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

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Research Staff: **A. Petrov**
Associated Members: **D. Knees**

Introductory Remarks

The main work on this project started in September 2006, when A. Petrov was employed as research staff in this MATHEON project.
In January 2008, D. Knees was associated to project C18.

Background of the Project

Shape-memory materials are metallic alloys having some surprising thermo-mechanical behavior, namely, strongly deformed materials regain their original shape after a thermal cycle (*shape-memory effect*). Moreover these alloys are *pseudo-elastic*, which means that they can retain an almost constant stress level over a large range of strains. These features for shape-memory alloys are not present in most of engineering materials and, thus, form the basis of innovative and commercially valuable applications. Nowadays, shape-memory materials are successfully used in many applications like for medical treatments (stents, dental braces) or in MEMS (actuators, valves, mini-grippers and positioners).

On the one hand, there exist many engineering models for phase transformations in solids (see e.g., [3, 6, 14]), which describe the principle effects but are usually restricted to very few phases and often the mathematics is restricted to one-dimensional situations. On the other hand, there is a rich mathematical literature on static problems involving microstructures (see e.g., [2, 13]). However, there are only very few models which combine the exact microscopic informations on the crystallographic level with complex hysteretic behavior of real 3D structures occurring for instance in micro-valves. For flexible isotropic models we refer to [1, 14], but the miniaturization generates the need to understand single-crystal models as well.

Here we follow the theory of energetic solutions for rate-independent material models established first in [11, 12, 4] and further developed in [10, 8, 9, 7]. This theory provides a flexible basis for incorporating many effects present in multifunctional materials, such piezoelectricity, ferromagnetism, magnetostriction, classical and twinning-induced plasticity, see [9, 25] for surveys on the applications. Moreover, the underlying models can be studied analytically by methods from the calculus of variations and hence allow for the derivation of limit models as well as for convergence analysis of numerical algorithms.

Report on the Period 09/2006–03/2008

The energetic formulation of rate-independent material models is based on two functionals, namely the stored-energy functionals $\mathcal{E}$ and the so-called dissipation distance $\mathcal{D}$. The state of the system is described by an elastic variable $u \in \mathcal{U}$ and an internal variable $z \in \mathcal{Z}$ and the classical evolution law is given as

$$\begin{array}{ll} \text{elastic equilibrium} & 0 = \mathrm{D}_u\mathcal{E}(t, u(t), z(t)), \\ \text{flow rule for internal variable} & 0 \in \partial_{\dot z}\mathcal{R}(z(t), \dot z(t)) + \mathrm{D}_z\mathcal{E}(t, u(t), z(t)). \end{array}$$

The energetic formulation is a weak form of the above system: it is given by the global stability condition (S) and the total energy balance (E):

$$\begin{array}{ll} \text{(S)} & \mathcal{E}(t, u(t), z(t)) \le \mathcal{E}(t, \widetilde{u}, \widetilde{z}) + \mathcal{D}(z(t), \widetilde{z}) \text{ for all } (\widetilde{u}, \widetilde{z}), \\ \text{(E)} & \mathcal{E}(t, u(t), z(t)) + \mathrm{Diss}_{\mathcal{D}}(z, [0, t]) = \mathcal{E}(0, u_0, z_0) + \int_0^t \partial_s\mathcal{E}(s, u(s), z(s))\,\mathrm{d}s. \end{array}$$

This formulation reflects also nicely the fact that the natural time discretization leads to the *incremental minimization problems*

$$(\mathrm{IMP})^\tau \qquad (u_k, z_k) \text{ minimizes } \mathcal{E}(k\tau, \cdot, \cdot) + \mathcal{D}(z_{k-1}, \cdot), \qquad (\tau > 0 \text{ is the time step})$$

which can be combined with space discretization as well.

The major advantage of this approach to the modeling shape-memory alloys lies in the fact that we do not need to assume smoothness in z. Hence $z(t, x)$ can be considered to lie in the Gibbs' simplex $Z = \mathrm{conv}\{e_1, ..., e_N\}$ of phase fractions. The corner e_j corresponds for to the j-th pure phase, whose well-known properties can be inserted into the model. Thus, it is possible to include all crystallographic information of single crystals. The properties of phase mixtures ($z \in Z$ not extremal) can be obtained by cross-quasiconvexification or by direct modeling, see [12, 8] and [19, 26], respectively.

The results obtained in the reporting period fall into four categories:

Modeling of Temperature-Induced Phase Transformations

The shape-memory effect is usually associated to the hysteretic behavior of the elastic deformation during thermal cycles. The energetic formulation for rate-independent systems was developed as a genuinely isothermal theory, since heat conduction is a rate-dependent effect. However, as it is done for many engineering applications, it is possible to assume that the time-dependent temperature distribution of a body can be considered as prescribed via given heat sources. In [19, 20, 26] it was shown that the energetic formulation can be used for different model classes in such cases as well.

