized by a significantly reduced complexity compared with real microstructures, leads to more efficient procedures. Therefore, we propose to construct such SSRVEs based on the minimization of a least-square functional considering the differences of suitable statistical measures characterizing the inclusion morphology of a given real microstructure and of the SSRVE. In 2D the construction of SSRVEs proves to be successfull in a series of numerical examples, cf. [3],[4].
The focus of our contribution is the extension of this method to the construction of three-dimensional SSRVEs. Therefore, we consider the phase fraction, the spectral density and the lineal-path function with respect to the inclusion phase for the evaluation of the least-square functional. As a target structure we use a real microstructure of a Dual-Phase steel which is obtained from 3D measurements based on Electron Backscatter Diffraction (EBSD) combined with a Focused Ion Beam (FIB), cf. [5].

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The maximal advance path constraint for the homogenization of materials with random network microstructures

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Network paths allow to formulate the constraints relating the macrodeformation of the materials with the random network microstructure to the microscopic deformation of one-dimensional strands constituting it. The latter incorporates reorientation and stretch [1] that both may be essentially non-affine [2].

In particular, specific paths that have the maximal advance in a certain direction, called maximal advance paths are considered. They are defined in the initial undeformed configuration of the network where all the chains have unit stretch and are oriented equally in all directions. The end-to-end vector of a path made by a large selection of chains from this assembly becomes a macroscopic object and deforms correspondingly. On the other hand this deformed path is composed of the deformed strands and is defined by the average of the microstretch vectors over the path. As a result the known macroscopic extension of such paths restrict the variation of the stretch in the network. Provided that the network at a given macrostretch strives to minimize its free energy the microdeformation of the filaments is found as a solution to a constraint minimization problem. The homogenized response of the material is then derived by the averaging over the relaxed network. The key question is then the free energy as a function of the microstretch distribution. Different generic energy terms are considered with respect to the uniqueness of the minima and the stability of the resulting homogenized material.

Finally, the numerical implementation of the developed model is proposed. This is based on the approximation of the variable microstretch on the microsphere of space orientations [2].

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