C18 Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys

A. Mielke

Requested funding

1 researcher position E13 TVöD (present funding: 1 researcher as well).

Background

Shape-memory alloys are used in medical treatments (stents, dental braces) or microelectromechanical systems (actuators, valves, mini-grippers and positioners) because of their pseudoelastic properties or the shape-memory effect. Both have their origin in microstructural phase transformations of the underlying crystallographic lattices. There exist many engineering models (see e.g., [BS96, AP02, Fré02]) for the evolution of phase transformations in solids that describe shape memory. This leads to phasefield models like those considered in the MATHEON projects C11, C14, C17, and Cf, where the phase-field vector $z = (z_1, ..., z_N)$ contains the volume fraction of each phase. The underlying quasistatic evolution is described by the equilibrium of elastic forces and the balance of internal forces:

$$0 = \mathcal{D}_u \mathcal{E}(t, u(t), z(t)), \quad 0 \in \partial_{\dot{z}} \mathcal{R}(z(t), \dot{z}(t)) + \mathcal{D}_z \mathcal{E}(t, u(t), z(t)).$$
(BE)

Here $u \in \mathcal{U}$ is the displacement, $\mathcal{E} : [0, T] \times \mathcal{U} \times \mathcal{Z} \to \mathbb{R}$ the energy functional, and \mathcal{R} the dissipation potential. Usually these models are restricted to very few phases and often the mathematics is restricted to one-dimensional or isotropic situations. However, complex multidimensional effects and anisotropies have to be taken into account for quantitative predictions in single crystals, see e.g., [Bha03]. So far, this is only understood in the static case, and there are only few mathematically acceptable models for explaining hysteresis under cyclic loading.

Since rate-independent material models are sufficiently close to the static case, they can take advantage of the well-developed techniques in the direct method of the calculus of variations, which led to the theory of *energetic solutions*, see [Mie05]. This provides a flexible basis for treating many multifunctional materials, such piezoelectricity, ferromagnetism, magnetostriction, and plasticity, see [Mie05, KMR05],[14].

References

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Highlights

The project brought two major achievements. Firstly, we generalized the theory by allowing for temperature-driven phase transformation, where temperature is treated as a given loading depending on space and time [6, 7]. Secondly, we developed a theory of Γ -convergence for rate-independent systems [10] providing a flexible framework to treat various approximation results. In particular, convergence results for finite-element approximations of phase transformation problems were established in [9],[17, 18], including quantitative convergence rate in the latter case.

Report

Project Head:

A. Mielke

Research Staff: A. Petrov (starting September 2006)

Associated Members: D. Knees

We have investigated rate-independent versions problem of (BE), where the dissipation potential $\mathcal{R}(z, \dot{z})$ is positively homogeneous of degree 1 in \dot{z} , while it is quadratic in \dot{z} in classical phase-field models. Since in nonconvex cases solutions may have jumps, one introduces the dissipation distance $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \to [0, \infty]$ associated with \mathcal{R} . Energetic solutions $(u, z) : [0, T] \to \mathcal{U} \times \mathcal{Z}$ satisfy the global stability condition (S) and the total energy balance (E):

$$\mathcal{E}(t, u(t), z(t)) \le \mathcal{E}(t, \tilde{u}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \text{ for all } (\tilde{u}, \tilde{z}) \in \mathcal{U} \times \mathcal{Z},$$
(S)

$$\mathcal{E}(t, u(t), z(t)) + \text{Diss}_{\mathcal{D}}(z, [0, t]) = \mathcal{E}(0, u(0), z(0)) + \int_{0}^{t} \partial_{s} \mathcal{E}(s, u(s), z(s)) \,\mathrm{d}s.$$
(E)

This formulation was introduced as the natural limit for solutions of the *incremental* minimization problems (where $\tau > 0$ is the time step):

$$(u_k, z_k)$$
 minimizes $\mathcal{E}(k\tau, \cdot, \cdot) + \mathcal{D}(z_{k-1}, \cdot)$ over $\mathcal{U} \times \mathcal{Z}$. (IMP) ^{τ}

The major advantage of the energetic approach is that we do not need to assume smoothness in z. Thus, precise crystallographic information of shape-memory single crystals can be included, while the properties of phase mixtures can be obtained by quasiconvexification or modeling, see [GMH02], and [6],[17].

