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Mini-Workshop: Analysis and computation of microstructures in finite plasticity

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Abstract. Plastic material behaviour is typically the result of the interaction of complex substructures on a microscopic scale. Common models of finite plasticity are based on macroscopic, phenomenological approaches and do not take into account any microstructural information. The miniworkshop focuses on the application of methods from the calculus of variations to models for microstructures in plasticity. In particular, the investigation of the relaxation of the underlying functional, corresponding to quasiconvexification of the energy density, allows us to gain interesting microscopic as well as macroscopic information.

Mathematics Subject Classification (2000): 49M20, 49J45, 74C15.

Introduction by the Organisers

The miniworkshop was attended by fourteen participants of whom twelve gave presentations. Additionally Kolumban Hutter from the University of Darmstadt, then at the research institute as a research-in-pairs fellow, agreed to give a talk on "Granular flows and avalanches". There was one discussion session chaired by Stefan Müller, during which the most important problems of the field which have to be addressed in the near future were identified. The individual talks lasted for one and a half hours in the average and were interlaced with lively discussions.

The main theme in the workshop was the variational formulation of crystal plasticity, in a rate-independent setting. For small time-intervals, this leads to a single variational problem, which is often referred to as the "first time step". One substantial difficulty arises from the fact that the resulting functional is not lower semicontinuous, leading to non-existence of minimizers. The corresponding

theory of relaxation has some analogies to the one developed in nonlinear elasticity. A second issue is the formulation of a theory that goes beyond small time intervals. In a framework where time is discretized, the functional at each time step depends on the minimizer at the previous one (assuming it exists). This leads to a sequence of coupled variational problems, and even the precise definition of the time-continuous limit is not yet completely understood.

The subjects treated ranged from the mathematical formulation of the variational problems and existence results for those, to analytical and numerical methods to determine their relaxation, and applications to various problems in mechanics and physics. Research in progress and sometimes of speculative nature was presented rather then established results. Specifically, the main questions treated were the following:

- *Relaxation.* How does one determine the relaxation of the single variational problem corresponding to the first time step? This links to the issue of determining, exactly or approximately, the quasiconvex envelope of an effective energy density. The talks addressed analytical approaches as well as numerical procedures and results, mainly on the calculation of laminated microstructures. A particularly complex open problem is that of physical softening, which in contrast to geometrical softening causes loss of coercivity of the potentials.
- *Time-continuous problem.* How can time-continuous evolution of microstructures and pattern-formation be described in a proper mathematical context? What is the appropriate concept of relaxation, and how can the relaxation be determined explicitly? What is a good material model for testing such formulations?
- *Singular perturbations.* What are the physically correct nonlocal extensions of the models, i.e., which of the various regularizing terms used are physically motivated? This class includes most singular perturbations, such as, e.g., surface-energy terms. In turn, how do these regularizations modify the structure of the model, and do they permit to explain quantitatively the experimentally observed microstructures, such as the so-called dislocation-walls?
- *Global vs. local optimization.* Do there exist more efficient and robust numerical algorithms than the global optimization procedures which currently have to be carried out? Is it possible to consider a physically-motivated local optimization procedure?
- *Experiment.* Is it possible to devise experimental tests for the theories developed?

During the miniworkshop progress could be made concerning some of these questions and interesting ideas where developed for the rest of them.

Mini-Workshop:
Analysis and computation of microstructures in finite plasticity

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Abstracts

Asymptotics of phase-field models of dislocations

Adriana Garroni

Single slip line tension energy: In collaboration with Stefan Müller ([3] and [4]) we consider a variational model for dislocations in a single slip plane and a single slip system proposed by Koslowki, Cuitiño and Ortiz [5]. We fix a slip plane ($\{x_3 = 0\}$) and we assigne the slip on this plane by imposing that the jump of the displacement must be given by $u\mathbf{b}$, where u is a scalar phase and $\mathbf{b}$ is the Burgers vector of the given system. The total energy can then be expressed in terms of the phase u and is given by a non local term (the long-range elastic interaction induced by the slip) and an interfacial potential which penalizes slips which are not multiples of the Burgers vector, i.e.,

$$E_\varepsilon = \int_Q\int_Q K(x-y)|u(x)-u(y)|^2 dx\, dy + \frac{1}{\varepsilon}\int_Q \operatorname{dist}^2(u,\mathbf{Z})\, dx\,,$$

where Q is the unit square in $\mathbf{R}^2$, ε is proportional to $|\mathbf{b}|$ and the kernel K satisfies $K(t) \approx |t|^{-3}$ as $t \to 0$. In addition we mimic the hardening effect, due to the interaction of the dislocations with inclusions of other materials or transversal dislocations, by adding a pinning condition on N_ε disks of radius εR. We assume that these disks are 'uniformely distributed' and 'well separated' in an appropriate sense.

It turns out that in order to get a compactness result the natural scaling for the energy is given by $E_\varepsilon/(\varepsilon N_\varepsilon)$. We then study the asymptotic behaviour of this energy in terms of Γ-convergence as $\varepsilon \to 0$ for all possible regimes for the number of obstacles N_ε. The most interesting regime is given by $N_\varepsilon \approx |\log\varepsilon|/\varepsilon$ for which the effect due to the competition between the multi-well potential and the non local regularization, and the effect of the obstacles are of the same order. Specifically we show that the limit of $E_\varepsilon/|\log\varepsilon|$ is the so called line-tension limit, i.e., the limit functional is defined on the space $BV(Q;\mathbf{Z})$, and is given by

$$\int_{S_u} \gamma(\nu_u)|[u]|\, d\mathcal{H}^1 + \int_Q D(u)\, dx,$$

where S_u is the jump set of u, with normal ν_u, $|[u]|$ is the jump of u, $\gamma(\nu_u)$ is an (anisotropic) line energy density, and $D(u)$ is a nonlinear potential quadratic at infinity which represents the limiting contribution of the obstacles.

The line tension energy density $\gamma(n)$ can be explicitly computed by means of the kernel K and gives the least energy for a transition from 0 to 1 with a flat interface orthogonal to n. Due to the logarithmic scale this transition does not depend on the precise shape of the profile and can be obtained by a mollification procedure.

Multi-slip line tension energy: In collaboration with S. Cacace ([2]) we consider a multi-phase variational model introduces by Koslowski and Ortiz [6] in

order to deal with the activation of several slip systems in a single slip plane. In this case the energy is defined on a multi-phase field and it is given by

$$F_\varepsilon = \int_Q\int_Q (u(x)-u(y))^t J(x-y)(u(x)-u(y))dx\,dy + \frac{1}{\varepsilon}\int_Q \mathrm{dist}^2(u,\mathbf{Z}^2)\,dx\,,$$

where $u : Q \to \mathbf{R}^2$ represents the slip on the plane $\{x_3 = 0\}$ and the matrix $J(t)$ is positive definite, $|J(t)| \approx |t|^{-3}$ as $t \to 0$, and it depends on the lattice structure of the crystal. Again, after a logarithmic rescaling, this energy shows a line tension effect in the limit. Namely we prove that there exist a subsequence $\varepsilon_k \to 0$ and a function $\phi : S^1 \times \mathbf{Z}^2 \to \mathbf{R}$ such that the sequence $F_{\varepsilon_k}/|\log \varepsilon_k|$ Γ-converges to the functional defined in $BV(Q,\mathbf{Z}^2)$ given by

$$\int_Q \phi(\nu_u,[u])\,d\mathcal{H}^1\,.$$

In this case the anisotropic line tension energy density can not be computed explicitly as in the scalar case. Precisely we show, with an example (for the cubic lattice), that the 'optimal interface' can develop microstructure and is not obtained with a one dimensional profile.

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A simple orthotropic finite elasto-plasticity model based on generalized stress-strain measures

JÖRG SCHRÖDER
(joint work with F. Gruttmann, J. Löblein)

In this paper we present a formulation of orthotropic elasto-plasticity at finite strains based on generalized stress-strain measures, which reduces for one special case to the so-called Green-Naghdi theory. The main goal is the representation of the governing constitutive equations within the invariant theory. Introducing additional argument tensors, the so-called structural tensors, the anisotropic constitutive equations, especially the free energy function, the yield criterion, the stress-response and the flow rule are represented by scalar-valued and tensor-valued isotropic tensor functions. For an introduction to the invariant formulation of anisotropic constitutive equations based on the concept of structural tensors and their representations as isotropic tensor functions see BOEHLER [1]. The proposed model is formulated in terms of generalized stress-strain measures in order to maintain the simple additive structure of the infinitesimal elasto-plasticity theory. In this work we formulate a model for anisotropic elasto-plasticity at large strains following the line of PAPADOPOULOS & LU [3, 4].

The nonlinear deformation map $\varphi_t : \mathcal{B} \rightarrow \mathcal{S}$ maps points $\mathbf{X}$ of the reference configuration $\mathcal{B}$ onto points $\mathbf{x}$ of the current configuration $\mathcal{S}$. Using the deformation gradient $\mathbf{F} := \text{Grad}\varphi_t$, with $\det\mathbf{F} > 0$, we define the generalized measures

$$\mathbf{E}^{(m)} := \frac{1}{2m}(\mathbf{C}^m - \mathbf{I}) \text{ for } m \neq 0, \quad \mathbf{E}^{(0)} := \frac{1}{2}\ln[\mathbf{C}] \text{ for } m = 0 \quad \text{with} \quad \mathbf{C} := \mathbf{F}^T\mathbf{F}.$$

The main assumption of this model is the additive split of the generalized measure into elastic and plastic parts, i.e.

$$\mathbf{E}^{(m)} = \mathbf{E}^{e(m)} + \mathbf{E}^{p(m)} \ .$$

Let us assume the existence of a free energy function $\psi = \psi^e(\mathbf{E}^{e(m)}) + \psi^{p,i}(e^{p(m)})$, where $e^{p(m)}$ is a scalar-valued internal variable associated to the plastic strains. In the following we focus on the strain measure defined by $m = 0$.

Here we use a representation of the free energy function and the flow rule which fulfill the material symmetry conditions with respect to the reference configuration a priori. For the orthotropic case we introduce the material symmetry group $\mathcal{G}_{orth}$, which elements are denoted by the unimodular tensors ${}^i\mathbf{Q}|i = 1, ...n$. The concept of material symmetry requires that the response functions have to be invariant under transformations on the reference configuration with elements of the symmetry group. In our special case the invariance requirement with respect to the material symmetry group is given by

$$\hat{\psi}^e(\mathbf{Q}^T\mathbf{E}^{e(m)}\mathbf{Q}) = \hat{\psi}^e(\mathbf{E}^{e(m)}) \quad \forall \ \mathbf{Q} \in \mathcal{G}_{orth} \subset \text{SO}(3), \ \mathbf{E}^{e(m)} \ , \tag{1}$$

where SO(3) characterizes the special orthogonal group; $\hat{\psi}$ is $\mathcal{G}_{orth}$-invariant. Similar ideas are assumed to be hold for the yield criterion. For the representation of these anisotropic functions, we have to extend the $\mathcal{G}_{orth}$-invariant functions to

functions which are invariant under the special orthogonal group. For this purpose we introduce the so-called structural tensors, which reflect the symmetry group of the considered material. The symmetry group of a material is defined by (1). An orthotropic material can be characterized by three symmetry planes, where the anisotropy can be described by two second-order tensors ${}^1\mathbf{M}, {}^2\mathbf{M}$ (defined with respect to the reference configuration) satisfying

$$\mathcal{G}_{orth} = \{\mathbf{Q} \in \mathrm{SO}(3),\ \mathbf{Q}^T {}^1\mathbf{M}\mathbf{Q} = {}^1\mathbf{M}, \mathbf{Q}^T {}^2\mathbf{M}\mathbf{Q} = {}^2\mathbf{M}\} \ .$$

For the orthotropic case the structural tensors are given by the dyadic products of the preferred directions ${}^1\mathbf{a}$ and ${}^2\mathbf{a}$ of the material

$${}^1\mathbf{M} := {}^1\mathbf{a} \otimes {}^1\mathbf{a} \quad \text{and} \quad {}^2\mathbf{M} := {}^2\mathbf{a} \otimes {}^2\mathbf{a} \ .$$

