USE OF GRADIENT POLYCONVEXITY IN THE MODELING OF RATE-INDEPENDENT EVOLUTION OF DIFFUSED PHASE IN SHAPE MEMORY ALLOYS

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1. Motivation and Background

Shape-memory alloys (SMAs) belong to the class of so-called smart materials which have wide range of important applications, especially in aerospace or mechanical engineering and human medicine. SMAs exhibit specific hysteretic stress/stain/temperature response, which is called a shape-memory effect or pseudoelasticity. The mechanism behind this behavior is connected with the so-called martensitic phase transformation; the material can exist in different phases which are separeted by a thin transition layer which stores a specific amount of interfacial energy; see e.g. [4].

Many interesting applications call for finite-strain models of SMAs which brings, however, many mathematical difficulties not presented in the small-strain regime. In particular, the constrain of local non-interpenetration of matter that involves determinant of deformation gradient and hence excludes convex or quasiconvex energies. The concept of polyconvexity, that allows for satisfactory existence theory for many hyperelastic solids, does not apply, however, for SMAs due to the presence of multiple stable phases.

One possible solution, c.f [1,2], consists in regularizing via the second gradient of deformation in which the energy is convex. This option corresponds to including interfacial energy effect that penalizes rapid spatial oscillations of deformation gradient (i.e. oscillations of phases). The resulting model falls into the class of so-called non-simple materials that, in comparison with 1st-gradient theories, allow for a wider class of possible boundary conditions; see [6].

2. Results

We consider interfacial energy of a different form, based on the concept of gradient polyconvexity, recently introduced in the context of hyperelastic materials in [3]:

Definition (Gradient Polyconvexity). *Let* $\hat{W} : \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3\times3} \times \mathbb{R}^3 \to \mathbb{R} \cup \{+\infty\}$ *be a lower semicontinuous function. The functional*

$$(1) \qquad I(y) = \int_\Omega \hat{W}(\nabla y, \nabla[\mathrm{Cof}\,\nabla y], \nabla[\det \nabla y])\,\mathrm{d}x,$$

defined for any measurable function $y : \Omega \to \mathbb{R}^3$ *for which the weak derivatives* ∇y, $\nabla[\mathrm{Cof}\,\nabla y]$, $\nabla[\det \nabla y]$ *exist and are integrable, is called* gradient polyconvex on a domain $\Omega \subset \mathbb{R}^3$ *(or* gradient polyconvex *for short) if the function* $\hat{W}(F, \cdot, \cdot)$ *is convex for every* $F \in \mathbb{R}^{3\times3}$.

Here $\hat{W}$ stands for stored energy density which is up to a multiplication by material density an isothermal restriction of Helmholtz free energy. Since determinant and cofactor measure the transformation of volumes and surfaces, respectively, the energy penalizes abrupt changes of these quantities. As opposed to the aforementioned approach that supposes coercivity of the energy in $|\nabla^2 y|^p$, for some $p \geq 1$, here only coercivity in $|\nabla[\mathrm{Cof}\,\nabla y]|^q$, for proper q, is assumed. As a consequence, the deformation y needs not to lie in Sobolev space $W^{2,p}(\Omega, \mathbb{R}^3)$. Indeed, for any $p \geq 1$ there exists a function (c.f. [3])

$$y \in W^{1,p}(\Omega; \mathbb{R}^3) \cap L^\infty(\Omega; \mathbb{R}^3) \setminus W^{2,1}(\Omega; \mathbb{R}^3)$$

such that

$$0 < \det \nabla y \in W^{1,\infty}(\Omega) \quad \text{and} \quad \operatorname{Cof} \nabla y \in W^{1,\infty}(\Omega; \mathbb{R}^{3 \times 3}).$$

Hence, the gradient polyconvexity allows for existence theory with weaker regularity assumptions on deformation. Moreover, since $\operatorname{Cof} \nabla y \in W^{1,q}$, its boundary value (and therefore the outer normal in deformed configuration) is well defined . In addition, the regularity still suffice for proving physically desirable properties of deformation such as local invertibility ($\det \nabla y > 0$) or global injectivity. Besides, the integrability of $\det^2 \nabla y$ in a Sobolev space $W^{1,r}(\Omega)$ is obtained for an appropriate $r \geq 1$. Concerning the modeling aspect of view, this special energy's dependence on the second gradient of deformation leads to a different form of hyperstress, a generalized form of stress occurring in higher-order gradient theories.

In a forthcoming paper, we extend the previous result for static problems in hyperelasticity to inelastic, isothermal processes. We treat the phase transformation as a dissipative rate-independent process, which is a justified assumption for many situations; see e.g. [7, 8]. We prove existence of *Energetic-solution* (c.f. [5] for a definition) driven by the Gibbs-type stored-energy potential $\mathcal{E}$ and the Rayleigh-type dissipation-energy pseudopotential $\mathcal{R}$; i.e. the activation criterion for the phase-transformation is purely energetic. We suppose that the state of the system is described, besides deformation y, by so-called internal variable z, denoting the vector of volume fractions of individual phases. The vector is determined by deformation gradient via a continuous mapping $\lambda : \mathbb{R}^{3 \times 3} \to \mathbb{R}^l$, where $l \in \mathbb{N}$ stands for the number of phases. The Gibbs-type potential is of the form

$$\mathcal{E}(t, y, z) = \begin{cases} I(y) - \langle \ell(t), y \rangle & \text{if } z = \lambda(\nabla y) \text{ a.e. in } \Omega, \\ +\infty & \text{otherwise,} \end{cases}$$

where t denotes time, I is as in (1) and $\ell(t)$ is a continuous linear functional of external forces at time t. Note that the functional depends on time only through loading $\ell(t)$, since we do not consider time-dependent Dirichlet data; nevertheless these can be effectively approximated by a penalty in Neumann boundary condition. The dissipation pseudopotential takes the form

$$\mathcal{R}(\dot{z}) = c \int_\Omega |\dot{z}| \, dx,$$

where $c > 0$ is tightly related to the amount of energy dissipated by the phase change. This specific choice of potentials $\mathcal{E}$ and $\mathcal{R}$ is a straightforward modification of the model summarized e.g. in [5].

References

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