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Gradient-enhanced model and its micromorphic regularization for simulation of Lüders-like bands in shape memory alloys

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ABSTRACT

Shape memory alloys, notably NiTi, often exhibit softening pseudoelastic response that results in formation and propagation of Lüders-like bands upon loading, for instance, in uniaxial tension. A common approach to modelling softening and strain localization is to resort to gradient-enhanced formulations that are capable of restoring well-posedness of the boundary-value problem. This approach is also followed in the present paper by introducing a gradient-enhancement into a simple one-dimensional model of pseudoelasticity. In order to facilitate computational treatment, a micromorphic-type regularization of the gradient-enhanced model is subsequently performed. The formulation employs the incremental energy minimization framework that is combined with the augmented Lagrangian treatment of the resulting non-smooth minimization problem. A thermomechanically coupled model is also formulated and implemented in a finite-element code. The effect of the loading rate on the localization pattern in a NiTi wire under tension is studied, and the features predicted by the model show a good agreement with the experimental observations. Additionally, an analytical solution is provided for a propagating interface (macroscopic transformation front) both for the gradient-enhanced model and for its micromorphic version.

1. Introduction

Due to their unique thermomechanical properties, shape memory alloys (SMAs) have gained wide applicability in engineering and medicine and thus attract significant research interest (Otsuka and Wayman, 1999). The underlying effects, notably pseudoelasticity and shape memory effect, result from the martensitic phase transformation and are accompanied by formation and evolution of martensitic microstructures at several scales (Bhattacharya, 2003). Numerous constitutive models have been developed to address various aspects of the complex behaviour of SMAs, from the atomistic to the macroscopic scale. A detailed overview of the constitutive models of SMAs available in the literature is beyond the scope of this paper, the reader is referred to recent reviews (e.g., Patoor et al., 2006; Lagoudas et al., 2006; Cisse et al., 2016).

It is commonly observed in the experiments that stress-induced pseudoelastic response of SMAs is accompanied by softening behaviour and strain localization. A typical example is the uniaxial tension of NiTi wires, strips and tubes (e.g., Shaw and Kyriakides, 1997; Sittner et al., 2005; Pieczyska et al., 2006; Favier et al., 2007; Daly et al., 2007; Zhang et al., 2010; Sedmák et al., 2016) in which transformation proceeds through nucleation and propagation of macroscopic transformation fronts so that the deformation pattern resembles Lüders bands. At low loading rates, i.e. in nearly isothermal conditions, the fronts propagate at an approximately constant load, thus a stress plateau is observed on the apparent stress–strain curve. A detailed study of the effect of the loading rate on the pattern of Lüders-like bands and on stress hysteresis in NiTi strips has been reported by Zhang et al. (2010). Localized deformation has been observed also in NiTi tubes under combined tension–torsion loading (Sun and Li, 2002) and under pure bending (Bechle and Kyriakides, 2014; Jiang et al., 2017a).

The typical mechanical response exhibiting a stress plateau is often incorrectly interpreted as the material response, while it is in fact the response of a specimen, which is related to nucleation and propagation of macroscopic transformation fronts. The actual material response involves softening, sometimes significant, which however cannot be directly observed due to localization phenomena. This has been very clearly illustrated by the careful experiment of Hallai and Kyriakides (2013), in which the intrinsic softening response of NiTi has been revealed by extracting it from the

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overall response of a uniformly deforming laminate composed of NiTi and steel sheets, the latter exhibiting a hardening elastoplastic response.

Implementation of the softening behaviour into a constitutive model usually does not constitute a difficulty. However, solution of the resulting boundary value problem is not immediate because the problem becomes ill-posed, which leads, for instance, to pathological mesh sensitivity. One way to regularize the problem is to enhance the model with non-local (Ahmadian et al., 2015) or gradient terms (Chang et al., 2006; Duval et al., 2011; Armattoe et al., 2014; Badnava et al., 2014; Alessi and Bernardini, 2015; León Baldelli et al., 2015). This introduces a characteristic length into the model so that diffuse transformation fronts are formed and a sharp transition from the transformed to non-transformed zone is penalized.

Note that a kind of regularization, which has a clear physical basis, is introduced by including the thermomechanical coupling and heat conduction. However, this regularization may be insufficient in nearly isothermal conditions, for instance, in the case of propagation of an existing macroscopic transformation front at a vanishingly small speed.

Interestingly, finite-element simulations of strain localization and Lüders-like bands in SMA strips and tubes under tension and tubes under bending have been successfully carried out by Jiang et al. (2017a–c) using an isothermal, plasticity-like softening model with no regularization. A mild mesh dependency of the results has been observed, which can be explained by the three-dimensional through-thickness effects (Mazière and Forest, 2015).