The results obtained in the reporting period fall into three overlapping areas.

• Modeling of Temperature-Induced Phase Transformations. The shape-memory effect is usually associated to the hysteretic behavior of the elastic deformation during thermal cycles. As it is done for many engineering applications, one can assume that the time-dependent temperature distribution of a body is prescribed via given heat sources (usually electrical heating). Hence, the temperature θ acts only as given loading in $\mathcal{E}(t, u, z) = \int_{\Omega} W(e(u), z, \theta_{appl}(t, x)) dx$. Such cases occur in practical applications, if each point in the body is sufficiently close to the surface, which allows immediate heat exchange with the environment. In [6, 7],[17] the energetic formulation was adapted to such cases under quite general conditions, including finite-strain elasticity.

• Γ -Limits and Numerical Convergence of Space-Time Discretizations. A general theory of Γ -limits for rate-independent processes was developed in [10] and applied to homogenization in elastoplasticity in [11]. For space-time discretized incremental problems $(IMP)_h^{\tau}$, where $\mathcal{U} \times \mathcal{Z}$ is replaced by a finite-element subspace $\mathcal{U}_h \times \mathcal{Z}_h$, one obtains approximants $(\bar{u}^{\tau,h}, \bar{z}^{\tau,h}) : [0,T] \to \mathcal{U}_h \times \mathcal{Z}_h$. In [9], [17, 19] the convergence of these approximations is established. Because of nonuniqueness one cannot hope to prove convergence of the full sequence. However, the set of approximants is precompact (giving a weak form of 'numerical stability'), and any limit of a converging subsequence is a solution of the continuous problem (giving a weak form of 'numerical consistency'). Because of the fully implicit nature of $(IMP)_h^{\tau}$ there are no restrictions on the length of the time step τ in terms of h.

For the Souza-Auricchio model [AP02], where \mathcal{E} is uniformly convex and smooth, the results from above were improved considerably. In [2] we showed that $(IMP)_h^{\tau}$ has unique solutions which converge to the desired continuous limits. More recently, we established the explicit error estimates

 $\|(\bar{u}^{\tau,h}(t), \bar{z}^{\tau,h}(t)) - (u(t), z(t))\|_{\mathcal{U} \times \mathcal{Z}} \le C(h^{\beta/2} + \tau^{1/2}) \text{ for } t \in [0,T],$

where the exponent $\beta \in (0, 1]$ is determined by the higher-order regularity of the static problem only, see [15],[18]. This seems to be the first rigorous error estimate for rateindependent evolution that does not need additional assumptions on the smoothness of the solutions to be approximated.

• Models Including Rate-Dependent Effects. Since rate independence is an idealization, we investigated how rate-independent models occur as limits of rate-dependent ones. For shape-memory materials such results are not yet available, but the following results in related fields are promising. In [5, 8, 12] dynamic elasto-visco-plastic models were investigated in the limit of a vanishing loading rate. In [13] a damped viscoelastic wave equation with an obstacle is studied. A nonconvex coupling between rate-independent damage and viscoelasticity was treated in [19]. In [3, 4] the vanishing-viscosity approach was used to obtain the rate-independent limit of crack propagation.

Research program for next funding period

The theory of fully rate-independent systems and its application to models for multifunctional materials is now developed fairly well.

