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Microstructures in Solids: From Quantum Models to Continua

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Abstract. The mathematical theory of solids was studied from the modern perspective of materials with microcstructures. The discussed topics ranged from experimental findings, via numerical simulations and mathematical modeling to the analysis of models with microstructures. A special emphasis was given to theories providing rigorous insight into and justification of the limit passage between different scales.

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Introduction by the Organisers

The design of modern materials, like multifunctional materials, and devices needs a deeper qualitative and quantitative understanding of material properties. However, the material behavior is influenced by effects on different length scales. For instance, the formation of single dislocations in a crystal is dominated by quantum and atomistic effects on a subnano-scale, whereas single-crystal plasticity has its origin in the motion and generation of thousands of dislocation lines on the micron scale. Similarly, phase transformations in shape-memory alloys or domain-wall formation in micromagnetics is generated via microstructures on different spatial scales. Formation of microcracks is one of the main origins of material failure, and the modeling of a crack tip involves length-scales over several decades.

The workshop brought together mathematicians and applied scientists and enabled them to discuss the relevant physical effects and their pertinence for the understanding of materials as well as the mathematical methods modeling the formation of microstructures and the effective description of small-scale effects

on larger scales. The talks concentrated on the following three main topics with special emphasis on their interaction:

- mathematical models for solids, in particular involving damage, fracture, plasticity and multifunctional materials;
- multiscale techniques, evolution of microstructures;
- computational and experimental aspects.

The discussed mathematical methods for multiscale problems included (two-scale and high-contrast) homogenization and analytical relaxation for models of crystal plasticity. Moreover, a new "uniformly Γ-equivalent" continuum theory for fracture was derived from a discrete model based on Lennard-Jones type interactions. For rate-independent systems the theory of Γ-convergence was shown to predict the creation and the evolution of microstructure from macroscopic states as well as providing a rigorous link between damage models and delamination of Griffith type. The passage from viscous kinetics to rate-independent dynamics was investigated via spatially random models, which give rise to a microscopic stick-slip motion.

The theory of dislocations was discussed from several points of view, namely as obstacles to crystallization in 3D, as a discrete origin to strain-gradient plasticity, and as a continuous transport theory for dislocation densities. Furthermore, a macroscopic model for non-associative plasticity in cam-clay was discussed analytically.

Effective descriptions of microstructures in nematic elastomers, elastoplastic materials, magnetic shape-memory alloys, solids undergoing phase transformations and ferroelectric materials were discussed in the framework of dissipative materials or using a special evolution law for simple or double laminates. The influence of rapid heating and cooling on microstructure formation was reported on the basis of recent experiments.

Size effects for microstructures in solids become relevant below the micron scale. The relevant multiscale modeling of the mechanical properties of metallic and biological polycrystals (e.g. chitin) was investigated using ab initio theory in conjunction with continuum homogenization. Similarly, progress in the understanding of interfacial cracks was obtained by combining quantum theory with macroscopic adhesion and strain-gradient models.

The foundations of such numerical approaches were investigated at several examples, like the statistically equivalent representative volume elements, a comparison of force-based atomistic/continuum hybrid models and the quasi-continuum methods and an effective numerical approach to gradient Young measures.

The stimulating discussion between the different research communities created many interesting links between previously disconnected research topics. The workshop initiated several new collaborations which will foster the progress of our understanding microstructures in solid materials.

Workshop: Microstructures in Solids: From Quantum Models to Continua

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Γ-convergence for local minimizers

Christopher J. Larsen
(joint work with Andrea Braides)

Γ-convergence is a key tool in studying approximations of energies, based on comparing global minimizers of an energy E and minimizers of approximate energies E_n. It is used in two main ways in applications: if E is a physical stored energy, it can sometimes be more convenient to find approximate energies that are more easily analyzed (see, e.g., [6, 2, 3, 5]). On the other hand, it can be that the physical energy has a natural small scale, such as atomistic energies, and one seeks a continuum model without a scale. In this case, the "true" physical energy is some E_n, with n large, and the limiting energy E is the approximation.

To study all stable states, one must also consider at least strict local minimizers, and for this Γ-convergence is generally not suitable. For this reason, we introduce new definitions of convergence (see [4]), based on coupling Γ-convergence with certain ideas of stability, with the hope that these will prove useful for studying (strict) local minimizers in a variety of situations. The stability we will use is based on the following:

Definition 1 (ε-slide and ε-stability)**.** *Let $E : X \to [0, +\infty]$ and $\varepsilon > 0$ with X a metric space. An* ε-slide *for E at u is a continuous function $\phi : [0, 1] \to X$ such that $\phi(0) = u$,*

$$\sup_{0 \le s < t \le 1} [E(\phi(t)) - E(\phi(s))] < \varepsilon$$

and $E(\phi(1)) < E(u)$.

We say that u is ε-stable *for E if no ε-slide at u exists, and* stable *if it is ε-stable for $\varepsilon > 0$ small enough (see* [7] *for motivation in the context of evolutions based on local minimization).*

Let $E_n : X \to [0, +\infty]$. A sequence $\{u_n\}$ is uniformly stable *for $\{E_n\}$ if, for all $\varepsilon > 0$ small enough, each u_n is ε-stable for E_n.*

Definition 2 (relative stability)**.** *We say that $\{E_n\}$ is* stable relative to E *if the following hold:*

(1) *If u has an ε-slide for E and $u_n \to u$, then each u_n has an ε-slide for E_n (for n large enough)*
(2) *If u is a strict local minimizer of E, then there exist $u_n \to u$ uniformly stable for $\{E_n\}$ (and so, by* (1)*, u is stable for E).*

To make this stability more meaningful, it will be coupled with Γ-convergence in the sequel.

Definition 3 (stable convergence)**.** *If $\{E_n\}$ is stable relative to E and Γ-converges to E, we say that it* stable converges *to E. Stable convergence will be denoted $E_n \xrightarrow{s} E$.*

Theorem 1. *Let $E_n \xrightarrow{s} E$.*

(i) *Let each stable point for E be a local minimizer. Then, if $u_n \to u$ and the u_n are uniformly stable for E_n, then u is a local minimizer of E;*

(ii) *Let each strict local minimizer for E be a stable point. Then, each strict local minimizer u of E is the limit of a sequence of uniformly stable points for E_n.*

We also give a stronger definition of convergence, strongly stable convergence (denoted $E_n \xrightarrow{s\text{-}s} E$) such that we have

Theorem 2. *If $E_n \xrightarrow{s\text{-}s} E$, then $(E_n + G) \xrightarrow{s} (E + G)$ for every continuous G such that $(E_n + G)$ is coercive.*

We also study some examples, including

Example 1. We consider the *Manhattan metric* function $\varphi : \mathbb{R}^2 \to \{1, 2\}$

$$\varphi(x_1, x_2) = \begin{cases} 1 & \text{if } x_1 \in \mathbb{Z} \text{ or } x_2 \in \mathbb{Z} \\ 2 & \text{otherwise,} \end{cases}$$

and the related scaled-perimeter functionals with forcing term f

$$E_n(A) = \int_A f(x)\, dx + \int_{\partial A} \varphi(nx)\, d\mathcal{H}^1$$

defined on Lipschitz sets A. By reasoning as in [1], it can be proved that the energies E_n Γ-converge to an energy of the form

$$E(A) = \int_A f(x)\, dx + \int_{\partial^* A} (|\nu_1| + |\nu_2|) d\mathcal{H}^1$$

defined on all sets of finite perimeter (ν denotes the normal to $\partial^* A$).

We show that actually $E_n \xrightarrow{s} E$.

Finally, we give a definition that is suitable for discrete-to-continuum problems.

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References

[1] L. Ambrosio and A. Braides, *Functionals defined on partitions of sets of finite perimeter, II: semicontinuity, relaxation and homogenization* J. Math. Pures. Appl. **69** (1990), 307–333.

[2] A. Braides, "Γ-convergence for Beginners", Oxford University Press, Oxford, 2002.

[3] A. Braides, *A handbook of Γ-convergence*, In "Handbook of Differential Equations. Stationary Partial Differential Equations", Volume 3 (M. Chipot and P. Quittner, eds.), Elsevier, 2006.

[4] A. Braides and C. J. Larsen, Γ-*convergence for stable states and local minimizers*, Ann. Scuola Norm. Sup. Pisa Cl. Sci., to appear.

[5] A. Braides and L. Truskinovsky, *Asymptotic expansions by Gamma-convergence*, Cont. Mech. Therm. **20** (2008), 21–62

[6] G. Dal Maso, "An Introduction to Γ-convergence", Birkhäuser, Boston, 1993.

[7] C. J. Larsen, *Epsilon-stable quasi-static brittle fracture evolution*, Comm. Pure Appl. Math. **63** (2010), 630–654.

On gradient descents in random wiggly energies

Timothy Sullivan
(joint work with Florian Theil)

In physics, engineering and other settings, it is important to understand the macroscopic behaviour of systems whose evolution is determined by microscale effects. It seems natural to consider these microscale effects to be random in nature (and, therefore, beyond the scope of classical averaging and homogenization theory) and to constitute some perturbation of a well-understood smooth structure. In the case of rate-*dependent* viscous systems, analysis of how the random microstructure determines the macroscopic behaviour can be found in the Green–Kubo relations and many further developments since their introduction in the 1950s. In the realm of rate-*independent* plasticity theory, there is a large literature (see, *e.g.*, [4]) surrounding rate-independent processes (or quasistatic evolutions) described by ordinary differential inclusions such as

$$\text{(1)} \qquad \begin{cases} \partial\Psi(\dot{z}(t)) \ni -\mathrm{D}E(t, z(t)), & \text{for all } t \in [0, T], \\ z_\varepsilon(0) = x_0, & \text{for some given } x_0 \in \mathbb{R}^n, \end{cases}$$

where Ψ is homogeneous of degree one, which have been very successful in modelling plastic effects with their associated structures of hysteresis loops, yield surfaces, stick-slip dynamics *& c.* Stick-slip evolutions such as the movement of a dislocation line in a crystalline structure or the Barkhausen effect in a ferromagnetic domain can be seen in this way, *cf.* [1] [2]. Our interest lies in rigorously obtaining the evolution of z in (1) as the limit as $\varepsilon \to 0$ of the (random) rate-dependent processes z_ε that satisfy

$$\text{(2)} \qquad \begin{cases} \dot{z}_\varepsilon(t) = -\dfrac{1}{\varepsilon}\nabla E_\varepsilon(t, z_\varepsilon(t)), & \text{for all } t \in [0, T], \\ z_\varepsilon(0) = x_0, & \text{for some given } x_0 \in \mathbb{R}^n, \end{cases}$$

where E_ε is a suitable (random) perturbation of the underlying energetic potential E. It should be noted that, typically, $E_\varepsilon \to E$ strongly whereas ∇E_ε does not converge as $\varepsilon \to 0$. It should also be noted that taking the limit as $\varepsilon \to 0$ results in a change from a dissipation potential that is homogenous of degree *two* in (2) to one of degree *one* in (1).

The convergence $z_\varepsilon \to z$ has been known since the 1990s in the case $n = 1$ with a periodic perturbation [1]. Periodic perturbations in $n = 2$ were considered in [3]; an undesirable feature of the periodic situation in $n \geq 2$ is that periodic "grid effects" introduce resonance zones for the limit process, where the dynamics consist of both sticking and slipping; these resonance zones have the structure of the complement of a Cantor set.

In order to dispense with the unnatural periodicity assumption and to avoid such anisotropic grid effects, we consider random perturbations of E. A result for $n = 1$ was reported in [6]; both the 1-dimensional case and the n-dimensional analysis outlined here are treated in detail in [5].

For simplicity, we consider the moving quadratic energetic potential $E(t, x) := \frac{1}{2}\langle Ax, x\rangle - \langle \ell(t), x\rangle$, where A is symmetric and positive-definite and ℓ is Lipschitz. The random perturbation $E_\varepsilon - E$ is a sum of prototypical *dent functions*

$$D_{\varepsilon,y}(x) := \frac{\sigma}{2} \min\left\{0, \frac{\|x - y\|_2^2}{\varepsilon} - 1\right\},$$

where y ranges over the points of a Poisson point process in $\mathbb{R}^n$ of intensity ε^{-p}, and $\sigma > 0$ is the magnitude of the dent's gradient at the edge of its support. It becomes apparent in the course of the proof that the constant-volume-fraction limit for the Poisson process (the case $p = n$) is not permissible; therefore, the $\varepsilon \to 0$ limit that we consider is a *dilute limit*, although limits arbitrarily close to the constant-volume-fraction limit are allowed.

Theorem 1. *In the notation used above, let* $\Psi := \sigma\|\cdot\|_2$. *Then, for all* $T > 0$ *and* $p \in (n - 1, n)$, *it holds that* $\lim_{\varepsilon\to 0} z_\varepsilon = z$ *in probability in* $\mathcal{C}^0([0, T]; \mathbb{R}^n)$ *with the uniform norm* $\|\cdot\|_\infty$*:* i.e., *for all* $\delta > 0$,

$$\lim_{\varepsilon\to 0} \mathbb{P}\left[\sup_{t\in[0,T]} \big\|z_\varepsilon(t) - z(t)\big\|_2 \geq \delta\right] = 0.$$

It follows from theorem 1 that, up to the extraction of suitable subsequences, $z_\varepsilon \to z$ uniformly on $[0, T]$, $\mathbb{P}$-almost surely.

The key step in the proof is to control the total variation of z_ε and thereby show that z_ε "nearly" satisfies the energy evolution inequality for the limit process z. More precisely, for $[a, b] \subseteq [0, T]$, define the *energy surplus* of $u\colon [a, b] \to \mathbb{R}^n$ by the following $\|\cdot\|_\infty$-lower-semicontinuous functional $\mathrm{ES}(\cdot, [a, b])\colon \mathrm{BV}([a, b]; \mathbb{R}^n) \to \mathbb{R}$:

$$\mathrm{ES}(u, [a, b]) := E(b, u(b)) - E(a, u(a)) + \int_a^b \big(\Psi(\dot{u}(t)) - (\partial_t E)(t, u(t))\big)\,\mathrm{d}t.$$

For the rate-independent limit process z, $\mathrm{ES}(z, [a, b]) \leq 0$ for all $[a, b] \subseteq [0, T]$. It can be shown that the random evolution z_ε has vanishing energy surplus in mean square:

$$\mathbb{E}\big[\mathrm{ES}(z_\varepsilon, [0, T])\big] \leq CT\varepsilon^{p-n+1},$$
$$\mathbb{V}\big[\mathrm{ES}(z_\varepsilon, [0, T])\big] \leq CT\varepsilon^{p-n+2}.$$

The tightness (compactness) of the family $(z_\varepsilon)_{\varepsilon>0}$ follows easily from this argument, and it is not hard to show that any uniform limit $\tilde{z}$ of $(z_\varepsilon)_{\varepsilon>0}$ must satisfy the stability constraint $\|\nabla E(t, \tilde{z}(t))\|_2 \leq \sigma$, which, together with the energy inequality, is the other condition that characterizes z.

It would be of interest to extend theorem 1 to more general energetic potentials E defined on possibly infinite-dimensional spaces, and to include the effects of a heat bath whose influence is of the same order as that of the microstructure E_ε.

References

[1] R. Abeyaratne, C.-H. Chu & R. D. James, Kinetics of materials with wiggly energies: theory and application to the evolution of twinning microstructures in a Cu-Al-Ni shape memory alloy, *Phil. Mag. A* **73** (1996), 457–497.

[2] N. Grunewald, Barkhausen effect: a stick-slip motion in a random medium, *Methods Appl. Anal.* **12**(1) (2005), 29–41.

[3] G. Menon, Gradient systems with wiggly energies and related averaging problems, *Arch. Ration. Mech. Anal.* **162**(3) (2002), 193–246.

[4] A. Mielke & F. Theil, On rate-independent hysteresis models, *NoDEA Nonlinear Differential Equations Appl.* **11**(2) (2004), 151–189.

[5] T. J. Sullivan, *Analysis of Gradient Descents in Random Energies and Heat Baths*, PhD thesis, University of Warwick, UK (2009).

[6] T. J. Sullivan & F. Theil, Deterministic stick-slip dynamics in a one-dimensional random potential, *Analysis and Numerics for Rate-Independent Processes, 25 February–3 March 2007*, ed. Martin Kružík. *Oberwolfach Reports* 11/2007 (2007) 62–65

Two-scale homogenization in strain gradient plasticity

Alessandro Giacomini

(joint work with Alessandro Musesti)

We provide a two-scale convergence approach for an homogenization result in strain gradient plasticity due to Fleck and Willis [4]. This result concerns the asymptotic behaviour of minimizers of the following energy

$$\mathcal{E}(u,p) - \int_\Omega f(x)\cdot u(x)\,dx,$$

where

$$\mathcal{E}(u,p) := \frac{1}{2}\int_\Omega \mathbb{C}(x)(Eu-p):(Eu-p)\,dx + \int_\Omega b(x)[|p|^2+\ell^2|\nabla p|^2]\,dx,$$

in the case the elastic and plastic moduli $\mathbb{C}$ and b oscillate. Here $\Omega\subset\mathbb{R}^N$ denotes the reference configuration of an elastoplastic body, Eu is the symmetrized gradient of the displacement $u:\Omega\to\mathbb{R}^N$, while $p:\Omega\to \mathrm{M}^N_D$ is the plastic strain, taking values in the space of deviatoric matrices. The constant ℓ, associated to the presence of the gradient of the plastic strain p, is an intrinsic length scale of the material. The deformation theory we consider is thus a *strain gradient deformation theory* [2, 3].

We consider the case of periodic oscillations, i.e., we consider

$$\mathbb{C}\in L^\infty(\mathbb{R}^N;\mathrm{Lin}(\mathrm{M}^N_{\mathrm{sym}};\mathrm{M}^N_{\mathrm{sym}})) \qquad \text{and} \qquad b\in L^\infty(\mathbb{R}^N)$$

such that for every $i=1,\dots,N$ and for a.e. $x\in\mathbb{R}^N$

$$\mathbb{C}(x+e_i)=\mathbb{C}(x) \qquad \text{and} \qquad b(x+e_i)=b(x).$$

Since oscillations occur on a scale ε, we accordingly rescale the intrinsic length scale to $\varepsilon\ell$. The energies then assume the following form

$$\mathcal{E}_\varepsilon(u,p) = \frac{1}{2}\int_\Omega \mathbb{C}\left(\frac{x}{\varepsilon}\right)(Eu-p):(Eu-p)\,dx + \int_\Omega b\left(\frac{x}{\varepsilon}\right)[|p|^2+\varepsilon^2\ell^2|\nabla p|^2]\,dx.$$

Assuming the coercivity estimates

$$\alpha|M|^2 \le \mathbb{C}(x)M : M \le \beta|M|^2, \qquad 0 < \alpha < \beta < +\infty$$

and $b(x) > c > 0$, $\mathcal{E}_\varepsilon$ turns out to be well defined on $H^1(\Omega;\mathbb{R}^N) \times H^1(\Omega;\mathrm{M}^N_D)$.

The family of minimizers of

$$(u,p) \mapsto \mathcal{E}_\varepsilon(u,p) - \int_\Omega f \cdot d\, dx$$

such that $u = \bar{u} \in H^1(\Omega;\mathbb{R}^N)$ on $\partial\Omega$ satisfy the following bound

$$\|u_\varepsilon\|_{H^1(\Omega;\mathbb{R}^N)} + \|p_\varepsilon\|_{L^2(\Omega;\mathrm{M}^N_D)} + \varepsilon\|\nabla p_\varepsilon\|_{L^2(\Omega;\mathbb{M}^N_D)} \le \tilde{C}.$$

As a consequence, the effective behaviour of the energies would be given in terms of the weak limit of the displacements in $H^1(\Omega;\mathbb{R}^N)$ and of the weak limit of the plastic strains in $L^2(\Omega;\mathrm{M}^N_D)$: the control on ∇p_ε in L^2 tends to vanish in the limit.

By means of an analysis involving two-scale convergence ([8, 1]), we show that the variational properties of $\mathcal{E}_\varepsilon$ are encoded in the two scale energy

$$\mathcal{E}(u,U,P) := \frac{1}{2}\int_{\Omega\times Y} \mathbb{C}(y)(Eu + E_yU - P) : (Eu + E_yU - P)\, dxdy + \int_{\Omega\times Y} b(y)[|P|^2 + \ell^2|\nabla_y P|^2]\, dxdy,$$

where Y denotes the unit cube in $\mathbb{R}^N$ centered at the origin,

$$u(x) \in H^1(\Omega;\mathbb{R}^N), \quad U(x,y) \in L^2(\Omega; H^1_{per,0}(Y;\mathbb{R}^N))$$

and

$$P(x,y) \in L^2(\Omega; H^1_{per}(Y;\mathrm{M}^N_D)).$$

In order to move toward a single scale setting, we introduce the functional

$$\mathcal{E}^{eff} : H^1(\Omega;\mathbb{R}^N) \times L^2(\Omega;\mathrm{M}^N_D) \to [0,+\infty[$$

defined by

$$\mathcal{E}^{eff}(u,p) := \min_{(U,P)} \Big\{ \mathcal{E}(u,U,P) : (U,P) \in L^2(\Omega; H^1_{per,0}(Y;\mathbb{R}^N)) \times L^2(\Omega; H^1_{per}(Y;\mathrm{M}^N_D)), \int_Y P(x,y)\, dy = p(x) \text{ for a.e. } x \in \Omega \Big\}.$$

We can now state our main results.

Theorem 1 (The homogenization result of Fleck and Willis). *For every $\varepsilon > 0$ let $(u_\varepsilon, p_\varepsilon)$ be the minimizer of*

$$(u,p) \mapsto \mathcal{E}_\varepsilon(u,p) - \int_\Omega f \cdot u\, dx$$

on $H^1(\Omega;\mathbb{R}^N) \times H^1(\Omega;\mathrm{M}^N_D)$ with $u = \bar{u}$ on $\partial\Omega$. Then for $\varepsilon \to 0$

$$u_\varepsilon \rightharpoonup u_0 \qquad \textit{weakly in } H^1(\Omega;\mathbb{R}^N)$$

and

$$p_\varepsilon \rightharpoonup p_0 \qquad \text{weakly in } L^2(\Omega;\mathrm{M}^N_D),$$

where (u_0,p_0) *is the unique minimizer of*

$$(u,p)\mapsto \mathcal{E}^{\mathit{eff}}(u,p)-\int_\Omega f\cdot u\,dx \tag{1}$$

on $H^1(\Omega;\mathbb{R}^N)\times L^2(\Omega;\mathrm{M}^N_D)$ *with* $u=\bar u$ *on* $\partial\Omega$. *Moreover*

$$\lim_{\varepsilon\to 0}\mathcal{E}_\varepsilon(u_\varepsilon,p_\varepsilon)=\mathcal{E}^{\mathit{eff}}(u_0,p_0).$$

The energy $\mathcal{E}^{\mathit{eff}}(u,p)$ turns out to be independent of ∇p. We have the following representation result involving a cell-type problem.

Theorem 2 (Representation formula for the effective energy). *For every* $(u,p)\in H^1(\Omega;\mathbb{R}^N)\times L^2(\Omega;\mathrm{M}^N_D)$ *we have*

$$\mathcal{E}^{\mathit{eff}}(u,p)=\int_\Omega F^{\mathit{eff}}(Eu(x),p(x))\,dx, \tag{2}$$

where for $(\bar A,\bar p)\in \mathrm{M}^N_{\mathrm{sym}}\times\mathrm{M}^N_D$

$$\begin{aligned} F^{\mathit{eff}}(\bar A,\bar p):=\min\Big\{&\frac12\int_Y \mathbb{C}(y)[\bar A+E_yU-P]:[\bar A+E_yU-P]\,dy\\ &+\int_Y b(y)[|P|^2+\ell^2|\nabla_y P|^2]\,dy : (U,P)\in H^1_{per,0}(Y;\mathbb{R}^N)\times H^1_{per}(Y;\mathrm{M}^N_D),\\ &\int_Y P(y)\,dy=\bar p\Big\}. \end{aligned} \tag{3}$$

Following the same two-scale approach, we can deal with the homogenization of strain gradient quasistatic evolutions. We concentrated on the model of Gurtin and Anand [5] in presence of linear isotropic hardening and neglecting the energetic strain gradient contribution. Following Mielke and Timofte [7], we show that the evolutions converge to a two-scale quasistatic evolution which is of strain gradient type in the microscopic variable y. The passage to a single scale setting entails loss of informations, and a description in terms of a quasistatic evolution for an ordinary plasticity theory seems not feasible. This is connected to the nonlocal effects (for example of memory-type) that can be induced by homogenization, as shown by Tartar [9].