Introducing the structural tensors as additional arguments in the free energy yields

$$\psi^e(\mathbf{E}^{e(m)}, {}^i\mathbf{M} | i = 1, 2) = \psi^e(\mathbf{Q}^T \mathbf{E}^{e(m)} \mathbf{Q}, \mathbf{Q}^T {}^i\mathbf{M}\mathbf{Q} | i = 1, 2) \ \forall\, \mathbf{Q} \ \in \ \mathrm{SO}(3) \ .$$

This is the definition of an isotropic scalar-valued tensor function in the arguments $(\mathbf{E}^{e(m)}, {}^1\mathbf{M}, {}^2\mathbf{M})$, thus ψ^e can be formulated in terms of the basic invariants $J_i = \mathrm{tr}[(\mathbf{E}^{e(m)})^i]$ for $i = 1, 2, 3$ and the mixed invariants $J_4 = \mathrm{tr}[{}^1\mathbf{M}\mathbf{E}^{e(m)}]$, $J_5 = \mathrm{tr}[{}^1\mathbf{M}(\mathbf{E}^{e(m)})^2]$, $J_6 = \mathrm{tr}[{}^2\mathbf{M}\mathbf{E}^{e(m)}]$, $J_7 = \mathrm{tr}[{}^2\mathbf{M}(\mathbf{E}^{e(m)})^2]$. Thus the free energy and the associated generalized stresses appear in the form

$$\psi = \psi^e(J_1, ..., J_7) + \psi^{p,i}(e^{p(m)}) \quad \rightarrow \quad \mathbf{S}^{(m)} := \partial_{E^{e(m)}} \psi^e \ .$$

Analogously, we formulate the anisotropic yield criterion function $\hat{\Phi}$ in terms of the deviatoric part of the generalized stresses, the structural tensors and a scalar-valued isotropic hardening function $\xi = \partial_{e^{p(m)}} \psi^{p,i}$

$$\hat{\Phi}(\mathrm{dev}\mathbf{S}^{(m)}, {}^1\mathbf{M}, {}^2\mathbf{M}, \xi) = \hat{\Phi}(\mathbf{Q}^T \mathrm{dev}\mathbf{S}^{(m)} \mathbf{Q}, \mathbf{Q}^T {}^1\mathbf{M}\mathbf{Q}, \mathbf{Q}^T {}^2\mathbf{M}\mathbf{Q}, \xi) \quad \forall\, \mathbf{Q} \in SO(3) \ .$$

This function is governed by the six invariants

$$\begin{array}{lll} I_1 = \mathrm{tr}[(\mathrm{dev}\mathbf{S}^{(m)})^2], & I_2 = \mathrm{tr}[{}^1\mathbf{M}(\mathrm{dev}\mathbf{S}^{(m)})^2], & I_3 = \mathrm{tr}[{}^2\mathbf{M}(\mathrm{dev}\mathbf{S}^{(m)})^2], \\ I_4 = \mathrm{tr}[{}^1\mathbf{M}\mathrm{dev}\mathbf{S}^{(m)}], & I_5 = \mathrm{tr}[{}^2\mathbf{M}\mathrm{dev}\mathbf{S}^{(m)}], & I_6 = \mathrm{tr}[(\mathrm{dev}\mathbf{S}^{(m)})^3]. \end{array}$$

In the following we consider a quadratic flow criterion function of the form

$$\Phi(I_1, I_2, I_3, I_4, I_5, \xi) \leq 0$$

and assume an associative flow rule and define the evolution of $e^{p(m)}$

$$\dot{\mathbf{E}}^{p(m)} = \lambda \partial_{S^{(m)}} \Phi \quad \text{and} \quad \dot{e}^{p(m)} = \sqrt{\frac{2}{3}} ||\dot{\mathbf{E}}^{p(m)}|| \ .$$

An example of the necking of a bar with an isotropic elasticity model and orthotropic yield function - with the preferred directions ${}^1\mathbf{a} = [1\ ,\ 0\ ,\ 0]^T$ and ${}^2\mathbf{a} = [0\ ,\ 1\ ,\ 0]^T$ lying in the cross-section area of the bar - is depicted in Figure 1. In this simulation we used the isotropic hardening function

$$\hat{\xi}(e^{p(m)}) = h e^{p(m)} + (Y^\infty - Y^0)(1 - \exp(-\delta e^{p(m)}))$$

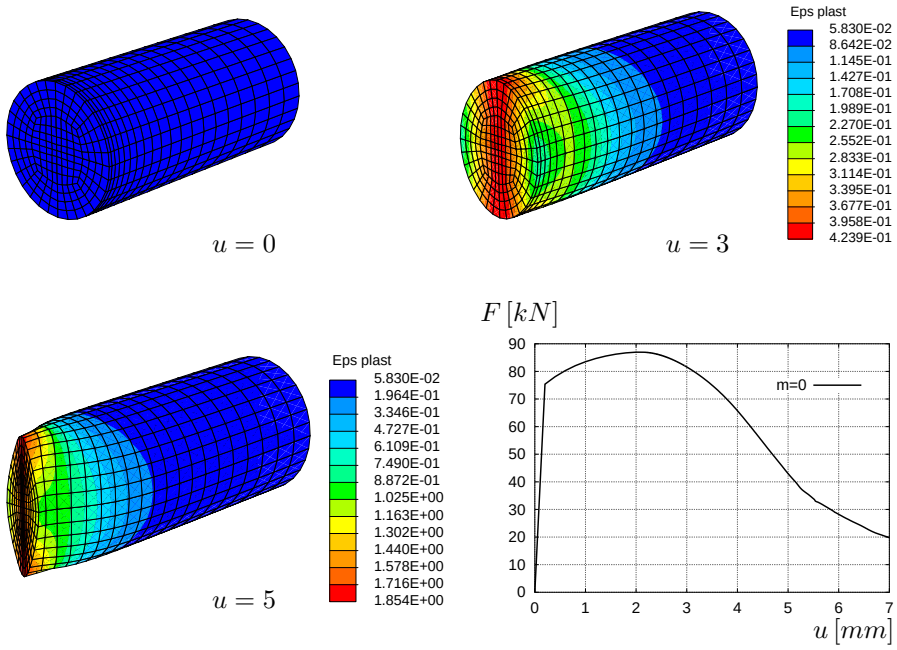

FIGURE 1. Necking of an orthotropic bar: equivalent plastic strains for different displacements u and load deflection curve [2].

with the hardening parameter $h = 0.12924\ GPa$ the yield stresses $Y^0 = 0.765\ GPa$, $Y^\infty = 1.03\ GPa$ and $\delta = 16.93$. More details of the orthotropic yield function

$$\Phi = \eta_1\, I_1 + \eta_2\, I_2 + \eta_3\, I_3 + \eta_4\, I_4^2 + \eta_5\, I_5^2 + \eta_6\, I_4 I_5 - \left(1 + \frac{\hat{\xi}(e^{p(m)})}{Y_{11}^0}\right)^2 \leq 0$$

are discussed in LÖBLEIN [2]. A circumstantial derivation of the tensor generators for the stresses and moduli as well as some representative numerical examples can be found in SCHRÖDER, GRUTTMANN & LÖBLEIN [5].

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Relaxation and evolution of microstructures – some conceptual ideas

Klaus Hackl

We investigate inelastic materials described by so-called internal or history- variables. Examples include elastoplastic but also damaged materials or those undergoing phase-transformations. By investigating associated potentials in a time-incremental setting it is possible to model the onset of the formation of microstructures but not their subsequent evolution, [1, 3, 6, 7, 8]. Here, some general ideas will be presented on how this problem could be treated.

In an isothermal setting the state of a general inelastic material will be defined by its deformation gradient $\boldsymbol{F} = \nabla \boldsymbol{\phi}$ an a collection of internal variables: $\boldsymbol{K}$. Denoting the specific Helmholtz free energy by $\Psi(\boldsymbol{F}, \boldsymbol{K})$ we introduce thermodynamically conjugate stresses by $\boldsymbol{P} = \frac{\partial \Psi}{\partial \boldsymbol{F}}$, $\boldsymbol{Q} = -\frac{\partial \Psi}{\partial \boldsymbol{K}}$. The evolution of $\boldsymbol{K}$ is then governed either by a so-called inelastic potential $J(\boldsymbol{K}, \boldsymbol{Q})$ or its Legendre-transform, the dissipation functional: $\Delta(\boldsymbol{K}, \dot{\boldsymbol{K}}) = \sup \{ \dot{\boldsymbol{K}} : \boldsymbol{Q} - J(\boldsymbol{K}, \boldsymbol{Q}) \mid \boldsymbol{Q} \}$. The evolution equations are then given in the two equivalent forms

$$\dot{\boldsymbol{K}} \in \frac{\partial J}{\partial \boldsymbol{Q}}, \qquad \boldsymbol{Q} \in \frac{\partial \Delta}{\partial \dot{\boldsymbol{K}}}. \tag{1}$$

The entire evolution problen can now be described in terms of two minimum principles, where we follow ideas presented in [2, 5, 8]. Considering the Gibbs free energy of the entire body $\mathcal{I}(t, \boldsymbol{\phi}, \boldsymbol{K}) = \int_\Omega \Psi(\nabla \boldsymbol{\phi}, \boldsymbol{K}) \, \mathrm{d}V - \ell(t, \boldsymbol{\phi})$ the deformation is given by the principle of minimum potential energy:

$$\boldsymbol{\phi} = \arg\min \{ \mathcal{I}(t, \boldsymbol{\phi}, \boldsymbol{K}) \mid \boldsymbol{\phi} = \boldsymbol{\phi}_0 \text{ on } \Gamma_\varphi \}. \tag{2}$$

Here Ω is the material body, Γ_φ a subset of its boundary and $\ell(t, \boldsymbol{\phi})$ the potential of external forces. On the other hand introducing the Lagrange functional $\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{K}, \dot{\boldsymbol{K}}) = \frac{d}{dt} \Psi(\nabla \boldsymbol{\phi}, \boldsymbol{K}) + \Delta(\boldsymbol{K}, \dot{\boldsymbol{K}})$ we can write the evolution equation (1) in the form

$$\dot{\boldsymbol{K}} = \arg\min \{ \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{K}, \dot{\boldsymbol{K}}) \mid \dot{\boldsymbol{K}} \}. \tag{3}$$

For rate-independent materials the principle (3) enables us to account for instantanious change of the value of $\boldsymbol{K}$, because it can be integrated to yield the balance law

$$\Psi(\nabla \boldsymbol{\phi}, \boldsymbol{K}_1) - \Psi(\nabla \boldsymbol{\phi}, \boldsymbol{K}_0) = -D(\boldsymbol{K}_0, \boldsymbol{K}_1), \tag{4}$$

where

$$D(\boldsymbol{K}_0, \boldsymbol{K}_1) = \inf \{ \int_0^1 \Delta(\boldsymbol{K}(s), \dot{\boldsymbol{K}}(s)) \, \mathrm{d}s \mid \boldsymbol{K}(0) = \boldsymbol{K}_0, \boldsymbol{K}(1) = \boldsymbol{K}_1 \} \tag{5}$$

is called dissipation-distance, [5]. When applied to a finite time-increment $[t_n, t_{n+1}]$ equation (4) gives rise to an approximate formulation, where $\boldsymbol{\phi}_{n+1}$ and $\boldsymbol{K}_{n+1}$ at

time t_{n+1} are determined for given loading at time t_{n+1} and value of the internal variables $\boldsymbol{K}_n$ at time t_n via the following principle:

$$(6)\quad \{\boldsymbol{\phi}_{n+1}, \boldsymbol{K}_{n+1}\} = \arg\min\Big\{ \int_\Omega \{\Psi(\nabla\boldsymbol{\phi}, \boldsymbol{K}) + D(\boldsymbol{K}_n, \boldsymbol{K})\}\,\mathrm{d}V - \ell(t_{n+1}, \boldsymbol{\phi}) \,\Big|\, \boldsymbol{\phi}, \boldsymbol{K} \Big\},$$

[2, 5]. Carrying out the minimization with respect to $\boldsymbol{K}$ in (6) beforehand gives the so-called condensed energy $\Psi^{\mathrm{cond}}_{\boldsymbol{K}_n}(\boldsymbol{F}) = \inf\big\{ \Psi(\boldsymbol{F}, \boldsymbol{K}) + D(\boldsymbol{K}_n, \boldsymbol{K}) \,\big|\, \boldsymbol{K} \big\}$ which has been used in the literature to calulate the onset of microstructures, [1, 3, 6, 7, 8]. This approach, however, is not suitable to describe the evolution of microstructures, because then the internal variables are already microstructured at the beginning of the time-increment as a result of a relaxation process in the preceeding time-increment. Or they are microstructured through the whole course of continuous evolution. Hence, they have to be given in the form of so-called Young–measures. We are going to give some concepts now, how such a formulation might be derived.

