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A gradient approach for the macroscopic modeling of superelasticity in softening shape memory alloys

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ABSTRACT

This paper presents a gradient approach for the quasi-static macroscopic modeling of superelasticity in softening shape memory alloys bars. The model is assumed to be rate-independent and to depend on a single internal variable. Regularization of the model is achieved through the free energy by assuming a quadratic dependance with respect to the gradient of the internal variable. The quasi-static evolution is then formulated in terms of two physical principles: a stability criterion which consists in selecting the local minima of the total energy of the system and an energy balance condition. Both homogeneous and non-homogeneous evolutions are investigated analytically for a family of material parameters. Non-homogeneous evolutions can be divided into three stages: the localized martensite nucleation followed by the propagation of the localized phase transformation front and finally the annihilation of the austenite phase. For each stage, the local phase field profile as well as the global stress–strain response are derived in closed-form. Due to the presence of an internal length related to the regularization, size effects are inherent with such non-local model. We show that for sufficiently long bars, snap-backs occur at the onset of localized phase transformation, leading to a time discontinuity in the quasi-static evolution.

1. Introduction

Quasi-static tensile tests performed on superelastic NiTi strips or wires at various speeds show that the martensitic phase transformation is a *non-homogeneous* process (Huo and Müller, 1993; Shaw and Kyriakides, 1995, 1997; Tobushi et al., 1993). It is characterized in the global response by a first elastic-hardening phase followed by a macroscopic instability: depending on the loading rate, one or several martensite localizations nucleate along the specimen and propagate at constant stress. Due to such non-homogeneous response, the extraction of the intrinsic response of SMA by means of a tensile test is a difficult task. Such underlying material response is nevertheless fundamental for an appropriate calibration of the macroscopic constitutive SMA models. Recently, Hallai and Kyriakides (2013) have been able to stabilize a homogeneous phase transformation in the case of a superelastic NiTi. By bonding stainless steel to the NiTi strip, instabilities in the NiTi specimen are avoided due to the hardening character of the stainless steel, thus leading to a *homogeneous* phase transformation. By subtracting the response of the stainless steel from the response of the bonded specimen, extraction of the (forward) intrinsic macroscopic behavior of the NiTi is then achieved. Stress–strain response during the phase transformation is non-monotonous, showing a significant softening part. Such result is consistent with the fact that the critical stress at which occurs the non-homogeneous phase transformation of NiTi corresponds approximatively to the Maxwell line associated to the softening intrinsic curve. Such experimental evidences emphasize the necessity to account for the softening behavior in the macroscopic modeling of SMAs in order to provide a correct modeling of their structural behavior and a better understanding of the localization phenomena (Song et al., 2012; Pham, 2014).

An important class of macroscopic superelastic SMA models for superelasticity is based on the description of the phase transformation by means of internal variables. Such models can be either derived from a micro-mechanical approach (Sun and Hwang, 1993a,b; Cherkaoui et al., 1998) or established phenomenologically by postulating the free energy as well as the dissipated potential with respect to the laws of thermodynamics (Auricchio and Sacco, 1997; Popov and Lagoudas, 2007; Zaki and Moumni, 2007; Song et al., 2012; Pham, 2014). However, most of these studies

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remain *local* in the sense that the constitutive behavior at a given point in space is function of the state variables of the same point only, being independent of the gradient of the state variables or of the state of other points. Such local approach is valid as long as the behavior does not show any sign of stress softening. As soon as the intrinsic behavior exhibits stress softening, local models are not any more mathematically well-posed and show a number of serious pathologies. In particular, an infinite number of austenite–martensite macroscopic interfaces can nucleate without any energy dissipation. This is in contradiction with the experimental results for which the number of localization is limited to one or two for very slow loading rate. From the numerical point of view, strong mesh sensitivities are observed and the propagation of the phase transformation cannot be handled correctly. To avoid such issues regularized models of SMA models must be considered. Following the seminal work of Ericksen (1975), this has been mainly done in the context of SMA by introducing either the gradient of the strain (Carr et al., 1985; Friedman and Sprekels, 1990; Shaw, 2002) or the gradient of the internal variable (Duval et al., 2011) in the constitutive equations and phase transformation criteria. Some of these works exhibit numerical examples illustrating the benefit of the regularization during the non-homogeneous phase transformation. However analytical and rigorous results are not always available on the properties of the localized solutions and their evolution. Such results are fundamental to better understand the impact of the regularization on the model behavior.