References

[1] Allaire G.: Homogenization and two-scale convergence. *SIAM J. Math. Anal.* **23** (1992), no. 6, 1482–1518.

[2] Fleck N.A., Hutchinson J.W.: Strain gradient plasticity. *Adv. Appl. Mech.* **33** (1997), 295–361.

[3] Fleck N.A., Hutchinson J.W.: A reformulation of strain gradient plasticity. *J. Mech. Phys. Solids.* **49** (2001), 2245–2271.

[4] Fleck N. A., Willis J. R.: Bounds and estimates for the effect of strain gradients upon the effective plastic properties of an isotropic two-phase composite. *J. Mech. Phys. Solids* **52** (2004), no. 8, 1855–1888.

[5] Gurtin M. E.; Anand L.: A theory of strain-gradient plasticity for isotropic, plastically irrotational materials. I. Small deformations. *J. Mech. Phys. Solids* **53** (2005), no. 7, 1624–1649.
[6] Mielke A.: *Evolution of rate-independent systems*. Evolutionary equations. Vol. II, 461–559, Handb. Differ. Equ., Elsevier/North-Holland, Amsterdam, 2005.
[7] Mielke A., Timofte A. M.: Two-scale homogenization for evolutionary variational inequalities via the energetic formulation. *SIAM J. Math. Anal.* **39** (2007), no. 2, 642–668
[8] Nguetseng G., A general convergence result for a functional related to the theory of homogenization. *SIAM J. Math. Anal.* **20** (1989), no. 3, 608–623.
[9] Tartar L.: Nonlocal effects induced by homogenization. *Partial differential equations and the calculus of variations, Vol. II, 925–938, Progr. Nonlinear Differential Equations Appl., 2*, Birkhäuser Boston, Boston, MA, 1989.

Towards uniformly Γ-equivalent theories in the context of fracture mechanics

Anja Schlömerkemper
(joint work with L. Scardia, C. Zanini)

The aim of our work is to rigorously derive continuum models for fracture mechanics from atomistic models. To get started, we study a one-dimensional chain of atoms with nearest and next-to-nearest neighbour interactions of Lennard-Jones type under certain boundary conditions and apply Γ-convergence methods.

Let J_1 and J_2 be the classical Lennard-Jones potentials, or more general interaction potentials of Lennard-Jones type, see [4] for details. Set $\lambda_n = \frac{1}{n}$, $n \in \mathbb{N}$ and let $u : \lambda_n\mathbb{Z} \cap [0,1] \to \mathbb{R}$ describe the deformation of the discrete chain with respect to the reference configuration $\lambda_n\mathbb{Z} \cap [0,1]$. We set $u^i = u(\lambda_n i)$ and identify u with its piecewise affine interpolation, so $u \in \mathcal{A}_n(0,1)$, the space of piecewise affine functions. Let the following three parameters ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$ be given. We consider the energy functional $H_n^\ell : \mathcal{A}_n(0,1) \to (-\infty, \infty]$ which is defined as

$$H_n^\ell(u) = \sum_{i=0}^{n-1} \lambda_n J_1\left(\frac{u^{i+1} - u^i}{\lambda_n}\right) + \sum_{i=0}^{n-2} \lambda_n J_2\left(\frac{u^{i+2} - u^i}{2\lambda_n}\right)$$

if u satisfies the boundary conditions $u^0 = 0, u^1 = \lambda_n u_0^{(1)}, u^{n-1} = \ell - \lambda_n u_1^{(1)}, u^n = \ell$ and is infinite else.

As shown in [4], the Γ-limit H_0^ℓ of H_n^ℓ as $n \to \infty$ involves the convexification of the effective potential

$$J_0(z) = J_2(z) + \frac{1}{2} \inf\big\{J_1(z_1) + J_1(z_2) : z_1 + z_2 = 2z\big\}.$$

The minimal value of the Γ-limit is $\min H_0^\ell = J_0^{**}(\ell)$ for all $\ell > 0$.

Since we are interested in describing fracture, the Γ-limit does not give a satisfactory answer. Indeed, we would like to obtain a boundary layer energy in the limit, i.e., a surface energy due to the opening of a crack. Therefore we derive [4]

the first order Γ-limit, H_1^ℓ. This has minimal values

$$\min H_1^\ell = \begin{cases} B\left(u_0^{(1)},\ell\right) + B\left(u_1^{(1)},\ell\right) - J_0(\ell) \\ -J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2} - \ell\right) & \text{if } \ell \le \gamma \\ B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma) + \beta_{\min} & \text{if } \ell > \gamma \end{cases}, \tag{1}$$

where γ is the minimum point of J_0, $B(\theta,\ell)$ is some boundary layer energy and $\beta_{\min} \neq 0$ involves boundary layer energies and depends on where the crack is located, see [4] for details. We remark that the first order development of the minimal values

$$\widetilde{m}(\ell) = \min H_0^\ell + \lambda_n \min H_1^\ell \tag{2}$$

shows a jump of order $\lambda_n\beta_{\min}$ at $\ell = \gamma$, see Figure 1 for a sketch. The jump

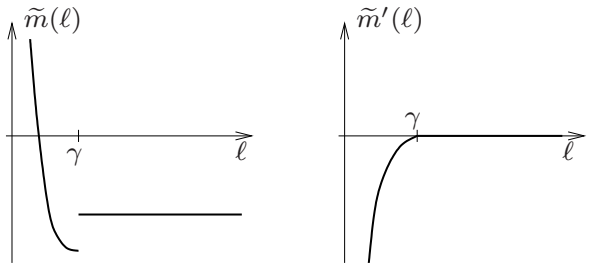

FIGURE 1. Behaviour of the development of minimal values in (2) in dependence of ℓ as well as the behaviour of the derivative.

at $\ell = \gamma$ is of the order λ_n, which means that our model contains an (internal) length parameter. This is what we expect to have in a model describing fracture. However, notice that at $\ell > \gamma$ the material breaks at zero tension. In order to overcome this, we derive a uniformly Γ-equivalent theory in the spirit of Braides and Truskinovsky [3].

To achieve this, we consider a blow up at $\ell = \gamma$ and generalise a Γ-convergence result by [2]. Let $\lambda_{n_j} \to 0$ and $\ell_j \to \ell$ as $j \to \infty$. Then the minimal value of the first order Γ-limit of H_n^ℓ is equal to (see [5])

$$\lim_{j\to\infty} \min \left\{ \alpha \int_0^1 |v'|^2\,dt + B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma) + \beta_0 \#(S_v \cap \{0\}) \right.$$
$$\left. + \beta_1 \#(S_v \cap \{1\}) + \beta_{\text{int}} \#(S_v \cap (0,1)) \ : v(0) = 0, v(1) = \frac{\ell_j - 1}{\sqrt{\lambda_{n_j}}} \right\}$$

with $\alpha = \frac{1}{2}J''(\gamma)$, where the scaling $v^i = \frac{u^i - \lambda_{n_j}\gamma i}{\sqrt{\lambda_{n_j}}}$ is considered and the β's again involve boundary layer energies. Furthermore, (1) is equal to

$$\lim_{j\to\infty} \min\left\{\frac{\alpha(\ell_j-\gamma)^2}{\lambda_{n_j}}, \beta_{\min}\right\} + B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma).$$

Hence the transition from elasticity 9described by the quadratic term in the minimum above) to fracture (corresponding to the constant value $\beta_{\min}$) depends on the rate of convergence of ℓ_j to γ with respect to λ_{n_j}, which is sketched in Figure 2.

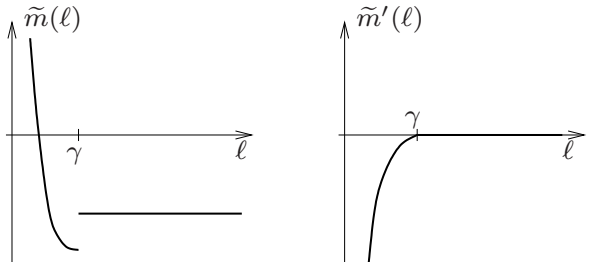

FIGURE 2. Blow up and failure curve at $\ell = \gamma$.

A uniformly Γ-equivalent theory is now obtained by taking an energy which is Γ-equivalent to the original energy for ℓ far from γ and an energy which is Γ-equivalent to the rectified one (obtained by blow-up) for ℓ close to γ, and by proving that these match at $\ell = \gamma$.
We show in [5] that the following functional G_n^ℓ is uniformly Γ-equivalent at first order to H_n^ℓ: If $\ell \le \gamma$, set

$$G_n^\ell(u) = \int_0^1 J_0(u')\,dt + \lambda_n\Big(B\big(u_0^{(1)}, \ell\big) + B\big(u_1^{(1)}, \ell\big) - J_0(\ell)\Big) - \lambda_n J_0'(\ell)\left(\frac{u_0^{(1)} + u_1^{(1)}}{2} - \ell\right),$$

and if $\ell > \gamma$, by a pull-back of variables $u(t) = \gamma t + \sqrt{\lambda_n} v(t)$, set

$$G_n^\ell(u) = J_0(\gamma) + \alpha\int_0^1 |u' - \gamma|^2 dt + \lambda_n\Big(B\big(u_0^{(1)}, \gamma\big) + B\big(u_1^{(1)}, \gamma\big) - J_0(\gamma)\Big) + \lambda_n\left(\beta_0 \#(S_u \cap \{0\}) + \beta_1 \#(S_u \cap \{1\})\right) + \lambda_n \beta_{int} \#(S_u \cap (0,1))$$

if $u(0) = 0$, $u(1) = \ell$, $[u] > 0$ on S_u, and ∞ else.

The qualitative behaviour of the minimal values of the equivalent theory G_n^ℓ is sketched in Figure 3. In particular, $\overline{m} : \ell \mapsto \min G_n^\ell$ is continuous. In future work we will investigate this and other Γ-equivalent theories further.

REFERENCES

[1] A. Braides and M. Cicalese, *Surface energies in nonconvex discrete systems*, Math. Models Methods Appl. Sci. **17** (2007), 985–1037.

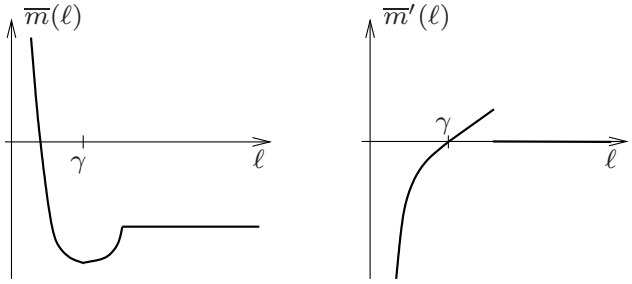

FIGURE 3. Behaviour of the minimal values and its derivatives of the uniformly Γ-equivalent theory in dependence of ℓ.

[2] A. Braides, A. Lew and M. Ortiz, *Effective cohesive behavior of layers of interatomic planes*, Arch. Rational Mech. Anal.**180** (2006), 151–182.
[3] A. Braides and L. Truskinvosky, *Asymptotic expansions by* Γ*-convergence*, Cont. Mech. Thermodyn. **20** (2008), 21–62.
[4] L. Scardia, A. Schlömerkemper, C. Zanini, *Boundary layer energies for nonconvex discrete systems*, submitted, MPI-MIS preprint 4/2009
[5] L. Scardia, A. Schlömerkemper, C. Zanini, *On uniformly* Γ*-equivalente theories for nonconvex discrete systems*, in preparation

Interfacial energy and size effects in evolving martensitic microstructures

STANISŁAW STUPKIEWICZ
(joint work with Henryk Petryk)

A fully three-dimensional model of evolving martensitic microstructure is proposed, which accounts for the interfacial energy and also for the dissipation related to annihilation of interfaces. The interfacial energy of two origins is considered, namely the atomic-scale energy of phase or twin boundaries and the elastic microstrain energy at microstructured interfaces. Accordingly, size effects can be studied quantitatively for a class of martensitic microstructures in shape memory alloys (SMA). Details of the approach can be found in [3, 4].

The total Helmholz free energy density Φ is assumed to comprise the size-independent bulk contribution Φ_{v} and several size-dependent interfacial energy contributions Φ_k

$$\Phi = \Phi_{\mathrm{v}} + \Phi_{\mathrm{i}}, \qquad \Phi_{\mathrm{i}} = \sum_k \Phi_k. \tag{1}$$

Each Φ_k originates from the interfacial energy at a specific scale which is integrated over all interfaces at this scale and divided by the volume of the corresponding representative element.

With regard to the martensitic transformation in polycrystalline SMA, the interfacial energy is considered at three scales, namely at the grain (or subgrain) boundaries attained by parallel martensitic plates, at the austenite-twinned martensite interfaces, and at the twin boundaries within the martensitic plates.

In general, the density (per unit area) of the interfacial energy γ_k can be a sum of the atomic-scale energy γ_k^{a} and elastic micro-strain energy γ_k^{e},

$$\gamma_k = \gamma_k^{\mathrm{a}} + \gamma_k^{\mathrm{e}}, \qquad \gamma_k^{\mathrm{e}} = \Gamma_k^{\mathrm{e}} h_k, \tag{2}$$

the latter is proportional to the spacing h_k of the laminated microstructure terminating at the interface. The proportionality factor Γ_k^{e} is a size independent quantity that can be estimated using the approach proposed in [1, 5] for the case of austenite-twinned martensite interfaces or a using an approximating function determined in [4], used here for the elastic micro-strain energy at the grain (subgrain) boundaries. The relevant atomic-scale interfacial energies are taken from the materials science literature.

Similarly to the free energy in (1), the dissipation increment ΔD is assumed as a sum of the size-independent bulk contribution ΔD_{v} and size-dependent interfacial contributions ΔD_k,

$$\Delta D = \Delta D_{\mathrm{v}} + \Delta D_{\mathrm{i}}, \qquad \Delta D_{\mathrm{i}} = \sum_k \Delta D_k. \tag{3}$$

The key assumption of the present model is that the negative increments of interfacial energy, which are associated with *annihilation* of interfaces, contribute to (size-dependent) dissipation, so that we have

$$\Delta D_k = \kappa_k(-\Delta\Phi_k)_+, \qquad (\psi)_+ = \begin{cases} \psi & \text{if } \psi > 0, \\ 0 & \text{if } \psi \le 0. \end{cases} \tag{4}$$

Here $0 \le \kappa_k \le 1$ is a coefficient that is expected to be close to unity at low scales and possibly smaller, but still close to unity, at higher scales. The bulk dissipation term includes all the remaining dissipation mechanisms and is assumed as $\Delta D_{\mathrm{v}} = f_{\mathrm{c}}|\Delta\eta|$, where η is the volume fraction of martensite and $f_{\mathrm{c}} > 0$ is the threshold value for the thermodynamic driving force $f = -\partial\Phi_{\mathrm{v}}/\partial\eta$.

The evolution of microstructure in an isothermal, quasi-static process is determined by minimization of the incremental energy supply [2]

$$\Delta E \;\to\; \min \qquad \text{subject to kinematical constraints,} \tag{5}$$

where, assuming kinematic control, the incremental energy is equal to

$$\Delta E = \Delta\Phi + \Delta D. \tag{6}$$

Note that the adopted dissipation function exhibits a limited path-independence [3] so that it automatically satisfies the essential symmetry restriction which is necessary for the minimization principle (5) to be applicable for finite increments [2, 3].

The above framework has been applied in [4] for the simulation of the pseudoelastic response of an idealized CuAlNi SMA polycrystal. Formation and evolution of a rank-three laminated microstructure of finite characteristic dimensions has been examined. The results illustrate also the effect of grain size of the macroscopic stress-strain response, including the hysteresis width, as well as on the characteristic dimensions such as twin spacing, plate thickness, and plate spacing.

References

[1] G. Maciejewski, S. Stupkiewicz, and H. Petryk, *Elastic micro-strain energy at the austenite–twinned martensite interface*, Arch. Mech. **57** (2005), 277–297.

[2] H. Petryk, *Incremental energy minimization in dissipative solids*, C.R. Mecanique **331** (2003), 469–474.

[3] H. Petryk and S. Stupkiewicz, *Interfacial energy and dissipation in martensitic phase transformations. Part I: Theory*, J. Mech. Phys. Solids **58** (2009), 390–408.

[4] H. Petryk, S. Stupkiewicz, and G. Maciejewski, *Interfacial energy and dissipation in martensitic phase transformations. Part II: Size effects in pseudoelasticity*, J. Mech. Phys. Solids **58** (2009), 373–389.

[5] S. Stupkiewicz, G. Maciejewski, and H. Petryk, *Low-energy morphology of the interface layer between austenite and twinned martensite*, Acta Mater. **55** (2007), 6292–6306.

Relaxation-based modeling of laminate microstructures in finite-strain crystal plasticity

Dennis M. Kochmann

(joint work with Klaus Hackl)

The non-quasiconvexity of the free energy density in finite-strain crystal plasticity gives rise to the formation of microstructures as minimizers of the governing minimum principles [1, 5]. Such microstructures form in plastically strained, crystalline solids and can be observed experimentally in terms of dislocation patterns. The specifics of these microstructures and their impact on the macroscopic material behavior can be determined by means of a relaxation of the energy and dissipation potentials involved.

In finite-strain plasticity models, the deformed state of a strained solid is generally described in terms of the displacement field $\boldsymbol{\phi}$ and a set of internal variables $\boldsymbol{K}$ which capture all microstructural characteristics. We denote the deformation gradient by $\boldsymbol{F} = \boldsymbol{\nabla}\boldsymbol{\phi}$ and the free energy density by $\Psi(\boldsymbol{F}, \boldsymbol{K})$. Furthermore, we introduce the total free energy stored in a deformed body Ω by

$$\mathcal{I}(t, \boldsymbol{\phi}, \boldsymbol{K}) = \int_\Omega \Psi(\nabla\boldsymbol{\phi}, \boldsymbol{K}) \mathrm{d}V - \ell(t, \boldsymbol{\phi}) \tag{1}$$

where $\ell(t, \boldsymbol{\phi})$ represents the potential of external forces. The microstructure development can then be determined from thermodynamic minimum principles [1, 5]. The actual displacement field follows from the principle of minimum potential energy, and the internal variables are determined from the principle of minimum dissipation potential. These principles are defined as

$$\boldsymbol{\phi} = \operatorname{argmin} \{ \mathcal{I}(t, \boldsymbol{\phi}, \boldsymbol{K}) \mid \boldsymbol{\phi} = \boldsymbol{\phi}_0 \text{ on } \partial\Omega \}, \tag{2}$$

$$\dot{\boldsymbol{K}} = \operatorname{argmin} \left\{ \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{K}, \dot{\boldsymbol{K}}) \;\middle|\; \dot{\boldsymbol{K}} \right\}, \tag{3}$$

respectively, with the dot denoting differentiation with respect to time, and with the introduced Lagrange functional

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{K}, \dot{\boldsymbol{K}}) = \frac{\mathrm{d}}{\mathrm{d}t} \Psi(\nabla\boldsymbol{\phi}, \boldsymbol{K}) + \Delta(\boldsymbol{K}, \dot{\boldsymbol{K}}). \tag{4}$$

$\Delta(\boldsymbol{K}, \dot{\boldsymbol{K}})$ represents the dissipation potential [1], which accounts for dissipation due to dislocation motion in the crystalline solid and must be specified.

To describe the formation of a particular type of microstructure, viz. simple laminates, we derive an approximation of the relaxed energy (i.e., of the quasiconvex envelope) by constructing a laminate of first order, characterized by N volume fractions λ_i with values $\boldsymbol{K}_i$ and $\boldsymbol{F}_i$, which are separated by parallel planes with common normal vector $\boldsymbol{b}$, so that we may write for each phase i [2]

$$\boldsymbol{F}_i = \boldsymbol{F}(\boldsymbol{I} + \boldsymbol{a}_i \otimes \boldsymbol{b}) \tag{5}$$

Hence, deformation gradients differ only by tensors of rank one, enforcing compatibility at laminate interfaces. We consider the normal vector $\boldsymbol{b}$ as inelastic (or dissipative), since any rotation of the laminate causes microstructural rearrangement and thus dissipation. In contrast, the amplitudes $\boldsymbol{a}_i$ can be changed purely elastically. Therefore, we define the (semi-)relaxed energy as

$$\Psi^{\mathrm{rel}}(\boldsymbol{F}, \lambda, \boldsymbol{K}, \boldsymbol{b}) = \inf \left\{ \sum_{i=1}^{N} \lambda_i \Psi(\boldsymbol{F}_i, \boldsymbol{K}_i) \;\middle|\; \boldsymbol{a}_i; \sum_{i=1}^{N} \lambda_i \boldsymbol{a}_i = \boldsymbol{0} \right\}, \tag{6}$$

where the abbreviations $\lambda = \{\lambda_1, \ldots, \lambda_N\}$ and $\boldsymbol{K} = \{\boldsymbol{K}_1, \ldots, \boldsymbol{K}_N\}$ are introduced, and the constraint accounts for the average laminate deformation to equal the overall deformation $\boldsymbol{F}$.

We apply the above formulation to an incompressible Neo-Hookean solid with one active slip system only (for illustrative purposes, the framework has been generalized to multiple slip systems) [2, 3]. The multiplicative split of the deformation gradient into elastic and plastic contribution, i.e., $\boldsymbol{F} = \boldsymbol{F}_{\mathrm{e}} \boldsymbol{F}_{\mathrm{p}}$, allows for the common flow rule of crystal plasticity: $\dot{\boldsymbol{F}}_{\mathrm{p}} \boldsymbol{F}_{\mathrm{p}}^{-1} = \sum_i \dot{\gamma}_i \, \boldsymbol{s}_i \otimes \boldsymbol{m}_i$. For a single active slip system $(\boldsymbol{s}, \boldsymbol{m})$, we conclude that $\boldsymbol{F}_{\mathrm{e}} = \boldsymbol{F}(\boldsymbol{I} - \gamma \, \boldsymbol{s} \otimes \boldsymbol{m})$ with plastic slip γ. The free energy density of an incompressible Neo-Hookean solid ($\det \boldsymbol{F} = 1$) follows as

$$\Psi(\boldsymbol{F}_{\mathrm{e}}, p) = \frac{\mu}{2} \left(\operatorname{tr} \boldsymbol{F}_{\mathrm{e}}^T \boldsymbol{F}_{\mathrm{e}} - 3 \right) + \kappa \, p^{\alpha}. \tag{7}$$

The second term accounts for hardening with p being a hardening variable, which is governed by the flow rule $\dot{p} = |\dot{\gamma}|$, and $\mu > 0$ and $\kappa > 0$ are the shear and hardening moduli, respectively. Furthermore, we assume dissipation of the type $\Delta(\dot{\gamma}) = r \, |\dot{\gamma}|$.

With this framework at hand, the minimization in (6) can be carried out analytically [2]. Besides, we have developed a suitable relaxed dissipation potential which accounts for a first-order laminate microstructure [2, 3].

Many approaches in the scientific literature make use of an effective (or condensed) energy functional to predict the formation of microstructures. However, this approach is not generally suitable for the description of their time-continuous evolution. Therefore, we establish a variational, incremental strategy, which is applicable both to monotonic and cyclic loading and which accounts for the exact microstructural changes during each time step. To this end, we incrementally solve the stationarity conditions of the minimum principle (3), where the energy density and dissipation potential are replaced by their relaxed counterparts. Our

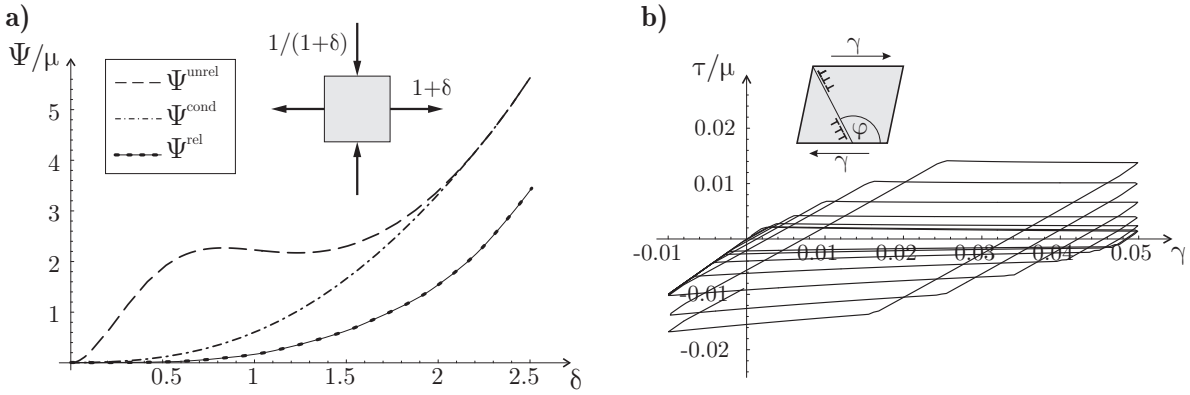

FIGURE 1. a) Comparison of the (normalized) unrelaxed energy Ψ^{unrel} and the relaxed energy for a tension-compression load path (from a condensed energy functional, Ψ^{cond}, and from the present approach, Ψ^{rel}), b) cyclic normalized stress-strain response for a simple shear test from the present approach. Results are for $\kappa = 0.005\mu$, $r = 0.001\mu$, $\varphi = 135°$, $\alpha = 2$.

numerical scheme includes in particular the possibility to update the hardening parameters during each time step (dependent on the existing microstructure at the beginning of the time step) [2, 3], furthermore possible laminate rotations [2], and cyclic loading [4].