Young-measures are probability–distributions $\lambda_{\boldsymbol{F}} \geq 0$ given for example for the deformation-gradient, i.e. on $\mathsf{GL}(d)$, and dependent on the material point. Thus they have the following properties: $\int \lambda_{\boldsymbol{F}}\ \mathrm{d}\boldsymbol{F} = 1$, $\int \lambda_{\bar{\boldsymbol{F}}}\,\bar{\boldsymbol{F}}\ \mathrm{d}\bar{\boldsymbol{F}} = \boldsymbol{F}$. Moreover in the case of the deformation-gradient, the probability-distribution has to be compatible, i.e. realizable by a deformation field $\boldsymbol{\phi}$. This means that $\frac{1}{\Omega_{\mathrm{rep}}}\int_{\Omega_{\mathrm{rep}}} \Psi(\nabla\boldsymbol{\phi})\,\mathrm{d}V = \int_{\mathsf{GL}(d)} \lambda_{\bar{\boldsymbol{F}}}\Psi(\bar{\boldsymbol{F}})\,\mathrm{d}\bar{\boldsymbol{F}}$ has to hold for all quasiconvex potentials Ψ. In this case we call $\lambda_{\boldsymbol{F}} \in \mathsf{GYM}$ a gradient Young-measure.

It is now, at least in principle, possible to define a relaxed energy and dissipation functional via cross-quasiconvexication as

$$(7)\quad \Psi^{\mathrm{rel}}(\boldsymbol{F}, \lambda_{\boldsymbol{K}}) = \inf\Big\{ \int \Lambda_{\bar{\boldsymbol{F}},\bar{\boldsymbol{K}}}\Psi(\bar{\boldsymbol{F}},\bar{\boldsymbol{K}})\,\mathrm{d}\bar{\boldsymbol{K}}\,\mathrm{d}\bar{\boldsymbol{F}} \,\Big|\, \int \Lambda_{\bar{\boldsymbol{F}},\bar{\boldsymbol{K}}}\ \mathrm{d}\bar{\boldsymbol{K}}\ \mathrm{d}\bar{\boldsymbol{F}} = 1,$$
$$\int \Lambda_{\bar{\boldsymbol{F}},\bar{\boldsymbol{K}}}\ \mathrm{d}\bar{\boldsymbol{K}} \in \mathsf{GYM}, \int \Lambda_{\bar{\boldsymbol{F}},\boldsymbol{K}}\ \mathrm{d}\bar{\boldsymbol{F}} = \lambda_{\boldsymbol{K}}, \int \Lambda_{\bar{\boldsymbol{F}},\bar{\boldsymbol{K}}}\,\bar{\boldsymbol{F}}\ \mathrm{d}\bar{\boldsymbol{K}}\ \mathrm{d}\bar{\boldsymbol{F}} = \boldsymbol{F}\Big\},$$

$$(8)\quad \Delta^*(\dot{\lambda}_{\boldsymbol{K}}) = \inf\Big\{ \int \Lambda_{\boldsymbol{K}_0,\boldsymbol{K}_1} D(\boldsymbol{K}_0,\boldsymbol{K}_1)\,\mathrm{d}\boldsymbol{K}_0\,\mathrm{d}\boldsymbol{K}_1 \,\Big|$$
$$\int \Lambda_{\boldsymbol{K}_0,\boldsymbol{K}_1}\ \mathrm{d}\boldsymbol{K}_0\,\mathrm{d}\boldsymbol{K}_1 = 1, \int \Lambda_{\boldsymbol{K}_0,\boldsymbol{K}_1}\ \mathrm{d}\boldsymbol{K}_0 = \dot{\lambda}_{\boldsymbol{K}}, \int \Lambda_{\boldsymbol{K}_0,\boldsymbol{K}_1}\ \mathrm{d}\boldsymbol{K}_1 = -\dot{\lambda}_{\boldsymbol{K}}\Big\}.$$

Related concepts have already been introduced in somewhat different settings in [6]. With these definitions we recover the original principles (2) and (3), with the only difference that the internal variables $\boldsymbol{K}$ have been replaced by the Young-measures $\lambda_{\boldsymbol{K}}$. However, we have to take care of the facts that $\lambda_{\boldsymbol{K}} \geq 0$ and $\int \lambda_{\boldsymbol{K}}\ \mathrm{d}\boldsymbol{K} = 1$. Introducing this constraints via Langrange- and Kuhn-Tucker-multipliers, respectively, the Lagrange functional in (3) assumes the form

$$(9)\quad \mathcal{L}(\boldsymbol{\phi}, \lambda_{\boldsymbol{K}}, \dot{\lambda}_{\boldsymbol{K}}) = \frac{d}{dt}\,\Psi^{\mathrm{rel}}(\nabla\boldsymbol{\phi}, \lambda_{\boldsymbol{K}}) + \Delta^*(\dot{\lambda}_{\boldsymbol{K}}) + \alpha\int \dot{\lambda}_{\boldsymbol{K}}\,\mathrm{d}\boldsymbol{K} - \int \beta_{\boldsymbol{K}}\dot{\lambda}_{\boldsymbol{K}}\,\mathrm{d}\boldsymbol{K},$$

and we get the Kuhn-Tucker conditions

$$\dot\lambda_{\boldsymbol{K}} \geq 0, \quad \beta_{\boldsymbol{K}} \geq 0, \quad \dot\lambda_{\boldsymbol{K}}\beta_{\boldsymbol{K}} = 0. \tag{10}$$

One main advantage of the present formulation is the fact, that it is possible to arrive at evolution equations for $\lambda_{\boldsymbol{K}}$. Thus we can avoid the solution of global minimization problems, as was required when calculating the onset of microstructions via the condensed energy, [1]. For this purpose we define thermodynamically conjugate forces: $q_{\boldsymbol{K}} = -\frac{\partial \Psi^{\mathrm{rel}}}{\partial \lambda_{\boldsymbol{K}}}$. Because of the two constraints mentioned above the evolution problem inherits an active set structure and a deviatoric structure. Therefore we introduce the active set $\mathcal{A} = \left\{ \boldsymbol{K} \,\middle|\, \lambda_{\boldsymbol{K}} > 0 \right\}$ and the active deviator $\mathrm{dev}_{\mathcal{A}}\, x_{\boldsymbol{K}} = x_{\boldsymbol{K}} - \left(\int_{\mathcal{A}} x_{\boldsymbol{K}}\, \mathrm{d}\boldsymbol{K}\right) \mathbf{1}$ as well as the restriction: $x_{\mathcal{A}} = (x_{\boldsymbol{K}})_{\boldsymbol{K}\in\mathcal{A}}$. We can once again define an inelastic potential via Legendre-tranform by

$$J^*(q_{\boldsymbol{K}}) = \inf \left\{ \int \dot\lambda_{\boldsymbol{K}} q_{\boldsymbol{K}}\, \mathrm{d}\boldsymbol{K} - \Delta^*(\dot\lambda_{\boldsymbol{K}}) \,\middle|\, \dot\lambda_{\boldsymbol{K}} \right\} = \chi(\Phi(q_{\boldsymbol{K}})), \tag{11}$$

which because of the rate-independence of the problem can be written in terms of the characteristic function χ of a yield-function Φ. With this notation we obtain the desired evolution equation

$$\dot\lambda_{\mathcal{A}} \in \mathrm{dev}_{\mathcal{A}} \left.\frac{\partial \Phi}{\partial q_{\boldsymbol{K}}}\right|_{\mathcal{A}} \tag{12}$$

along with the consistency condition

$$\frac{\partial \Delta^*}{\partial \dot\lambda_{\boldsymbol{K}}} - \mathrm{dev}_{\mathcal{A}}\, q_{\boldsymbol{K}} \geq 0 \quad \text{for} \quad \boldsymbol{K} \notin \mathcal{A}. \tag{13}$$

Here the inequality (13) plays the role of a switch determining when an inactive constraint becomes active again. An evolution equation of the type presented in (12) is applied to polycrystalline shape-memory-alloys in [4].

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Some existence results in finite-strain plasticity

Alexander Mielke

Most theories of finite-strain elastoplasticity are based on Kröner and Lee's assumption of the multiplicative decomposition $\mathbf{F} = \mathbf{F}_{\rm elast}\mathbf{P}$, where $\mathbf{F} = \mathrm{D}\boldsymbol{\varphi}$ is the gradient of the deformation $\boldsymbol{\varphi} : \Omega \to \mathbb{R}^d$. The plastic tensor $\mathbf{P}$ and additional hardening variables $p \in \Pi$ are taken to be internal parameters. Moreover, the modeling is usually done in the rate-independent setting. This note concerns the implications of these two basic axioms.

Right from the beginning we emphasize that $\mathbf{F}$ and $\mathbf{P}$ should not be considered as elements of the linear space $\mathbb{R}^{d\times d}$ but rather as elements of Lie groups, namely

$$\mathbf{F} \in \mathrm{GL}^+(d) = \{\mathbf{A} \in \mathbb{R}^{d\times d} \mid \det \mathbf{A} > 0\} \text{ and } \mathbf{P} \in \mathrm{SL}(d) = \{\mathbf{A} \in \mathbb{R}^{d\times d} \mid \det \mathbf{A} = 1\}.$$

Thus, the geometric nonlinearities of finite-strain plasticity can be understood in the sense of Lie groups.

The constitutive laws of associate plasticity are given in terms of a stored energy density $W(x, \mathbf{F}, \mathbf{P}, p)$ and a dissipation potential $R(\mathbf{P}, p, \dot{\mathbf{P}}, \dot{p})$. The basic axioms of multiplicative plasticity (cf. [Mie02, Mie03, GA04]) lead to the following special form of the constitutive laws

$$\begin{aligned} W(x, \mathbf{F}, \mathbf{P}, p) &= \widetilde{W}(x, \mathbf{F}_{\rm elast}, p) \text{ with } \mathbf{F}_{\rm elast} = \mathbf{F}\mathbf{P}^{-1} \in \mathrm{GL}^+(d) \text{ and} \\ R(\mathbf{P}, p, \dot{\mathbf{P}}, \dot{p}) &= \widetilde{R}(x, p, \boldsymbol{\xi}, \dot{p}) \text{ with } \boldsymbol{\xi} = \dot{\mathbf{P}}\mathbf{P}^{-1} \in \mathrm{sl}(d) = \mathrm{T}_{\mathbf{1}}\mathrm{SL}(d). \end{aligned}$$

Rate-independence means 1-homogeneity of R in the rates, i.e., $\widetilde{R}(x, p, \gamma\boldsymbol{\xi}, \gamma\dot{p}) = \gamma\widetilde{R}(x, p, \boldsymbol{\xi}, \dot{p})$ for $\gamma \geq 0$. The dissipation potential R is in one-to-one correspondence with the elastic domains $\mathbb{E}(x, p)$ (whose boundary is the yields surface) via Legendre-Fenchel transform in $(\boldsymbol{\xi}, \dot{p})$, namely $\chi_{\mathbb{E}(x,p)} = \mathcal{L}\widetilde{R}(x, p, \cdot)$.