Numerical Convergence of Space-Time Discretizations

The incremental minimization problem $(\mathrm{IMP})^\tau$ can be combined with space-discretization by simply restricting the minimization to finite-element subspaces $\mathcal{V}_h = \mathcal{U}_h \times \mathcal{Z}_h$. This will give rise to approximants $(\overline{u}^{\tau,h}, \overline{z}^{\tau,h}) : [0, T] \to \mathcal{V}_h$. In [28, 29, 26] the question of convergence of these approximations is addressed. Since in general the functional $\mathcal{E}$ need not be convex, the energetic solutions are not unique. Nevertheless it is possible to show that the set of approximants is precompact (numerical stability) and that any accumulation point (limit of a subsequence) is a solution of the continuous problem (numerical consistency). Because of the fully implicit nature of $(\mathrm{IMP})^{\tau,h}$ there are no restrictions on the length of the time step τ.

In [15] the isotropic model developed in [1, 14] was investigated. There the solutions of $(\mathrm{IMP})^\tau$ are unique and certain convergence rate estimates could be derived.

Γ-Limits and Microstructures

A general theory of Γ-limits for rate-independent processes was developed in [21]. It concerns the case that the functionals $\mathcal{E}_\varepsilon$ and $\mathcal{D}_\varepsilon$ depend on a small parameter ε. Under suitable conditions it is shown that solutions $(u_\varepsilon, z_\varepsilon)$ converge to solutions (u_0, z_0) for the Γ-limit functionals $\mathcal{E}_0$ and $\mathcal{D}_0$. This theory has applications in numerics (where $\varepsilon = h$) and in systems forming microstructure. In [17] the evolution of gradient-Young measure is studied to describe the evolution of microstructures due to formation of sequential laminates. In [29] localization phenomena in damage are treated.

Models Including Rate-Dependent Effects

Since rate-independence is an idealization it is necessary to investigate in what sense rate-independent models occur as limits of rate-dependent ones. The papers [18, 22, 27] were devoted to elasto-(visco) plastic models and established the convergence results for the solutions of kinetic evolutionary variational inequalities for limit of a vanishing loading rate. The limit is the classical rate-independent plasticity problem (with hardening).

In [23] some new mathematical results on existence for a damped wave equation with an obstacle and for full viscoelasticity are given. In [29] mainly a rate-independent model for damage was treated, however, it also provides some first considerations about the coupling of kinetic terms to nonconvex, rate-independent material behavior.

Finally, [16] uses the method of *vanishing viscosity* to approach the rate-independent limit of crack propagation from a viscous modeling. It is shown that in general the limits of viscous solutions are different from the energetic solutions, and a precise characterization is provided.

Outlook

In the following two years we want to investigate the following topics:

- So far most existence results rely on the fact that the stored-energy functional contains a regularizing term $\int_\Omega \sigma|\nabla z|^2 \,\mathrm{d}x$ with $\sigma > 0$, while for applications on the micro-scale this value is still so small that it is desirable to treat the limit $\sigma = 0$. In this case one loses compactness and it is not clear whether and who microstructure develops.
- It is important to derive conditions for uniqueness of solutions. Only then it is possible to prove convergence of the whole sequence of approximants. In turn this is necessary to obtain explicit convergence rates for space-time discretizations.
- The coupling of the rate-independent material behavior to a full energy balance including heat conduction is an important issue to widen the applicability of the theory.
- The recently started cooperation with a group at ICM Warsaw on polycrystalline effects and grain boundaries will be cocntinued.
- The structure of the incremental minimization problems $(\mathrm{IMP})^\tau$ has to be analyzed further to decide which techniques from other MATHEON projects (e.g., C13 or C17) provide effective algorithms for solving these problems, see e.g., [5].
- It is planned to develop a software tool for the simulation of MEMS.

References

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Project Statistics

Refereed Publications

[15] F. Auricchio, A. Mielke, and U. Stefanelli. A rate-independent model for the isothermal quasi-static evolution of shape-memory materials. *M^3AS Math. Models Meth. Appl. Sci.*, 18(1):125–164, 2008.

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Book Chapter and Edited Book

[24] Analysis and numerics for rate-independent processes. *Oberwolfach Rep.*, 4(1):591–665, 2007. Abstracts from the workshop held February 25–March 3, 2007, Organized by Gianni Dal Maso, Gilles Francfort, Alexander Mielke and Tomáš Roubíček.

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Submitted Articles

[26] A. Mielke, L. Paoli, and A. Petrov. On the existence and approximation for a 3D model of thermally induced phase transformations in shape-memory alloys. *SIAM J. Math. Anal.*, 2008. Submitted. WIAS preprint 1307.

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[30] A. Mielke and A. M. Timofte. Modeling and analytical study for ferroelectric materials. *Mech. Advanced Materials Structures*, 13:457–462, 2006.

Further Publications

[31] A. Mielke. A mathematical framework for generalized standard materials in the rate-independent 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.