Figure 1 illustrates two important characteristics of the results obtained from the present approach which has been combined with a suitable numerical scheme. From Figure 1a it becomes apparent that the present approach gives rise to a considerable reduction of energy, compared to the results from using a condensed energy functional. This stems in particular from the incremental updates of the hardening variables due to volume fraction changes [2]. Besides, the possibility of an incremental laminate rotation is accounted for by the present approach and might yield further decreases of the energy. Figure 1b demonstrates the stress-strain hysteresis obtained from a cyclic simple shear test. Such cyclic tests show a gradual degeneration of the stress-strain hysteresis as well as an elastic-shakedown effect with some interesting characteristics of persistent slip bands. Within a certain number of load cycles, an almost steady laminate is formed, which consists of one elastically deforming phase with high volume fraction (80-90%) and one phase which concentrates plastic slip in a low volume fraction (10-20%). The specifics of the steady-state laminate as well as the number of load cycles to arrive at that state highly depend on the chosen hardening modulus κ.

REFERENCES

[1] C. Carstensen, K. Hackl, A. Mielke, *Non-convex potentials and microstructures in finite-strain plasticity*, Proc. Royal Soc. London **458** (2002), 299–317.

[2] K. Hackl, D.M. Kochmann, *Relaxed potentials and evolution equations for inelastic microstructures*, in: Daya Reddy, B. (ed.), Theoretical, Computational and Modeling Aspects of Inelastic Media (2008), IUTAM Bookseries, Springer, Berlin, 27–39.

[3] D.M. Kochmann, K. Hackl, *Time-continuous evolution of microstructures in finite plasticity*, in: Hackl, K. (ed.), Variational Concepts with Applications to the Mechanics of Materials, IUTAM Bookseries, Springer, Berlin, in press (2010).
[4] D.M. Kochmann, K. Hackl, *Influence of Hardening on the Cyclic Behavior of Laminate Microstructures in Finite Crystal Plasticity*, Techn. Mech. (2010), in press.
[5] M. Ortiz, E.A. Repetto, *Nonconvex energy minimization and dislocation structures in ductile single crystals*, J. Mech. Phys. Solids **47** (1999), 397–462.

Force-based atomistic/continuum hybrid models

Christoph Ortner

(joint work with Matthew Dobson, Mitchell Luskin, C. Makridakis, Endre Süli)

The motivation for atomistic/continuum hybrid models is that the accuracy of an atomistic model for a defect can, in principle, be combined with the efficiency of a continuum model of the elastic "far field". Despite several creative attempts [5, 9, 10], significant obstacles remain to the development of efficient and accurate hybrid coupling energies. The force-based approach [1, 6, 8] has become very popular because it provides a simple and efficient method for coupling two physics models without the development of a consistent coupling energy.

Consider a simple atomistic energy functional

$$\mathcal{E}(y) = \varepsilon \sum_{\ell=-N+1}^{N} \sum_{r=1}^{R} \big[\phi(\varepsilon^{-1}(y_{\ell+r} - y_\ell)) - f_\ell y_\ell\big],$$

where the displacement $u = y - x$ ($x = (x_\ell) = (\varepsilon\ell)$) is $2N$-periodic and has zero mean, $\varepsilon = 1/N$, and $y'_\ell = \varepsilon^{-1}(y_\ell - y_{\ell-1})$. The *local QC approximation* of $\mathcal{E}$ is the short-ranged functional

$$\mathcal{E}^c(y) = \varepsilon \sum_{\ell=-N+1}^{N} \big[W(y'_\ell) - f_\ell y_\ell\big],$$

where $y'_\ell = \varepsilon^{-1}(y_\ell - y_{\ell-1})$ and

$$W(t) = \sum_{r=1}^{R} \phi(rt).$$

Thus, in the local QC model a non-local second neighbour interaction is replaced by a local nearest-neighbour interaction, which subsequently makes it possible to remove degrees of freedom for an efficient computational algorithm. For the sake of simplicity of notation we will ignore this step (the formulation and analysis in [7] does consider coarse-graining).

The QCF operator is defined as

$$\mathcal{F}_\ell(y) = \begin{cases} -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}(y)}{\partial y_\ell}, & \ell = -K, \dots, K, \\ -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}^c(y)}{\partial y_\ell}, & \text{otherwise}, \end{cases}$$

where the index set $\mathcal{A} = \{-K, \dots, K\}$ is the *atomistic region*, and $\mathcal{C} = \{-N + 1, \dots, N\} \setminus \mathcal{A}$ is the *continuum region*.

The linearized QCF operator $D\mathcal{F}(Bx)$ (linearized at a perfect lattice Bx) was the subject of detailed studies in [2, 3]. In [7] these analyses were extended to the case of finite deformations. Under suitable technical assumptions it was shown that, if y_a is a "sufficiently stable" atomistic equilibrium, and if y_a is "smooth" in the continuum region $\mathcal{C}$ then a solution y_{qc} of the QCF system

$$\mathcal{F}(y) = f$$

exists and satisfies the error estimate

$$\|y_a' - y_{qc}'\|_{\ell^\infty} \leq C\varepsilon^2(\|y_a''\|^2_{\ell^\infty(\tilde{\mathcal{C}})} + \|y_a'''\|_{\ell^\infty(\tilde{\mathcal{C}})}), \tag{1}$$

where

$$\tilde{\mathcal{C}} = \mathcal{C} \cup (\mathcal{C} + R) \cup (\mathcal{C} - R).$$

The main tool in the proof of (1) is the following "weak form" of the QCF operator: Let $(\cdot, \cdot)_\varepsilon$ denote the weighted ℓ^2-inner product, then

$$\begin{aligned}(\mathcal{F}(y), u)_\varepsilon = \varepsilon \sum_{\ell \in \mathcal{A}} \sigma^a_\ell(y) u'_\ell + \varepsilon \sum_{\ell \in \mathcal{C}} \sigma^c_\ell(y) u'_\ell \\ - u_K(\sigma^a_{K+1}(y) - \sigma^c_{K+1}(y)) + u_{-K}(\sigma^a_{-K}(y) - \sigma^c_{-K}(y)),\end{aligned}$$

where the "stress functions" σ^a_ℓ and σ^c_ℓ are given by

$$\sigma^c_\ell(y) = DW(y'_\ell), \quad \text{and} \quad \sigma^a_\ell(y) = \sum_{r=1}^{R} \sum_{k=\ell-r}^{\ell-1} \phi'\big(\varepsilon^{-1}(y_{k+r} - y_k)\big).$$

An analysis of these stress functions leads to stability estimates and quasi-optimal consistency error estimates that are then used to establish (1).

However, the interface terms cause considerable technical difficulties, especially for the generalization of the results to higher dimensions. Moreover, we see that the QCF method does not impose the desirable "zero-flux" transmission condition on the A/C interface. Hence, in [7] we also propose a new force-based coupling scheme:

$$(S^{qc}(y), u) = \varepsilon \sum_{\ell \in \mathcal{A}} \sigma^a_\ell(y) u'_\ell + \varepsilon \sum_{\ell \in \mathcal{C}} \sigma^c_\ell(y) u'_\ell,$$

which has superior theoretical properties: in particular, sharper stability estimates and positivity of the linearization.

References

[1] M. Dobson and M. Lusin, *Analysis of a force-based quasicontinuum approximation*, M2AN Math. Model. Numer. Anal., 42(1):113–139, 2008.

[2] M. Dobson, M. Luskin, and C. Ortner, *Sharp stability estimates for the force-based quasicontinuum method*, to appear in Multiscale Modellin & Simulation.

[3] M. Dobson, M. Luskin, and C. Ortner, *Stability, instability, and error of the force-based quasicontinuum approximation*, to appear in Arch. for Rat. Mech. Anal.

[4] M. Dobson, M. Luskin, and C. Ortner, *Iterative methods for the force-based quasicontinuum approximation*, arXiv:0910.2013v1.

[5] W. E, J. Lu, and J. Yang, *Uniform accuracy of the quasicontinuum method*, Phys. Rev. B, **74**(21):214115 (2004).
[6] S. Kohlhoff and S. Schmauder, *A new method for coupled elastic-atomistic modelling*, Atomistic Simulation of Materials: Beyond Pair Potentials, Eds.: V. Vitek, D.J. Srolovitz, Plenum Press, New York, London, pp. 411-418 (1989).
[7] C. Makridakis, C. Ortner, and E. Süli, *Analysis of force-based quasicontinuum approximations*, in preparation.
[8] V. B. Shenoy, R. E. Miller, E. B. Tadmor, D. Rodney, R. Phillips, and M. Ortiz. An adaptive finite element approach to atomic-scale mechanics — the quasicontinuum method, *J. Mech. Phys. Solids*, 47(3):611–642 (1999).
[9] T. Shimokawa, J. Mortensen, J. Schiotz, and K. Jacobsen, *Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region*, Phys. Rev. B, **69**(21):214104 (2004).
[10] E. B. Tadmor, R. Phillips, and M. Ortiz, *Quasicontinuum analysis of Defects in Solids.* Phil. Mag. A 73(6):1529–1563, 1996.

From Electrons to Atoms to Continuae at Interfaces

Siegfried Schmauder

Shear at metal/ceramic interfaces plays an important role during deformation and fracture in a number of materials. High-strength materials, such as metal-matrix composites consist of internal interfaces between ceramic (e.g. SiC or Al_2O_3) particles or filaments within a metallic host. In microelectronics packaging, interfaces between metallic (Cu and/or Al) interconnects and SiO_2, carbide/nitride (TiCN) or oxide (Al_2O_3) ceramics are commonplace, and impact the performance and longevity of solid state devices. Despite their widespread use, a basic understanding of these interfaces has been elusive. For example, given a particular metal/ceramic interface, it is not yet possible to accurately predict such fundamental properties as its fracture energy. In most of the cases, improvements in interface properties proceed via a costly and time consuming trial-and-error process in which numerous materials are evaluated until suitable performance is obtained. Computational methods provide a wide range of possibilities to study the fracture behaviour of such metal/ceramic interfaces:

In the first part of the presented work, the deformation behaviour of niobium single crystals has been simulated using crystal plasticity theory. An automatic identification procedure has been proposed to identify the crystal plasticity parameters for each family of slip systems and simulation results of the mechanical behaviour of single crystal niobium are compared with the experiment. Good agreement between the experimental and simulation results was found. The second part presents effects of the different niobium single crystalline material orientations on crack initiation energies of the bicrystal niobium/sapphire four-point-bending-test specimens for a stationary crack tip. The trends of crack initiation energies are found to be similar to those observed during experiments. In the third part, crack propagation analyses of niobium/alumina bicrystal interface fracture have been performed using a cohesive modelling approach for three different orientations of

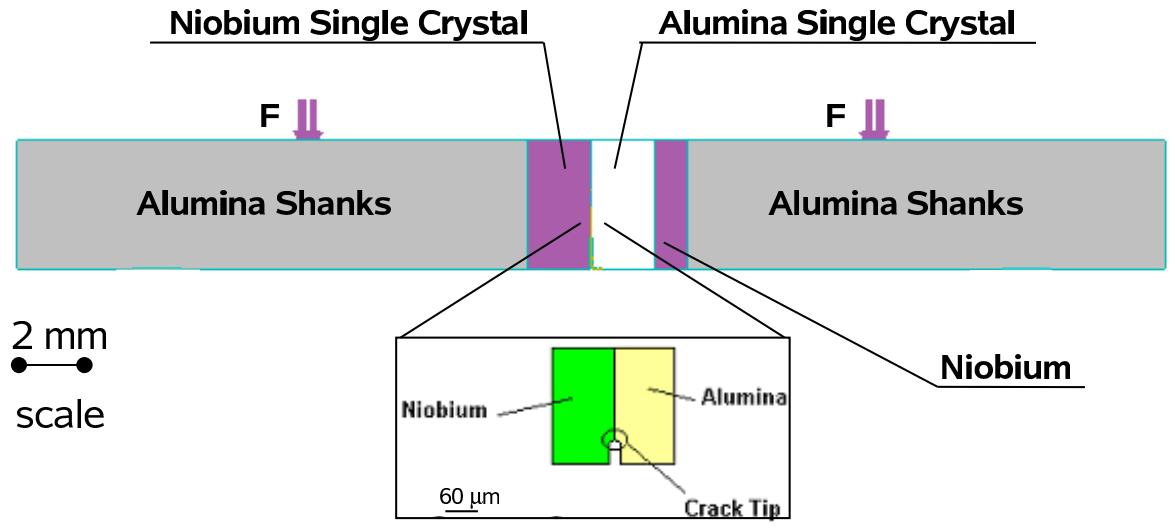

FIGURE 1. Simulated metal/ceramic interface fracture problem in the frame of crystal plasticity (CP) theory.

single crystalline niobium. Parametric studies have been performed to study the effect of different cohesive law parameters, such as work of adhesion and cohesive strength, where work of adhesion is the area under the cohesive law curve while cohesive strength is the peak stress value of the cohesive law. The results show that cohesive strength has a stronger effect on the macroscopic fracture energy as compared to work of adhesion. Cohesive model parameters are identified for different combinations of cohesive strength and work of adhesion by applying a scale bridging procedure based on ab initio data of work of adhesion taken from literature. In the last part, a correlation among the macroscopic fracture energy, cohesive strength, work of adhesion and yield stress of niobium single crystalline material will be derived.

REFERENCES

[1] A. Siddiq, S. Schmauder, *Simulation of hardening in high purity niobium single crystals during deformation*, STEEL GRIPS **3** (2005), 281-286.

[2] A. Siddiq, S. Schmauder, *Interface fracture analyses of a bicrystal niobium/alumina specimen using cohesive modelling approach*, Simul. Modell. Mater. Sci. & Engng. **14** (2006), 1015-1030.

[3] A. Siddiq, S. Schmauder,*Modelling of crystal plasticity effects on the crack initiation energies of a bi-crystal interface (Nb/Al_2O_3)*, CAMES **14** (2007), 67-78.

[4] A. Siddiq, S. Schmauder, Y. Huang, *Fracture of bicrystal metal/ceramic interfaces: A study via the mechanism-based strain gradient crystal plasticity theory*, Int. Journal of Plasticity **23** (2007), 665-689.

Micromechanical modeling of martensitic microstructures

Klaus Hackl

Shape memory alloys can be described in a uniform way relying on energetic considerations only. We present a micromechanically motivated model for polycrystalline shape memory alloys based on work presented in [3, 5, 6]. Micromechanical models for the monocrystalline case can be found in [1, 2]. The model studied here is based on energy minimization and includes hysteretic effects via a simple dissipation ansatz which is homogeneous of first order. It is capable of reproducing important aspects of the material behavior such as pseudoelasticity and pseudoplasticity. The influence of anisotropies in the crystalline texture as well as in the elastic constants of the austenite and the martensitic variants are also discussed.

We adopt the hypothesis that, at the microscopic level, the material choses the crystallographic variant which corresponds to the lowest energy

$$\bar{W}^j(\boldsymbol{\varepsilon}) = \min_{i=0,\dots,n} \left[W^j(\boldsymbol{\varepsilon}, \mathbf{i}_i) \right] \tag{1}$$

for a given strain. Here, n is the number of martensitic variants and $\mathbf{i}_i$ are the unit vectors in $n+1$-dimensional variant space. Furthermore, the energy at every microscopic material point will also depend on the orientation of the crystallite it lies in. In order to take the crystal orientations into account, the continous texture of an idealized polycrystal is approximated by a large, but finite number of orientations $j = 1, \dots, N$ each of which is charactarized by a rotational tensor $\mathbf{R}^j$. The energy of each variant within each crystal orientation in dependence of the corresponding linearized strain $\boldsymbol{\varepsilon}_i^j$ is assumed to have the linear elastic form

$$W^j\left(\boldsymbol{\varepsilon}_i^j, \mathbf{i}_i\right) = \left(\boldsymbol{\varepsilon}_i^j - \boldsymbol{\eta}_i^j\right) : \mathbb{C}_i^j : \left(\boldsymbol{\varepsilon}_i^j - \boldsymbol{\eta}_i^j\right) + \alpha_i, \tag{2}$$

where the so-called chemical energy α_i differs only between austenite and martensite and the transformation strain $\boldsymbol{\eta}_i^j$ is given by $\boldsymbol{\eta}_i^j = \mathbf{R}_i^T \cdot \boldsymbol{\eta}_i \cdot \mathbf{R}_i$, $\boldsymbol{\eta}_i$ being the transformation strain of phase i in a single crystal. Since the energy formulation given by (1) is clearly non-quasiconvex, the mesoscopic energy is calculated via relaxation methods. For simplicity, we employ straightforward convexification to obtain a lower bound which is then used as an estimate W^{rel} for the unknown quasiconvex hull of the energy density. The quality of this estimate is validated by comparison to an upper bound. The latter bound is based on derivations concerning the energy density of polycrystals by [12] in combination with a lamination upper bound presented in [3], for details see [6]. In order to close the formulation, hysteretic aspects of the material behavior are included into the model via the dissipation ansatz

$$\Delta\left(\dot{\boldsymbol{\lambda}}, ||\boldsymbol{\lambda}_0||\right) = r(||\boldsymbol{\lambda}_0||) \sqrt{\sum_{j=1}^{N} \xi^j \sum_{i=0}^{n} \left(\dot{\lambda}_i^j\right)^2}, \tag{3}$$

where ξ^j is the volume fraction of the jth crystallite, which remains constant within in the temperature range of interest, and λ_i^j is the percentage of the ith crystallographic variant within that crystallite. Furthermore we make an ansatz

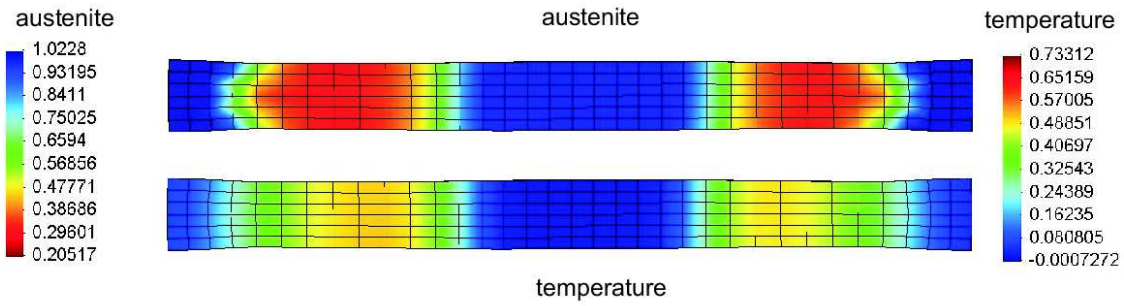

FIGURE 1. Distribution of the austenite phase (top) and the corresponding temperature field, setting room temperature to zero (bottom).

for the dissipation coefficient $r(||\boldsymbol{\lambda}_0||)$ in order to account for varying energy costs, depending on the average amount of austenite $||\boldsymbol{\lambda}_0||$.

Using the variational procedure found among others in [4, 8, 9, 10, 11] we derive evolution equations by minimizing the total power

$$\mathcal{L}\left(\boldsymbol{\lambda}, \dot{\boldsymbol{\lambda}}\right) = \frac{\mathrm{d}}{\mathrm{d}t} W^{rel}\left(\boldsymbol{\varepsilon}, \boldsymbol{\lambda}\right) + \Delta\left(\dot{\boldsymbol{\lambda}}\right) \tag{4}$$

with respect to $\dot{\lambda}$ for fixed $\boldsymbol{\varepsilon}$.

In order to simulate entire specimens made of shape memory alloys and to account for the coupling in between phase transition and temperature, we genralize the formulation introduced above by maximizing the entropy production Σ under the constraint of energy-consevation. The entropy production is formulated as

$$\Sigma = \Delta\left(\dot{\boldsymbol{\lambda}}\right) + \frac{\alpha_{therm}}{2}|\boldsymbol{q}|^2, \tag{5}$$

where $\boldsymbol{q}$ denotes the heat-flux. Using a finite element approach the displacement and the temperature field is solved together with a field function which serves as regularization to circumvent mesh dependence due to Δ being a functional of the internal variables. A typical result displaying the distributions of temperature and volume content of austenite is given in Figure 1. We validate the model by comparing the martensite orientation distribution functions it predicts to those measured by synchrotron diffraction experiments, see [7] and references therein. For this purpose, we simplify the formulation by assuming, on the one hand, that the elasticity tensor $\mathbb{C}_i^j$ is the same for all crystal orientations and variants and, on the other hand, that transformation occurs mainly in the stress plateau, which is characteristic for phase transitions in shape memory alloys.

REFERENCES

[1] T. Bartel, K. Hackl, *A novel approach to the modelling of single-crystalline materials undergoing martensitic phase-transformations*, Materials Science and Engineering: A, **481-482** (2008) 371-/375.

[2] T. Bartel, K. Hackl, *A micromechanical model for martensitic phase-transformations in shape-memory alloys based on energy-relaxation*, ZAMM, **89** (2009) 792/809.

[3] S. Govindjee, K. Hackl, R. Heinen, *An Upper Bound to the Free Energy of Mixing by Twin-Compatible Lamination for n-variant Martensitic Phase Transformations*, Contin. Mech. Thermodyn. **18 (7-8)** (2007) 443-453.
[4] K. Hackl, F.D. Fischer, *On the relation between the principle of maximum dissipation and inelastic evolution given by dissipation potentials*, Proc. Royal Soc. London A **464** (2007), 117–132.
[5] K. Hackl, R. Heinen, *A micromechanical model for pretextured polycrystalline shape-memory alloys including elastic anisotropy.* Contin. Mech. Thermodyn. **19 (8)** (2008) 499-510.
[6] K. Hackl, R. Heinen, *An upper bound to the free energy of n-variant polycrystalline shape memory alloys.* J. Mech. Phys. Solids 56 **9** (2008) 2832-2843.
[7] K. Hackl, R. Heinen, W.W. Schmahl, and M. Hasan, *Experimental verification of a micromechanical model for polycrystalline shape memory alloys in dependence of martensite orientation distributions*, Mat. Sci. Eng. A., **481** (2008) 347–350.
[8] A. Mielke, *Finite elastoplasticity, Lie groups and geodesics on SL(d)*, In "Geometry, Dynamics, and Mechanics, P. Newton, A. Weinstein, P. Holmes (eds), Springer–Verlag"(2002) 61–90.
[9] A. Mielke, *Deriving new evolution equations for microstructures via relaxation of variational incremental problems*, Comp. Meth. Appl. Meth. Eng. **193, No. 48-51** (2004) 5095–5127.
[10] A. Mielke, *A mathematical framework for generalized standard materials in the rate-independent case*, in: R. Helmig, A. Mielke, and B. Wohlmuth (eds.), Multifield problems in solid and fluid mechanics. (2006) 399–428.
[11] M. Ortiz, E.A. Repetto, *Nonconvex energy minimisation and dislocation in ductile single crystals*, J. Mech. Phys. Solids, **47**, 2 (1999) 397–462.
[12] V.P. Smyshlyaev, J.R. Willis, *A 'non-local' variational approach to the elastic energy minimization of martensitic polycrystals*, Proc. R. Soc. Lond. A, **454** (1989) 1573–1613.

Fast evolution of microstructures due to recovery during heat treatment of metals

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(joint work with J. Pilch)

Thermomechanical properties of metals depend, in addition to basic characteristics as elastic constants, crystal structure and mobility of crystal defects, phase transformations, also on the initial microstructure (grain size, texture, density of dislocation defects, grain boundary misorientations etc.) which is given to the metal by the final processing. Typically, this includes hot/cold working passes followed by final heat treatment. During the final heat treatment, the heavily deformed microstructure of the metal resulting from the final cold work is recovered by thermally driven recovery processes taking place during the heat treatment. This heat treatment is conventionally preformed by exposing the metal to temperatures 200C-600C for several minutes or hours.

