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

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Requested funding

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

Background

Shape-memory alloys are used in medical treatments (stents, dental braces) or micro-electromechanical systems (actuators, valves, mini-grippers and positioners) due their pseudoelastic properties or the shape-memory effect. Both have their origin in microstructural phase transformations of the underlying crystallographic lattices. Most engineering models (see e.g. [BS96, AP02, Fré02]) for the evolution of the phase transformations in solids use phase-field variable z, which may be scalar, vector or tensor-valued. The underlying quasistatic evolution is described by the equilibrium of elastic forces and the balance of internal forces:

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

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. The models in MATHEON projects C11, C14, C17, C28, and C32 also fall into this class. Usually the elastic effects are modeled only very coarsely, but for multi-dimensional models for shape-memory alloys the complex anisotropies and relations between the transformation strains have to be taken into account, 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.
Rate-independent material models are sufficiently close to the physics and have the advantage that the well-developed techniques in the calculus of variations are applicable, 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],[15].

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Highlights

In a first step we generalized the existence theory by allowing for temperature-driven phase transformation, where temperature is treated as a given loading depending on space and time [6, 8].
Secondly, we developed a theory of Γ-convergence for rate-independent systems [11] providing a flexible framework to treat various approximation results, like convergence results for finite-element methods for phase transformation problems, see [10, 7] and [18] for quantitative convergence rates.
The project head is invited to give a plenary lecture on the bi-annual SIAM Conference on *Mathematical Aspects of Materials Science* in May 2010.

Report

Project Head: A. Mielke
Research Staff: A. Petrov (starting September 2006)
Associated Member: D. Knees (up to May 2009)

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):

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

$$\mathcal{E}(t,u(t),z(t))+\mathrm{Diss}_{\mathcal{D}}(z,[0,t])=\mathcal{E}(0,u(0),z(0))+\textstyle\int_0^t\partial_s\mathcal{E}(s,u(s),z(s))\,\mathrm{d}s.\tag{E}$$

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

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

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, 7].

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 as given loading in $\mathcal{E}(t,u,z)=\int_\Omega W(e(u),z,\theta_{\mathrm{appl}}(t,x))\mathrm{d}x$. Such cases occur in practical applications, if each point in the body is sufficiently close to the surface, which allows for fast heat exchange with the environment. In [6, 8, 7] the energetic formulation was adapted to such cases under general conditions, including finite-strain elasticity.

• *Γ-Limits and Numerical Convergence of Space-Time Discretizations.* A theory of Γ-limits for rate-independent processes was developed in [11] and applied to homogenization in plasticity in [12]. For space-time discretized incremental problems $(\mathrm{IMP})_h^\tau$, 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 [10, 7], [19] the convergence of subsequences of these approximations is established, since nonuniqueness prevents convergence of the full sequence. The set of approximants is precompact (weak form of 'numerical stability'), and any limit of a converging subsequence is a solution of the continuous problem (weak form of 'numerical consistency'). The fully implicit nature of $(\mathrm{IMP})_h^\tau$ has no stability restrictions on the length of the time step τ in terms of h.
For the model in [AP02], where $\mathcal{E}$ is convex and smooth, the results from above were improved considerably. In [2] we showed that $(\mathrm{IMP})_h^\tau$ has unique solutions converging to the continuous ones. Recently, we established the explicit error estimates

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

where $\beta\in(0,1]$ is determined by the higher-order regularity of the static problem only, see [17, 18]. This is the first rigorous error estimate for rate-independent evolution that works without assuming additional smoothness for the solutions.

• *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, 9, 13], dynamic elasto-visco-plastic models were investigated in the limit of a vanishing loading rate. In [14] a damped viscoelastic wave equation with an obstacle is studied, and convergence of its numerical approximation is under investigation. A nonconvex coupling between rate-independent dam-

age 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 applications 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. 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 $(\mathrm{IMP})^{\tau,h}$. Because of the inherent nonsmoothness of rate-independent problems one needs to apply nonsmooth Newton methods, where we will use the expertise of C17 and C28. Preliminary 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 re-orientation 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 (TWinning Induced Plasticity). Since twinning and 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. Here we will use the expertise of C11.

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 C31, where the numerical solution of nonsmooth and nonconvex minimization problems is studied using adaptive finite-element methods. This and the convergence theory is needed for the longterm goal of establishing a software tool.
We plan to use the numerical schemes developed in C17 and C28 involving a nonsmooth Newton methods for solving the time-incremental problem $(\mathrm{IMP})^{\tau,h}$.

C32 (Knees/Kraus) on damage evolution will use similar modeling techniques, and we will cooperate on models having rate-independent as well as viscous dissipation.

External cooperation *Mathematics*: G. Francfort (Paris), A. Garroni (Roma), L. Paoli (Saint-Etienne), T. Roubíček (Praha), M. Schatzman (Lyon), U. Stefanelli (Pavia). *Engineering and material science*: F. Auricchio (Pavia), S. Govindjee (Berkeley), K. Hackl (Bochum), P. Šittner (Praha), J. Zeman (Praha).

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Publications related to the project

Books

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