Numerical Analysis and Software Development. For practical applications it is now desirable to develop a software tool, which can be used to test the different modeling options and to compare the model predictions with experimental data. Hence, the first major task of the new period will be to finish the software that we develop since late 2008. At the beginning we will start with the well-established Souza-Auricchio model [AP02] and provide a simulation of a small benchmark for a micro-valve. The key problem in the numerical algorithm is the effective calculation of the minimizers in the space-time discretized minimization problem $(IMP)^{\tau,h}$. Because of the inherent nonsmoothness of rate-independent problems one needs to apply nonsmooth Newton methods, where we will use the expertise of C13 and C17. First theoretical investigations show that this should work nicely for the convex Souza-Auricchio model. However, for more general single-crystal problems one has to expect local minimizers and indefinite second derivatives. Thus, more advanced techniques are needed, and we plan to use a technique involving viscous regularization. For the latter one still needs to investigate how the viscosity should be chosen in dependence of the spatial discretization.

Improvement of the models for shape-memory materials. In a next step we have to improve the modeling class to allow for direct comparison with experiments and to make it usable in practical applications. Here we have to push forward the theoretical understanding, the numerical analysis as well as the software development. The following features have to be addressed:

- treatment of the anisotropy of the phases possibly with different elastic constants;
- derivation of suitable models for the effective energy of mixed phases (cf. [GMH02]) via upper and lower bounds of the cross-quasiconvexification,
- coupling to a full energy balance including heat conduction;
- provide a theoretical basis for the vanishing-viscosity approach in the context of phase transformations;
- introducing other rate-dependent effects such as kinetic terms and interior relaxation mechanisms like viscoplastic effects;
- develop corresponding models for single-crystals and poly-crystals.

The last topic is related to a cooperation with ICM Warsaw, where the influence of grain boundary movement and reorientation is investigated.

Models including other effects. Recent experimental evidence shows that martensitic phase transformations in steel occur in most cases in combination with plastic effects. Such materials are called TWIP steels (for TWinning Induced Plasticity). Since the twinning and the plastic flow can be modeled as rate-independent processes, we want to apply our expertise in this novel field to derive suitable models for such materials and to include these models into our simulation tool.

Software

Based on the MATLAB program [CK02] we started to develop a software tool for simulating the behavior of shape-memory materials. First results are expected in 2009, and a general version should be available in the middle of the next period.

Cooperation

Internal MATHEON cooperation The projects has common interests with project C13, where the numerical solution of nonsmooth and nonconvex minimization problems is

studied using adaptive finite-element methods. These methods and the converge theory is needed in for the longterm goal of establishing a software tool.

We plan to use the numerical schemes developed in C17 involving a nonsmooth Newton methods for solving the time-incremental problem $(IMP)^{\tau,h}$.

Project Cf (Knees-Kraus, damage evolution) will use similar modeling techniques and we will cooperate on models having rate-independent as well as viscous dissipation.

Cooperation with ICM Warsaw Recently a cooperation with a group at the ICM in Warsaw (M. Gokieli, P. Rybka) was started to model polycrystalline effects, in particular the influences of grain boundaries and their movement.

External cooperation The project has strong cooperations within the *mathematical community*: G. Francfort (Paris), A. Garroni (Roma), L. Paoli (Saint-Etienne), T. Roubíček (Praha), M. Schatzman (Lyon), U. Stefanelli (Pavia). Applications are done together with *engineers* and *material scientists*: F. Auricchio (Pavia), S. Govindjee (Berkeley), K. Hackl (Bochum), P. Šittner (Praha), J. Zeman (Praha).

External funding

Public funding A. Mielke was granted the Project *Regularizations and relaxations of time-continuous problems in plasticity* within the DFG Research Unit FOR 797 "Analysis and computation of microstructure in finite plasticity" (one PostDoc for 2007-2010, possible extension to 2013).

D. Knees (together with Ch. Kraus) was granted the Project *Modellierung von Schädigungsprozessen* within "Wettbewerb der Leibniz-Gemeinschaft" (two PreDocs and one PostDoc for 2009-2011).

Publications related to the project

Books

 R. Helmig, A. Mielke, and B.I. Wohlmuth, editors. Multifield Problems in Solid and Fluid Mechanics, volume 28 of Lecture Notes in Applied and Computational Mechanics. Springer-Verlag, Berlin, 2006.