We have developed a nonconventional method of heat treatment by electric current which allows for performing heat treatments of thin filaments made of cold worked NiTi shape memory alloy and setting their functional mechanical properties in much shorter time interval of few milliseconds. The filament is heated by electric current pulse to temperatures as high as 1000C and the recovery processes take place under stresses as high as 600MPa. In this way, NiTi filaments with

carefully controlled nanosized microstructures were prepared and their functional superelastic properties were investigated.

Experimental evidence on the fast evolution of microstructures during the heat treatment of thin NiTi wires determined from in-situ mechanical, electric resistance and synchrotron X-ray studies during the fast heat treatment [1] is reported in this talk. It is interesting to see that the recovery processes responsible for microstructure evolution normally considered to proceed for minutes or hours in fact can complete within microseconds. Next, experimental information on the microstructures observed in wide range of differently treated NiTi wires by transmission electron microscopy and X-ray diffraction was presented and confronted with the functional superelastic properties of these wires determined from thermomechanical testing experiments. A microstructure-property relationship for superelastic NiTi wires was established and discussed. It is suggested that the microstructure yielding best superelastic properties is partially polygonized and recrystallized with grain size in the range 20-50 nanometers.

In order to obtain information on the stress induced transformation process responsible for the superelasticity, the microstructures in NiTi wires subjected to 10 tensile cycles were also investigated by transmission electron microscopy. It was found that in wires having microstructures with grain size larger than 100 nm, large density of slip dislocations was created by cycling. These dislocations are thought to be responsible for the accumulated plastic strains, since no residual martensite particles were found by TEM in the microstructure of the cycled wires. It was concluded that the slip activity is largely suppressed in microstructures having small grain size under 50 nm but stress induced transformation is not. The microstructure control by heat treatment can thus be very effective in setting unique mechanical properties of metals in which various deformation mechanisms become active upon straining.

References

[1] B. Malard, J. Pilch, P. Sittner, V. Gartnerova, R. Delville, C. Curfs, D. Schryvers, *Microstructure and functional property changes in thin NiTi wires shape set by electric current – high energy X-ray and TEM investigations*, Functional Materials Letters **2** (2009), 45-54.

Statistically Similar Representative Volume Elements based on Lineal-Path Functions

Daniel Balzani

(joint work with Jörg Schröder, Dominik Brands)

1. Introduction

For the prediction of the mechanical behavior of micro-heterogeneous materials the FE^2-method provides a suitable numerical tool, see e.g. Smit et al. [8], Miehe et al. [4], Schröder [5]. In this context a micromechanical boundary

value problem is solved at each macroscopic Gauss point, where the discretization of a representative volume element (RVE) reflecting the real microstructure is taken into account. In this context see e.g. [6], where also eigenstress distributions are taken into account at the microscale. Here, a method is proposed for the construction of more efficient statistically similar RVEs (SSRVEs) that are characterized by a much less complexity than usual RVEs. This method is based on a general least-square functional taking into account the squared differences of some suitable statistical measures characterizing the inclusion phase morphology, that are computed for a given real (complex) microstructure and the SSRVE, cf. [3], [2], [7]. Optimizing this least-square functional leads to certain problems such as a non-smooth energy surface and the existence of numerous local minima as shown in [1]. To overcome these problems a moving-frame algorithm combining a line-search strategy is given in [2]. In [3] it turns out that simple scalar-valued statistical measures are not enough to characterize e.g. macroscopic anisotropy appropriately. In this contribution it is shown that even the spectral density does not suffice and significantly improved results are obtained by taking into account the lineal-path function.

2. Least-Square Functions for the Construction of SSRVEs

For the construction of SSRVEs we consider an optimization problem, where the general objective functional taking into account the summation of individual least-square functionals

$$\mathcal{L}(\boldsymbol{\gamma}) \to \min \quad \text{with} \quad \mathcal{L}(\boldsymbol{\gamma}) = \sum_{L=1}^{n_{sm}} \omega^{(L)} \mathcal{L}_{SM}^{(L)}(\boldsymbol{\gamma}) \tag{1}$$

is minimized. ω denotes an appropriate weighting factor and $\mathcal{L}_{SM}$ is the squared difference of a statistical measure computed for a reference target structure (which can be interpreted as an usual RVE) and the SSRVE parameterized by splines such that the sampling point coordinates enter the general vector $\boldsymbol{\gamma}$ representing the degrees of freedom of the optimization problem. In this contribution we analyze three different statistical measures, the volume fraction, the spectral density, and the lineal-path function, see e.g. Torquato [9] for the definition of the lineal-path function. Then the resulting least-square functionals are

$$\mathcal{L}_V(\boldsymbol{\gamma}) = \left(1 - \frac{\mathcal{P}_V^{SSRVE}(\boldsymbol{\gamma})}{\mathcal{P}_V^{real}}\right)^2 , \tag{2}$$

$$\mathcal{L}_{SD}(\boldsymbol{\gamma}) = \frac{1}{N_x\, N_y} \sum_{m=1}^{N_x} \sum_{k=1}^{N_y} \left(\mathcal{P}_{SD}^{real}(m,k) - \mathcal{P}_{SD}^{SSRVE}(m,k,\boldsymbol{\gamma})\right)^2 , \tag{3}$$

$$\mathcal{L}_{LP}(\boldsymbol{\gamma}) = \frac{1}{N_x\, N_y} \sum_{m=1}^{N_x} \sum_{k=1}^{N_y} \left(\mathcal{P}_{LP}^{real}(m,k) - \mathcal{P}_{LP}^{SSRVE}(m,k,\boldsymbol{\gamma})\right)^2 . \tag{4}$$

Here, we compare the results obtained from minimizing the two different objective functions $\mathcal{L}_1$ and $\mathcal{L}_2$ given by

$$(5)\quad \mathcal{L}_1(\boldsymbol{\gamma}) := \omega_V \mathcal{L}_V + \omega_{SD}\mathcal{L}_{SD} \quad \text{and} \quad \mathcal{L}_2(\boldsymbol{\gamma}) := \omega_V \mathcal{L}_V + \omega_{SD}\mathcal{L}_{SD} + \omega_{LP}\mathcal{L}_{LP}\,,$$

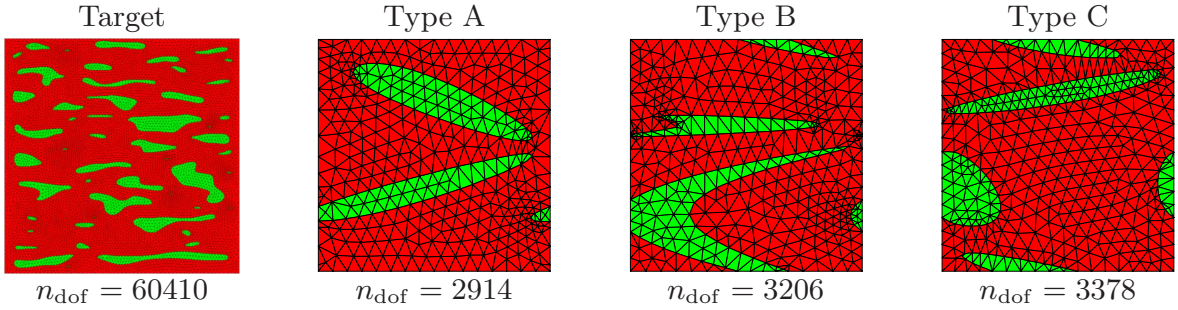

FIGURE 1. Considered target structure and resulting SSRVEs from minimizing the least-square functional $\mathcal{L}_2$.

where we set the weighting factors to $\omega_V = \omega_{SD} = 1$ and $\omega_{LP} = 10$. We consider three different types of SSRVEs: Type A takes into account two inclusions with 3 spline-sampling points each, Type B two inclusions with 4 sampling points each and Type C three inclusions with 3 sampling points each. All inclusions are not permitted to intersect with themselves or with the other ones and at the boundary of the SSRVE we ensure that a periodic extension is possible. The microstructure shown in Fig. 1 (left) serves as a target structure. Then, the two objective functions are minimized using the method proposed in [3] and as an example Fig. 1 shows the resulting SSRVEs obtained from minimizing $\mathcal{L}_2$. When discretizing the microstructures with Finite Elements obviously much less elements are required for the SSRVEs leading to much more efficient numerical micro-macro procedures. In order to estimate the quality of the individual SSRVEs we compare the mechanical response of the SSRVEs with the response of the target structure in three different virtual experiments: uniaxial tension in horizontal and vertical direction and simple shear. For this purpose we define the mechanical error measure $r^{(i)} = \frac{\sigma_i^{\text{real}} - \sigma_i^{\text{SSRVE}}}{\sigma_i^{\text{real}}}$ evaluated in a number of n calculated stress-strain situations i. To estimate the mechanical quality in simple identificators we define the errors $\widetilde{r}_x$, $\widetilde{r}_y$ and $\widetilde{r}_{xy}$ for the three different virtual experiments

$$(6)\quad \widetilde{r} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}[r^{(i)}]^2} \quad \text{with} \quad r^{(i)} := r\left(\frac{i}{n}\frac{\triangle l_{\max}}{l_0}\right) \quad \text{and} \quad \widetilde{r}_{\phi} = \frac{\widetilde{r}_x + \widetilde{r}_y + \widetilde{r}_{xy}}{3}$$

representing an overall mechanical error $\widetilde{r}_{\phi}$. The results are given in Table 1 and we observe that with decreasing values of the minimized objective function the overall mechanical error decreases, too. For both objective functions we observe that Type C leads to the best mechanical correspondence and conclude that more than two inclusions are required for a good representation by a SSRVE. Furthermore, we observe that the mechanical errors for objective function $\mathcal{L}_2$ are more uniformly

distributed for the three experiments and that the overall mechanical error is significantly lower (0.7 vs. 1.1). We conclude that a much more suitable SSRVE can be constructed when adding the lineal-path function as a statistical measure.

SSRVE	$\mathcal{L}$ [$\times 10^{-3}$]	$\widetilde{r}_x$ [%]	$\widetilde{r}_y$ [%]	$\widetilde{r}_{xy}$ [%]	$\widetilde{r}_{\varnothing}$ [%]
Objective function $\mathcal{L}_1$:					
A	2.98	2.43 ± 0.86	1.72 ± 0.40	5.06 ± 2.07	3.07
B	1.17	1.14 ± 0.39	0.97 ± 0.44	4.38 ± 1.85	2.17
C	0.84	0.14 ± 0.15	0.09 ± 0.06	3.08 ± 1.24	1.10
Objective function $\mathcal{L}_2$:					
A	4.31	2.37 ± 0.60	1.19 ± 0.29	2.61 ± 1.15	2.06
B	1.58	7.20 ± 2.97	1.99 ± 0.55	4.59 ± 2.04	4.59
C	1.31	0.53 ± 0.36	0.07 ± 0.08	1.51 ± 0.66	0.70

TABLE 1. Results of optimization and comparison of mechanical response

REFERENCES

[1] D. Balzani and J. Schröder. Reconstruction of statistically similar microstructures for FE^2-simulations in elasto-plasticity. In *Proceedings of the International Symposium of Plasticity 2009*. Neat press,ISBN: 0-9659463-9-8, 2009.

[2] D. Balzani, J. Schröder, and D. Brands. FE^2-simulation of microheterogeneous steels based on statistically similar rve's. In *Proceedings of the IUTAM Symposium on Variational Concepts with applications to the mechanics of materials, September 22-26, 2008, Bochum, Germany*, 2009. in press.

[3] B. Balzani, D. Brands, J. Schröder, and C. Carstensen. Sensitivity Analysis of Statistical Measures for the Reconstruction of Microstructures based on the Minimization of generalized Least-Square Functionals. *Technische Mechanik*, in press, 2010

[4] C. Miehe, J. Schröder, and J. Schotte. Computational homogenization analysis in finite plasticity. simulation of texture development in polycrystalline materials. *Computer Methods in Applied Mechanics and Engineering*, 171:387–418, 1999.

[5] J. Schröder. *Homogenisierungsmethoden der nichtlinearen Kontinuumsmechanik unter Beachtung von Stabilitätsproblemen*. Bericht aus der Forschungsreihe des Institut für Mechanik (Bauwesen), Lehrstuhl I, 2000. Habilitationsschrift.

[6] J. Schröder, D. Balzani, H. Richter, H.P. Schmitz, L. Kessler. Simulation of Microheterogeneous Steels based on a Discrete Multiscale Approach. Proceedings of the 7th International Conference and Workshop on Numerical Simulation of 3D Sheet Metal Forming Processes (NUMISHEET), September 1-5, Interlaken, Switzerland, Part A, 379-383, 2008

[7] J. Schröder, D. Balzani & D. Brands. A FE^2-Homogenization Technique for Two-Phase Steels based on Statistically Similar Representative Volume Elements. Proceedings of the International Symposium of Plasticity 2009, St. Kitts, USA, January 3-8, NEAT press

[8] R.J.M. Smit, W.A.M. Brekelmans, and H.E.H. Meijer. Prediction of the mechanical behavior of nonlinear heterogeneous systems by multi-level finite element modeling. *Computer Methods in Applied Mechanics and Engineering*, 155:181–192, 1998.

[9] T. Torquato. Random heterogeneous materials. microstructure and macroscopic properties. Springer, 2002

From discrete dislocations to strain gradient crystal plasticity

Marc Geers
(joint work with Ron Peerlings, Marcel Brekelmans, Tuncay Yalcincaya)

Miniaturization has become an important industrial drive in the development of engineering micro- and nanosystems. At the level of most microsystems, metallic structures and films are used ranging from sizes of a few microns or below to hundreds of microns. Within this context, considerable research efforts were done to characterize metallic materials a range where size effects have a dominating contribution. The present talk departs from a general classification of different size effects, related to different underlying physical mechanisms in the crystalline microstructure [1]. Among these, first-order size effects, processing induced size effects [2], interfacially controlled size effects and strain gradient (lattice curvature driven) size effects are briefly addressed.

In order to address all these possible size effects, an enriched crystal plasticity model is required, which has to be further extended to cover all known physical mechanisms in a multi-phase polycrystal. Emphasis is put on the formulation, thermodynamics and physics of strain gradient crystal plasticity models, for which the models presented by Gurtin [3] and Evers and Bayley et al. [4, 5, 6] are taken as reference. Whereas the thermodynamical model presented by Gurtin looks substantially different from the phenomenological-physical model of Evers-Bayley, it is shown that an intrinsic duality between the two models exists [7], as already emphasized by Kuroda et al [8]. This duality implies the thermodynamical consistency of the Evers-Bayley approach on the one hand, and provides a clear physical interpretation of the micro-stress vectors and the assumed free energy terms in the Gurtin model. Particular emphasis is given on the meaning and interpretation of the related boundary conditions in both models. As a result of this analysis, it becomes evident that the physical short-range interactions between dislocations have to be accounted for in the free energy.

The most important topic of this contribution concerns the need for an energetic strain gradient contribution, which is demonstrated on the basis of an idealized pile-up problem. The critical role of the underlying discreteness is thereby addressed, and the vanishing continuum limit (for the stress) is discussed in detail [9]. It is shown that a corrective internal dislocation interaction stress has to be accounted for in the viscous slip law, which emanates from a defect energy. The energetic dislocation interaction terms can be approximated in a deterministic manner, using a nearest neighbour approach [10]. The duality between the resulting back stress in a deterministic setting and the one obtained from a statistical mechanics approach (e.g. from Groma et al. [11]) is advocated, and its implications on future steps to be taken in strain gradient crystal models are addressed. The generalization to a complete crystal plasticity model with all its slip systems is discussed, using an analytical integration scheme of the induced dislocation stresses [4, 5].

In the context of the presented models, the following challenges are briefly outlined:

- identifying higher-order terms and boundary conditions in a consistent manner from discrete dislocation solutions
- properly handling dislocation screening in a continuum model, based on the dislocation interactions (and the induced fine scale fluctuations)
- the general solution of an idealized pile-up problem, with a variable slip plane spacing
- the mathematical interpretation of the analytical solution based on the stress fields of distributed discrete dislocations on multiple slip systems, for which the defect energy cannot be determined trivially.

The talk concludes with some recent work on a non-convex strain gradient plasticity model, for which the extended slip law has been derived in a thermodynamical setting. The resulting problem has a structure that partially compares with phase field models with a non-convex free energy. An example is presented, revealing the time-dependent patterning of slip in a simple 1D setting.

References

[1] M.G.D. Geers, W.A.M. Brekelmans, P.J.M. Janssen, *Size effects in miniaturized polycrystalline FCC samples: Strengthening versus weakening*, International Journal of Solids and Structures **43** (2006), 7304–7321.

[2] P.J.M. Janssen, J.P.M. Hoegnagels, Th.H. de Keijser, M.G.D. Geers, *Processing induced size effects in plastic yielding upon miniaturisation*, Journal of the Mechanics and Physics of Solids **56** (2008), 2687–2706.

[3] M.E. Gurtin, *A finite-deformation, gradient theory of single-crystal plasticity with free energy dependent on densities of geometrically necessary dislocations*, International Journal of Plasticity **52** (2008), 702–725.

[4] L.P. Evers, W.A.M. Brekelmans, M.G.D. Geers, *Non-local crystal plasticity model with intrinsic SSD and GND effects*, Journal of the Mechanics and Physics of Solids **52** (2004), 2379–2401.

[5] C.J. Bayley, W.A.M. Brekelmans, M.G.D. Geers, *A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity,*, International Journal of Solids and Structures **43** (2006), 7268–7286.

[6] M.G.D. Geers, W.A.M. Brekelmans, C.J. Bayley, *Second-order crystal plasticity: internal stress effects and cyclic loading*, Modelling ans Simulation in Materials Science and Engineering **15** (2007), S133–S145.

[7] I. Ertürk, J.A.W. van Dommelen, M.G.D. Geers, *Energetic dislocation interactions and thermodynamical aspects of strain gradient crystal plasticity theories*, Journal of the Mechanics and Physics of Solids **57** (2009), 1801–1814.

[8] M. Kuroda, V. Tvergaard, *On the formulations of higher-order strain gradient crystal plasticity model*, Journal of the Mechanics and Physics of Solids **56** (2008), 1591–1608.

[9] A. Roy, R.H.J. Peerlings, M.G.D. Geers, Y. Kasyanyuk, *Continuum modeling of dislocation interactions: why discreteness matters?*, Materials Science and Engineering A **486** (2008), 653–661.

[10] M.G.D. Geers, R.H.J. Peerlings, J.P.M. Hoefnagels, Y. Kasyanyuk, *On a Proper Account of First- and Second-Order Size Effects in Crystal Plasticity*, Advanced Engineering Materials **11**(3) (2009), 143–147.

[11] I. Groma, F.F. Csikor, M. Zaiser, *Spatial correlations and higher-order gradient terms in a continuum description of dislocation dynamics*, Acta Materialia **51**(5) (2003), 1271–1281.

Conservation laws and Hamilton-Jacobi equations in the theory of plasticity

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In a metallic thin film the plastic yield limit is higher than in a bulky body of the same material. One of the explanations is that the movement of dislocation lines, is restricted in thin films by geometrical reasons. Standard mathematical models of plasticity and viscoplasticity do not reflect this observation. Here we summarize a systematic study in [2] of the continuous theory of dislocations [3] to deduce a refined mathematical model, which, as we hope, accounts for the influence of the geometrical dimensions on the inelastic behavior of the metallic body. We first formulate a classical crystallographic model, which can be found for example in [1, 4], sketch the investigations in [2] and state the model resulting from these investigations.

We need some definitions and notations. We assume that all deformations are small and we use a quasistatic model. Let $\Omega \subseteq \mathbb{R}^3$ be a bounded open set with sufficiently smooth boundary $\partial\Omega$ representing the crystalline body. Assume that there are k slip planes with unit normal vectors g_s and Burgers vectors b_s, $s = 1, \dots, k$. The vector b_s must be orthogonal to g_s. We do not require that all g_s are different. By T_e we denote a positive number (time of existence), which can be chosen arbitrarily large. $\mathcal{S}^3$ denotes the set of symmetric 3×3–matrices. Unknown are the displacement $u(x,t) \in \mathbb{R}^3$ of the material point x at time t, the Cauchy stress tensor $T(x,t) \in \mathcal{S}^3$ and the slips $\varepsilon_p^s(x,t) \in \mathbb{R}$ along the s–th slip plane in the direction of b_s. The equations of the standard model are

$$-\mathrm{div}_x\, T = 0\,, \tag{1}$$

$$T = D\big(\varepsilon(\nabla_x u) - \varepsilon_p\big), \tag{2}$$

$$\partial_t \varepsilon_p^s = f_s\big(|b_s|\, m_s : T\big)\,, \quad s = 1, \dots k, \tag{3}$$

$$\varepsilon_p = \sum_{s=1}^{k} m_s \varepsilon_p^s\,, \tag{4}$$

which must be satisfied in $\Omega \times [0, T_e]$. Standard initial and traction boundary conditions are

$$\varepsilon_p^s(x,0) = \varepsilon_p^{s(0)}(x), \quad x \in \Omega \tag{5}$$

$$T(x,t)n(x) = \gamma(x,t), \quad (x,t) \in \partial\Omega \times [0, T_e). \tag{6}$$

Here we use the notation

$$\mathrm{div}_x\, T = \textstyle\sum_{j=1}^{3} \big(\partial_{x_j} T_{ij}\big)_{i=1,2,3}\,.$$

$\nabla_x u$ denotes the 3×3–matrix of first order partial derivatives of u, and

$$\varepsilon(\nabla_x u) = \hat{a}\big(\nabla_x u + (\nabla_x u)^T\big) \in \mathcal{S}^3$$

is the linear strain tensor. We write A^T for the transpose of a matrix A. With the unit vectors $\hat{b}_s = b_s/|b_s|$ we define the symmetric tensors

$$m_s = \varepsilon(\hat{b}_s \otimes g_s) = \hat{a}(\hat{b}_s \otimes g_s + g_s \otimes \hat{b}_s) \in \mathcal{S}^3.$$

$\varepsilon_p(x,t) \in \mathcal{S}^3$ is the plastic strain tensor, and $D : \mathcal{S}^3 \to \mathcal{S}^3$ is a symmetric, positive definite linear mapping, the elasticity tensor. For $x \in \partial\Omega$ we denote by $n(x)$ the exterior unit normal vector to $\partial\Omega$, and $\varepsilon_p^{*(0)} : \Omega \to \mathbb{R}$, $\gamma : \partial\Omega \times [0, T_e) \to \mathbb{R}^3$ are the given initial data and the given boundary traction, respectively. The constitutive functions $f_s : \mathbb{R} \to \mathbb{R}$ must satisfy

$$s \cdot f_s(s) \geq 0, \quad \text{for all } s \in \mathbb{R}.$$

A typical choice is $f_s(s) = c_s|s|^{\gamma_s} s$ with constants $c_s > 0$ and $\gamma_s > 1$.

This completes the formulation of the standard model. The constitutive equation (3) consists of a system of ordinary differential equations, which are independent of the dislocation density and the geometrical dimensions of the body Ω. This is different for the model obtained from the continuous theory of dislocations, where the dislocation density enters the constitutive equations explicitly. This model is based on an evolution equation for the dislocation density $\rho(x,t)$. To formulate this evolution equation, we use four conditions, which determine the form of the evolution equation rather precisely. These conditions are:

(1) Since $\rho(\cdot,t)$ must be a rotation field for all times t, the evolution equation must have the form

$$\partial_t \rho = \mathrm{rot}_x \alpha[T, \rho, b],$$

with a suitable function α.

(2) The Clausius-Duhem inequality $\partial_t \psi + \mathrm{div}_x q \leq 0$ must hold.

(3) The evolution equation must be such that the dislocation density $t \mapsto \rho_{\ell(t)}$ to a single dislocation line driven by the Peach-Koehler force $F(x,t) = \tau(x,t) \times T(x,t)b$ is a distribution solution. Here τ denotes a unit tangent vector to the dislocation line.

(4) Plastic deformations must be volume conserving. This means that the plastic part h_p of the displacement gradient must satisfy the equation

$$\mathrm{trace}\, h_p(x,t) = 0.$$

The model obtained in this way consists of the equations (1), (2), (4)–(6) with (3) replaced by the equations

$$\partial_t \varepsilon_p^s = f_s(|b_s| m_s : T)\, |\nabla_{g_s} \varepsilon_p^s|, \quad s = 1, \ldots, k, \tag{7}$$

where ∇_{g_s} denotes the tangential gradient to the slip plane with normal vector g_s. The constitutive equations (7), which have the form of Hamilton-Jacobi equations, differ from the constitutive equations (3) only by the term

$$\nabla_{g_s} \varepsilon_p^s = g_s \times \nabla_x \varepsilon_p^s = -\mathrm{rot}\ (g_s \varepsilon_p^s).$$

This term is just the density of dislocations with Burgers vector b_s lying in the slip plane with normal g_s. In the constitutive equation (7) the slip rate is therefore proportional to the dislocation density.