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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.

• For certain model classes it is possible to study smooth or nonsmooth convex minimization problems with a leading order quadratic functional. For the future, it is planned to test whether in these cases the numerical schemes developed in C17 (relying on nonsmooth Newton methods) can be used efficiently.

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 Academic Cooperation

On the one hand this project has strong cooperations within the *mathematical community*: G. Francfort (Paris), A. Garroni (Roma), M. Gokieli (ICM Warszawa), M. Kružík (Praha), M.D.P. Monteiro-Marques (Lisbon), L. Paoli (Saint-Etienne), T. Roubíček (Praha), P. Rybka (Warszawa), M. Schatzman (Lyon 1), U. Stefanelli (Pavia).

On the other hand, the application side is done together with *engineers* and *material scientists*: F. Auricchio (Pavia), S. Govindjee (Zürich), K. Hackl (Bochum), P.M. Mariano (Firenze), J.A.C. Martins (Lisboa), Ch. Miehe (Stuttgart), P. Šittner (Praha), J. Zeman (Praha).

Contributed Talks

D. Knees

02/06/2008 *On global spatial regularity in elasto-plasticity, Seminar on Material Modeling*
WIAS-Materialmodellierungsseminar. WIAS Berlin

A. Mielke

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

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

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

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

A. Petrov

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

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

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

07/24/2007 *Thermally driven phase transformation in shape-memory alloys*
WIAS-Materialmodellierungsseminar. Weierstrass Institute for Applied Analysis and Stochastics, Berlin

02/26/2008 *Thermally driven phase transformation in shape-memory alloys*
Workshop "Analysis and Numerics of Rate-Independent Processes". February 26–March 2, 2007, Mathematisches Forschungsinstitut Oberwolfach

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

Invited and Plenary Talks

A. Mielke

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

02/21/2008 *Modeling of multifunctional materials: how to describe evolving microstructures in solids*
Workshop "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

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

04/19/2007 *On the energetic formulation of rate-independent processes and applications*
6th MULTIMAT meeting, Marie Curie Research Training Network. April 19–21, 2007, Institute of Physics & Mathematical Institute, Academy of Sciences of the Czech Republic, Praha, Czech Republic

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

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

Outreach

03/20/2007 *Warum sind modern Materialien schlau?* (A. Mielke)
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 Lectures** at the newly established Hausdorff-Center in Bonn. This included a series of 12 lectures (8–23. January 2008)

Awards and Grants

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 2006-2009, possible extension to 2012).

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).

Other Activities

The informations and publications mentioned in this report and some additional material are available on the following web site:
`http://www.wias-berlin.de/research-groups/pde/projects/matheonC18.html`

Workshop & conference organization

- 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 Theory 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.
- Oberwolfach Conference 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.

Guests of C18 at WIAS

- T. Roubíček, Charles University, Praha, Czech Republic. January 21–February 18, 2008.
- L. Paoli, Université de Saint-Etienne, France. January 7– February 7, 2008.
- T. Roubíček, Charles University, Praha, Czech Republic. September 6–16, 2007.
- L. Paoli, Université de Saint-Etienne, France. June 11–29, 2007.
- G. Francfort, Université de Paris-Nord, France. March 29–April 1, 2007.
- A. Garroni, Università di Roma "La Sapienza", Italy. March 29–April 1, 2007.
- T. Roubíček, Charles University, Praha, Czech Republic. January 15–February 15, 2007.
- T. Roubíček, Charles University, Praha, Czech Republic. August 21–September 21, 2006.

Guests talks in WIAS (selection of some relevant talks)

- P.M. Mariano, De Giorgi Center Pisa and Università di Firenze, Italy. *Gross scale effects of atomic rearrangements in quasicrystals: some results and open problems.* February 15, 2008.
- T. Roubíček, Charles University, Praha, Czech Republic. *Mathematical techniques for rate-independent processes.* February 6, 2008.
- L. Paoli, Université de Saint-Etienne, France. *The existence and application for 3D model of thermally-induced phase transformations in shape-memory alloys.* January 29, 2008.
- F. Cagnetti, SISSA Trieste, Italy. *A vanishing viscosity approach to fracture growth in a cohesive zone model with prescribed crack path.* September 19, 2007.
- T. Roubíček, Charles University, Praha, Czech Republic. *Rate-independent processes in viscous solids and their thermodynamics.* September 12, 2007.
- P. Neff, TU Darmstadt. August 27, 2007. Minimale Cosserat-Rotationen und Synthetische Reproduktion einer Nano-Einkerbung.
- L. Paoli, Université de Saint-Etienne, France. *Asymptotics for some vibro-impact problem with linear dissipation term.* June 13, 2007.
- T. Roubíček, Charles University, Praha, Czech Republic.
Gradient estimates for heat equation with L^1*-data and applications to thermomechanical systems.* February 7, 2007.