The classical plasticity equations consist of the elastic equilibrium problem and the flow rule $0 \in \partial_{\dot{\mathbf{P}},\dot{p}} R + \mathrm{D}_{\mathbf{P},p} W$. A weaker form of these differential form is the *energetic formulation* which is solely base on the *energy functional*

$$\mathcal{E}(t, \boldsymbol{\varphi}, \mathbf{P}, p) = \int_\Omega \widetilde{W}(x, \mathbf{F}_{\rm elast}, p)\,\mathrm{d}x - \langle \ell(t), \boldsymbol{\varphi}\rangle$$

and the *dissipation distance* $\mathcal{D}((\mathbf{P}_0, p_0), (\mathbf{P}_1, p_1)) = \int_\Omega D(x, (\mathbf{P}_0, p_0), (\mathbf{P}_1, p_1))\,\mathrm{d}x$, where $D : \Omega\times(\mathrm{SL}(d)\times\Pi)^2 \to [0, \infty]$ is defined via

$$\begin{aligned} D(x, (\mathbf{P}_0, p_0), (\mathbf{P}_1, p_1)) = \inf \Big\{ \int_{s=0}^{1} R(x, p, \dot{\mathbf{P}}\mathbf{P}^{-1}, \dot{p})\,\mathrm{d}s \;\Big|\; (\mathbf{P}(0), p(0)) = (\mathbf{P}_0, p_0), \\ (\mathbf{P}(1), p(1)) = (\mathbf{P}_1, p_1),\ (\mathbf{P}, p) \in \mathrm{C}^1([0, 1]; \mathrm{SL}(d)\times\Pi),\ \Big\} \end{aligned}$$

The calculation of D is a difficult task as it involves the geodesic curves on $\mathrm{SL}(d)\times\Pi$ with respect to the Riemannian or Finslerian metric R. For some special cases, like von Mises plasticity this can be done, see [Mie02, HMM03].

By $\mathcal{F} \subset \mathrm{W}^{1,p}(\Omega; \mathbb{R}^d)$ we denote the set of kinematically admissible deformation and by $\mathcal{Z}$ the set of all internal states $(\mathbf{P}, p) : \Omega \to \mathrm{SL}(d)\times\Pi$. A function $(\boldsymbol{\varphi}, \mathbf{P}, p) :$

$[0,T] \to \mathcal{F}\times\mathcal{Z}$ is called *energetic solution* for the above problem, if for all $t \in [0,T]$ the global stability condition (S) and the energy balance (E) hold:

$$\text{(S)}\ \forall\,(\widetilde{\boldsymbol{\varphi}},\widetilde{\mathbf{P}},\widetilde{p}) \in \mathcal{F}\times\mathcal{Z}\colon \mathcal{E}(t,\boldsymbol{\varphi}(t),\mathbf{P}(t),p(t)) \le \mathcal{E}(t,\widetilde{\boldsymbol{\varphi}},\widetilde{\mathbf{P}},\widetilde{p})+\mathcal{D}(\mathbf{P}(t),p(t),\widetilde{\mathbf{P}},\widetilde{p}),$$

$$\begin{aligned}\text{(E)}\quad &\mathcal{E}(t,\boldsymbol{\varphi}(t),\mathbf{P}(t),p(t)) + \mathrm{Diss}_{\mathcal{D}}((\mathbf{P},p),[0,T]) \\ &\qquad = \mathcal{E}(0,\boldsymbol{\varphi}(0),\mathbf{P}(0),p(0)) + \textstyle\int_0^t \partial_s\mathcal{E}(s,\boldsymbol{\varphi}(s),\mathbf{P}(s),p(s))\,\mathrm{d}s\end{aligned}$$

The solvability of this weak formulation is still an open problem, except for a few special cases in space dimension 1, see [Mie04b].

However, it is quite natural to consider a fully implicit time incremental problem (IP) and for some simpler material models the convergence of solutions of (IP) for step size going to 0 to solutions of (S) & (E) is established, see [MTL02, Mie05b, FM05]. For finite-strain plasticity already the solvability for (IP) is a major problem under current investigation, since formation of microstructure is to be expected in many cases, see [OR99, ORS00, CHM02].

$$\text{(IP)}\qquad (\boldsymbol{\varphi}_k,\mathbf{P}_k,p_k) \in \operatorname*{Argmin}_{(\widetilde{\boldsymbol{\varphi}},\widetilde{\mathbf{P}},\widetilde{p})\in\mathcal{F}\times\mathcal{Z}} \mathcal{E}(t_k,\widetilde{\boldsymbol{\varphi}},\widetilde{\mathbf{P}},\widetilde{p}) + \mathcal{D}(\mathbf{P}_k,p_k,\widetilde{\mathbf{P}},\widetilde{p}).$$

The major observation is that the incremental problem consists of k successive minimization steps, which was first observed in [OR99].

In [Mie04b] an existence result is established under the assumption that the so-called *condensed potential*

$$W_p^{\mathrm{cond}}(\mathbf{F}) = \min_{\widetilde{\mathbf{P}},\widetilde{p}}\ W(\mathbf{F}\widetilde{\mathbf{P}}^{-1},\widetilde{p})+D(\mathbf{1},p,\widetilde{\mathbf{P}},\widetilde{p})$$

is polyconvex. This assumption is very hard to check but an example for dimension $d = 2$ was established with the help of [Mie05a]. Imposing suitable coercivity assumptions, which show that exponential hardening is needed, it is then shown that (IP) has solutions.

To avoid the difficult assumptions on W^{cond} it is possible to introduce regularizing terms into $\mathcal{E}$ via $\mathcal{E}^{\mathrm{reg}} = \mathcal{E} + \int_\Omega \kappa|(\mathrm{curl}\mathbf{P})\mathbf{P}^{\mathsf{T}}|^{q_C}\,\mathrm{d}x$. This case is analyzed in [MM05] via $\mathcal{A}$–quasiconvexity and a special identity for the minors of the product $\mathrm{D}\boldsymbol{\varphi}\mathbf{P}^{-1}$. Assuming that the semicondensed potential

$$(\mathbf{F}_{\mathrm{elast}},\mathbf{P}) \mapsto \min_{\widetilde{p}} W(\mathbf{F}_{\mathrm{elast}},\widetilde{p}) + D(\mathbf{P}_0,p_0,\mathbf{P},\widetilde{p})$$

is polyconvex and coercive with suitable exponents, it is possible to show that (IP) is solvable.

In many situations without regularization (IP) does not have solutions. In these situations one needs to relax the problem to find effective equations or one needs to find evolution equations for the associated microstructure, which often can be described by (sequential) laminates. In the mechanics literature this is described, e.g., in [AMO03, ML03, BCHH04]. For an attempt to provide a mathematical underpinning to these procedures we refer to [Mie04a, KMR05] and for the complete analysis in a very special case see [CT05].

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Constitutive parameters for a nonlinear Cosserat model. A numerical study.

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(joint work with I. Münch, W.Wagner)

The presented nonlinear Cosserat model is an elastic two-field minimization problem with respect to the deformation $\varphi : \Omega \mapsto \mathbb{R}^3$ and independent rotations $\overline{R} : \Omega \mapsto \mathrm{SO}(3,\mathbb{R})$, subject to boundary conditions. More precisely, one minimizes

$$I(\varphi,\overline{R}) = \int_\Omega W(\nabla\varphi,\overline{R}) + \mu\, L_c^2\, \|\nabla\overline{R}\|^2 \,\mathrm{dV} \mapsto \min\,.(\varphi,\overline{R})\,. \tag{1}$$

Frame-indifference of the strain energy implies the representation $W(F,\overline{R}) = \hat{W}(F^T\overline{R})$. The most simple quadratic, isotropic representation of $\hat{W}$ is given by

$$\hat{W}(\overline{U}) = \mu\|\operatorname{sym}\overline{U}\|^2 + \mu_c\|\operatorname{skew}(\overline{U})\|^2 + \frac{\lambda}{2}\operatorname{tr}\left[\overline{U} - \mathbb{1}\right]^2. \tag{2}$$

Here, μ,λ are the usual Lamé constants of isotropic elasticity, while $\mu_c \geq 0$ is an additional parameter, called the Cosserat couple modulus. $L_c > 0$ introduces a length scale into the model to the effect that smaller structures behave comparatively stiffer than larger structures.

The value of the Cosserat couple modulus in applications to solid material is controversial. More about the modelling, application and mathematical treatment can be found in [2, 1], where a more general approach, the so called micromorphic model, is dealt with at length.

The author has investigated this minimization problem from an analytical point of view. These investigations suggest that the couple modulus μ_c should be zero - contrary to what is usually assumed. Here I present numerical calculations which show the influence of μ_c and the internal length scale L_c on the stress-strain response. These numerical results suggest as well that taking $\mu_c > 0$ is inconsistent with any observed real material behaviour since it would lead to unbounded tangent stiffness for arbitrarily small material samples.

In the case of $\mu_c = 0$ and $L_c = 0$ an analytical development shows the existence of a lamination microstructure solution with arbitrary many sharp interfaces in the simple glide problem. This shows that for $\mu_c = 0$ the role of the rotationfield $\overline{R}$ is to relax the material response.

For $\mu_c = 0$ and $L_c > 0$ the compression test on a rectangular specimen shows a nonclassical response: it is energetically favourable to twist the specimen in the middle of the height.

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Applied relaxations in rank connected systems

Sanjay Govindjee

Many materials admit morphological (phase) transformations under mechanical/electrical/thermal loadings. In certain cases, these phenomena are attractive for designing novel engineering systems. One impediment, however, to effective design with such materials is the lack of a general purpose (constitutive) model suitable for use in solving boundary value problems using analysis software such as finite element programs. Recently, however, there has been a concerted effort in the development of such models for macro-scale modeling. Most approaches have been moving toward a common generalized thermodynamic framework employing varying degrees of internal variables. In shape memory alloys, for example, several promising models utilizing internal variables to describe single martensitic variants and some with multiple variants have appeared. In this work we exploit some recent results in quasi-convexity theory in a general multivariant framework for single crystals that is based upon lattice correspondence variants. These results are based upon some simple energy bounds which we are able to show are quite tight under certain common circumstances. Example computations are shown and are correlated to detailed theoretical results and non-trivial experimental data on single crystal Copper based alloys with orthorhombic and monoclinic martensitic structures.

At a mesoscopic scale the phenomena we wish to describe is geometrically enormously complex. At the macroscopic scale we likewise observe a very rich variety of phenomena. However at the microscale, the phenomena we are interested in is very elementary. It is a diffusionless phase transformation from one crystalline lattice symmetry to another. Given to considerations of group algebra, we note that the number of allowed transformation is finite and of order 3 to 12. Our desire is to base our model on only the simple microscopic symmetry changes. If we account properly for the energetics of these microscopic symmetry changes it is our hope that we can produce a model that self-assembles in a natural way to produce the rich variety of phenomena seen at the macroscopic scales. The essence of our modeling approach is to construct a model from a few very basic physical observations/mechanisms combined with a generic seemingly "universal" thermodynamic structure. Our tool of choice to transition from the microscale to the macroscale is quasi-convex relaxation.

The model framework employed is a classical thermodynamically mediated gradient decent framework (with a maximum entropy production character) as described in [5] or its zero dissipation limiting case as described in [8]. Central to this framework is the need for an explicit or efficient to evaluate implicit expression for the free energy of the material. The simplest and most natural choice for this (omitting for simplicity thermal terms) is [9, 2, 10, 3] $W(U) = \min_{\alpha=1,\cdots,N} W_\alpha(U)$, where U is the right stretch tensor and α indexes through the different symmetry variants. $W_\alpha(\cdot)$ is the appropriately centered variant (free) energy. Such an

energy density is well-known not to be quasi-convex and thus will lead to an overall system of equations ill-suited for our objectives. Following along the lines of [10, 12] in [6, 7] we replace this energy density by its partial quasiconvexification. This produces a model that accurately models the physics of the actual material response and in particular naturally respects the need for the rank connected laminated microstructures as has been recognized for some time (see e.g. [14]). This relaxation, however, does lead to issues of efficiency and thus there is some need for the use of approximations to the relaxation. In particular, one can employ lamination upper bounds combined with efficient search algorithms [1] or one can utilize lower bounds as developed in [6, 7]. One advantage of the lower bounds is that they are in closed algebraic form and are thus very efficient. Second, these bounds are provably exact for a wide range of actual physical systems. In cases where they are not exact their error is computably reasonable from an engineering perspective.