One can interpret this result as follows: In a bulky solid metallic body normally a high number of dislocation lines can be found in every part of the body. In this case the dislocation density is everywhere different from zero and does not vary much. Therefore it can be replaced by a constant, in which case the equations (7) take the form of the standard equations (3). The standard model can therefore be used in most cases and yields accurate results in simulations. In a situation however, where the number of dislocations is small, or where the movement of dislocations is restricted by various reasons, the refined constitutive equations (7) must be used to obtain accurate results.

Since (7) is a system of partial differential equations, boundary conditions for the functions ε_p^s must be added to get a complete model. For a discussion of these boundary conditions we must refer the reader to [2].

References

[1] H.-D. Alber, *Materials with memory - Initial-boundary value problems for constitutive equations with internal variables*, Lecture Notes in Mathematics, **1682**, Springer, Berlin (1998).

[2] H.-D. Alber, *A viscoplastic model based on the continuous theory of dislocations and an evolution equation for the dislocation density*, Manuscript in preparation.

[3] E. Kröner, *Dislocation theory as a physical field theory*, Meccanica, **31** No.5 (1996), 577–587.

[4] L. Méric, P. Poubanne, G. Cailletaud, *Single crystal modeling for structural calculations. Part 1 - model presentation*, Trans. ASME J. Engrg. Mat. Technol., **113** (1991), 171–182.

Plasticity with hardening and softening: the Cam-Clay model in soil mechanics

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(joint work with Antonio DeSimone and Francesco Solombrino)

Cam-Clay plasticity is a phenomenological model used to describe the inelastic behaviour of fine grained soils. Some of its interesting features are its nonassociative character, and that it may lead to both hardening and softening behaviour, depending on the loading conditions. The variables considered in the model are the displacement $u(t,x)$, the elastic and plastic strains $e(t,x)$ and $p(t,x)$, the stress $\sigma(t,x)$, and two internal variables $z(t,x)$ and $\zeta(t,x)$. All these functions are defined for positive time t and for x in the reference configuration Ω, a bounded open set in $\mathbb{R}^n$, $n \geq 2$, with Lipschitz boundary. As it is typical in plasticity, the stress is constrained to lie in a convex set $K(\zeta)$ of the space $\mathbb{M}^{n\times n}_{sym}$ of symmetric $n\times n$ matrices, whose size is controlled by a scalar parameter ζ and whose boundary represents the yield surface. Given a time-dependent body force $f(t,x)$, and denoting the normal cone to $K(\zeta)$ at σ by $N_{K(\zeta)}(\sigma)$, the equations summarising the model are

(a) constitutive equations: $\sigma(t,x) = \mathbb{C}e(t,x)$ and $\zeta(t,x) = V(z(t,x))$,
(b) additive decomposition: $\frac{1}{2}(\nabla u(t,x) + \nabla u(t,x)^T) = e(t,x) + p(t,x)$,
(c) equilibrium condition : $-\text{div}\ \sigma(t,x) = f(t,x)$,
(d) stress constraint: $\sigma(t,x) \in K(\zeta(t,x))$,

(e) flow rule: $\dot{p}(t,x) \in N_{K(\zeta(t,x))}(\sigma(t,x))$,
(f) evolution of the internal variable: $\dot{z}(t,x) = \varrho \star [(\varrho \star \operatorname{tr} \sigma(t,\cdot)) \operatorname{tr} \dot{p}(t,\cdot)](x)$,

accompanied by suitable boundary conditions. In the previous equations, $\mathbb{C}$ is the isotropic elasticity tensor, V is a nondecreasing globally Lipschitz function satisfying $V(z) \geq \zeta_{min} > 0$ for every $z \in \mathbb{R}$, div is the divergence operator with respect to the space variable, ϱ is a smooth convolution kernel, and $\star$ denotes the convolution with respect to the space variable. In the typical applications, $\partial K(\zeta)$ are homothetic ellipsoids passing through the origin in the space $\mathbb{M}^{n\times n}_{sym}$; more in general, we assume that $K(\zeta) = \zeta K(1)$ for every $\zeta \geq \zeta_{min}$ and that $K(1)$ is a compact convex body in $\mathbb{M}^{n\times n}_{sym}$ containing 0.

The convolution kernel in the evolution of the internal variable has been introduced for technical reasons: it ensures that a very weak convergence of σ and $\dot{p}$ implies strong convergence of the corresponding z. From the point of view of mechanics, the convolution gives a nonlocal character to the evolution law for the internal variable: it implies that the size of the yield surface at a point x is affected by pressure and volumetric plastic strain rate in a small neighborhood of x, which is not physically implausible.

The study of the spatially homogeneous case (see [1] and [3]) shows that, for many initial data, the problem has no smooth solutions. We introduce a notion of generalized solution, based on a viscoplastic approximation of Duvaut-Lions type. Given a viscosity parameter $\varepsilon > 0$, the corresponding viscoplastic evolution $u_\varepsilon(t,x)$, $e_\varepsilon(t,x)$, $p_\varepsilon(t,x)$, $z_\varepsilon(t,x)$, $\sigma_\varepsilon(t,x)$, $\zeta_\varepsilon(t,x)$ satisfies (a), (b), (c), and (f); condition (d) is dropped, while (e) is replaced by

(e_ε) regularized flow rule: $\dot{p}_\varepsilon(t,x) = N^\varepsilon_{K(\zeta_\varepsilon(t,x))}(\sigma_\varepsilon(t,x))$,

where $N^\varepsilon_K(\sigma,\zeta) := \frac{1}{\varepsilon}\big(\sigma - \pi_{K(\zeta)}(\sigma)\big)$ and $\pi_{K(\zeta)}$ is the projection onto $K(\zeta)$. The existence of a viscoplastic evolution is obtained using a fixed point argument.

An energy estimate allows us to prove the existence of change of variables $t = t^\circ_\varepsilon(s)$, uniformly Lipschitz with respect to s, such that the rescaled functions $p^\circ_\varepsilon(s,x) := p_\varepsilon(t_\varepsilon(s),x)$ are uniformly Lipschitz with respect to s, in a suitable function space. This idea has already been used in [4, 5, 6] for rate independent dissipative problems in finite dimension. The authors of the last two papers have used the same idea to study a similar problem in infinite dimension [7].

The Ascoli-Arzelà Theorem provides the existence of a subsequence (not relabelled), such that

$$t^\circ_\varepsilon(s) \to t^\circ(s) \quad \text{and} \quad p^\circ_\varepsilon(s,\cdot) \rightharpoonup p^\circ(s,\cdot)\,,$$

the latter in a weak topology. A further argument, based on the uniqueness of the solution to an auxiliary variational problem, shows that

$$e^\circ_\varepsilon(s,\cdot) := e_\varepsilon(t_\varepsilon(s),\cdot) \rightharpoonup e^\circ(s,\cdot) \quad \text{and} \quad u^\circ_\varepsilon(s,\cdot) := u_\varepsilon(t_\varepsilon(s),\cdot) \rightharpoonup u^\circ(s,\cdot)\,.$$

The compactness ensured by the presence of the convolutions in the evolution law for the internal variable allows to prove that

$$z^\circ_\varepsilon(s,x) := z_\varepsilon(t_\varepsilon(s),s) \to z^\circ(s,x)\,,$$

uniformly with respect to x. It is then easy to see that (a), (b), (c) are satisfied by the limit functions. As for (f), it holds only in a weak form since, in general, the limit $p^\circ(s,\cdot)$ is just a measure and this requires an *ad-hoc* definition for the derivative.

Condition (d) is satisfied in the limit only for those values of s for which $t^\circ(s)$ is not locally constant. Condition (e) is replaced by

(e^{ext}) extended flow rule: $\dot p^\circ(s,x) \in N^{ext}_{K(\zeta^\circ(s,x))}(\sigma^\circ(s,x))$,

where $N^{ext}_{K(\zeta)}(\sigma) := N_{K(\zeta)}(\sigma)$ (the normal cone to $K(\zeta)$ at σ) if $\sigma \in K(\zeta)$, while $N^{ext}_{K(\zeta)}(\sigma) := \{\lambda\big(\sigma - \pi_{K(\zeta)}(\sigma)\big) : \lambda \ge 0\}$ if $\sigma \notin K(\zeta)$. This result follows from an energy-dissipation balance, which presents two main differences with respect to the case of perfect plasticity [2]: first, the set K, and hence the plastic dissipation, depend now on $\zeta^\circ(s,x)$; second, there is an additional dissipative term,

$$\int_0^S \int_\Omega \big(\sigma^\circ(s,x) - \pi_{K(\zeta^\circ(s,x))}(\sigma^\circ(s,x))\big) : \dot p^\circ(s,x)\, dx\, ds\,, \tag{1}$$

which accounts for viscous dissipation in those intervals where $t^\circ(s)$ is locally constant (the colon denotes the scalar product between matrices). A similar term appears in [5], where a different evolution problem with nonconvex energy is studied through a viscosity approximation and time rescaling.

References

[1] G. Dal Maso, A. DeSimone, *Quasistatic evolution problems for Cam-Clay plasticity: examples of spatially homogeneous solutions*, Math. Models Methods Appl. Sci. **19** (2009), 1–69.

[2] G. Dal Maso, A. DeSimone, M.G. Mora, *Quasistatic evolution problems for linearly elastic-perfectly plastic materials*, Arch. Ration. Mech. Anal. **180** (2006), 237–291.

[3] G. Dal Maso, F. Solombrino, *Quasistatic evolution for Cam-Clay plasticity: the spatially homogeneous case*, Netw. Heterog. Media **5** (2010), 97–132.

[4] M. Efendiev, A. Mielke, *On the rate-independent limit of systems with dry friction and small viscosity*, J. Convex Anal. **3** (2006), 151–167.

[5] A. Mielke, R. Rossi, G. Savaré, *Modeling solutions with jumps for rate-independent systems on metric spaces*, Discrete Contin. Dynam. Systems **25** (2009), 585–615.

[6] A. Mielke, R. Rossi, G. Savaré, *BV-solutions of the viscosity approximation of rate-independent systems*, WIAS Preprint, Berlin, 2009.

[7] R. Rossi: *Interazione di norme L^2 e L^1 in evoluzioni rate-independent*, Lecture given at the "XIX Convegno Nazionale di Calcolo delle Variazioni", Levico (Trento), February 8-13, 2009.

Analytical aspects of relaxation for models in crystal plasticity

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(joint work with Sergio Conti, Georg Dolzmann)

Modern mathematical approaches to plasticity lead to a sequence of non-convex variational problems [5] for which the standard methods of the calculus of variations are not applicable. In order to derive information about macroscopic material behavior one has to study the relaxation of the single incremental problems, which

amounts to calculating quasiconvex envelopes. In this contribution we consider geometrically nonlinear crystal elasto-plasticity in two dimensions with one active slip system and restrict to investigating the first time step under monotone loading. Our focus is on the question of whether systems with an elastic energy leading to large penalization of small elastic strains can be well-approximated by a model based on the assumption of rigid elasticity [1, 4].
To be more precise let $\Omega \subset \mathbb{R}^2$ be the reference configuration of a two-dimensional elasto-plastic body, $u : \Omega \to \mathbb{R}^2$ the total deformation of the sample and $F = \nabla u$ the deformation gradient. Accounting for finite strains yields a multiplicative decomposition of F into an elastic part $F_{\rm el}$ and a plastic one $F_{\rm pl}$, i.e. $F = F_{\rm el}\, F_{\rm pl}$. The single slip system is characterized by the slip direction $s \in \mathbb{S}^1$ and the slip-plane normal $m \in \mathbb{S}^1$ with $s \perp m$. Further let γ denote the slip strain along (s, m). Then the system energy density consists of the three components $W_{\rm el}(F_{\rm el}) + W_{\rm pl}(F_{\rm pl}) + {\rm Diss}(F_{\rm pl})$, where $W_{\rm el}(F_{\rm el})$ is the elastic energy density and the sum of plastic and dissipated energy density is given by

$$W_{\rm pl}(F_{\rm pl}) + {\rm Diss}(F_{\rm pl}) = \begin{cases} |\gamma|^p & \text{if } \ F_{\rm pl} = \mathbb{I} + \gamma s \otimes m \\ \infty & \text{else,} \end{cases}$$

with $p = 1$ and $p = 2$ describing models without hardening and with linear hardening, respectively. If we choose

$$W_{{\rm el},\varepsilon}\,(F_{\rm el}) = \frac{1}{\varepsilon}\ {\rm dist}^2\big(F_{\rm el}, {\rm SO}(2)\big), \qquad \varepsilon > 0$$

as the elastic energy density and optimize over all possible decompositions of F with plastic component $F_{\rm pl} = \mathbb{I} + \gamma s \otimes m$, we end up with the condensed energy density

$$W_\varepsilon(F) = \inf_{\gamma \in \mathbb{R}} \Big\{ \frac{1}{\varepsilon}\ {\rm dist}^2\big(F\,(\mathbb{I} - \gamma\ s \otimes m)\,, {\rm SO}(2)\big) + |\gamma|^p \Big\},$$

which is the object of our interest. Notice that the multiplicative decomposition of F combined with the pointwise minimization over the internal variables $F_{\rm pl}$ and γ results in non-standard growth for W_ε.
Considering the limit $\varepsilon \to 0$ in $W_{{\rm e},\varepsilon}(F_{\rm el})$ leads to an elastically rigid energy density and hence a simplified single-slip model. In [2, 3] the relaxation of the corresponding energy density W was determined explicitly by proving the subsequent representation formulas for the quasiconvex envelopes,

$$W_1^{\rm qc}(F) = \begin{cases} \sqrt{|F|^2 - 2} & \text{if } F \in \mathcal{N} \\ \infty & \text{else,} \end{cases} \qquad W_2^{\rm qc}(F) = \begin{cases} |Fm|^2 - 1 & \text{if } F \in \mathcal{N} \\ \infty & \text{else,} \end{cases}$$

for $p = 1$ and $p = 2$, respectively. Here $\mathcal{N} = \{F \in \mathbb{M}^{2\times 2} |\ \det F = 1,\ |Fs| \le 1\}$ is the quasiconvex hull of the set where W is finite. Thus, under the hypothesis of rigid elasticity macroscopic material behavior is analyzed completely. Now let us summarize the results for the model with elastic energy.
In absence of hardening one can find curves along which W_ε grows merely sublinearly. Exploiting these directions in a subtle construction of appropriate rank-one lines gives rise to this result.

Theorem 1 ([1, Theorem 1]). *If $p = 1$ and $\varepsilon > 0$, the quasiconvex envelope of W_ε vanishes identically on $\mathcal{N}$, i.e. $W_\varepsilon^{\mathrm{qc}}(F) = 0$ for all $F \in \mathcal{N}$.*

Even if the pointwise limit $\lim_{\varepsilon\to 0} W_\varepsilon(F) = W(F)$ for all $F \in \mathbb{M}^{2\times 2}$ might suggest the opposite, W is not a good approximation to W_ε, just compare the statement of Theorem 1 to W_1^{qc}. In terms of physics these findings reveal very soft material behavior in response to a large class of applied loads.
The regularizing effect of linear hardening, however, renders an approximation result via Γ-convergence possible.

Theorem 2 ([4, Theorem 1.1]). *Let $p = 2$ and $X = \{u \in W^{1,1}(\Omega;\mathbb{R}^2) \mid \int_\Omega u = 0\}$ be endowed with the strong L^1-topology. For $\varepsilon > 0$ we define the energy functionals $E_\varepsilon : X \to \overline{\mathbb{R}}$ and $E : X \to \overline{\mathbb{R}}$ by $E_\varepsilon[u] = \int_\Omega W_\varepsilon(\nabla u)\,\mathrm{d}x$ and*

$$E[u] = \begin{cases} \int_\Omega W_2^{\mathrm{qc}}(\nabla u)\,\mathrm{d}x, & \text{if } u \in W^{1,2}(\Omega;\mathbb{R}^2) \cap X, \nabla u \in \mathcal{N} \text{ a.e. in } \Omega \\ \infty, & \text{else.} \end{cases}$$

Then, E_ε Γ-converges to E in X as $\varepsilon \to 0$ and the corresponding compactness result holds.

The proofs of compactness and the lower bound are widely based on careful algebraic estimates exploiting the anisotropic structure of W_ε. The crucial point is the recovery of the incompressibility constraint in the limit. For this purpose Conti, Dolzmann and Müller [6] recently developed a generalization of the classical div-curl lemma for sequences whose div and curl are compact as functionals on Lipschitz functions. For the construction of the recovery sequence we use local laminates with position-dependent period and orientation.

References

[1] S. Conti, G. Dolzmann and C. Klust *Relaxation of a class of variational models in crystal plasticity*, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **465** (2009), 1735–1742.

[2] S. Conti and F. Theil *Single-slip elastoplastic microstructures*, Arch. Ration. Mech. Anal. **178** (2005), 125–148.

[3] S. Conti *Relaxation of single-slip single-crystal plasticity with linear hardening*, Multiscale Materials Modeling, Fraunhofer IRB, Freiburg (2006), 30–35.

[4] S. Conti, G. Dolzmann and C. Kreisbeck *Asymptotic behavior of crystal plasticity with one slip system in the limit of rigid elasticity*, in preparation.

[5] M. Ortiz and E. A. Repetto *Nonconvex energy minimization and dislocation structures in ductile single crystals*, J. Mech. Phys. Solids **2** (1999), 397–462.

[6] S. Conti, G. Dolzmann and S. Müller *The div–curl lemma for sequences whose divergence and curl are compact in $W^{-1,1}$*, submitted to C. R. Acad. Sci. Paris Sér. I Math.

Macroscopic modeling of Magnetic Shape Memory Alloys

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(joint work with F. Auricchio, A.-L. Bessoud, A. Reali)

In the last decade a new class of materials called magnetic shape memory alloys (MSMAs) has been intensively investigated. MSMAs are metallic alloys presenting

the superlastic and shape memory effects along with a *giant* magnetostrictive behavior (up to 5-8%) which is the effect of the ferromagnetic nature of martensites. In particular, the martensitic phase in MSMAs presents the classical ferromagnetic texture of magnetic domains. This mesostructure can be modified by magnetic domain wall motion, magnetization rotation, and martensitic variant reorientation. We are focusing here on the *magnetically uniaxial* case, that is to say that martensites are assumed to present just one magnetic *easy axis*. This is specifically the case of cubic-to-tetragonal martensitic transformations (as in Ni_2MnGa, FePd, FePt among others).

We aim at presenting a novel 3D description of the constitutive response of MSMAs as the effect of changes in the internal magnetic field $\boldsymbol{H}$, the total strain $\boldsymbol{\sigma}$, and the absolute temperature T. The linearized (small) strain $\boldsymbol{\varepsilon}$ is additively decomposed into $\boldsymbol{\varepsilon} = \mathbb{C}^{-1}{:}\boldsymbol{\sigma} + \boldsymbol{z}$ where $\mathbb{C}$ is the elasticity tensor whereas $\boldsymbol{z} \in \mathbb{R}^{3\times 3}_{\mathrm{dev}}$ is the inelastic (or transformation) part and shall be regarded as the descriptor of the martensitic structure of the material. Given variant $\boldsymbol{z}$, we obtain the corresponding (directed) easy axis as

$$\mathcal{A}\boldsymbol{z} := \frac{1}{3} m_{\mathrm{sat}} (1,1,1)^{\top} + \mathbb{A}{:}\boldsymbol{z}$$

where m_{sat} is the saturation magnetization, $\mathbb{A}$ is a 3-tensor of components

$$\mathbb{A}_{iii} = -\frac{2}{3}\sqrt{\frac{2}{3}}\frac{m_{\mathrm{sat}}}{\varepsilon_L}, \quad \mathbb{A}_{ijj} = \frac{1}{3}\sqrt{\frac{2}{3}}\frac{m_{\mathrm{sat}}}{\varepsilon_L}, \quad \mathbb{A}_{ijk} = 0$$

for $i,j,k = 1,2,3,\ i \neq j \neq k,$, and ε_L is the maximal strain modulus due to alignment of martensitic variants. In particular, we have that $\mathcal{A}\boldsymbol{z}_i = m_{\mathrm{sat}}\boldsymbol{e}_i$ (coordinate vector) for all pure variants $\boldsymbol{z}_i$ obtained by compression along the respective coordinate directions. A second internal variable is the local (signed) proportion $\alpha \in [-1,1]$ of magnetic domains oriented in the direction of the (directed) easy axis. Additional modeling details and motivation are reported in [1] and the reader is referred to [2, 3] for some relevant modeling discussions.

Our main modeling ansatz is that of directly connecting magnetic and mechanical variables by prescribing the magnetization $\boldsymbol{M}$ of the material in terms of $\boldsymbol{z}$ and α as

$$\boldsymbol{M} = \alpha\mathcal{A}\boldsymbol{z}.$$

In particular, we assume that the magnetic anisotropy of the material is sufficiently strong so that the magnetization stays rigidly attached to the easy axes of the martensitic variants and no magnetization rotation occurs [5]. Note that the specific form of $\mathcal{A}$ is compatible with material symmetries and yields the natural constraint $|\boldsymbol{M}| \leq m_{\mathrm{sat}}$.

We prescribe the Gibbs free energy density of the material (of a constant and normalized density) as

$$\begin{aligned} G(\boldsymbol{\sigma},\boldsymbol{H},T,\boldsymbol{z},\alpha) := &-\frac{1}{2}\boldsymbol{\sigma}{:}\mathbb{C}^{-1}{:}\boldsymbol{\sigma} - \boldsymbol{\sigma}{:}\boldsymbol{z} + \beta(T)|\boldsymbol{z}| + \frac{h}{2}|\boldsymbol{z}|^2 + I_{\varepsilon_L}(\boldsymbol{z}) \\ &+ \frac{1}{2\delta}\alpha^2 + I_{[-1,1]}(\alpha) - \mu_0 \boldsymbol{H}\cdot\alpha\mathcal{A}\boldsymbol{z}. \end{aligned} \tag{1}$$

The first line in (1) is exactly the Gibbs energy of the well-known *Souza-Auricchio model* for non-magnetic SMAs [4]. In particular, $T \mapsto \beta(T) \geq 0$ is a specific function of the temperature, $h > 0$ is a hardening modulus, and I_{ε_L} is the *indicator function* of the ball $\{\boldsymbol{z} \in \mathbb{R}^{3\times 3}_{\rm dev} \ : \ |\boldsymbol{z}| \leq \varepsilon_L\}$.

The second line in (1) describes the magnetic behavior of the material. The term $-\mu_0 \boldsymbol{H}\cdot\alpha\mathcal{A}\boldsymbol{z}$ is nothing but the classical *Zeeman energy* term. Note that $\boldsymbol{H}$ stands here for the *internal* magnetic field. In particular, $\boldsymbol{H}$ corresponds to the sum of the applied external field and the corresponding induced demagnetization field. The indicator function $I_{[-1,1]}$ is constraining the scalar α to take values in $[-1, 1]$ and $1/\delta$ is a hardening parameter.

As for the dissipative character of the model, we assume that the inelastic strain $\boldsymbol{z}$ dissipates energy whereas the variable α is non-dissipative. This is of course disputable as the dissipation in α is, for instance, the basic dissipative mechanism in ferromagnetic materials. Still, experiments show that, at small strains, the dissipation in α is negligible with respect to that in $\boldsymbol{z}$. Eventually, the dissipation function associated with $\boldsymbol{z}$ is given by

$$D(\dot{\boldsymbol{z}}) = \sup\left\{\boldsymbol{g}:\dot{\boldsymbol{z}} \ \middle| \ F(\boldsymbol{g}) \leq 0\right\} = \begin{cases} R|\dot{\boldsymbol{z}}| & \text{if } \dot{\boldsymbol{z}} \in \mathbb{R}^{3\times 3}_{\rm dev} \\ \infty & \text{else} \end{cases}$$

Moving from these considerations, the internal variable α can be directly obtained as a function of $\boldsymbol{H}$ and $\boldsymbol{z}$ as $\alpha = \max\left\{-1, \min\left\{1, \delta\mu_0 \boldsymbol{H}\cdot\mathcal{A}^*\boldsymbol{z}\right\}\right\}$.

