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Analysis of localization phenomena in Shape Memory Alloys bars by a variational approach

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Dedicated to the memory of
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ABSTRACT

Localization of the phase transformations in Shape Memory Alloys (SMA) wires are well known. Several experimental and theoretical studies appeared in the last years. In this work the problem is addressed by means of a variational approach within the framework of the modeling of rate-independent materials by the specification of a non-local free energy and a dissipation function, focusing attention on the basic case of isothermal conditions. General expressions are given for a rather broad class of models, whereas a simple model is studied in detail. A full stability analysis of both homogeneous and non-homogeneous solutions is carried out analytically, showing that stable non-homogeneous solutions have necessarily to occur if the bar is longer than an internal length determined by the constitutive parameters. The analysis also shows that snap-back phenomena may occur both in the nucleation and the coalescence phase, depending on another material length which is also function of the number of transformation fronts. This helps to explain why the second stress drop associated to coalescence is much more difficult to observe experimentally. Closed form expressions are given for the phase fraction profiles of both single and multiple localizations as well as nucleation and propagation stresses. A comparison between the prediction of the model with experimental data finally shows a good agreement both in terms of global response and in the spatio-temporal evolution of the transformation domains.

1. Introduction

Shape Memory Alloys (SMA) exhibit a complex thermomechanical behavior induced by the occurrence of phase transformations between Austenite and one or more variants or groups of variants of Martensite (Patoor, 2006; Lagoudas et al., 2006). This is reflected at the macroscopic scale by their peculiar functional properties known as pseudoelasticity, one or two-way shape memory effect (Lagoudas, 2008; Lexcellent, 2013). Such properties are nowadays widely known and are exploited by an increasing number of applications like, among the others: biomedical devices, aerospace structures, mechanical components, MEMS as well as civil engineering structural elements or devices (Schwartz, 2002; Schwartz, 2008).

While the basic properties of SMA were known since 1960s, Shaw and Kyriakides (1995) first noticed the occurrence of non-homogeneous strain fields associated with the localization of the phase transformations at the macroscopic scale in NiTi superelastic wires. Further experimental investigations then provided ample confirmation that, during tensile tests under displacement control, NiTi wires or stripes tend to transform through the nucleation, growth and propagation of macroscopic domains observable at the macroscopic scale in the form of bands with striking similarity with Lüders phenomena observed in other types of metals (Shaw, 1997; Shaw and Kyriakides, 1997; Iadicola and Shaw, 2002; Churchill et al., 2009). This phenomenology was confirmed by Sun and coworkers in fine-grained polycrystalline NiTi microtubes where an additional level of complexity arises with respect to the possibility of formation of cylindrical or helix-shaped domains (Sun and Li, 2002; Feng and Sun, 2006; Hallai and Kyriakides, 2013). Recent experiments show qualitatively similar behavior also for SMA tubes subject to bending (Bechle and Kyriakides, 2014).

Further experimental analyses pointed out the importance of the thermomechanical coupling (Iadicola and Shaw, 2002; Shaw, 2000; Sun et al., 2012; Depriester et al., 2014). The latent heat released or absorbed during phase transformations is localized at the domains and this generates a non-uniform temperature field that, given the temperature dependence of the nucleation stress, usually gives rise to the formation of multiple domains. Since the

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actual temperature field is determined by the concomitant effect of the latent heat and the heat exchanged with the environment, the thermomechanical coupling is strongly related to the loading rate. For each loading rate the maximum number of fronts and the corresponding spacing has been estimated in He and Sun (2010).

The occurrence of localized phase transformations is reflected on the overall response of the sample by stress peaks that can be interpreted as the difference between the nucleation and propagation stresses emerging as an outcome of material instability. The fact that SMA tend to show unstable softening behavior is known since the first thermodynamic equilibrium analyses in Fu et al. (1993) and has recently been observed experimentally in Hallai and Kyriakides (2013).

A large number of constitutive models, able to describe many features of the complex response of SMA, are available in the scientific literature (Patoor, 2006; Lagoudas et al., 2006; Lagoudas, 2008; Bernardini and Pence, 2002; Bernardini and Pence, 2009) but most of them cannot model the occurrence of localized phase transformations. However, over the years, various different approaches have been used to describe the localizations in SMA.

The first attempts to model this phenomenology go back to Shaw and Kyriakides (1997) where FEM analyses based on standard 3-dimensional plasticity models were carried out to model the loading phase of SMA strips, later extended to take into account the thermomechanical coupling (Shaw, 2000). In Shaw (2002), and Chang et al. (2006) a 1-dimensional nonlocal model for SMA bars based on two internal variables and a free energy depending on the strain gradient was proposed. Numerical simulations showed the ability of the model to describe the localized responses in tensile tests of SMA wires. Another approach based on a series-asymptotic expansion method originating from the work of Dai and Cai (2006) led to interesting analytical results in the study of phase transformations and the instability of SMA circular cylindrical wires (Song et al., 2013; Song and Dai, 2015). Implicit nonlocal gradient models were proposed in Duval et al. (2011), Armattoe (2014) through the introduction of an internal length parameter that determines the nonlocality of the model through a partial differential equation. The model was then implemented in FEM codes and numerical results showed a good agreement with the experiments.