This modeling framework has been tested on a number of copper based alloys and shown to be physically accurate for both macroscopic system response as well as various secondary and tertiary experimental features. For tetragonal Nickel-Aluminum alloys it has been shown that our approximate lower bound relaxed energy matches very closely to the approximate upper bound relaxed energy and that it is exact for a wide spectrum of physically relevant situations. The approximate lower bound has similarly been computed to be very accurate for a monoclinic Copper-Aluminum-Nickel based alloy. The overall framework has been tested on the polycrystalline estimate of [4] and shown to be accurate for Nickel-Aluminum. The framework has been further tested against the orthorhombic tension loading/unloading test data of [11]. It has reproduced well the overall system response, the variant production, and tertiary features of the displacement mapping observed. Lastly, we have tested out framework against the tension/torsion monoclinic test data of [13]. The model while failing to reproduce the actual induced response of these multiaxial tests does accurately reproduced the driving forces when driven with the experimentally measured displacement field.

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Single-slip elastoplastic microstructures

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(joint work with Sergio Conti)

1. Introduction

We study rate-independent evolution of elastoplastic bodies. We consider the simplest case where the kinematics is maximally restricted in the sense that only one slip system is active and the only allowed elastic deformations are rigid body rotations, within the standard framework of crystal plasticity. Approximate solutions are constructed by considering sequences that minimize the sum of elastic energy and dissipated energy in the limit, the only source of dissipation being plastic deformation. The corresponding variational problems are denoted *incremental problems*. Due to the interplay of the directional dependence of the plastic deformation with the rotational invariance of the elastic part a minimizer does not, in general, exist. Minimizing sequences develop fine scale oscillations, which are analogous to microstructures found in models for solid-solid phase-transitions. Regular lamellar structures between phases with a different plastic deformation have been observed at large strains in a wide variety of metals, see e.g. [1, 2] and references therein.

The lack of minimizers for the incremental problems leads to instabilities in numerical algorithms that attempt to follow the time-continuous evolution of the elastoplastic deformation. A standard approach to overcome this difficulty is to consider a relaxed evolution problem where the original incremental problem is replaced by the lower semicontinuous envelope, see e.g. [1, 3, 4, 5].

The main objectives of this paper are (i) to demonstrate rigorously that a simple multi-dimensional model predicts the formation of a single-laminate microstructure; and (ii) to give a partial justification of numerical methods that are based on the computation of the relaxation of the incremental problems.

The first objective is achieved by determining an explicit formula for the quasiconvex envelope of the first incremental problem in the case where only one slip system is active (in two directions) and the elastic strains are negligible. The latter corresponds to the assumption that the elastic energy is infinite whenever the elastic part of the deformation gradient (in a multiplicative decomposition) is not a rotation. We show that microstructure states can approximate a variety of affine deformations of the type $y(x) = Fx$. In particular, in two dimensions this is possible for F in a relatively open subset of the volume-preserving affine maps $\{F : \det F = 1\}$. We show that the relaxation is achieved by first-order laminates (Theorem 1).

The second objective is achieved by considering the evolution problem that is associated to the relaxed incremental problem. We construct explicit solutions for the relaxed evolution problem that can not be interpreted as simple single-slip motions. These solutions correspond to time-evolving microstructure. In addition we prove that there exist sequences of approximate solutions for the original single-slip model that not only converge weakly to the relaxed solution, but also have the property that the associated plasticity-induced dissipation converges to the dissipation predicted by the relaxed system. The analysis is based on the construction of Lipschitz maps that form a perfect laminate except on a compact set with arbitrarily small measure.

Our analysis has nontrivial implications also for crystals with several slip systems. In particular, one can see that in two dimensions, three slip systems generate an effective response which is identical to Tresca plasticity (i.e. to the response obtained by assuming infinitely many slip systems).

2. Main results

We work within the framework of perfectly rigid, multiplicative crystal plasticity theory without hardening. More precisely, we assume that for deformations $y : \Omega \to \mathbb{R}^d$ the deformation gradient $F = \nabla y$ admits a multiplicative decomposition $F = F_\mathrm{e}F_\mathrm{p}$ where $F_\mathrm{e}, F_\mathrm{p} \in \mathbb{R}^{d\times d}$ are the elastic and the plastic strain tensor. The total elastic energy is given by $\int_\Omega W_\mathrm{e}(F_\mathrm{e})\,\mathrm{d}x$ where

$$W_\mathrm{e}(F_\mathrm{e}) = \begin{cases} 0 & \text{if } F_\mathrm{e} \in SO(d) \\ \infty & \text{else.} \end{cases}$$

For the sake of simplicity we assume that only one slip system is active, characterized by the vectors $s, m \in \mathbb{R}^d$, the slip direction and the slip-plane normal which form a pair of orthogonal unit vectors. The plastic dissipation which occurs when the plastic strain tensor changes from F_0 to F_p is given by $\int_\Omega W_\mathrm{p}(F_\mathrm{p}, F_{\mathrm{p}0})\,\mathrm{d}x$,

where

$$W_{\mathrm{p}}(F_{\mathrm{p}}, F_{p0}) = \begin{cases} |\gamma_2 - \gamma_1| & \text{if there exists } \gamma_1, \gamma_2 \in \mathbb{R} \text{ such that} \\ & F_{\mathrm{p}} = \mathrm{Id} + \gamma_2 s \otimes m \text{ and } F_{\mathrm{p}0} = \mathrm{Id} + \gamma_1 s \otimes m, \\ \infty & \text{else.} \end{cases}$$

After discretizing the rate-independent evolution problem in time one is confronted with the task to solve the *incremental problems* which consist in minimizing the energy

$$\int_\Omega W_{\mathrm{ep}}(\nabla y; \nabla y(t_k))\,\mathrm{d}x\,, \tag{1}$$

where $y(t_k)$ is the deformation at time t_k and

$$W_{\mathrm{ep}}(F, F_0) = \begin{cases} |s \cdot F_{\mathrm{p}}(F) F_{\mathrm{p}}^{-1}(F_0) m| & \text{if } F_{\mathrm{p}}(F) \text{ and } F_{\mathrm{p}}(F_0) \text{ are defined,} \\ \infty & \text{else.} \end{cases}$$

We used the convention

$$F_{\mathrm{p}}(F) = \begin{cases} R^T F & \text{if there exists } R \in SO(d), \gamma \in \mathbb{R} \\ & \text{such that } F = R(\mathrm{Id} + \gamma s \otimes m), \\ \text{undefined,} & \text{else.} \end{cases}$$

It can be checked that γ_1 and γ_2 are uniquely determined by F and F_0, hence W_{ep} is well defined.

Theorem 1. *In two dimensions, the quasiconvex envelope of $W_{\mathrm{ep}}(\cdot, F_0)$ is given by*

$$W^{\mathrm{qc}}(F, F_0) = \begin{cases} \lambda_{\max}(F F_{\mathrm{p}}^{-1}(F_0)) - \lambda_{\min}(F F_{\mathrm{p}}^{-1}(F_0)) & \textit{if } F, F_0 \in N^{(2)} \\ \infty, & \textit{else} \end{cases} \tag{2}$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the maximal and minimal singular values of $F F_{\mathrm{p}}^{-1}(F_0)$, and

$$N^{(2)} = \{F \in \mathbb{R}^{2\times 2} \mid \det F = 1, |Fs| \le 1\}.$$

The rank-one convex and the polyconvex envelopes, W^{rc} and W^{pc}, also agree with W^{qc}.

Note that $N^{(2)}$ is a three-dimensional set whereas the set where W_{ep} assumes finite values is two-dimensional, hence the the quasiconvexification leads to a non-trivial extension of the kinematics.

Since W_{ep} is strongly singular (the set where it assumes finite values has measure 0) the quasiconvex envelope increases if we go from two to three dimensions. In particular the formation of three-dimensional elastoplastic microstructures cannot be described within the framework of the single slip model.

Theorem 2. *In three dimensions, the function $W_{\rm ep}(\cdot, F_0)$ is quasiconvex. Its rank-one convex and polyconvex envelopes are given by*

$$W^{\rm pc}(F,F_0) = W^{\rm rc}(F,F_0) = \begin{cases} \lambda_{\max}(FF_{\rm p0}^{-1}) - \lambda_{\min}(FF_{\rm p0}^{-1}) & \text{if } F, F_0 \in N^{(3)} \\ \infty, & \text{else} \end{cases}$$

where $F_{\rm p0} = F_{\rm p}(F_0)$, $\lambda_{\max}$ and $\lambda_{\min}$ are the maximal and minimal nonnegative singular values of $FF_{\rm p0}^{-1}$, and

$$N^{(3)} = \{F \in \mathbb{R}^{3\times 3} \mid \det F = |F(s\wedge m)| = |\operatorname{cof} F(s\wedge m)| = 1, |Fs| \le 1\}.$$

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Microstructure and relaxation in single-crystal plasticity

Sergio Conti

We consider single-crystal plasticity in the limiting case of infinite latent hardening, which signifies that the crystal must deform in single slip at all material points. This requirement introduces a nonconvex constraint, leading to the formation of fine-scale structures. We restrict attention throughout to the deformation theory of plasticity, which is appropriate for monotonic proportional loading and confers the boundary value problem of plasticity a well-defined variational structure analogous to elasticity.

We first study a scale-invariant (local) problem, within a linearized framework. Precisely, let $\{s_i \otimes m_i\}_{i=1,\dots N}$ be a set of slip systems, each (s_i, m_i) being an orthormal pair in $\mathbb{R}^3$. Let $u : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ be the deformation, $\gamma : \Omega \to \mathbb{R}^N$ be the set of internal variables. We consider single-slip, i.e. assume that at each material only one of the γ_i is nonzero. Precisely, γ takes values in the set

$$\Gamma_s = \left\{\gamma \in \mathbb{R}^N : \exists j, \gamma_i = 0 \ \ \forall i \neq j\right\} . \tag{1}$$

We focus on the condensed energy

$$W_{\rm cond}(\epsilon) = \min_{\gamma\in\Gamma_s} \left\{ \frac{1}{2}(C(\epsilon - \epsilon_p(\gamma)), \epsilon - \epsilon_p(\gamma) + \tau|\gamma| \right\} , \tag{2}$$

where the plastic strain takes the form

$$\epsilon_p(\gamma) = \sum_{i=1}^{N} \gamma_i \frac{s_i \otimes m_i + m_i \otimes s_i}{2} \tag{3}$$

(at this stage, only one term in the sum is nonzero). The variational problem amounts at minimizing

$$E[u] = \int_\Omega W_{\text{cond}} \left(\frac{\nabla u^T + \nabla u}{2} \right) dx \tag{4}$$

subject to appropriate boundary conditions. We show that the quasiconvex envelope of W_{cond} equals its convex envelope. This determines also the relaxation of $E[u]$.

Theorem 1 (joint work with M. Ortiz, see [5])**.** *The quasiconvex envelope of the function W_{cond} equals its convex envelope*

$$W^{**}_{\text{cond}}(\epsilon) = \min_{\gamma \in \mathbb{R}^N} \left\{ \frac{1}{2}(C(\epsilon - \epsilon_p(\gamma)), \epsilon - \epsilon_p(\gamma) + \tau \sum_{i=1}^{N} |\gamma_i| \right\} \tag{5}$$

(both functions of strain are understood to be composed with projection onto symmetric matrices).

We remark that $W^{**}_{\text{cond}}(\epsilon)$ corresponds to the case of zero latent hardening. This means that, by developing microstructures in the form of sequential laminates of finite depth, crystals can *beat* the single-slip constraint, i. e., the relaxed constitutive behavior is indistinguishable from multislip ideal plasticity.