In this paper we consider a regularized model for a SMA bar with stress-softening regularized through the introduction of an internal length and an energy dissipation depending on the gradient of the phase-field. We derive a fully analytical solution of the one-dimensional evolution problem including explicit expressions for the homogeneous and localized response and a full description of the nucleation phase and the propagation of the phase-transformation front. Moreover we show that global strain–stress response can exhibit a snap-back depending on the ratio between the length of the bar and the introduced internal length. The regularization introduces a scale-effect, as classical in damage and fracture (Bazant and Pijaudier-Cabot, 1989; Pham et al., 2011). Our model is formulated in the framework of the variational theory of rate-independent standard processes (Halphen and Nguyen, 1975; Mielke, 2005). The cornerstone of this framework is the minimization (in a certain sense) of the total energy of the system. Such minimizing technique proves to be a particularly powerful tool for non-convex problems such as phase transformation, plasticity or fracture. Although it has been widely used at the microscopic scale to account for the formation of martensite domains, self-accommodation as well as shape-memory effect (Ball and James, 1989; Puglisi and Truskinovsky, 2000; Ren and Truskinovsky, 2000; Bhattacharya, 2003), such minimization approach can be also extended to macroscopic scale to deal with the evolution of stress-softening SMAs. In our context, the quasi-static evolution is required to verify a local stability criterion and an energy balance condition, requiring the continuity of the total energy with respect to the loading parameter. This framework has proved its efficiency in many areas which involve stress-softening issues such as brittle fracture (Bourdin et al., 2008), damage (Pham et al., 2011), or coupled damage-plasticity (Alessi et al., 2014). This work can be regarded as an extension of Pham (2014), where a local SMA model is formulated and analyzed in the same framework.

The paper is organized as follows. In Section 2, we introduce the energetic formulation of the one dimensional non-local superelastic model of SMA with gradient of the phase transformation variable. Section 3 presents the study of a one dimensional bar submitted to a tensile test. The associated evolution problem is formulated in terms of a stability criterion based on the selection of *local* minima of the total energy and an energy balance. The strong formulation in terms of Kuhn–Tucker conditions is then derived under specific hypothesis. In Section 4, we present the homogeneous evolution of the bar and calibrate our model according to published experimental data. Section 5 is devoted to the analysis of solution involving the localization of the phase field. The localization profile as well as the associated global stress–strain response are derived for a class of material functions and discussed. Conclusions are drawn in Section 6.

The following notations are used: the dependence on the time parameter t is indicated by a subscript whereas the dependence on the spatial coordinate x is indicated classically by parentheses, *e.g.* $x \mapsto u_t(x)$ stands for the displacement field at time t. In general, the material functions of the phase transformation variable are represented by sans serif letters, like E, G or R. The prime denotes either the derivative with respect to x or the derivative with respect to the phase transformation variable, the dot stands for the time derivative, *e.g.* $u_t'(x) = \partial u_t(x)/\partial x$, $\mathsf{E}'(\alpha) = d\mathsf{E}(\alpha)/d\alpha$ or $\dot{u}_t(x) = \partial u_t(x)/\partial t$.

2. Gradient model of SMA with an internal variable

Macroscopic phase transformation processes are usually understood as rate-independent processes. The main source of rate-dependency usually comes from the heat release during the austenitic–martensitic phase transformation which has an autocatalytic effect. However, by enforcing sufficiently slow elongation rate ($\sim 10^{-5}\,\mathrm{s}^{-1}$ to $10^{-4}\,\mathrm{s}^{-1}$), the system can be considered as isothermal and fully rate-independent. Such quasi-static hypothesis will be considered in this article. The modeling of the macroscopic superelastic behavior of SMA will be done within the *standard* framework (Halphen and Nguyen, 1975) for which the material behavior admits an energetic formulation. The standard model we will consider is based on a single scalar internal variable z which will account both for the phase transformation as well as the transformation strain due to the oriented martensite (Pham, 2014). We assume that z belongs to the interval $[0,1]$, with $z=0$ and $z=1$ representing a fully transformed state of austenite and martensite, respectively. The formulation of the standard model starts here by postulating directly the form of the strain work density at a material point. In a non-local setting, we assume that this material point is described by its strain state ε, the phase field z and its gradient z'. Hence, let us call $W(\varepsilon,z,z')$ the strain work required to transform a material point from the reference state $(0,0,0)$ to a state (ε,z,z'). This quantity depends not only on the final state (ε,z,z') but also on the history of the loading because of the dissipative nature of the transformation. For standard models of dissipative processes and for *homogeneous* evolutions (no effect of gradient *i.e.* $z'=0$), the strain work can be decomposed as follows

$$W(\varepsilon,z,0) = \phi(\varepsilon,z) + \mathcal{D}(z,\dot{z}), \tag{1}$$

where $\phi(\varepsilon,z)$ and $\mathcal{D}(z,\dot{z})$ represent the local free energy and the total dissipated energy, respectively. Under the small strain assumption, the free energy is taken as a quadratic function of ε which is cast under the following form

$$\phi(\varepsilon,z) = \frac{1}{2}\mathsf{E}(z)(\varepsilon - \mathsf{p}(z))^2 + \mathsf{G}(z). \tag{2}$$

The free energy is a *state function* which does not depend on the history of the loading and which involves four material functions of the internal variables, namely the Young's modulus of the mixture of austenite–martensite $z \mapsto \mathsf{E}(z)$, the phase transformation strain $z \mapsto \mathsf{p}(z)$ and the latent energy released (or absorbed) during the forward (or the backward) phase transformation $z \mapsto \mathsf{G}(z)$. For the following developments it is useful to introduce also the compliance function $\mathsf{S}: z \mapsto 1/\mathsf{E}(z)$. The total dissipated energy $\mathcal{D}(z,\dot{z})$ depends on the history of the loading. For rate-independent processes, its time