In this work, the study of the localization phenomena in pseudoelastic SMA bars, arising in tensile tests under displacement control, is addressed by using a variational approach within the framework of a global energetic formulation for rate-independent dissipative materials modeled by the constitutive specification of a free energy and a dissipation function (Mielke and Theil, 2004; Mielke, 2011; Auricchio et al., 2008; Frost et al., in press).

The evolution problem is stated by means of three energetic requirements: two of them reflect the first and second law of thermodynamics, the third one is a directional stability condition based on the minimization of the energy injection that would be needed to realize virtual radial continuation processes from a given state. The latter plays a role analogous to other criteria that provide restrictions on the dissipative behavior (like e.g. in Halphen and Nguyen (1975), Valery (1995), Ziegler et al. (1987)) but it offers the possibility to be interpreted in terms of stability as done, from slightly different perspectives in the important works (Fedelich and Ehrlacher, 1997; Petryk, 2005; Nguyen, 1984). Moreover, the approach is amenable to a robust numerical implementation by means of Incremental Energy Minimization (Petryk, 2003) that will be discussed in forthcoming works.

The energetic criteria are stated in a global spatial and temporal form as proposed by Mielke and coworkers to obtain a derivative-free formulation able to deal with very weak smoothness requirements (Mielke and Theil, 2004; Mielke, 2011). The present analysis is however carried out without taking full advantage of the generality in Mielke and Theil (2004) working instead with differential stability conditions in the spirit of Marigo and coworkers who successfully applied this type of criteria to the study of gradient damage models (Pham, 2010; Pham and Marigo, 2010; Pham et al., 2011) and coupled damage and plasticity models (Alessi et al., 2014; Alessi et al., 2015). An application of this approach to SMA has recently appeared in León Baldelli et al. (2015) on the basis of a rather different constitutive model. Moreover, with respect to León Baldelli et al. (2015), here the complete stability analysis of both homogeneous and non-homogeneous response is discussed.

The energetic formulation is described in Section 2 with reference to isothermal conditions which are a good approximation of the actual behavior only for very slow loading rates. This choice is done as the main motivation of the work is to show the applicability of the energetic approach in the most basic setting. The extension of the formulation to a full non-isothermal setting that properly takes into account the very important influence of the thermomechanical coupling is presently under development.

Section 2 also shows how the combined use of first-order directional stability and energy balance yields transformation criteria and kinetics both in variational and strong form. The discussion is referred to a class of SMA models characterized by the free energy functions proposed in Bernardini (2001), Bernardini and Masiani (2014) modified by the introduction of a nonlocal term proportional to the gradient of the Martensite fraction. The constitutive information is then completed by a positively homogeneous dissipation function as in Rajagopal and Srinivasa (1999), Bernardini and Pence (2002). In this framework, various SMA models with different levels of detail can be studied by using specific expressions for the effective elastic moduli, interaction energy and driving force thresholds as a function of the Martensite fraction.

The attention is then restricted to the simplest version of the model specified by a constant elastic modulus, quadratic interaction energy and constant driving force thresholds, as described in Section 3. The consideration of more elaborate versions of the model, taking into account heterogeneity of the elastic properties of the phases, micromechanically derived interaction energies, non-constant driving force thresholds as well as tension–compression asymmetry, will be considered in forthcoming works.

In Section 4 the spatially homogeneous solutions are studied. Since the adopted free energy is non-convex in the internal variables, homogeneous phase transformations are accompanied by softening. The study of their stability then reveals that such solutions become unstable when the length of the bar exceeds an internal length ℓ_s determined by the dependence of the free energy density on the gradient of the phase fraction.

Given the instability of the homogeneous transformations, localized Martensite fraction profiles may develop, provided that the length of the bar L is greater than a second internal length ℓ ($< \ell_s$), corresponding to the support of a half-localization. Due to the nonlocality of the model, the transformation criteria turn out to be to integro-differential equations that can be solved with the stress as a parameter. The stress is then computed from the knowledge of the average value of the Martensite fraction. Section 5 and Appendix A discuss general properties of localized phase fraction profiles offering closed form expressions for the basic cases of boundary and inner localizations.

Section 6 discusses in detail the response of the bar when a single localization nucleates at the fixed end, grows and then propagates towards the other end. Explicit expressions are given for the nucleation and propagation stresses and it turns out that the corresponding stress drop is completely determined by the interaction energy and the local transformation strain. The analysis also shows that snap-back instabilities may occur depending on the length of