In a second step, we include dislocation line energies into the model. This introduces a length scale into the problem, and different regimes lead to distinct types of microstructure patterns. For simplicity, we focus on the case of antiplane shear, with two slip systems, and consider a cubic grain $\Omega_L = (0, L)^3$ contained in an infinite polycrystal (matrix material). Precisely, we seek a deformation $u : \Omega_L \to \mathbb{R}$ and a plastic strain $F^p : \Omega_L \to \mathbb{R}^3$ which minimize the free energy

$$E(u, F^p) = \int_{\Omega_L} |\nabla u - F^p|^2 dx + \sigma \int_{\Omega_L} |\nabla \times F^p| + \mu \, \|u - \gamma x_1\|^2_{H^{1/2}(\partial\Omega_L)} \tag{6}$$

subject to the side conditions $F^p_1 = \pm F^p_2$ and $F^p_3 = 0$ a.e.. We remark that here u is a scalar and F^p a vector. The three terms in the energy represent the elastic energy, the energy of the dislocation cores, and the elastic energy of the matrix. The qualitative material behavior can be understood determining the scaling of the infimum energy.

Theorem 2 (joint work with M. Ortiz, see [5]). *There are universal constants c, c' such that*

$$cE_0\left(\tilde{\sigma},\mu\right) \leq \frac{1}{L^3\gamma^2}\inf E(u,F^{\mathrm{p}}) \leq c' E_0(\tilde{\sigma},\mu)$$

where the infimum is taken among all u and F^{p} which obey the side condition, $\tilde{\sigma} = \sigma/\gamma L$, and

$$E_0(\tilde{\sigma},\mu) = \min\left(1,\mu,\mu^{1/2}\tilde{\sigma}^{1/2},\tilde{\sigma}^{2/3}\right).$$

The four regimes correspond to different macroscopic material behavior. In particular, the first one corresponds to elastic response, and the third one to onset of plastic response, characterized by the formation of a laminar structure. The yield stress scales as $L^{-1/2}$, in agreement with the experimentally known Hall-Petch scaling law in polycrystals.

The third part of this talk was devoted to the relaxation of a geometrically nonlinear problem with linear hardening. We consider the single-slip model from [3, 1], which takes the form

$$W_{BCHH}(F) = \min_{\gamma\in\mathbb{R}, F=F_e(\mathrm{Id}+\gamma s\otimes m)} U_e(\det F_e) + \frac{\mu}{2}|F_e|^2 + \tau|\gamma| + \frac{h}{2}\gamma^2 \tag{7}$$

Here s and m are a fixed pair of orthonormal vectors in $\mathbb{R}^2$, $F\in\mathbb{R}^{2\times 2}$, U_e is a convex function with minimum at 1, and the plastic strain takes the single-slip form $\mathrm{Id}+\gamma s\otimes m$.

First, we consider a corresponding 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. Precisely,

Theorem 3. *The quasiconvex envelope of the function*

$$W_r(F) = \begin{cases} \gamma^2 & \text{if } F = Q(\mathrm{Id}+\gamma s\otimes m) \quad \text{for some } Q\in SO(2)\,,\ \gamma\in\mathbb{R}\,,\\ \infty & \text{else.}\end{cases} \tag{8}$$

is given by

$$W_r^{qc}(F) = \begin{cases} |Fm|^2 - 1 & \text{if } \det F = 1 \text{ and } |Fs|\leq 1\,,\\ \infty & \text{else.}\end{cases} \tag{9}$$

The corresponding result for the case without hardening (i.e., with $|\gamma|$ instead of γ^2 in (8)) had been previously treated in [4, 6].

We then refine the analysis, by means of a coupled analytical-numerical method (joint work with C. Carstensen and A. Orlando, see [2]). This permits to determine analytically a second laminate which has "good" energy, and furnishes an upper bound on the relaxed energy. Subsequent numerical optimization of the laminate results in very good quantitative agreement with previous work by Bartels, Carstensen, Hackl and Hoppe [1], which had required a significantly higher

numerical effort. The main advantage of the present approach is that the analytical step gives a good starting condition for the numerical relaxation, permitting to limit numerical analysis to a low-dimensional, local minimization.

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Minimizing paths and incremental minimum problems for inelastic solids

Michael Ortiz

The classical theory of continuum thermodynamics and constitutive relations provides a useful framework for the formulation of the initial boundary value problem for general inelastic solids. The motions of the body are described by a time-dependent deformation mapping $\varphi : B\times[a,b] \to \mathbb{R}^3$, where $B \subset \mathbb{R}^3$ is the reference configuration and $[a,b]$ is the time interval elapsed during the motion; and obey conservation laws and the first and second laws of thermodynamics, namely:

$$\dot{R} = 0\,, \qquad \text{in } B\,, \tag{1a}$$

$$R\dot{V} = \mathrm{Div}P + RB\,, \qquad \text{in } B\,, \tag{1b}$$

$$PN = \bar{T}\,, \qquad \text{on } \partial_T B\,, \tag{1c}$$

$$PF^T = FP^T\,, \qquad \text{in } B\,, \tag{1d}$$

$$\dot{E} = P\cdot\dot{F} + RQ - \mathrm{Div}H\,, \qquad \text{in } B\,, \tag{1e}$$

$$H\cdot N = \bar{H}\,, \qquad \text{on } \partial_N B\,, \tag{1f}$$

$$\dot{\Gamma} \equiv \dot{N} - \frac{RQ}{\Theta} + \mathrm{Div}\frac{H}{\Theta} \geq 0\,, \qquad \text{in } B\,, \tag{1g}$$

where R is the mass density per unit undeformed volume; $V = \dot{\varphi}$ is the material velocity; B is the body force density per unit mass; N is the unit outward normal; P is the first Piola-Kirchhoff stress tensor; $\bar{T}$ are the applied tractions over the traction boundary $\partial_T B$; E is the internal energy per unit undeformed volume; N is the entropy per unit undeformed volume; Θ is the absolute temperature; Q is the distributed heat source per unit mass; and H is the outward heat flux; $\bar{H}$ is the prescribed outward heat flux over the Neumann boundary $\partial_N B$; $F = \nabla\varphi$ is

the deformation gradient and $\dot{\Gamma}$ is the internal entropy production rate per unit undeformed volume.

In addition, we suppose that the *local thermodynamic state* of an infinitesimal material neighborhood is defined by: the local deformation gradient $F \in GL_+(3,\mathbb{R}) \equiv$ the Lie group of invertible and orientation-preserving linear transformations in $\mathbb{R}^3$; the local entropy density per unit undeformed volume $N \in \mathbb{R}$; and a collection $Z \in M$ of additional or *internal variables*. The set M in which Z take values varies depending on the material class and cannot be specified universally for all solids. Depending on the nature of the internal variables, M may be: a vector space; a manifold, e.g., if the internal processes are subject to holonomic constraints; or a Lie group, e. g., if the internal variables are naturally composed by multiplication. The internal energy density and the absolute temperature are functions of the local state, i.e.,

$$E = E(F, N, Z)\,, \tag{2a}$$

$$\Theta = \Theta(F, N, Z)\,. \tag{2b}$$

The equilibrium stresses and the thermodynamic driving forces conjugate to the internal variables are, by definition,

$$P^e \equiv \partial_F E(F, N, Z)\,, \tag{3a}$$

$$Y \equiv -\partial_Z E(F, N, Z)\,. \tag{3b}$$

The viscous or non-equilibrium stress is then

$$P^v \equiv P - P^e\,. \tag{4}$$

A theorem of Coleman and Noll [2] then shows that (2b) is necessarily of the form

$$\Theta = \partial_N E(F, N, Z)\,, \tag{5}$$

and that all processes must comply with the dissipation inequality

$$\Theta\dot{\Gamma} = Y \cdot \dot{Z} + P^v \cdot \dot{F} - \frac{1}{\Theta} H \cdot \nabla\Theta \geq 0\,. \tag{6}$$

Alternatively, we may introduce the Helmholtz free energy by applying the Legendre transformation

$$A(F, \Theta, Z) = \inf_N \{E(F, N, Z) - \Theta N\}\,, \tag{7}$$

in terms of which the equilibrium relations take the form

$$N = -\frac{\partial A}{\partial \Theta}(F, \Theta, Z)\,, \tag{8a}$$

$$P^e = \frac{\partial A}{\partial F}(F, \Theta, Z)\,, \tag{8b}$$

$$Y = -\frac{\partial A}{\partial Z}(F, \Theta, Z)\,. \tag{8c}$$

In order to obtain a closed set of governing equations defining well-posed initial boundary-value problems the equilibrium relations summarized above need to be supplemented with appropriate kinetic relations enabling the determination of P^v,

$\dot{Z}$ and H. A special form of the kinetic relations is obtained by postulating the existence of a kinetic potential $\Delta(\dot{F}, \dot{Z}, G; F, N, Z)$ such that

$$P^v = \partial_{\dot{F}} \Delta(\dot{F}, \dot{Z}, G; F, N, Z)\,, \tag{9a}$$

$$Y = \partial_{\dot{Z}} \Delta(\dot{F}, \dot{Z}, G; F, N, Z)\,, \tag{9b}$$

$$-H = \partial_{G} \Delta(\dot{F}, \dot{Z}, G; F, N, Z)\,, \tag{9c}$$

i.e., a function that acts as joint potential for the viscosity law, rate-sensitivity and the heat conduction law.

Formally, a time-discretized incremental problem having a variational structure can be derived by recourse to minimizing paths, in the vein of *deformation theories* of plasticity [4, 3, 7, 1]. In particular, we envision a sequence of times $t_0, \ldots, t_n$, $t_{n+1}, \ldots$, and seek to characterize the state (φ, Θ, N, Z) of the solid at those times. For simplicity, here we confine our attention to the quasistatic, isothermal case. The general case including heat conduction is treated in [8]. Assume that the state $(\varphi_n, \Theta_n, N_n, Z_n)$ is known, and that the temperature Θ and the entropy N are given in the interval (t_n, t_{n+1}). We wish to consistently approximate the state (φ_{n+1}, Z_{n+1}) at time t_{n+1} as the solution of an extremum problem. By a consistent approximation we mean that the limits of the divided differences $\{(\varphi_{n+1} - \varphi_n)/\Delta t, (Z_{n+1} - Z_n)/\Delta t)\}$ as $\Delta t = t_{n+1} - t_n$ tends to zero satisfy the rate field equations at t_n. To this end, introduce the incremental functional

$$\Phi_n[\varphi_{n+1}, Z_{n+1}] = \inf_{\text{paths}} \int_{t_n}^{t_{n+1}} \left\{ \int_B (\dot{A} + \Delta)\, dV + G(\dot{\varphi}, \Theta) \right\} dt \tag{10}$$

where the subscript n signifies that $\Phi_n[\varphi_{n+1}, Z_{n+1}]$ depends parametrically on the initial conditions, the functional

$$G(\dot{\varphi}, \Theta) \equiv - \int_B RB \cdot \dot{\varphi}\, dV - \int_{\partial_T B} \bar{T} \cdot \dot{\varphi}\, dS + \int_B RQ \log \frac{\Theta}{\Theta_0}\, dV - \int_{\partial_N B} \bar{H} \log \frac{\Theta}{\Theta_0}\, dS \tag{11}$$

collects the power of the forcing terms, and the minimum is taken over all admissible *paths* joining (φ_n, Z_n) at time t_n to (φ_{n+1}, Z_{n+1}) at time t_{n+1}. The fundamental properties of the incremental potential Φ_n may be ascertained as follows. Integration of the perfect differential $\dot{A}$ gives

$$\Phi_n[\varphi_{n+1}, Z_{n+1}] = \int_B (A_{n+1} - A_n)\, dV + \inf_{\text{paths}} \int_{t_n}^{t_{n+1}} \left\{ \int_B \Delta\, dV + G(\dot{\varphi}, \Theta) \right\} dt\,. \tag{12}$$