We have proved existence of *energetic solutions* for both the constitutive relation problem and the three-dimensional quasi-static evolution problem ($\boldsymbol{H}$ given). Moreover, we have checked the reduction of this model to the Souza-Auricchio non-magnetic one by means of a rigorous Γ-convergence argument.

References

[1] A.-L. Bessoud and U. Stefanelli. Magnetic Shape Memory Alloys: three-dimensional modeling and analysis. *Preprint IMATI-CNR*, 27PV09/20/0, 2009, available at `http://www.imati.cnr.it/ulisse/pubbl.html`

[2] L. Hirsinger and C. Lexcellent. Internal variable model for magneto-mechanical behaviour of ferromagnetic shape memory alloys Ni-Mn-Ga *J. Phys. IV*, 112 (2003) 977–980.

[3] B. Kiefer and D.C. Lagoudas. Modeling the coupled strain and magnetization response of magnetic shape memory alloys under magnetomechanical loading. *J. Intell. Mater. Syst. Struct.*, 20 (2009), 143–170.

[4] A. C. Souza, E. N. Mamiya, and N. Zouain. Three-dimensional model for solids undergoing stress-induces transformations. *Eur. J. Mech. A Solids*, 17 (1998), 789-806.

[5] R. Tickle and R. D. James. Magnetic and magnetomechanical properties of Ni_2MnGa, *J. Magn. Magn. Mater.*, 195 (1999) 627–638.

Microstructures in Nematic Elastomers

Antonio DeSimone

Nematic elastomers consist of networks of cross–linked polymeric chains, each of which contains nematic rigid rod-like molecules (nematic mesogens). The interaction between nematic order and the underlying rubbery solid results in unusual

elastic properties. These arise from material instabilities (elastic shear banding) which are closely reminiscent of mechanical twinning in crystalline solids.

We have presented some analytical and computational results which reproduce rather well the available experimental evidence on nematic elastomers. Our analysis is conducted both in the framework of finite deformations and using linearized kinematics.

The basic formula for the analysis of the large deformation regime is the energy density

$$W(\mathbf{F}) = \frac{1}{2}\mu a^{1/3}\left(\lambda_{\min}^2 + \lambda_{\mathrm{mid}}^2 + \frac{1}{a}\lambda_{\max}^2 - 3a^{-1/3}\right), \quad \text{if } \det\mathbf{F} = 1 \tag{1}$$

and $W(\mathbf{F}) = +\infty$, if $\det\mathbf{F} \neq 1$. Here $\mu > 0$ and $a > 1$ are material parameters, $\lambda_{\max} \geq \lambda_{\mathrm{mid}} \geq \lambda_{\min}$ are the ordered singular values of the deformation gradient $\mathbf{F}$ (principal stretches). The counterpart of (1) in the small strain regime is

$$\varphi(\mathbf{E}) = \mu\left[(e_{\max} - \gamma)^2 + (e_{\mathrm{mid}} + \frac{1}{2}\gamma)^2 + (e_{\min} + \frac{1}{2}\gamma)^2\right], \quad \text{if } \mathrm{tr}\,\mathbf{E} = 0 \tag{2}$$

and $\varphi(\mathbf{E}) = +\infty$, if $\mathrm{tr}\,\mathbf{E} \neq 0$. Here $0 < \gamma << 1$ is a material parameter ($a^{1/3} = 1 + \gamma$), while $e_{\max} \geq e_{\mathrm{mid}} \geq e_{\min}$ are the ordered eigenvalues of the linear strain $\mathbf{E}$ (principal strains). Energy (2) is obtained from

$$\varphi(\mathbf{E}) = \inf_{\mathbf{n}\in S^2} \Phi(\mathbf{E}, \mathbf{n}), \tag{3}$$

where

$$\Phi(\mathbf{E}, \mathbf{n}) = \mu|\mathbf{E} - \mathbf{E}_0(\mathbf{n})|^2, \quad \text{if } \mathrm{tr}\,\mathbf{E} = 0 \tag{4}$$

and $\Phi(\mathbf{E}, \mathbf{n}) = +\infty$ if $\mathrm{tr}\,\mathbf{E} \neq 0$. This last expression was obtained in [6] by Taylor expansion of the classical trace formula of Warner and Terentjev [8].

We have reported on recent results including an explicit formula for the quasiconvex hull of (2) obtained in [2], which is the small-strain counterpart of the result in [5], and a justification of (2) and of its quasi-convex hull as the small-strain Γ-limit of (1), see [1].

Knowledge of the quasiconvex hull of (2) has been used to set up efficient finite-element simulations of the mechanical response arising from global enengy minimizers, in the same spirit as it was done in [3] in the large deformation regime.

A model for the dynamics of nematic elastomers in the small strain regime is available [4] and it has been validated against experimental evidence [7]. This allows us now to explore the issue of the dynamic accessibility of global energy minimizers.

References

[1] V. Agostiniani, A. DeSimone *Gamma-convergence of energies for nematic elastomers in the small strain limit*, forthcoming (2010).

[2] P. Cesana, *Relaxation of multi-well energies in linearized elasticity and applications to nematic elastomers*, Arch. Rat. Mech. Anal., in press (2010).

[3] S. Conti, A. DeSimone, and G. Dolzmann, *Soft elastic response of stretched sheets of nematic elastomers: a numerical study*, J. Mech. Phys. Solids **50** (2002), 1431–1451.

[4] A. DeSimone, A. DiCarlo, and L. Teresi, *Critical voltages and blocking stresses in nematic gels*, Eur. Phys. J. E **24** (2007), 303–310.
[5] A. DeSimone, G. Dolzmann, *Macroscopic response of nematic elastomers via relaxation of a class of* SO(3)*-invariant energies*, Arch. Rat. Mech. Anal. **161** (2002), 181–204.
[6] A. DeSimone, L. Teresi, *Elastic energies for nematic elastomers*, Eur. Phys. J. E **29** (2009), 191-204.
[7] A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi, *Dynamics of Electro-Opto-Mechanical Effects in Swollen Nematic Elastomers*, Macromolecules **41** (2008), 9389–9396.
[8] M. Warner, E. Terentjev, *Liquid Crystal Elastomers*, Clarendon Press, Oxford 2003.

Multiscale modeling of the mechanics of metallic and biological polycrystals using ab initio theory in conjunction with continuum homogenization

Dierk Raabe

We introduce concepts to predict and experimentally validate elasto-plastic crystal mechanical problems using multiscale models which proceed in part from the level of quantum mechanics. The presentation starts with an concise introduction to crystal plasticity finite element modeling with examples from small and large scales. Concerning the use of quantum mechanical models two main examples will be presented thereafter. The first one is the study of the effective elastic properties of polycrystals using a quantum mechanical approach in conjunction with different types of continuum-based mechanical homogenization schemes (Hershey; fast Fourier transform approaches; finite element method). The predictions are compared to experimentally observed elastic constants considering measured crystallographic textures and microstructures. As example materials we use a set of beta-Ti-Nb alloys (BCC) with different composition and Zener anisotropy ratios . In a first step the elastic single crystal constants are for all alloys (BCC crystal structure) calculated using an ab-initio approach based on density functional theory (DFT) in the generalized gradient approximation (GGA-PBE96). In the second step these constants are used as input data for the calculation of the effective polycrystal stiffness using different homogenization methods. As second example we propose a hierarchical model for the prediction of the elastic properties of mineralized lobster cuticle using ab initio calculations. The prediction of the elastic properties of chitin and the ensuing hierarchical homogenization are performed in a bottom-up order in order to identify the cuticle properties at all hierarchy levels. The mechanically relevant parts of lobster cuticle consist of planes reinforced with chitin-protein fibers embedded in a matrix consisting of calcium carbonate nanoparticles and proteins. The planes are stacked over each other and gradually rotate along the normal direction of the cuticle to form a twisted plywood structure. In addition, the cuticle has a canal pore system which pierces it through its thickness. The canals have the shape of twisted ribbons with elliptical cross section and are arranged in a hexagonal array so that the cuticle resembles a honeycomb-like structure. We compare the model predictions to experimental data for the Young moduli and the Poisson's ratios of wet lobster endocuticle. It

is found that the dominant factors determining the cuticle stiffness are the mineral content, the specific microstructure of the mineral-protein matrix and the in-plane area fraction of the pore canals.

References

[1] W.A. Counts, M. Friak, D. Raabe, J. Neugebauer, *Using ab intio calculations in designing bcc Mg-Li alloys for ultra light-weight applications*, Acta Mater. **57** (2009), 69–76.

[2] W.A. Counts, M. Friak, D. Raabe, J. Neugebauer, *Theory-guided bottom-up design of beta-titanium alloys as biomaterials based on first principles calculations: theory and experiments*, Acta Mater. **55** (2007), 4475–4487.

From kinetic relations to kinetic equations

Lev Truskinovsky
(joint work with Anna Vainchtein)

In this talk we discussed the concept of *kinetic equations* representing a natural extension of the more conventional notion of a *kinetic relation*. Algebraic kinetic relations, widely used to model dynamics of dislocations, cracks and phase boundaries, link the instantaneous value of the velocity of a defect with an instantaneous value of the driving force. The new approach [1] generalizes kinetic relations by implying a relation between the velocity and the driving force which is nonlocal in time. To make this relations explicit one needs to integrate the system of kinetic equations.

We illustrate the difference between kinetic relation and kinetic equations by working out in full detail a prototypical model of an overdamped defect in a one-dimensional discrete lattice. We show that the minimal nonlocal kinetic description containing now an internal time scale is furnished by a system of two ordinary differential equations coupling the spatial location of defect with another internal parameter that describes configuration of the core region. The aim of these equations is to capture the transient phases of the defect evolution in response to nonsteady driving.

Martensitic phase boundaries are particularly convenient for the demonstration of the main principles of our approach because these plane defects may be adequately represented already in one-dimensional models. To emphasize ideas we consider the simplest case of a phase boundary with overdamped dynamics. At the microscale, the analysis of the non-steady evolution of the core region of such phase boundaries requires a study of a dynamical system with an infinite number of degrees of freedom representing different atomic bonds. The key to our method is the assumption that the dynamics of only a few bonds located in the core region has to be resolved fully. The other bonds remain confined to their respective potential wells, and their relaxation can be treated as instantaneous.

To be more specific, consider an infinite chain of particles, connected to their nearest neighbors (NN) through viscoelastic springs and to their next-to-nearest neighbors (NNN) by elastic springs. Suppose that in the undeformed configuration

the NN and NNN springs have lengths ε and 2ε, respectively. Let $u_n(t)$ denote the displacement of nth particle at time t with respect to the reference configuration. We associate with the deformation of nth NN spring a discrete measure of strain $w_n = (u_n - u_{n-1})/\varepsilon$. For the viscoelastic NN springs we assume the following constitutive relation for the force:

$$f_{\mathrm{NN}}(w, \dot{w}) = \phi'_{\mathrm{NN}}(w) + \xi \dot{w}, \tag{1}$$

where $\xi > 0$ is the viscosity coefficient. To describe martensitic phase transitions the energy $\phi_{\mathrm{NN}}(w)$ must be at least a double-well potential; to obtain explicit solutions, we assume that this function is biquadratic:

$$\phi_{\mathrm{NN}}(w) = \begin{cases} \frac{1}{2}\mu w^2, & w \le w_c \\ \frac{1}{2}\mu(w-a)^2 + \mu a\left(w_c - \dfrac{a}{2}\right), & w \ge w_c. \end{cases} \tag{2}$$

To simplify calculations further, we assume that the NNN interactions are linearly elastic: $f_{\mathrm{NNN}}(\hat{w}) = 2\gamma\hat{w}$. Here we defined $\hat{w}_n = (w_{n+1} + w_n)/2$ as the strain in the NNN spring connecting $(n+1)$th and $(n-1)$th particles.

The dynamics of the chain is governed by the following system of ordinary differential equations:

$$\begin{aligned} \rho\varepsilon\ddot{u}_n =& \mu[w_{n+1} - w_n - \theta(w_{n+1} - w_c)a + \theta(w_n - w_c)a] \\ &+ \gamma(w_{n+2} + w_{n+1} - w_n - w_{n-1}) + \xi(\dot{w}_{n+1} - \dot{w}_n). \end{aligned} \tag{3}$$

Here $\rho > 0$ is the mass density of the chain and $\theta(x)$ is the unit step function. To ensure stability of the chain we require that $E = \mu + 4\gamma > 0$ where E is the homogenized macroscopic elastic modulus; we also assume that the NNN interactions are of ferromagnetic type, meaning that $\gamma \le 0$. Our main interest is the overdamped limit when $\xi >> \varepsilon\sqrt{\rho E}$. Then the dimensionless system equations reads

$$\dot{w}_n - \dot{w}_{n+1} = \hat{\sigma}(w_{n+1}) - \hat{\sigma}(w_n) + D(w_{n+2} + w_{n+1} - w_n - w_{n-1}), \tag{4}$$

where $\hat{\sigma}(w) = w - \theta(w - w_c)$ is the normalized macroscopic stress-strain law. The dimensionless parameter $D = -\gamma/E \ge 0$ measures the relative strength of NN and NNN interactions. The system (4) can be "integrated"

$$\dot{w}_n = D(w_{n+1} - 2w_n + w_{n-1}) - \hat{\sigma}(w_n) + \sigma. \tag{5}$$

where $\sigma = \sigma(t)$ is the time-dependent applied stress.

Our goal is to approximate this *infinite-dimensional* dynamical system of a gradient flow type by a *finite-dimensional* reduced dynamical system of the same type

$$\dot{\boldsymbol{\nu}} = -\boldsymbol{\alpha}\nabla\Phi(\boldsymbol{\nu}; G(t)), \tag{6}$$

where $\boldsymbol{\alpha}$ is the effective mobility matrix. The gradient is taken with respect to the order parameter $\boldsymbol{\nu} \in \mathbb{R}^K$ where the integer-valued parameter K defines the dimensionality of the reduced system. After the solution of the vector equation (6) is known, the approximation of the dynamics of the discrete field should be recoverable from the auxiliary relations $w_n(t) = w_n(\nu_1(t), \ldots, \nu_K(t))$ describing the recovery of relaxed "non-order-parameter" variables.

Assume first that G is given and minimize the energy with respect to all strain variables other than w_{-1}, w_0 and w_1. We obtain the following recovery relations

$$w_n = \begin{cases} w_c + G + 1/2 + (w_{-1} - w_c - G - 1/2)e^{\lambda(n+1)}, & n \le -1 \\ w_0, & n = 0 \\ w_c + G - 1/2 + (w_1 - w_c - G + 1/2)e^{\lambda(1-n)} & n \ge 1. \end{cases} \tag{7}$$

The remaining variables $w_{-1}(t)$, $w_0(t)$ and $w_1(t)$ satisfy the equations

$$\begin{aligned} \dot{w}_{-1} &= (-2D - 1 + e^{-\lambda}D)w_{-1} + Dw_0 + (w_c + G + 1/2)(1 + D(1 - e^{-\lambda})) \\ \dot{w}_0 &= (-2D - 1)w_0 + Dw_1 + Dw_{-1} + w_c + G + 1/2 \\ \dot{w}_1 &= (-2D - 1 + e^{-\lambda}D)w_{-1} + Dw_0 + (w_c + G - 1/2)(1 + D(1 - e^{-\lambda})) \end{aligned} \tag{8}$$

One can see that the equations governing the dynamics of $w_{-1}(t)$ and $w_1(t)$ differ only by a constant term in the right hand side. This allows us to reduce (8) to a two-dimensional system for

$$x(t) = w_0(t), \quad y(t) = \frac{w_{-1}(t) + w_1(t)}{2}. \tag{9}$$

The two variables: $x(t)$, describing the dynamics of the transforming spring, and $y(t)$, describing the average strain in the core region, must satisfy the following system of equations:

$$\dot{x} = (-2D - 1)x + 2Dy + w_c + G + 1/2 \tag{10}$$

$$\dot{y} = Dx + (-2D - 1 + e^{-\lambda}D)y + (w_c + G)(1 + D(1 - e^{-\lambda})). \tag{11}$$

This system of kinetic equations can be reformulated as a gradient flow (6) and turns out to be an excellent approximation of the full infinite-dimensional dynamics not only for $G = \text{const}$ but also in a wide range of non-steady regimes when $G = G(t)$ (see [1] for the details).

References

[1] L. Truskinovsky and A. Vainchtein, *Beyond kinetic relations*, Continuum Mechanics and Thermodyanmics (2010), in print.

Pinning of interfaces in random media

Patrick W. Dondl
(joint work with Nicolas Dirr, Michael Scheutzow)

Problems of interface evolution in heterogeneous media arise in a large number of physical models. Common to such models is a regularizing operator, for example line tension, and the competition between an external applied driving force F and a force field $f(x, y)$ describing the inhomogeneities. Assuming a viscous law for the relation between the driving force and the velocity of the interface, an important question is whether rate independent hysteresis can emerge from the interaction between the heterogeneous force field and the regularizing operator.

Here, we consider a model for the evolution of an interface through a random field of obstacles. Let $n \in \mathbb{N}, n \geq 1$. Let $(\Omega, \mathcal{F}, \mathbf{P})$ be a probability space, $\omega \in \Omega$. We model the interface as the graph $(x, u(x,t,\omega))$ of a function $u\colon \mathbb{R}^n \times \mathbb{R} \times \Omega \to \mathbb{R}$ moving through a field $f(x,y,\omega)$ of (soft) random obstacles and driven by a constant force F. More precisely, we consider the semi-linear PDE

$$\partial_t u(x,t,\omega) = \triangle u(x,t,\omega) + f(x, u(x,t,\omega), \omega) + F \quad \text{on } \mathbb{R}^n, \tag{1}$$

$$u(x,0,\omega) = 0. \tag{2}$$

The random nonlinearity f is constructed in the following way: We consider the obstacle function $\phi \in C^\infty(\mathbb{R}^n \times \mathbb{R})$ to have the properties $\phi \leq 0$, $\phi(x,y) = 0$ for $||(x,y)|| > r_1$, $\phi(x,y) \leq -1$ for $||(x,y)||_\infty \leq r_0$, with $r_1 > \sqrt{n} r_0 > 0$, thus fixing a 'shape' for the individual obstacles. Here, $||\cdot||$ denotes the Euclidean norm on $\mathbb{R}^{n+1}$, $||\cdot||_\infty$ denotes the maximum-norm. The heterogeneity f is now given as the sum over individual obstacles with centers $\{(x_k(\omega), y_k(\omega))\}_{k\in\mathbb{N}}$, and strength $f_k(\omega) \geq 0$, i.e.,

$$f(x,y,\omega) = \sum_k f_k(\omega)\phi(x - x_k(\omega), y - y_k(\omega), \omega).$$

The laws of x_k, y_k, and f_k will be specified below.

In the physics literature, a parabolic semi-linear equation with random input like (1) is sometimes called Quenched Edwards-Wilkinson model. It is motivated in the following way: A very basic model for an interface (phase boundary, dislocation line in its slip plane etc) moving through an array of random obstacles (e.g. impurities, other dislocation lines) in an over-damped limit (inertial effects are neglected) is the gradient flow of the area functional plus a random bulk term. If so-called inner variations are considered, the resulting evolution law is *forced mean curvature flow*, where the forcing is random. The model is called "quenched," because the random field does not explicitly depend on time. For forced mean curvature flow and applications, in particular in the case of periodic forcing, we refer to [1, 2, 5, 7]. If the interface is a graph and the gradient is sufficiently small, the evolution by forced mean curvature flow for the graph can be approximated heuristically by the semi-linear parabolic PDE (1). These kinds of problems have found considerable interest in the physics community, see e.g. [6].

The goal is to construct, for some $F > 0$, a stationary supersolution v to (1) satisfying $v \geq 0$. If such a supersolution exists, by the comparison principle for parabolic equations, the evolving solution u will always remain below v—the interface is pinned. Such pinning of an interface leads to a rate independent hysteresis in the physical system.

We first pose a condition on the distribution of obstacles. The condition basically states that there is a uniform lower bound for finding an obstacle of some strength (also bounded from below) in a box of volume 1, independent of its shape or position, and independently for pairwise disjoint boxes.

Condition 1. *We assume from now on that the random distribution of obstacle sites* $\{(x_k, y_k)\}_{k\in\mathbb{N}} \subset \mathbb{R}^n \times [r_1, \infty)$ *and strength* $\{f_k\}_{k\in\mathbb{N}} \subset [0, \infty)$ *satisfy*

(1) (x_k, y_k) *are distributed according to an* $n+1$*-dimensional Poisson process on* $\mathbb{R}^n \times [r_1, \infty)$ *with intensity* $\lambda > 0$.
(2) f_k *are i.i.d. strictly positive random variables which are independent of* $\{x_k, y_k\}$.

Note that there are no obstacles crossing the line $\{y = 0\}$, so at $t = 0$ the interface with initial condition (2) only sees the external driving force. We thus have $\partial_t u \geq 0$ for all times.

Theorem 1 below depends crucially on the existence of an infinite cluster of open sites in $\mathbb{Z}^{n+1}$ that is the graph of a Lipschitz function, for site percolation with $\mathbf{P}\{\text{Site open}\} > p_c$ independently for all sites. This result is proved in [3].

The following result asserts the existence of a stationary positive supersolution to (1).

Theorem 1 (Existence of a pinned solution)**.** *If Condition 1 is satisfied, then there exists* $F^* > 0$ *and a positive* $v\colon \mathbb{R}^n \times \Omega \to [0, \infty)$ *so that* $0 \geq \triangle v(x, \omega) + f(x, v(x, \omega), \omega) + F^*$ *a.s., i.e., any solution to* (1) *with initial condition* (2) *gets pinned.*

The proof consists of a piecewise construction of the supersolution, and an amount of tedious, but simple, algebra. It can be found in [4].

References

[1] P. Cardaliaguet, P.-L. Lions, and P. E. Souganidis. A discussion about the homogenization of moving interfaces. *J. Math. Pures Appl. (9)*, 91(4):339–363, 2009.
[2] B. Craciun and K. Bhattacharya. Effective motion of a curvature-sensitive interface through a heterogeneous medium. *Interfaces Free Bound.*, 6(2):151–173, 2004.
[3] N. Dirr, P. W. Dondl, G. R. Grimmett, A. E. Holroyd, and M. Scheutzow. Lipschitz percolation. *Electronic Communications in Probability*, 15, 2010.
[4] N. Dirr, P. W. Dondl, and M. Scheutzow. Pinning of interfaces in random media. *arXiv:0911.4254v1 [math.AP]*, 2009.
[5] N. Dirr and N. K. Yip. Pinning and de-pinning phenomena in front propagation in heterogeneous media. *Interfaces Free Bound.*, 8(1):79–109, 2006.
[6] M. Kardar. Nonequilibrium dynamics of interfaces and lines. *arXiv:cond-mat/9704172v1 [cond-mat.stat-mech]*, 1997.
[7] G. N. Dirr, G. Karali and N. K. Yip. Pulsating wave for mean curvature flow in inhomogeneous medium. *European Journal of Applied Mathematics*, 19:661–699, 2008.

An efficient approach to numerical solutions of multi-well variational problems

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(joint work with Sören Bartels)

Let the specimen representing an elastic body occupy a domain $\Omega \subset \mathbb{R}^n$. The stress-free parent austenite is a natural state of the material which makes it, in the context of continuum mechanics, a canonical choice for the reference configuration. As usual, $y\colon \Omega \to \mathbb{R}^n$ denotes the *deformation* and $u\colon \Omega \to \mathbb{R}^n$ the *displacement*,

which are related to each other via the identity $y(x) = x + u(x)$, where $x \in \Omega$. Hence the *deformation gradient* is $F := \nabla y = \mathbb{I} + \nabla u$. Here, $\mathbb{I} \in \mathbb{R}^{n\times n}$ is the identity matrix and ∇ the gradient operator.