Refereed publications

- [2] F. Auricchio, A. Mielke, and U. Stefanelli. A rate-independent model for the isothermal quasistatic evolution of shape-memory materials. M³AS Math. Models Meth. Appl. Sci., 18(1):125– 164, 2008.
- [3] D. Knees, A. Mielke, and C. Zanini. On the inviscid limit of a model for crack propagation. M³AS Math. Models Meth. Appl. Sci., 18:1529–1569, 2008.
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- [6] A. Mielke. A model for temperature-induced phase transformations in finite-strain elasticity. IMA J. Applied Math., 72:644–658, 2007.
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- [9] A. Mielke and T. Roubíček. Numerical approaches to rate-independent processes and applications in inelasticity. *Math. Model. Numer. Anal.*, 2009. In press. WIAS Preprint 1169.
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- [11] A. Mielke and A.M. Timofte. Modeling and analytical study for ferroelectric materials. Mech. Advanced Materials Structures, 13:457–462, 2006.
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- [13] A. Petrov and M. Schatzman. Mathematical results on existence for viscoelastodynamic problems with unilateral constraints. SIAM J. Appl. Anal, 40(5):1882–1904, 2009.

Proceedings

[14] A. Mielke. A mathematical framework for generalized standard materials in the rateindependent case. In R. Helmig, A. Mielke, and B.I. Wohlmuth, editors, *Multifield Problems* in Solid and Fluid Mechanics, volume 28 of Lecture Notes in Applied and Computational Mechanics, pages 351–379. Springer-Verlag, Berlin, 2006. WIAS Preprint 1123.

- [15] A. Mielke, L. Paoli, A. Petrov, and U. Stefanelli. Error control for space-time discretizations of a 3D model for shape-memory materials. In K. Hackl, editor, *Proceedings of IUTAM Symposium* on Variational Methods in Mechanics. Springer, 2009. In press.
- [16] A. Petrov. Thermally driven phase transformation in shape-memory alloys. In G. Dal Maso, G. Francfort, A. Mielke, and T. Roubíček, editors, *Oberwolfach Reports*, volume 11, pages 605–607, Oberwolfach, 2007.

Submitted articles

- [17] A. Mielke, L. Paoli, and A. Petrov. On existence and approximation for a 3D model of thermallyinduced phase transformations in shape-memory alloys. *SIAM J. Math. Anal.*, 2009. Submitted. WIAS preprint 1330.
- [18] A. Mielke, L. Paoli, A. Petrov, and U. Stefanelli. Error estimates for space-time discretizations of a rate-independent variational inequality. *SIAM J. Numer. Anal.*, 2009. Submitted. WIAS preprint 1405.
- [19] A. Mielke, T. Roubíček, and J. Zeman. Complete damage in elastic and viscoelastic media and its energetics. *Comput. Methods Appl. Mech. Engrg.*, 2008. Submitted. WIAS preprint 1285.

Talks

Invited and Plenary Talks

A. Mielke

09/26/2008: Construction of solutions for finite-strain plasticity with gradient regularization, IU-TAM Symposium on Variational Concepts with Applications to the Mechanics of Materials. September 22–26, 2008, Bochum, Germany.

09/22/2008: Global energetic solutions for finite-strain plasticity, ISIMM Meeting STAMM XVI: Symposium on Trends in Applications of Mathematics to Mechanics. September 21–24, 2008, Università degli Studi di Trento, Centro Internazional per la Ricerca Matematica, Levico, Italy.

06/21/2008: Lie groups in plasticity at finite strains, Workshop "Applied Dynamics and Geometric Mechanics". July 21–25, Mathematisches Forschungsinstitut, Oberwolfach, Germany.

03/03/2008: Analysis of rate-independent material models (4 lectures), Nečas Center for Mathematical Modeling, Charles University Praha, Czech Republic.