Taking variations with respect to the independent variables and enforcing stationarity gives

$$\int_B P^e_{n+1}\cdot\delta F_{n+1}\,dV+\int_{t_n}^{t_{n+1}}\int_B\left[\partial_{\dot F}\Delta\cdot\delta\dot F+\partial_F\Delta\cdot\delta F\right]\,dV\,dt$$
$$+\int_{t_n}^{t_{n+1}}\left[\int_B RB\cdot\delta\dot\varphi\,dV+\int_{\partial_T B}\bar T\cdot\delta\dot\varphi\,dS\right]\,dt=0\,, \tag{13a}$$

$$-\int_B Y_{n+1}\cdot\delta Z_{n+1}\,dV+\int_{t_n}^{t_{n+1}}\int_B\left(\partial_{\dot Z}\Delta\cdot\delta\dot Z+\partial_Z\Delta\cdot\delta Z\right)\,dV\,dt=0\,. \tag{13b}$$

Integration by parts with respect to time and localization of the result gives

$$\mathrm{Div}\left[-\frac{d}{dt}\left(\partial_{\dot F}\Delta\right)+\partial_F\Delta\right]+R\dot B=0\,,\qquad\text{in } B\,, \tag{14a}$$

$$\left[-\frac{d}{dt}\left(\partial_{\dot F}\Delta\right)+\partial_F\Delta\right]\cdot N=\dot{\bar T}\,,\qquad\text{on } \partial_T B\,, \tag{14b}$$

$$-\frac{d}{dt}\left(\partial_{\dot Z}\Delta\right)+\partial_Z\Delta=0\,,\qquad\text{in } B\,, \tag{14c}$$

in the interval $t\in(t_n,t_{n+1})$, and

$$\mathrm{Div}(P^e_{n+1}+\partial_{\dot F_{n+1}}\Delta_{n+1})+RB_{n+1}=0\,,\qquad\text{in } B\,, \tag{15a}$$

$$(P^e_{n+1}+\partial_{\dot F_{n+1}}\Delta_{n+1})\cdot N=\bar T_{n+1}\,,\qquad\text{on } \partial_T B\,, \tag{15b}$$

$$Y_{n+1}=\partial_{\dot Z_{n+1}}\Delta_{n+1}\,,\qquad\text{in } B\,, \tag{15c}$$

at time t_{n+1}. Eqs. (14a – 14c) determine the minimizing paths. The remaining eqs. (15a – 15c) are the Euler-Lagrange equations of the functional Φ_n. Evidently, eqs. (15a – 15c) are the rate field equations expressed at time t_{n+1}. *Therefore, the critical points of Φ_n satisfy the rate field equations at time t_{n+1} with rates computed from the corresponding minimizing paths.*

An additional requirement of stability leads to the incremental minimum problem

$$\inf_{\varphi_{n+1},Z_{n+1}}\Phi_n[\varphi_{n+1},Z_{n+1}]\,, \tag{16}$$

whereby the stable states at time t_{n+1} are identified with the minimizers of Φ_n. As noted by Ortiz *et al.* [5, 6], minimization with respect to the internal state Z_{n+1} yields a reduced potential $\Phi_n[\varphi_{n+1}]$, and the subsequent minimum problem is indistinguishable from that of an elastic material. However, it should be carefully noted that the incremental functional Φ_n reflects both the *energetics* as well as the *kinetics* of the material. A manifestation of the kinetic character of Φ_n is its parametric dependence on the initial conditions at time t_n. Alternatively, we may regard the incremental functional Φ_n as changing between time steps. This incremental nature of Φ_n allows for irreversible behavior, path dependency and hysteresis, as required.

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Challenges in the computation of rank-one convex envelopes

Georg Dolzmann

The characterization of the relaxed functional

$$\mathcal{F}^{\mathrm{qc}}(u) = \int_\Omega W^{\mathrm{qc}}(Du)\,\mathrm{d}x$$

requires the knowledge of the quasiconvex envelope of the free energy density W given by

$$W^{\mathrm{qc}} = \sup\{g \le W : g \text{ quasiconvex}\}.$$

There are very few examples with physical relevance where the relaxed energy density has been obtained explicitly. One therefore needs to resort to an approximation of the quasiconvex envelope by the rank-one convex envelope W^{rc} of the energy density defined by

$$W^{\mathrm{rc}} = \sup\{g \le W : g \text{ rank-one convex}\}. \tag{1}$$

Here a function $g : \mathbb{M}^{m\times n} \to \mathbb{R}$ from the space of all real $m \times n$ matrices into the real numbers is said to be rank-one convex if g is convex on all rank-one lines of the form $t \mapsto F + tR$ with F, $R \in \mathbb{M}^{m\times n}$ and $\operatorname{rank}(R) = 1$. Equivalently, W^{rc} can be defined as an infimum over all finite laminates,

$$W^{\mathrm{rc}}(F) = \inf\Big\{\sum_{i=1}^{N} \lambda_i W(F_i) : (\lambda_i, F_i) \text{ satisfies } H_N\Big\}, \tag{2}$$

see [2] for more information.

The following paragraphs discuss important open problems related to analytical and numerical questions in this context.

1. How to compute W^{rc}? There are two fundamentally different strategies based on the two representations of W^{rc}.

(a) If one is interested in the values of the energy density W^{rc} in a small set of matrices, then one can use an *on the fly* algorithm where one optimizes (2) over a special class of laminates, typically first or second order laminates.

(b) If one needs the values of W^{rc} on a large set of matrices, for example if one combines the computation of the relaxed energy with a finite element discretization in space, then a more systematic approach based on (1) following the ideas in [7] may be advantageous.

The implementation proposed in [3, 6] uses an equidistant mesh $\mathcal{G}_h = h\mathbb{Z}^{m\times n}$ in the space of all matrices and restricts the computation to a finite box $Q_M = [-M, M]^{m\times n} \cap \mathcal{G}_h$. The idea is to compute an approximation W_h^{rc} that is convex on a set of rank-one directions $\mathcal{R}_h$ that correspond to vectors of rank-one in the cube Q_M. The advantage of this approach is that the approximation is an upper bound for W^{rc} and that one can obtain an explicit error estimate [6]. Let

$$\mathcal{R}_h = \big\{ha \otimes b : a \in \mathbb{Z}^m,\, b \in \mathbb{Z}^n,\, \|a\|_\infty,\, \|b\|_\infty \le h^{-1/3}\big\}.$$

If the infimum in (2) is attained for a finite N and if there exists a rank-one convex function g such that $W \ge g$ and $W = g$ on $\mathbb{M}^{m\times n} \setminus Q_{M/2}$, then

$$\|W^{\mathrm{rc}} - W_h^{\mathrm{rc}}\|_{\infty;Q_M} \le Ch^{1/3}.$$

A recent modification of the algorithm [1] provides an error estimate of order $\mathcal{O}(h)$. The extension of the algorithm described in [4] computes simultaneously a microstructure that leads to the relaxed energy.

2. Find sufficient conditions such that W^{rc} can be computed with a laminate of finite order. There is no condition known that allows one to estimate the number N in the definition (2) of W^{rc} in terms of properties of W that are easy to check. A related difficulty is that there is no criterion known that ensures that the matrices needed in the computation of W^{rc} by (2) lie in a ball with a given finite radius. The examples in [5] show that there exist minimizers u of functionals with quasiconvex energy densities which have unbounded gradients.

3. Use frame indifference and/or material symmetry in an efficient way. Most examples of physical importance lead to stored energy densities which satisfy the fundamental principle of material frame indifference, $W(F) = W(RF)$ with $R \in \mathrm{SO}(n)$ where $\mathrm{SO}(n)$ is the group of all proper rotations. From an algorithmic point of view one can reduce the amount of storage needed since the energy depends only on the symmetric part of the deformation gradient. However, the implementation of the approach in [3, 6] is not straight-forward since rank-one lines in the space of all matrices do not correspond to straight lines in the space of symmetric parts in the polar decomposition $F = RU$. It seems to be an open problem to describe an efficient algorithm that computes an interpolation with suitable convexity properties of a function given on $\mathcal{G}_h$

4. Combine numerical relaxation with a finite element minimization of the total energy in the system. The ultimate challenge is to determine the effective energy of the variational problem: Minimize

$$\mathcal{F}(u) = \int_\Omega W(Du)\,\mathrm{d}x$$

from a joint relaxation and minimization in the sense that one minimizes

$$\mathcal{F}_h(u) = \int_\Omega W_h^{\mathrm{rc}}(DU)\,\mathrm{d}x$$

where $U \in S^1$ is a finite element function (e.g. continuous and affine on the elements of a regular triangulation).

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Rate-independent damage at large strains

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(joint work with A. Mielke)

We consider damage in the context of nonlinear elasticity at large strains, which is certainly a relevant concept especially because damaged materials may allow indeed for very large deformations. On the other hand, only materials with quasiconvex stored energy of a polynomial growth $p > 3$, as Ogden's type materials, are analyzed. Moreover, we consider damage as a *rate-independent* process, as standardly applied to concrete, filled polymers, or filled rubbers. Being rate-independent, it is necessarily an *activated* process, i.e. to trigger a damage the mechanical stress must achieve a certain activation threshold. We consider the *isotropic damage* that can be described by a scalar parameter $z \in [0,1]$ and neglect any other rate dependent processes like viscosity and inertia. In accord to some engineering literature and for mathematical reasons, our model involves also the *gradient of damage*, expressing certain nonlocality in the sense that damage of a particular spot is to some extent influenced by its surrounding.

At a fixed time, the state of the system is considered as $q = (u, \zeta)$ where $u : \Omega \to \mathbb{R}^3$ is the *deformation* considered on the reference body configuration

$\Omega \subset \mathbb{R}^3$, and $\zeta : \Omega \to [0,1]$ is a distribution of *damage*; $\zeta(x) = 1$ means 100% quality of the material, 0 means that the material is completely damaged at the current point $x \in \Omega$, and $0 < \zeta(x) < 1$ means that some portion of material is already damaged due to, e.g., microcracks or microvoids.

The *stored energy* density $\varphi(x, F, z)$ is then a function of deformation gradient $F = \nabla u$ and the damage variable z:

$$\varphi(F, z) := \varphi_0(F) + z\varphi_1(F). \tag{1}$$

Dissipative mechanisms are routinely described by a (pseudo)*potential of dissipative forces*, here denoted by R, as a function of the rate of $q = q(t)$. The only dissipation of energy we consider is due to the damage and, on the microscopical level, it is related with irreversible structural changes of the material starting with microcracks and ending by its complete disintegration. We describe it by a single phenomenological parameter $d > 0$ having the meaning of a specific energy (per volume, i.e. in physical units Jm^{-3} =Pa) needed for complete damage of the unit volume of the material, i.e. the energy needed to switch $\zeta(x)$ from 1 to 0.

The classical formulation of the quasi-static problem consists in the balance of Piola-Kirchoff stress and the activated evolution of the damage parameter described by a complementarity problem:

$$-\mathrm{div}\big(\varphi_0'(\nabla u) + \zeta\varphi_1'(\nabla u)\big) = 0, \tag{2a}$$

$$\frac{\partial \zeta}{\partial t} \le 0, \tag{2b}$$

$$\zeta\varphi_1(\nabla u) - r_\zeta \le d + \kappa\,\mathrm{div}\big(|\nabla\zeta|^{r-2}\nabla\zeta\big), \tag{2c}$$

$$\frac{\partial \zeta}{\partial t}\Big(d - \zeta\varphi_1(\nabla u) + \kappa\,\mathrm{div}\big(|\nabla\zeta|^{r-2}\nabla\zeta\big) + r_\zeta\Big) = 0 \tag{2d}$$

on the reference domain Ω, here $\kappa > 0$ is a so-called factor of influence of damage and $r > 3$, and $r_\zeta \in \partial\chi_{[0,+\infty)}(\zeta)$ is an additional force balancing the natural constraint $\zeta \ge 0$; the notation $\chi_{[0,+\infty)}$ stands for the indicator function of $[0, +\infty)$.

This system is completed by time-dependent hard-device loading, i.e. time-dependent Dirichlet boundary conditions $u|_\Gamma = w_{\mathrm{D}}(t)$ are prescribed on some part Γ of the boundary $\partial\Omega$ while zero normal stress is considered on the rest. Due to the damage gradient term, some boundary conditions (here of Neumann's type) should be considered also for ζ.