In this work, a gradient-enhancement is introduced into a simple one-dimensional model of pseudoelasticity in SMAs. The starting point here is a one-dimensional small-strain version of the model of pseudoelasticity developed by Stupkiewicz and Petryk (2013), however, the approach is general and can be applied to virtually any macroscopic model, including extension to a three-dimensional model. The main focus of this work, and its original contribution, is a micromorphic regularization of the gradient-enhanced model and its energy-based incremental formulation. To this end, a new degree of freedom is introduced into the model that can be interpreted as a micromorphic counterpart of the volume fraction of martensite. The micromorphic approach adopted here is similar to that of Mazière and Forest (2015) that has been developed for modelling of softening–hardening plasticity leading to formation of Lüders bands in metals. The resulting micromorphic model is suitable for a direct finite-element implementation based on the incremental energy minimization approach combined with the augmented Lagrangian treatment of the resulting non-smooth minimization problem. An analytical solution is also provided for a propagating phase transformation interface (macroscopic transformation front) both for the gradient-enhanced model and for the micromorphic one. Finally, a thermomechanically coupled model is formulated and implemented in a finite-element code. Using this model, uniaxial tension of a NiTi wire is simulated, and the effect of loading rate on the localization pattern is studied. The results obtained show a good agreement with the experiment.

2. One-dimensional model of pseudoelasticity

In order to concentrate on the most essential features, i.e. on the gradient enhancement and its micromorphic regularization, the model discussed in this paper is restricted to one-dimensional pseudoelastic response in tension at small strain. A sequence of isothermal models is discussed first, starting from a local model, through its gradient-enhanced version, to finally arrive at a micromorphic model. Subsequently, the most essential thermomechanical coupling terms are accounted for, thus leading to a coupled thermomechanical model. The isothermal local model discussed below is essentially a one-dimensional version of the general three-dimensional model of Stupkiewicz and Petryk (2013).

Despite the model is one-dimensional, in the notation we will use ∇ and $\nabla\cdot$ to denote the gradient and divergence, respectively, so that the structure of the model resembles that of the corresponding three-dimensional model to be developed in the future. Clearly, in one-dimension, the two operations reduce to the usual spatial derivative.

2.1. Local model

The total strain $\varepsilon = e(u)$, where $e(u) = \nabla u$ and u denotes the displacement, is decomposed into its elastic ε_e and inelastic (transformation) ε_t parts,

$$\varepsilon = \varepsilon_e + \varepsilon_t, \qquad \varepsilon_t = \eta\bar{\epsilon}_t, \qquad 0 \le \eta \le 1, \tag{1}$$

where η denotes the volume fraction of martensite, and $\bar{\epsilon}_t$ is a model parameter. Here, we rely on the assumption that, in the pseudoelastic regime, martensite is fully oriented, and $\bar{\epsilon}_t$ is its transformation strain. Since only tension is considered, we have $\bar{\epsilon}_t > 0$.

The function specifying the Helmholtz free energy (per unit volume) in isothermal conditions is adopted in the following form (cf. Stupkiewicz and Petryk, 2013),

$$\phi(\varepsilon, \eta) = \phi_0 + \Delta\phi_0\eta + \frac{1}{2}E(\varepsilon - \eta\bar{\epsilon}_t)^2 + \frac{1}{2}H\eta^2, \tag{2}$$

where ϕ_0 is the free energy of austenite in a stress-free state, $\Delta\phi_0$ is the chemical energy, E is the Young's modulus, and H is the parameter controlling the hardening or softening associated with increasing η. We assume here that H is non-negative, $H \ge 0$, because for $H < 0$ a softening response is obtained, as shown later, and the problem is then ill-posed. A negative hardening parameter will be admitted in the gradient-enhanced model discussed in Section 2.2.

The Helmholtz free energy functional $\Phi[u, \eta]$ is obtained by integrating ϕ over the body domain B,

$$\Phi[u, \eta] = \int_B \phi(e(u), \eta)\,\mathrm{d}V, \tag{3}$$

and the potential energy is defined as

$$\mathcal{E}[u, \eta] = \Phi[u, \eta] + \Omega[u], \tag{4}$$

where $\Omega[u]$ is the potential energy of external loads, which are assumed conservative.

In the incremental (finite-step) formulation, the rate-independent dissipation is governed by the following dissipation potential,

$$\Delta D(\Delta\eta) = f_c|\Delta\eta|, \qquad f_c > 0, \qquad \Delta\eta = \eta - \eta_n, \tag{5}$$

and its global counterpart,

$$\Delta\mathcal{D}[\eta] = \int_B \Delta D(\eta - \eta_n)\,\mathrm{d}V, \tag{6}$$

where f_c is the critical driving force, and η_n is the martensite volume fraction at the end of the previous step. Note that quantities without a subscript refer to the current time instant $t = t_{n+1}$.

The incremental solution, i.e. the *fields* of displacement u and volume fraction η at the current instant t_{n+1}, are determined by minimization of the *global* incremental potential $\Pi[u, \eta]$ (cf., Petryk, 2003; Stupkiewicz and Petryk, 2013),

$$\{u, \eta\} = \arg\min_{u,\eta} \Pi[u, \eta], \tag{7}$$

where

$$\Pi[u, \eta] = \mathcal{E}[u, \eta] - \mathcal{E}[u_n, \eta_n] + \Delta\mathcal{D}[\eta] + \mathcal{I}[\eta], \tag{8}$$