The total stored energy in the bulk occupying, in its reference configuration, the domain Ω, is then

$$V(y) := \int_\Omega \varphi(\nabla y(x))\,\mathrm{d}x. \tag{1}$$

A common variational principle in continuum mechanics is the *minimisation of the stored energy*. Due to the coexistence of several variants at low temperature, φ has multiple minima and thus a multi-well character. We consider an isothermal situation with several variants coexisting. Here φ is a nonnegative multi-well energy density with zeros precisely at $\mathrm{SO}(n)U_\ell$, $\ell = 0, \ldots, M$, where $\mathrm{SO}(n)$ denotes the group of proper rotations in n dimensions and U_ℓ the stretch matrices of particular material phases/variants. Due to nonconvexity, minimising sequences of V tend to develop, in general, finer and finer spatial oscillations of their gradients. In other words, the deformation gradient often tends to develop spatial oscillations due to the lack of (quasi-)convexity of the stored energy density. These oscillations are difficult to model in full detail. The oscillations correspond to the development of fine microstructures when the stored energy is to be minimised. The minimum of V, under specific boundary conditions for y, is usually not attained in a space of functions. Therefore one needs to extend the notion of a solution. *Young measures* are here an appropriate tool. They are capable of recording, on a mesoscopic level, the limit information of the finer and finer oscillating deformation gradient as we move towards the macroscopic scale. This can be described, for a current macroscopic point $x \in \Omega$, by a probability measure ν_x on the set of deformation gradients, that is, matrices in $\mathbb{R}^{n\times n}$. Then the mesoscopic stored energy reads

$$\bar{V}(y, \nu) := \int_\Omega \int_{R^n \times n} \varphi(A)\nu_x(\mathrm{d}A)\,\mathrm{d}x\ ,$$

where $\nu = \{\nu_x\}_{x\in\Omega}$ is a gradient Young measure with the first moment ∇y and the set of all gradient Young measures is denoted by $\mathcal{G}(\Omega; \mathbb{R}^{n\times n})$.

Dissipation due to phase transitions. In order to describe dissipation due to transformations we adopt the (to some extent rather simplified) standpoint that the amount of dissipated energy associated with a particular phase transition between austenite and a martensitic variant or between two martensitic variants can be described by a specific energy (of the dimension $\mathrm{J/m^3} = \mathrm{Pa}$). For an explicit definition of the transformation dissipation, we need to identify the particular phases or phase variants. To this behalf, we define a continuous mapping $\mathcal{L}\colon \mathbb{R}^{n\times n} \to \triangle$, where

$$\triangle := \left\{ \zeta \in \mathbb{R}^{1+M} \;\middle|\; \zeta_\ell \geq 0 \text{ for } \ell = 0, \ldots, M \text{ and } \sum_{\ell=0}^{M} \zeta_\ell = 1 \right\}$$

is a simplex with $M+1$ vertices, with M being the number of martensitic variants. Here $\mathcal{L}$ is related with the material itself and thus has to be frame indifferent. We

assume, beside $\zeta_\ell \geq 0$ and $\sum_{\ell=0}^{M} \zeta_\ell = 1$, that the coordinate ζ_ℓ of $\mathcal{L}(F)$ takes the value 1 if F is in the ℓ-th (phase) variant, that is, F is in a vicinity of the ℓth well $\mathrm{SO}(n)U_\ell$ of φ, which can be identified by the stretch tensor $F^\top F$ being close to $U_\ell^\top U_\ell$. If $\mathcal{L}(F)$ is not in any vertex of $\triangle$, then it means that F is in the spinodal region where no definite phase or variant is specified. We assume, however, that the wells are sufficiently deep and the phases and variants are geometrically sufficiently far from each other so that the tendency for minimisation of the stored energy will essentially prevent F to range into the spinodal region. Thus, the concrete form of $\mathcal{L}$ is not important as long as $\mathcal{L}$ enjoys the properties listed above. We remark that $\mathcal{L}$ plays the role of what is often called vector of *order parameters* or a vector-valued *internal variable*.

For two states q_1 and q_2, with $q_j = (y_i, \nu_i, \lambda_i)$ for $j = 1, 2$, we now define the dissipation due to martensitic transformation which "measures" changes in the volume fraction $\lambda \in L^\infty\left(\Omega; \mathbb{R}^{M+1}\right)$. This dissipation is given by

$$\mathcal{D}\left(q_1, q_2\right) := \int_\Omega \left|\lambda_1(x) - \lambda_2(x)\right|_{\mathbb{R}^{M+1}} \mathrm{d}x \ , \tag{2}$$

where $\lambda_j(x) := \int_{\mathbb{R}^{n\times n}} \mathcal{L}(s)\nu_{j,x}(\mathrm{d}s)$ and $|\cdot|_{\mathbb{R}^{M+1}}$ is a norm on $\mathbb{R}^{M+1}$.

In experiments, the specimen is subjected to external loads. In order to simplify our exposition, we consider only dead body forces and surface forces. We assume that we are given two disjoint sets $\Gamma_0, \Gamma_1 \subset \partial\Omega$, where the $(n-1)$-dimensional Hausdorff measure of Γ_0 is positive. We consider Dirichlet boundary conditions $y = y_0$ on Γ_0 for some prescribed (time-independent) mapping y_0. As for the surface forces acting on Γ_1, we define a linear functional

$$L(q) := \int_\Omega f(x) \cdot y(x) \,\mathrm{d}x + \int_{\Gamma_1} g(x) \cdot y(x) \,\mathrm{d}S \ , \tag{3}$$

where $f\colon \Omega \to \mathbb{R}^n$ and $g\colon \Gamma_1 \to \mathbb{R}^n$ are the densities of volume and surface forces acting on the material, respectively. Below, we write $L = L(t, q)$ to indicate the possibility of temporally changing forces.

From now on let $y \in \mathbb{Y}\left(\Omega; \mathbb{R}^n\right) := \left\{y(t) \in W^{1,p}\left(\Omega; \mathbb{R}^n\right) \,\middle|\, y = y_0(t) \text{ on } \Gamma_0\right\}$ and $\mathcal{Q} := \mathbb{Y}\left(\Omega; \mathbb{R}^n\right) \times \mathcal{G}(\Omega; \mathbb{R}^{n\times n}) \times L^\infty(\Omega; \mathbb{R}^{M+1})$. We introduce

$$\mathbb{Q} := \left\{q \in \mathcal{Q} \,\middle|\, \lambda = \mathcal{L} \bullet \nu,\, \nabla y = \mathbb{I} \bullet \nu\right\} \ ,$$

where, for almost all $x \in \Omega$, $[\mathcal{L} \bullet \nu](x) := \int_{\mathbb{R}^{n\times n}} \mathcal{L}(s)\nu_x(\mathrm{d}s)$; $\mathbb{I} \bullet \nu$ is defined analogously.

The existence of a rate-independent evolution [4] commonly proceeds via time-discretisation. Thus, in a first step, a sequence of incremental problems is defined. We employ a time discretization $0 = t_0 < \ldots < t_n = T$ via a time step $\tau > 0$, chosen in such a way that $N = T/\tau \in \mathbb{N}$. Let an initial state $q_\tau^0 \in \mathbb{Q}$ be given. For $1 \leq k \leq N$ we find $q_\tau^k \in \mathbb{Q}$ by solving

$$\text{minimize } \mathcal{I}(t_k, q) + \mathcal{D}\left(q_\tau^{k-1}, q\right), \text{ subject to } q \in \mathbb{Q} \ . \tag{4}$$

In this contribution, we propose to replace the set of gradient Young measures in this minimization by the set of Young measures satisfying the Jensen inequality

for all minors only. A suitable discretization then leads to a linear programming problem with linear constraints [1] for which the first order optimality conditions are known and we use them in an effective numerical algorithm [2] for its solution [3].

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References

[1] S. Bartels, *Reliable and efficient approximation of polyconvex envelopes*, SIAM J. Numer. Anal. **43** (2005), 363–385.

[2] C. Carstensen, T. Roubíček, *Numerical approximation of Young measures in nonconvex variational problems*, Num. Math. **84** (2000), 395–415.

[3] S. Bartels, M. Kružík, *An effective numerical approach to rate-independent problems*, in preparation.

[4] A. Mielke, T. Roubíček, *A rate-independent model for inelastic behavior of shape-memory alloys*, Multiscale Model. Simul. **1** (2003), 571–597.

From Damage to Delamination in Nonlinearly Elastic Materials at Small Strains

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(joint work with Alexander Mielke and Tomáš Roubíček)

Damage means the creation and growth of cracks and voids on the micro-level of a solid material. This phenomenon can be described by means of so-called continuum damage mechanics, which was introduced by L.M. Kachanov in 1958, see e.g. [1] in english. Within this approach an inner variable, the damage variable $z : [0,T] \times \Omega \to [0,1]$, is incorporated to the constitutive law, where it reflects the changes in the elastic behaviour due to damage. Here, $[0,T]$ denotes a time interval and $\Omega \subset \mathbb{R}^d$ the reference domain of the body. Moreover, $z(t,x) = 1$ stands for no damage and $z(t,x) = 0$ for complete damage in the point $(t,x) \in [0,T] \times \Omega$. With similar ideas also the delamination, i.e. the micro-cracking, of a compound along an interface Γ_{C} can be described. Then, $z : [0,T] \times \Gamma_{\mathrm{C}} \to [0,1]$ denotes the delamination variable, which accounts for the constitution of the bonding along the interface. In many engineering contributions (e.g. in [2]) an interface is understood as the limit of a thin medium following its own constitutive law. This was our motivation to mathematically rigorously perform such a limit passage in order to obtain a delamination model as the limit of damage models [3, 4]. We consider a three-specimen-sandwich-structure, where the outer two constituents are perfectly unbreakable and the middle component experiences partial damage. This means that there is a lower bound $\varepsilon^\gamma \in (0,1)$ for a positive γ, such that $z(t,x) \in [\varepsilon^\gamma, 1]$ for a.e. $(t,x) \in [0,T] \times \Omega_{\mathrm{D}}^\varepsilon$. As $\varepsilon \to 0$ the lower bound on the damage variable as well as the thickness 2ε of the damageable component $\Omega_{\mathrm{D}}^\varepsilon$ tend to 0, so that the limit model describes delamination along the interface Γ_{C}. The limit passage is done in a double limit. Since the damage model contains a

regularization $\int_{\Omega_{\mathrm{D}}^\varepsilon} \frac{\kappa}{\varepsilon}|\nabla z|^r \,\mathrm{d}x$, $r \in (d,\infty)$, the first limit $\varepsilon \to 0$ leads to a model involving the delamination gradient. Due to this, the delamination variable can attain values between 0 and 1. This property differs from those of crack-models based on Griffith' fracture criterion [5], as studied e.g. in [6, 7, 8]. To overcome this discrepancy the gradient is suppressed in a second limit $\kappa \to 0$. In fact, this second limit model is of Griffith-type. In particular, both delamination models incorporate transmission and unilateral contact conditions along the interface:

$$z\llbracket u \rrbracket = 0 \quad \text{and} \quad \llbracket u \cdot \mathrm{n}_1 \rrbracket \geq 0 \quad \text{a.e. on } \Gamma_{\mathrm{C}}\,, \tag{1}$$

which result from the following ansatz for the stored energy density on $\Omega_{\mathrm{D}}^\varepsilon$

$$W_{\mathrm{D}}(e,z) := zW(e) + |\max\{-e_{11},0\}|^p\,. \tag{2}$$

Here, $W : \mathbb{R}^{d\times d}_{\mathrm{sym}} \to \mathbb{R}$ is a convex, coercive stored energy density, e is the linearized strain tensor and e_{11} its' 11-component. The multiplicative link between the damage variable and the strains is a common ansatz for damage in engineering, but it leads to a lack of uniform coercivity as $\varepsilon \to 0$. This complicates the derivation of the transmission condition and requires the assumption $r > d$. Moreover, the unilateral contact condition can be obtained due to the anisotropic term.

The analysis is done using the so-called energetic formulation. This approach is solely based on an energy functional $\mathcal{E}_\varepsilon^\kappa : [0,T] \times \mathcal{Q} \to \mathbb{R} \cup \{\infty\}$ and on a dissipation potential $\mathcal{R}_\varepsilon : \mathcal{Z} \to [0,\infty]$ which takes into account the evolution of the inner variable. Thereby $\mathcal{Q} = \mathcal{U} \times \mathcal{Z}$ is a suitable state space with $\mathcal{U}$ as the set of admissible displacements and $\mathcal{Z}$ as the set of admissible inner variables being Banach spaces in our setting. Rate-independence is featured by the positive 1-homogeneity of $\mathcal{R}_\varepsilon$, i.e. $\mathcal{R}_\varepsilon(0) = 0$ and $\mathcal{R}_\varepsilon(\alpha v) = \alpha\mathcal{R}_\varepsilon(v)$ for all $\alpha \in (0,\infty]$ and all $v \in \mathcal{Z}$. Moreover, the damage process is assumed to be unidirectional, i.e. healing is forbidden. With a constant $\varrho > 0$, this is featured by

$$\mathcal{R}_\varepsilon(v) := \int_{\Omega_{\mathrm{D}}^\varepsilon} R_\varepsilon(v(x))\,\mathrm{d}x\,, \quad \text{where} \quad R_\varepsilon(v) := \begin{cases} \frac{\varrho}{\varepsilon}|v| & \text{if } \varrho \leq 0\,, \\ \infty & \text{else}\,. \end{cases}$$

Under the assumption of $\mathcal{E}_\varepsilon^\kappa$ being convex with respect to the linearized strain tensor $e(u) := \frac{1}{2}(\nabla u + \nabla u^\top)$ the existence of so-called energetic solutions was proven in [9]. Thereby, an energetic solution $q = (u,z) : [0,T] \to \mathcal{Q}$ for a rate-independent system $(\mathcal{Q}, \mathcal{E}_\varepsilon^\kappa, \mathcal{R}_\varepsilon)$ is characterized by satisfying the global stability condition (S) and the global energy balance (E) for all $s,t \in [0,T]$:

$$\text{(S)} \qquad \text{for all } \tilde{q} = (\tilde{u},\tilde{z}) \in \mathcal{Q} \text{ holds}: \quad \mathcal{E}_\varepsilon^\kappa(t,q(t)) \leq \mathcal{E}_\varepsilon^\kappa(t,\tilde{q}) + \mathcal{R}_\varepsilon(\tilde{z}-z(t))\,,$$

$$\text{(E)} \qquad \mathcal{E}_\varepsilon^\kappa(t,q(t)) + \mathrm{Diss}_{\mathcal{R}_\varepsilon}(z,[s,t]) = \mathcal{E}_\varepsilon^\kappa(s,q(s)) + \textstyle\int_s^t \partial_\xi \mathcal{E}_\varepsilon^\kappa(\xi,q(\xi))\,\mathrm{d}\xi \quad \text{with}$$

$$\mathrm{Diss}_{\mathcal{R}_\varepsilon}(z,[s,t]) := \sup\Big\{ \textstyle\sum_{j=1}^N \mathcal{R}_\varepsilon(z(\xi_j)-z(\xi_{j-1})) \,\big|\, s=\xi_0<\ldots<\xi_N=t,\, N\in\mathbb{N}\Big\}.$$

The convergence of the systems is proven using the abstract result [10, Th. 3.1], which states the convergence of (subsequences of) energetic solutions of the approximating systems to an energetic solution of the limit system. Compared to the original notion of Γ-convergence of static functionals, in the context of rate-independent processes it is not sufficient, if the energy functionals and the

dissipation potentials Γ-converge. Rather the properties (S) & (E) have to be preserved under convergence. Amongst other properties this can be guaranteed by the validity of Γ-lim inf-inequalities for $\mathcal{E}_\varepsilon^\kappa$ and $\mathcal{R}_\varepsilon$, the convergence of the partial time-derivatives of the energy functionals and the existence of so-called mutual recovery sequences. The last property is extraordinarily difficult to verify in our setting, not only due to the discontinuity of the dissipation potential but also due to the fact that conditions (1) require a strong interplay between the sequence of damage/delamination variables and the sequence of the displacements.

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References

[1] L.M. Kachanov, *Introduction to Continuum Damage Mechanics*, Kluwer Academic Publishers (1990).
[2] O. Allix: *Interface Damage Mechanics: Application to Delamination* in *Continuum Damage Mechanics of Materials and Structures*, eds.: O. Allix and F. Hild, Elsevier (2002), 295–325.
[3] M. Thomas: *Rate-independent Damage Processes in Nonlinearly Elastic Materials*, PhD Thesis, Humboldt-Universität zu Berlin (2009).
[4] A. Mielke, T. Roubíček and M. Thomas: *From Damage to Delamination* (in preparation).
[5] A.A. Griffith: *The Phenomena of Rupture and Flow in Solids*, Phil. Trans. R. Soc. Lond. A **221** (Jan. 1921), 163–198.
[6] G. Dal Maso and R. Toader: *A Model for the Quasi-Static Growth of Brittle Fractures: Existence and Approximation Results*, Arch. Ration. Mech. Anal. **162:2** (2002), 101–135.
[7] G. Francfort and C. Larsen: *Existence and Convergence for Quasi-Static Evolution in Brittle Fracture*, Comm. Pure Appl. Math. **56:10** (2003), 1465–1500.
[8] A. Giacomini: *Ambrosio-Tortorelli approximation for quasi-static evolution of brittle fractures*, Calc. Var. **22** (2005), 129–172.
[9] M. Thomas and A. Mielke *Rate-independent Damage Processes in Nonlinearly Elstic Materials – Existence and Regularity Results*, ZAMM **90:2** (2010), 88–112.
[10] A. Mielke, T. Roubíček and U. Stefanelli: Γ-*limits and relaxations for rate-independent evolutionary problems*, Calc. Var. PDE *31:3* (2008), 387–416.

Across multiscales in solid mechanics via Γ-convergence in the context of quasistatic evolution

Tomáš Roubíček

This contribution addresses the quasistatic initial-value problem for the following equality/inclusion:

$$\partial\mathcal{R}\Big(\frac{\mathrm{d}z}{\mathrm{d}t}\Big)+\partial_z\mathcal{E}(t,u,z)\ni 0,\qquad \partial_u\mathcal{E}(t,u,z)=0,\qquad z(0)=z_0, \tag{1}$$

with $u\in\mathcal{U}$ a "fast" variable, $z\in\mathcal{Z}$ a "slow" variable with an activated evolution, $\mathcal{U}$ and $\mathcal{Z}$ Banach spaces, $\mathcal{E}:[0,T]\times\mathcal{U}\times\mathcal{Z}\to\mathbb{R}\cup\{\infty\}$ a stored-energy potential, $\mathcal{R}:\mathcal{Z}\to\mathbb{R}^+\cup\{\infty\}$ a convex (positively) homogeneous degree-1 dissipation pseudopotential, "∂" denoting (partial) subdifferentials or Gâteaux differentials. Due to the mentioned homogeneity degree-1, the problem (1) is rate independent in

the sense that any monotone rescaling of time scale does not influence its (set of) solution(s). We will briefly refer to (1) as the $(\mathcal{U}\times\mathcal{Z},\mathcal{E},\mathcal{R},z_0)$-problem.

If also $\mathcal{E}(t,\cdot,\cdot)$ is convex, the usual definition of weak solution to (1) is essentially equivalent to the so-called *energetic formulation*, i.e. beside the initial condition $z(0)=z_0$, the couple (u,z) is to satisfy the *energy equality* and *stability*:

$$\text{(2a)}\quad \mathcal{E}\big(T,u(T),z(T)\big)+\mathrm{Var}_{\mathcal{R}}(z;0,T)=\mathcal{E}\big(0,u_0,z_0\big)+\int_0^T\partial_t\mathcal{E}(t,u(t),z(t))\,\mathrm{d}t,$$

$$\text{(2b)}\quad \forall v\in\mathcal{Z},\ \ t\in[0,T]:\qquad \mathcal{E}\big(t,u(t),z(t)\big)\le\mathcal{E}\big(t,u(t),v\big)+\mathcal{R}\big(v-z(t)\big)$$

with $\mathrm{Var}_{\mathcal{R}}(z;0,T)$ denoting the variation of $z:[0,T]\to\mathcal{Z}$ with respect to $\mathcal{R}$ defined as $\sup_{0\le t_0<t_1<\ldots<t_I\le T}\sum_i\mathcal{R}(z(t_i)-z(t_{i-1}))$. The energetic formulation (2), invented by Mielke at al. [12, 13], works also in the nonconvex case, is derivative-free, and expresses a competition between minimisation of stored energy and maximisation of dissipation. This is an applicable concept for a lot of activated processes in mechanics (as plasticity, damage, delamination, or phase transformation).

Considering of sequences of functionals $\{\mathcal{E}_n\}_{n\in\mathbb{N}}$ and $\{\mathcal{R}_n\}_{n\in\mathbb{N}}$, it was observed in [9] that their Γ-convergence respectively to some $\mathcal{E}$ and $\mathcal{R}$ does not ensure convergence of the corresponding energetic solutions of $(\mathcal{U}\times\mathcal{Z},\mathcal{E}_n,\mathcal{R}_n,z_0)$-problems towards energetic solutions of $(\mathcal{U}\times\mathcal{Z},\mathcal{E},\mathcal{R},z_0)$-problem, and disclosed that this goal needs the (Γ-lim inf)-parts combined with a so-called *mutual-recovery-sequence* (MRS) condition, i.e. for any sequence $(t_n,u_n,z_n)\to(t,u,z)$ and for any $(\widetilde{u},\widetilde{z})\in\mathcal{U}\times\mathcal{Z}$, one is to find another sequence $\{(\widetilde{u}_n,\widetilde{z}_n)\}_{n\in\mathbb{N}}$ such that

$$\text{(3)}\qquad \limsup_{n\to\infty}\big(\mathcal{E}_n(t_n,\widetilde{u}_n,\widetilde{z}_n)+\mathcal{R}_n(\widetilde{z}_n-z_n)-\mathcal{E}_n(t_n,u_n,z_n)\big)\le\mathcal{E}(t,\widetilde{u},\widetilde{z})+\mathcal{R}(\widetilde{z}-z)-\mathcal{E}(t,u,z).$$

Explicit construction of mutual recovery sequences $\{(\widetilde{u}_n,\widetilde{z}_n)\}_{n\in\mathbb{N}}$ thus represents the main task. In accord to [8], one can distinguish several typical cases:

(A) unidirectional processes (i.e. $\mathcal{R}=\mathcal{R}_0+\delta_K$ with $\mathcal{R}_0$ continuous and K a cone) and $\mathcal{E}(t,\cdot,\cdot)$ quadratic; then a so-called binomial trick applies – a prominent example is the linearised plasticity and a nontrivial illustration of this technique is limit of the hardening model towards the perfect-plasticity Prandtl-Reuss model if hardening parameters approach 0, cf. [2].

(B) unidirectional processes with general nonquadratic $\mathcal{E}(t,\cdot,\cdot)$; this may, in general, be very difficult and an explicit construction of MRS's is to be made case by case; an example is passage from a partial damage to a complete damage [4, 11], or from adhesive delamination [5] or from a damage on a thin layer [10] to a Griffith-type brittle delamination [14].

(C) $\mathcal{R}$ is continuous in the topology in which the sub-level sets of $\mathcal{E}(t,\cdot,\cdot)$ are compact – then and recovery sequence for $\{\mathcal{E}_n\}_{n\in\mathbb{N}}$ serves as a MRS.

Situation for (C) occurs, e.g., in *multiscale* modelling: the sequence $\{\mathcal{E}_n\}$ typically arises by some higher-gradient theory that vanishes with $n\to\infty$ and the minimisers typically develop a microstructure (often modelled by Young measures solving *relaxed problems*). The relaxed problems can effectively be solved on a "mesoscopical"-level and simultaneously justified from a "microscopical"-level by

higher-gradient-type regularizations. This concerns e.g. models of shape-memory alloys on microscopical level in [1] limited to mesoscopical level [3, 6, 7].

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References

[1] M.Arndt, M.Griebel, T.Roubíček: Modelling and numerical simulation of martensitic transformation in shape memory alloys. *Continuum Mech. Thermodyn.* **15** (2003), 463-485.
[2] S.Bartels, A.Mielke, T.Roubíček: Small-strain plasticity in the limit of vanishing hardening. In preparation.
[3] B.Benešová: Modeling of shape-memory alloys on the mesoscopic level. In: Proc. Conf. *ESOMAT, Prague, 2009*, P.Šittner et al. (Eds.), EDP Sciences, , 03003,pp1-7, 2009.
[4] G.Bouchitté, A.Mielke, T.Roubíček: A complete damage problem at small strains. *Zeitschrift angew. Math. Phys.* **60** (2009), 205-236.
[5] M.Kočvara, A.Mielke, T.Roubíček: A rate-independent approach to the delamination problem. *Math. and Mech. of Solids* **11** (2006), 423-447.
[6] M.Kružík, A.Mielke, T.Roubíček: Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in CuAlNi. *Meccanica* **40** (2005), 389-418.
[7] A.Mielke, T.Roubíček: A rate-independent model for inelastic behavior of shape-memory alloys. *Multiscale Modeling and Simulation* **1** (2003), 571-597.
[8] A.Mielke, T.Roubíček: Numerical approaches to rate-independent processes and applications in inelasticity. *Math. Modelling Numer.Anal.* **43** (2009), 395-428.
[9] A.Mielke, T.Roubíček, U.Stefanelli: Γ-limits and relaxations for rate-independent evolutionary problems. *Calc. Var. P.D.E.* **31** (2008), 387-416.
[10] A.Mielke, T.Roubíček, M.Thomas: From damage to delamination in nonlinearly elastic materials at small strain. In preparation.
[11] A.Mielke, T.Roubíček, J.Zeman: Complete damage in elastic and viscoelastic media and its energetics. *Comp. Methods Appl. Mech. Engr.* **199** (2010), 1242–1253
[12] A.Mielke, F.Theil: On rate-independent hysteresis models. *Nonlin. Diff. Eq. Appl.* **11** (2004) 151–189 (Accepted July 2001).
[13] A.Mielke, F.Theil, V.I.Levitas: A variational formulation of rate-independent phase transformations using an extremum principle. *Archive Rat. Mech. Anal.* **162** (2002) 137–177.
[14] T.Roubíček, L.Scardia, C.Zanini: Quasistatic delamination problem. *Continuum Mech. Thermodynam.*, **21** (2009), 223-235.