The energetics involves the overall Gibbs' *stored energy*

$$G(t,u,\zeta) := \begin{cases} \displaystyle\int_\Omega \varphi\big(\nabla u(x), \zeta(x)\big) + \frac{\kappa}{r}|\nabla\zeta(x)|^r\,\mathrm{d}x & \text{if } u|_\Gamma = w_{\mathrm{D}}(t),\ \zeta \ge 0 \text{ a.e.,} \\ +\infty & \text{otherwise,} \end{cases} \tag{3}$$

and the *dissipation* rate

$$R(\dot q) := \int_\Omega \varrho(\dot\zeta(x))\,\mathrm{d}x \quad \text{where} \quad \varrho(\dot z) := \begin{cases} -d\dot z & \text{if } \dot z \le 0, \\ +\infty & \text{otherwise,} \end{cases} \tag{4}$$

here $\dot q = (\dot y; \dot\zeta)$ stands for the rate of q. The *energetic solution* $q : [0,T] \to Q := W^{1,p}(\Omega;\mathbb{R}^3) \times L^1(\Omega)$ to (2) on a fixed time interval $[0,T]$ is required to satisfy the *stability* condition

$$\forall \tilde q \in Q: \quad G\big(t,q(t)\big) \le G(t,\tilde q) + R\big(\tilde q - q(t)\big), \tag{5}$$

for all $0 \le t \le T$, and the *energy equality*

$$G(t,q(t)) + \mathrm{Var}_R(q;s,t) = G(s,q(s)) + \int_s^t P(\theta,q(\theta))\,\mathrm{d}\theta \tag{6}$$

$$\text{with} \quad P(t,q) \equiv P(t,u,\zeta) := \int_\Omega \varphi_F'\big(\nabla u(x),\zeta(x)\big) : \nabla \frac{\partial u_{\mathrm D}}{\partial t}(t,x)\,\mathrm{d}x.$$

for any $0 \le s < t \le T$ where the total variation $\mathrm{Var}_R(q;s,t) := \sup \sum_{i=1}^j R(q(t_i) - q(t_{i-1}))$ with the supremum taken over all $j \in \mathbb{N}$ and over all partitions of $[s,t]$ in the form $s = t_0 < t_1 < ... < t_{j-1} < t_j = t$, and eventually q is required also to satisfy a prescribed *initial condition* $q(0) = 0$.

Main assumptions are p-polynomial coercivity and growth both for φ_0 and φ_1 which are to be polyconvex, the p-growth for φ_0' and φ_1', and qualification of the Dirichlet loading $w_{\mathrm D} \in W^{1,1}(0,T;W^{1,\infty}(\Omega;\mathbb{R}^3))$. The coercivity of φ_0 means that only an incomplete damage is considered now.

Existence of an energetic solution $q \in \mathrm{B}([0,T];W^{1,p}(\Omega;\mathbb{R}^3)) \times (\mathrm{BV}([0,T];L^1(\Omega)) \cap L^\infty(W^{1,r}(\Omega)))$ with "B(·)" and "BV(·)"denoting the spaces of bounded and bounded-variation functions, respectively, is proved by a convergence of approximate solutions q_τ with $q_\tau|_{(\tau(k-1),\tau k]} = q_\tau^k$ solving the following recursive minimization problem

$$\left\{\begin{array}{ll} \text{Minimize} & G(t_\tau^k,q) + R(q - q_\tau^{k-1}) \\ \text{subject to} & q \equiv (u,\zeta) \in Q; \end{array}\right. \tag{7}$$

existence of q_τ^k is by the direct method. Of course, we put $q_\tau^0 = q_0$ a given initial condition. This suggests, after a further spatial discretization, a constructive computational strategy.

A-priori estimates that can be obtained are the following:

$$\big\|u_\tau\big\|_{L^\infty(0,T;W^{1,p}(\Omega;\mathbb{R}^3))} \le C_1, \quad \text{and} \tag{8a}$$

$$\big\|\zeta_\tau\big\|_{\mathrm{BV}([0,T];L^1(\Omega)) \cap L^\infty(0,T;W^{1,r}(\Omega))} \le C_2, \tag{8b}$$

$$\big\|t \mapsto G_\tau(t,q_\tau(t))\big\|_{\mathrm{BV}([0,T])} \le C_3. \tag{8c}$$

with G_τ defined like in (3) but with a piecewise constant approximation of $w_{\mathrm D}$. Moreover, a discrete stability and two-sided energy estimate can be derived.

Convergence can then be shown by the methodology developed in [1, 2], i.e. selecting a subsequence converging weakly* in the topologies indicated in (8) and, by Banach-space-valued Helly's selection principle, even pointwise in time for all quantities under the BV-estimates in (8). Then a limit passage in the discrete stability and two-sided energy estimate goes through, using various sophisticated

techniques, e.g. Tikhonov's (non-sequential) compactness of a product of a countable number of copies of a (weakly compact) ball in $W^{1,p}(\Omega;\mathbb{R}^3)$ or an approximation of Lebesgue integrals by Riemann's sums.

The contribution is based on [3] where several generalizations are considered: ζ may act nonlinearly in (1), beside the hard-loading device also a prescribed-trajectory impact of an ideally rigid body is considered, and eventually some ideas are outlined for a complete damage.

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Analysis of damage models

Gilles A. Francfort

Rate independence is a shared feature of many constitutive behaviors for solids, from brittle fracture, to associated elasto-plasticity, damage or phase transformation. The material is assumed to be described by a free energy and a dissipation potential. In the case of brittle damage, the free energy $W(F,z)$ is a function whose first entry is the gradient of the deformation u, a $\mathbb{R}^N$-valued vector, and whose second entry is an internal variable (in $[0,1]$) that measures the state of damage in the material, so that $W \searrow$ with z. The dissipation potential $\mathcal{D}$, associated to the rate of change of z, is chosen such that $\mathcal{D}(\dot{z}(t)) \geq 0$, $\mathcal{D}$ is convex with $\mathcal{D}(0) = 0$. This ensures the positivity of the mechanical dissipation. In all that follows we take

$$\mathcal{D}(s) = \begin{cases} ks, \ s \geq 0 \\ \infty, \quad \text{else,} \end{cases}$$

the last condition translating the irreversibility of the process.

Consider a domain $\Omega \in \mathbb{R}^N$, occupied by such a material, clamped throughout its boundary, and submitted to, say, time dependent body loads $f(t)$. If we assume that inertia is negligible, then the material will follow a quasi-static evolution.

Quasi-static evolution for a damaging material can then be schematically written as follows:

$$\begin{cases} -\mathrm{div} D_F W(Du(t), z(t)) = f(t) \\ u(t) = U(x)(\text{given}) \text{ on } \partial\Omega \\ -D_z W(Du(t), z(t)) \in \partial\mathcal{D}(\dot{z}(t)) + \partial\mathbb{I}_{[0,1]}(z(t)) \\ z(0) = z_0 \text{ (initial condition).} \end{cases}$$

where $\mathbb{I}_{[0,1]}$ denotes the indicatrix function of $[0,1]$.

Defining the potential energy at time t as $E(t,v,\zeta) := \int_\Omega W(Dv,\zeta)dx - \int_\Omega f.vdx$ and the dissipation as $D(\zeta) := k\int_\Omega \zeta dx$. one can show that this problem is equivalent (modulo regularity) to the following variational evolution [1]

- $(u(t), z(t))$ satisfies a first order necessary condition of local (unilateral) minimality for the functional

$$E(t,v,\zeta) + D(\zeta)$$

among all $v = 0$ on $\partial\Omega$ and $1 \geq \zeta \geq z(t)$ (we do not specify the functional dependence at this point);
- $\frac{d}{dt}\Big(E(t,u(t),z(t)) + D(z(t))\Big) = -\int_\Omega \dot{f}(t).u(t)dx.$

The necessary optimality condition is difficult to manipulate, so that, here as in many related works, it is replaced by a global minimality requirement. This requirement acts as a (certainly often too drastic) selection principle among potential evolution paths. As such the problem can be viewed as a time-indexed sequence of constrained minimization problems.

We further simplify the evolution by assuming brutal partial damage, that is that

- $z(t) \equiv \chi(t) \in \{0,1\}$, where $\chi(t)$ becomes the characteristic function of the (unique) damaged state;
- W corresponds to a linearized model, i.e. $W(e,\chi) := 1/2(\chi A_w + (1-\chi)A_s)e.e$ where the symmetric entry e will only see the symmetrized gradient of u and $A_w \leq A_s$ are elasticity tensors;
- $A_w > 0$ (the damage is not total).

The natural way to approach this problem is use a time-stepping method over the interval of investigation $[0,T]$. At the first time step t_0, the problem becomes: minimize, over $(v,\ \chi)$,

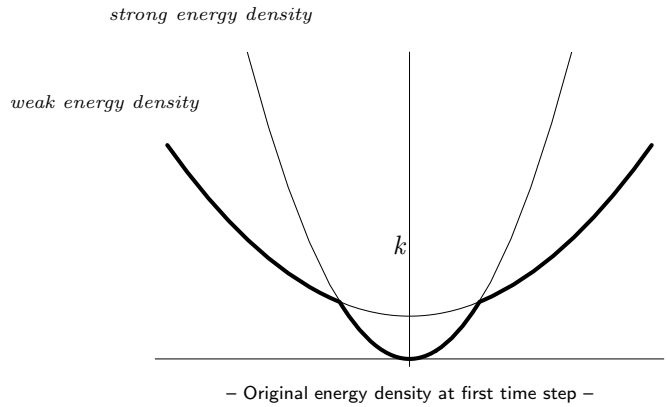
$$\int_\Omega \left[\frac{1}{2}(\chi A_w + (1-\chi)A_s)e(v).e(v) + k\chi\right]\ dx - \int_\Omega f_0.vdx$$

with $f_0 := f(0)$. It is straightforward to eliminate χ in the minimization process, and we are thus left with the minimization over v of

$$\int_\Omega W(t_0, e(v))\ dx - \int_\Omega f_0.vdx,$$

where

$$W(t_0, e) := \min\left\{\frac{1}{2}A_w e.e + k, \frac{1}{2}A_s e.e\right\}.$$



But the energy density $W(t_0, \cdot)$ is not convex, and the infimum

$$I(t_0) := \inf_v \int_\Omega W(t_0, e(v))\, dx - \int_\Omega f_0.v dx$$

is generically not attained. It is by now classical that

$$I(t_0) = \min_v \int_\Omega QW(t_0, e(v))\, dx - \int_\Omega f_0.v dx$$

where $QW(t_0, \cdot)$ is the quasi-convex envelope of $W(t_0, \cdot)$. That quasiconvexification process produces carefully tailored fine mixtures of the original two phases throughout the domain (those mixtures vary from point to point).

From the standpoint of the evolution problem, this is a source of trouble because, in a nutshell, the optimal microstructure for the relaxation process at the next time step will generically be mutually incompatible with that formed at the previous step due to the irreversibility constraint which imposes monotonicity of the associated characteristic function.

In [2], we propose a method which removes this obstacle and permits to pursue the analysis beyond the first time step, thus reconciling the formation of microstructures (necessary for relaxation) with the irreversible character of their creation. We then obtain a well-posed time-continuous evolution process for brittle damage in a linearly elastic material; the internal damage variable is the volume fraction $\Theta(t)$ of the strong (undamaged) material, while the corresponding stiffness $A(t)$ is well-defined as a function of $\Theta(t)$ and of the solution $u(t)$ (although possibly non-unique). In doing so, we have in effect replaced a model of brutal damage with a richer one of progressive damage.

Finally, we show that the obtained evolution is not too low in the sense that we can exhibit, for any solution of the relaxed evolution, a sequence of non-relaxed evolutions (associated to a sequence $\chi_n(t) \overset{t}{\nearrow}$ of characteristic functions of the

damaged material) which have asymptotically (as $n \nearrow \infty$) the same volume fraction of damaged material and same elastic stiffness $A(t)$ as the relaxed evolution, and this for almost all times. In particular, the associated energy sequence is asymptotically that of the relaxed evolution.

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