02/21/2008: Modeling of multifunctional materials: how to describe evolving microstructures in solids, Workshop on "Mathematics for Key Technologies and Innovation". February 21–22, 2008, Warsaw, Poland.

01/17/2008: Numerical approaches to rate-independent material models, IUTAM Symposium on Theoretical, Modeling and Computational Aspects of Inelastic Media. January 13–18, 2008, Cape Town, South Africa.

11/17/2007: Global existence for rate-independent gradient plasticity at finite strain, Workshop on Rate-Independence, Homogenization and Multiscaling. November 15–17, 2007, Centro di Ricerca Matematica Ennio De Giorgi, Pisa, Italy.

10/27/2007: Modeling of hysteresis in shape-memory alloys via microstructure evolution, European Conference on Smart Systems. October 26–28, 2006, Roma, Italy.

10/02/2007: Modeling of rate-independent hysteresis effects in materials (4 lectures), Workshop on Structures of the mechanics of complex bodies. October 1–6, 2007, Centro di Ricerca Matematica Ennio De Giorgi, Pisa, Italy.

04/19/2007: On the energetic formulation of rate-independent processes and applications, 6th MUL-TIMAT meeting. April 19–21, 2007, Academy of Sciences of the Czech Republic, Praha, Czech Republic.

06/20/2006: Gamma convergence for evolutionary problems, Workshop "Applications of Asymptotic Analysis". June 18–24, 2006, Mathematisches Forschungsinstitut Oberwolfach, Germany.

A. Petrov

09/24/2008: Error estimates for space-time discretizations of a 3D model for shape-memory materials, IUTAM Symposium on Variational Concepts with Applications to the Mechanics of Materials. September 22–26, 2008, Bochum, Germany.

02/26/2007: Thermally driven phase transformation in shape-memory alloys, Workshop "Analysis and Numerics of Rate-Independent Processes". February 26–March 2, 2007, Mathematisches Forschungsinstitut Oberwolfach, Germany.

Contributed Talks

D. Knees

04/01/2008: On the inviscid limit of a model for crack propagation, 79th Annual Meeting of GAMM. March 31–April 4, 2008, Bremen, Germany.

A. Mielke

02/10/2009: BV solutions and parametrized solutions for rate-independent systems, 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics. February 9–13, 2009, Gdańsk, Poland.

04/21/2008: Multiscale modeling for shape-memory alloys: How to describe evolving microstructures in solids, Graduate School Seminar, Aachen Institute for Advanced Study in Computational Engineering Science, Aachen, Germany.

04/02/2008: Wiggly energy landscapes and the origin of rate-independent friction, 79th Annual Meeting of GAMM. March 31–4 April, 2008, Bremen.

01/25/2008: Rate-independent pseudo-elasticity as vanishing-viscosity limit for a chain with random, 7th GAMM Seminar on Microstructures. January 25–26, 2008, Bochum, Germany.

10/2007: Gamma convergence for evolutionary problems (4 lectures), Autumn School "Analysis of Multiphase Problems". October 8–12, 2007, Nečas Center for Mathematical Modeling and Institute of Information Theory and Automation, Praha, Czech Republic.

10/05/2007: Gamma convergence and relaxation of rate-independent material models, International Conference on Multifield Problems, Minisymposium on Material Modeling and Multiscale Problems. October 4–6, 2006, Stuttgart, Germany.

07/18/2007: Existence of energetic solutions in finite-strain plasticity, 6th International Congress on Industrial and Applied Mathematics (ICIAM), Minisymposium "Mathematical Aspects of Material Science". July 16–20, 2007, ETH Zürich and University of Zürich, Switzerland.

06/21/2007: Local versus global stability in rate-independent processes, Joint International Meeting UMI-DMV, Minisymposium "Phase transitions and hysteresis in free boundary problems". June 18–22, 2007, Università degli Studi di Perugia, Dipartimento di Matematica e Informatica, Italy.

09/08/2006: Evolution of microstructures in shape-memory alloys, Polish-German Workshop "Modeling Structure Formation". Interdisciplinary Center for Mathematical and Computational Modeling, Warsaw, Poland.