Continuum and discrete dynamic models with high contrast via "non-classical" homogenization

Valery P. Smyshlyaev

Classical homogenization when specialized to dynamic problems corresponds to a low frequency regime, where the wavelength is much larger than the size of the heterogeneity. Taking as an example linear elastic matrix-inclusion periodic composite with uniformly positive and uniformly bounded (in other words, moderately contrasting) elasticity tensors and densities, the resulting homogenized equations are well known to describe waves in an "effective" uniform medium retaining all the "classical" properties (the uniform positivity, symmetry of the elasticity tensor, etc). Such a classical effective medium hence propagates waves of any frequency in any direction, with appropriate speeds and polarizations (generally three, in three

dimensions). Classical homogenization is hence intrinsically incapable of accounting for such effects as dispersion and localization due to the micro-heterogeneity (in particular due to the so-called "micro-resonances"). Remark that the classical homogenization has numerous variants, for linear and nonlinear, vector and scalar, (non-)periodic and stochastic, continuum and discrete models, with the common feature being a uniform ellipticity and boundedness (i.e. non-degeneracy) which ensures the compactness properties for the solutions $u^\varepsilon(x,t)$ as $\varepsilon \to 0$ and their ultimate (weak) convergence to homogenized solutions $u_0(x,t)$.

One way to account further for the effect of the heterogeneity on dynamics, still within the low-frequency regime, is to incorporate higher order terms into the homogenization, i.e. to seek correctors to the homogenized equation with respect to the small parameter ε which is in this context the ratio of the heterogeneity (e.g. the size of the periodicity cell) and the wavelength (say in the matrix). One way for achieving this was proposed (in a static context) in our earlier work [1] via a hybrid of two-scale asymptotic and variational approaches, which resulted in a well-posed higher-order in ε homogenized equation with higher-order error bounds obtained. The higher-order terms display the dependence on higher derivatives of the macroscopic strain, consistently with phenomenologically used "strain-gradient" models (we refer to our earlier work [2] and further references therein for homogenization of such models). This was extended to some nonlinear regimes [3] and to the "beyond all orders" (exponential) homogenization [4].

Allowing higher contrasts in the components' properties extends dramatically the range of the effects observed via developing an appropriate version of a "non-classical" homogenization. Consider e.g. the case when the densities are comparable but the inclusion is considerably softer than the matrix, with the underlying small parameter of the contrast δ (which is crudely the ratio of the stiffnesses). Because of the high contrast, the same frequency would generate highly contrasting wavelengths λ_I and λ_M in the inclusions and the matrix respectively (in fact, $\lambda_I/\lambda_M \sim \delta^{1/2}$). Hence, increasing the frequency (equivalently, decreasing the wavelengths) from "very low" up we eventually reach such a regime when the wavelength in the matrix is still much larger than the periodicity size (i.e.. still a "low frequency" regime for an observer in the matrix), while the wavelength in the inclusions already becomes comparable to the size of the inclusion (equivalently, the "resonance" regime). Selecting the macroscale ("order one") comparable to λ_M, corresponds to $\varepsilon \sim \lambda_I/\lambda_M \sim \delta^{1/2}$, or $\delta \sim \varepsilon^2$, which is a "critical" scaling extensively studied in the literature (sometimes called "double porosity"-type scaling, for its appearance in models of flow in fractured porous rocks).

Setting $\delta = \varepsilon^2$ one observes that, asymptotically for $\varepsilon \to 0$, the solution $u^\varepsilon(x,t)$ retains (although in the inclusion only) the dependence on the "fast" variable, i.e.

$$u^\varepsilon(x,t) \sim \begin{cases} u_0(x,t) & \text{in matrix} \\ u_0(x,t) + v(x,x/\varepsilon,t) & \text{in inclusion,} \end{cases}$$

where $v(x,y,t)$ is periodic in the "microscopic variable" y, being supported on the inclusion and vanishing on its boundary. One then ends up with (u_0, v) solving

a coupled "two-scale" limit problem, see [10] and further references therein. The limit problem allows an equivalent (two-scale) variational formulation with a corresponding well-defined two-scale self-adjoint limit operator, having an explicitly described limit spectrum displaying (upon an uncoupling) a band-gap structure. The convergence is rigorously established by means of two-scale spectral and operator convergence and associated (two-scale) compactness, cf. [11, 12]. The uncoupling of the limit problem in the frequency domain displays highly nonlinear dependence of the macroscopic solution on the spectral parameter (i.e. the frequency). This gives rise to both the band-gap effect (the presence of ranges of frequencies for which waves fail to propagate i.e. stay localized, see e.g. [7, 8] with analysis of localized modes emerging due to defects in high-contrast periodic media) and high dispersion in the bands (close to their right ends, i.e. the eigenfrequencies of the inclusions or "micro-resonances", see [9]). An effect of high contrasts not only in frequency but also in density is addressed in [13], and the effect of nonlinearity (including non-convexity) is studied in detail in [14] in the context of variational (static) problems. One can consider similar high-contrast discrete models, with (in particular) a hybrid two-scale limit system: a continuum homogenized matrix coupled to discrete microresonances in the "inclusions".

If the uncoupling is done in the time domain rather than in the frequency domain, the nonlinear dependence on frequency translates (e.g. via the Laplace transform) into the time-nonlocality, i.e. to the well-known memory effect via homogenization. (See also e.g. [5] for other instances of the memory effect via homogenization.) Analogous *spatial* nonlocality was observed and analyzed in [6] in the case of highly anisotropic fibers. By analogy with the temporal nonlocality linked to the dispersion and band-gap effect in the frequency domain, one can expect a link of the spatial nonlocality to similar effects on the wavevectors (since the wavevector is a Fourier dual of the spatial variable just as the frequency is the Fourier dual of the time). This was explored to some extent in [10], and indeed an effect of a "directional localization" could be observed this way: certain frequency ranges fail propagating in certain ranges of directions while can propagate in other directional ranges. It was also noticed in [10] that the case of highly anisotropic fibers considered in [6] could be regarded as a particular case of a *"partial" degeneracy* (of the stiffness tensor, in the context of elasticity): while the fiber is "soft" in the cross-sectional directions, it remains "stiff" along the fiber. This motivates a generalization for "partially" high contrasts, see [10] for the case of inclusions with such properties. This allows viewing from a unified viewpoint the classical homogenization, the "fully" high-contrast one, and all the intermediate cases.

Mathematically, the introduction of the partially high contrast poses, in the context of a two-scale asymptotic analysis, an interesting challenge of accounting for the microscopically partially constrained kinematics coupled to the macroscopic fields. This requires appropriately modifying the two-scale convergence technique and results in the two-scale effective equations explicitly involving projectors accounting for the kinematic constraints. A more systematic study of related general mathematical constructions and of their rigorous analysis is performed in [15].

References

[1] V.P. Smyshlyaev, K.D. Cherednichenko, *On rigorous derivation of strain gradient effects in the overall behaviour of periodic heterogeneous media*, J. Mech. Phys. Solids **48** (2000), 1325–1357.

[2] V.P. Smyshlyaev, N.A. Fleck, *The role of strain gradients in the grain size effect for polycrystals*, J. Mech. Phys. Solids **44** (1996), 465–495.

[3] K.D. Cherednichenko, V.P. Smyshlyaev, *On full two-scale expansion of the solutions of nonlinear periodic rapidly oscillating problems and higher-order homogenised variational problems*, Arch. Rat. Mech. Anal **174** (2004), 385–442.

[4] V. Kamotski, K. Matthies and V.P. Smyshlyaev, *Exponential homogenisation of linear second order elliptic PDEs with periodic coefficients* SIAM J. Math. Anal. **38** (2007), 1565–1587.

[5] Z. Abdessamad, I. Kostin, G. Panasenko, V.P. Smyshlyaev, *Memory effect in homogenization of viscoelastic Kelvin-Voigt model with time dependent coefficients*, Math. Models Meth. Appl. Sci. **19** (2009), 1603–1630.

[6] K.D. Cherednichenko, V.P. Smyshlyaev, V.V. Zhikov, *Non-local homogenised limits for composite media with highly anisotropic periodic fibres*, Proc. R. Soc. Edinb **136** (2006), 87–114.

[7] I.V. Kamotski, V.P. Smyshlyaev, *Localised eigenstates due to defects in high contrast periodic media via homogenisation*, Preprint (2006), http://www.bath.ac.uk/math-sci/bics/preprints/BICS06_3.pdf

[8] M. Cherdantsev, *Spectral convergence for high-contrast elliptic periodic problems with a defect via homogenization*, Mathematika **55** (2009), 29–57.

[9] V.P. Smyshlyaev, P. Kuchment, *Slowing down and transmission of waves in high contrast periodic media via non-classical homogenization*, Waves 2007 Proceedings, 200–202.

[10] V.P. Smyshlyaev, *Propagation and localization of elastic waves in highly anisotropic composites via homogenization*, Mechanics of Materials **41** (2009), 434–447.

[11] V.V. Zhikov, *On an extension and an application of the two-scale convergence method*, Sbornik Math. **191** (2000), 973–1014.

[12] V.V. Zhikov, *Gaps in the spectrum of some elliptic operators in divergent form with periodic coefficients* (in Russian), Algebra Anal. **16** (2004), 34–58. English transl.: St. Petersburg Math. J. **16** (2005), 773–790.

[13] N.O. Babych, I.V. Kamotski, V.P. Smyshlyaev, *Homogenization in periodic media with doubly high contrasts*, Networks and Heterogeneous Media, **3** (2008), 413–436.

[14] M. Cherdantsev, K.D. Cherednichenko, *Two-scale Gamma-convergence and its application to homogenisation of high-contrast variational integrals*, Preprint (2010).

[15] I.V. Kamotski, V.P. Smyshlyaev, *Homogenization of degenerate PDEs and applications to localization of waves*, in preparation (2010).

The Time-Dependent von Kármán Plate Equation as a Limit of 3d Nonlinear Elastodynamics

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(joint work with Helmut Abels and Stefan Müller)

The present contribution concerns the rigorous derivation of two-dimensional dynamic models for a thin elastic plate starting from three-dimensional nonlinear elastodynamics. Let $\Omega_h = \Omega' \times (-\frac{h}{2}, \frac{h}{2})$ be the reference configuration of a thin plate, where $\Omega' \subset \mathbb{R}^2$ is a bounded Lipschitz domain and $h > 0$. The plate is

made of a hyperelastic material whose energy potential $W\colon \mathbb{R}^{3\times 3} \to [0,+\infty]$ is continuous and satisfies the following natural conditions:

(1) $W(RF) = W(F)$ for every $R \in SO(3), F \in \mathbb{R}^{3\times 3}$ (frame indifference),

(2) $W = 0$ on $SO(3)$, $W(F) \geq C\,\mathrm{dist}^2(F, SO(3))$, $C > 0$,

(3) W is smooth in a neighbourhood of $SO(3)$.

The dynamic equation of nonlinear elasticity reads as

$$\partial_\tau^2 w - \mathrm{div}_x DW(\nabla w) = f^h \quad \text{in } [0,\tau_h]\times\Omega_h, \tag{4}$$

where $w\colon [0,\tau_h]\times\Omega_h \to \mathbb{R}^3$ is the deformation of the plate and $f^h\colon [0,\tau_h]\times\Omega_h \to \mathbb{R}^3$ is an external body force applied to the plate. We focus on the case where $f^h(\tau,x) = h^\alpha f(\tau,x')e_3$, where $\alpha \geq 3$ and $f \in L^2((0,+\infty);L^2(\Omega'))$.

Let w^h be a solution to (4) on $[0,\tau_h]\times\Omega_h$. To discuss its limiting behaviour as $h \to 0$, it is convenient to rescale Ω_h to the fixed domain $\Omega = \Omega'\times(-\frac{1}{2},\frac{1}{2})$ and to rescale time by setting $t = h\tau$. According to this change of variables, we set

$$y^h(t,x) := w^h\big(\tfrac{t}{h},(x',hx_3)\big)$$

for every $(t,x) \in (0,T_h)\times\Omega$, where $T_h := h\tau_h$. Using the notation

$$\nabla_h\psi := \big(\nabla'\psi \,|\, \tfrac{1}{h}\partial_3\psi\big), \quad \mathrm{div}_h\Phi := \mathrm{div}'\Phi' + \tfrac{1}{h}\partial_3\Phi_3$$

for any $\psi \in H^1(\Omega)$, $\Phi \in H^1(\Omega;\mathbb{R}^{3\times 3})$, the scaled deformations y^h satisfy

$$h^2\partial_t^2 y^h - \mathrm{div}_h DW(\nabla_h y^h) = h^\alpha g e_3 \quad \text{in } (0,T_h)\times\Omega, \tag{5}$$

where $g(t,x') := f\big(\frac{t}{h},x'\big)$ for every $(t,x) \in (0,+\infty)\times\Omega'$. We also assume that the following initial conditions hold:

$$y^h|_{t=0} = \bar{w}^h, \qquad \partial_t y^h|_{t=0} = \tfrac{1}{h}\hat{w}^h \tag{6}$$

together with the mixed Neumann–clamped boundary conditions

$$y^h|_{\partial\Omega'\times(-\frac{1}{2},\frac{1}{2})} = \begin{pmatrix} x' \\ hx_3 \end{pmatrix}, \qquad DW(\nabla_h y^h)e_3\big|_{x_3=\pm\frac{1}{2}} = 0, \tag{7}$$

or, assuming $\Omega' = (-L,L)^2$, the mixed Neumann–periodic boundary conditions

$$\begin{gathered} \Big(y^h(t,x) - \begin{pmatrix} x' \\ hx_3 \end{pmatrix}\Big)\Big|_{x_\alpha=-L} = \Big(y^h(t,x) - \begin{pmatrix} x' \\ hx_3 \end{pmatrix}\Big)\Big|_{x_\alpha=L} \quad \alpha = 1,2, \\ DW(\nabla_h y^h)e_3\big|_{x_3=\pm\frac{1}{2}} = 0. \end{gathered} \tag{8}$$

If $\alpha > 3$, we prove that, under suitable regularity assumptions on g and appropriate scaling and regularity of the initial data $\bar{w}^h$, $\hat{w}^h$, for every $T > 0$ there exists $h_0 > 0$ such that for every $h \in (0,h_0)$ equation (5), supplemented by the initial conditions (6) and the boundary conditions (8), has a unique strong solution defined on $[0,T]$. If $\alpha = 3$, assuming in addition that g and the initial data are small enough, we show that (5), supplemented by (6) and (8), has a unique strong solution on $[0,T]$ for every $h \in (0,1)$ ([1, Theorem 3.1]).

Assuming that W is differentiable with Lipschitz continuous derivative and that

$$\tfrac{1}{2}\int_\Omega |\hat{w}^h|^2\,dx + \int_\Omega W(\nabla_h \bar{w}^h)\,dx \le Ch^{2\alpha-2}, \tag{9}$$

we prove ([2, Theorem 2.1]) that, if y^h is a weak solution to (5) on $[0,T]$, satisfying (6), the boundary conditions (7) or (8), and the energy inequality, then $y^h \to (x',0)$ in $L^\infty([0,T];H^1(\Omega;\mathbb{R}^3))$. Moreover, the in-plane and out-of-plane displacements

$$u^h(t,x') := \frac{1}{h^{\alpha-1}}\int_{-\frac{1}{2}}^{\frac{1}{2}} \big((y^h)' - x'\big)\,dx_3, \qquad v^h(t,x') := \frac{1}{h^{\alpha-2}}\int_{-\frac{1}{2}}^{\frac{1}{2}} y_3^h\,dx_3$$

converge in a suitable sense to a limit displacement (u,v). If $\alpha = 3$, (u,v) is a solution to the dynamic von Kármán plate equations

$$\begin{cases} \partial_t^2 v + \frac{1}{12}\mathrm{div}\big[\mathrm{div}\mathcal{L}_2((\nabla')^2 v)\big] - \mathrm{div}\big[\mathcal{L}_2(\mathrm{sym}\nabla' u + \frac{1}{2}\nabla' v\otimes\nabla' v)\nabla' v\big] = g, \\ \mathrm{div}\big[\mathcal{L}_2(\mathrm{sym}\nabla' u + \frac{1}{2}\nabla' v\otimes\nabla' v)\big] = 0, \end{cases}$$

in $[0,T]\times\Omega'$, and satisfies the boundary conditions $u|_{\partial\Omega'} = 0$, $v|_{\partial\Omega'} = 0$, $\nabla' v|_{\partial\Omega'} = 0$, or, respectively, periodic boundary conditions, and the initial conditions $v|_{t=0} = \bar{w}_3$, $\partial_t v|_{t=0} = \hat{w}_3$. Here $\mathcal{L}_2$ is the linear form associated with the quadratic form $Q_2 : \mathbb{R}^{2\times 2} \to \mathbb{R}$ defined by $Q_2(G) = \mathcal{L}_2 G : G := \min_{F''=G} Q_3(F)$, where $Q_3(F) := D^2W(\mathrm{Id})F : F$, while F'' denotes the 2×2-submatrix of F defined by $F''_{ij} = F_{ij}$ for $1 \le i,j \le 2$. The limiting initial values $\bar{w}_3$ and $\hat{w}_3$ are the limits of suitably scaled averages of $\bar{w}_3^h$ and $\hat{w}_3^h$, whose existence is guaranteed by the scaling condition (9).

If $\alpha > 3$, the limit in-plane displacement u is equal to 0, while the out-of-plane displacement v is a solution to the dynamic linear plate equation

$$\partial_t^2 v + \tfrac{1}{12}\mathrm{div}\big[\mathrm{div}\mathcal{L}_2((\nabla')^2 v)\big] = g \qquad \text{in } [0,T]\times\Omega'$$

and satisfies the boundary conditions $v|_{\partial\Omega'} = 0$, $\nabla' v|_{\partial\Omega'} = 0$, or, respectively, periodic boundary conditions, and the initial conditions $v|_{t=0} = \bar{w}_3$, $\partial_t v|_{t=0} = \hat{w}_3$.

References

[1] H. Abels, M.G. Mora, S. Müller, *Large time existence for thin vibrating plates*, Preprint SISSA, Trieste, Italy.

[2] H. Abels, M.G. Mora, S. Müller, *The time-dependent von Kármán plate equation as a limit of 3d nonlinear elasticity*, Preprint SISSA, Trieste, Italy.

A variational approach to the Hamiltonian boundary value problem: existence and approximation

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(joint work with Hartmut Schwetlick)

We consider the conservative dynamical system

$$\frac{d^2q(t)}{\mathrm{d}t^2} = -\nabla V(q)\ , \tag{1}$$

where V is a smooth potential on $Q \subset \mathbb{R}^n$, and

$$q(0) = q_a \text{ and } q(T) = q_b \tag{2}$$

with $q_a, q_b \in Q$ and $T > 0$; we assume that the total energy E, defined as the sum of kinetic and potential energy, is fixed, so T has to be determined.

A motivation for the analysis of this problem comes from Molecular Dynamics and other problems with complex energy landscapes. For example, q_a and q_b can be different conformational states of a molecule; then the Newtonian equations of motion (1) describe the vibrations of one conformation, followed by a rapid transition to the energetic well containing the other conformation, and vibrations in that well. This example illustrates two typical difficulties: the state space Q can be high-dimensional (for example, $n \approx 400$ for relatively simple models of DNA motion); the timescale T will be very long in comparison to the temporal scale of typical vibrations.

The problem of solving (1) with periodic boundary conditions has a long history, including existence results by Seifert [5], Weinstein [6], Rabinowitz [3].

The boundary value problem (1)–(2) is less studied. An existence result with additional differential-geometric assumptions on the underlying metric is due to Gordon [2].

We present an alternative existence result, where the *a priori* estimates depend on physical quantities, notably the total energy E and the potential energy V. The method we employ resembles so-called string methods, but the particular setting we use allows us to prove the convergence of a suitable approximation.

The setting we use is that of Jacobi and Maupertuis; according to this classical principle, trajectories to (1) with total energy E are suitably re-parametrised geodesics with respect to the *Jacobi metric*

$$g_{ij}(q) := 2(E - V(q))\delta_{ij}(q) \; ; \tag{3}$$

we recall that geodesics are critical points γ of

$$L[\gamma] := \int_0^\tau \sqrt{g_{ij}(\gamma(s))\dot\gamma^i(s)\dot\gamma^j(s)}\,\mathrm{d}s \; , \tag{4}$$

where $q = q(s)$, $q(0) = q_a$, $q(\tau) = q_b$. For Jacobi's metric, this is

$$L[\gamma] := \int_0^\tau \sqrt{2(E - V(q))\,\langle \dot q, \dot q\rangle}\,\mathrm{d}s \; . \tag{5}$$

Physical time can then be recovered via the explicit formula

$$t = \int_0^\tau \sqrt{\frac{\langle \dot q, \dot q\rangle}{2(E-V)}}\,\mathrm{d}s \; . \tag{6}$$

The advantage of the variational method (5) is its elliptic nature; the existence of periodic solution is thus often studied in this setting [5, 6]. An argument going back to Birkhoff [1] can in this case provide a constructive existence proof.

We provide a similar result for the boundary value problem, but with a different focus: Given q_a and q_b, bounds can be given on the choice for E such that the

existence of a trajectory can be guaranteed. The argument uses discrete curvature bounds to obtain a neighbourhood of q_a and q_b which is invariant under a flow.

While in principle such an argument is not hard once a curvature bound yielding an invariant region is found, we choose to complicate the proof so that it yields in the end a constructive convergent approximation by line segments. Line segments are Euclidean geodesics, so it is natural to use piecewise constant approximations of the Jacobi metric (3). The computation of the length is then in principle simple. However, care has to be taken of the scaling. It can be shown that locking and other artificial effects can be avoided if three different scales are considered: one for the discretisation width ϵ_0 of polygonal approximations for γ, a finer one for the step width of the Birkhoff step and an even finer one for the computation of the length.

Unlike the continuous (original) Birkhoff step, the argument requires a grid refinement, even a sequence of refinements $\epsilon_k := 2^{-k}\epsilon_0$ (and suitable refinements of the two other scales involved). It can then be shown that the Birkhoff procedure stops on every discrete level k after finitely many steps, yielding a limit polygon γ_k. It can be shown that $\gamma_k \to \gamma \in C^{1,1}$ as $k \to \infty$, where γ is a geodesic graph.

We close by remarking that, rather than relying on a Birkhoff procedure, a parabolic flow with an artificial time can be used as a steepest descent procedure to the elliptic limit associated with (5). A numerical implementation shows that this is an efficient string method [4]; a theoretical underpinning of this flow in form of a convergence proof is however missing.

The homogenisation of this problem (that is, the computation of effective Hamiltonians for potentials V_ϵ with wiggly contributions in the limit $\epsilon \to 0$) was also mentioned as open problem in the discussion at the meeting. Also, the result presented here is deterministic. Extensions to a stochastic setting (e.g., within the Freidlin-Wentzell theory or for thermostats) are presently not available.

References

[1] G. D. Birkhoff, *Dynamical systems*. With an addendum by Jurgen Moser. American Mathematical Society Colloquium Publications, Vol. IX. American Mathematical Society, Providence, R.I. (1966).

[2] W. B. Gordon, *The existence of geodesics joining two given points*, J. Differential Geometry **9** (1974), 443–450.

[3] P. H. Rabinowitz, *Periodic solutions of Hamiltonian systems*, Comm. Pure Appl. Math. **31** (1978), 157–184.

[4] H. Schwetlick, J. Zimmer, *Calculation of long time classical trajectories: Algorithmic treatment and applications for molecular systems*, J. Chem. Phys. **130** (2009), 124106.

[5] H. Seifert, *Periodische Bewegungen mechanischer Systeme*, Math. Z. **51** (1948), 197–216.

[6] A. Weinstein, *Periodic orbits for convex Hamiltonian systems*, Ann. of Math. (2) **108** (1978), 507–518.

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