07/07/2006: Multiple scales and Gamma limits in rate-independent material models, Berlin-Leipzig Seminar on Analysis and Probability Theory, University of Leipzig, Germany.

A. Petrov

02/10/2009: On existence for viscoelastodynamic problems with unilateral boundary conditions, 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics. February 9–13, 2009, Gdańsk, Poland.

01/17/2009: On the error estimates for space-time discretizations of rate-independent processes, 8th GAMM Seminar Microstructures "Theoritical, Computational and Experimental Aspects". January 16–17, 2009, Regensburg, Germany.

04/01/2008: Existence and approximation for 3D model of thermally-induced phase transformations in shape-memory alloys, 79th Annual Meeting of the International Association of Applied Mathematics and Mechanics. March 31–April 4, 2008, Bremen, Germany.

03/17/2008: Some mathematical results for a 3D model of thermally-induced phase transformations in shape-memory alloys, Workshop MATHEON-ICM Workshop on Free Boundaries and Material Modeling. March 17–18, 2008, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany.

07/18/2007: On the convergence for kinetic variational inequality to quasi-static variational inequality with application to elastic-plastic systems with hardening, 6th International Congress on Industrial and Applied Mathematics (ICIAM). July 16–20, 2007, ETH Zürich and University of Zürich, Switzerland.

10/27/2008: Mathematical results on the stability of quasi-static paths of elastic-plastic systems with hardening, European Conference on Smart Systems. October 26–28, 2006, Roma, Italy.

Outreach

December 6, 2008: Project C18, contributed to the MATHEON-Adventskalender.

June 2008: Differential, energetic and metric formulations for rate-independent processes, A. Mielke was invited to give a series of 6 lectures in the context of a course entitled Nonlinear PDEs and Applications organized by the CIME foundation in Certrao, Italy (22–28 June 2008).

03/20/2007: A. Mielke, Warum sind moderne Materialien schlau? MathInside — Mathematik (nicht nur) für Schüler. Urania, Berlin.

Jan. 2007: *Modeling and analysis of rate-independent processes*, A. Mielke was invited to give the first **Lipschitz Lecture Series** at the newly established Hausdorff-Center in Bonn (12 lectures from 8–23 January 2008).

Other Activities See also

http://www.wias-berlin.de/research-groups/pde/projects/matheonC18.html

Workshop & conference organization

- Workshop on *Microstructures in Solids*. Mathematisches Forschungsinstitut Oberwolfach March 15–19, 2010. Org.: A. Mielke and M. Ortiz.
- MATHEON–ICM Workshop on Free Boundaries and Material Modeling. WIAS Berlin, March 17–18, 2008. Organized by D. Knees, C. Kraus and A. Mielke.
- Workshop on Rate-Independence, Homogenization and Multiscaling. Centro di Ricerca Matematica Ennio De Giorgi, Pisa, Italy. November 15–17, 2007. Organized by A. Visintin and A. Mielke.
- Autumn School on Analysis of Multiphase Problems. Institute of Information The-

ory and Automation, Praha, Czech Republic. October 8–12, 2007. Organized by T. Roubíček and A. Mielke.

- Conference on Structures of the Mechanics of Complex Bodies. Centro di Ricerca Matematica Ennio De Giorgi, Pisa, Italy. October 1–7, 2007. Organized by Wing Kam Liu, P. M. Mariano, A. Mielke.
- Workshop on Analysis and Numerics for Rate-Independent Processes. Mathematisches Forschungsinstitut Oberwolfach February 25–March 3, 2007. Organized by G. Dal Maso, G. Francfort, A. Mielke and T. Roubíček.
- Sixth GAMM Seminar on Microstructure. WIAS Berlin. January 12–13, 2007. Organized by A. Mielke and S. Conti.
- Polish-German Workshop at ICM, Warszawa. September 7–8, 2006. Organized by M. Gokieli, M. Niezgodka, and A. Mielke.