European Journal of Mechanics A/Solids 52 (2015) 1–11

Contents lists available at ScienceDirect

European Journal of Mechanics A/Solids

journal homepage: www.elsevier.com/locate/ejmsol

A phenomenological model for the magneto-mechanical response of single-crystal magnetic shape memory alloys

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ARTICLE INFO

Article history:
Received 19 December 2013
Accepted 24 December 2014
Available online 10 January 2015

Keywords:
Magnetic shape memory alloys
Discretization
Numerical simulation

ABSTRACT

We advance a three-dimensional phenomenological model for the magneto-mechanical behavior of magnetic shape memory alloys. Moving from micromagnetic considerations, we propose a thermodynamically consistent constitutive relation which is able to reproduce the magnetically-induced martensitic transformation in single crystals. Existence results for the constitutive relation problem as well as for the corresponding quasi-static evolution system are illustrated and convergence of time- and space–time-discretizations are recorded. Eventually, we present algorithmic considerations and we numerically test the model in order to assess its ability in reproducing the typical response of magnetic shape memory alloys, as well as in recovering standard shape-memory and pseudo-elastic behaviors when no magnetic field is present.

1. Introduction

Shape memory alloys (SMAs) are *active* materials: reversible strains as large as 10–12% can be induced by either thermal or mechanical stimuli (Frémond, 1987). This unique behavior is at the basis of a variety of innovative applications ranging from sensors and actuators, to Aerospace, Biomedical, and Seismic Engineering (Duerig TW and Pelton AR editors, 2003), just to mention a few hot application fields. Correspondingly, the interest for the efficient modeling, analysis, and control of SMAs behavior has triggered an intense research activity (Roubíček, 2004). Without any claim of completeness, we shall refer to Auricchio and Sacco (1997), Falk and Konopka (1990), Govindjee and Miehe (2001), Helm and Haupt (2003), Lagoudas et al. (2006), Levitas (1998), Peultier et al. (2006), Popov and Lagoudas (2007), Raniecki and Lexcellent (1994), Reese and Christ (2008) and Thamburaja and Anand (2001) for a collection of SMA modeling results.

Some SMAs (Ni_2MnGa, NiMnInCo, NiFeGaCo, FePt, FePd, among others) are called *magnetic* shape memory alloys (MSMAs) as they feature a specific ferromagnetic behavior entailing a so-called *giant* magnetostrictive response. For instance, the 10% magnetostrictive strain of a Ni_2MnGa single crystal (at a 1–3 MPa activation stress under the effect of a 1 T magnetic field) compares very favorably with the maximal 0.2% strain (at 60 MPa stress and 0.2 T field) in polycrystalline *TerFeNOL-D*, one of the highest performing magnetostrictive materials available to date.

The magnetic-induced strains in MSMAs are the macroscopic effect of the orientation of the ferromagnetic martensitic variants of the material. In particular, the martensitic phase in MSMAs presents the classical ferromagnetic texture of magnetic domains. This mesostructure changes under the influence of an external magnetic field by magnetic-domain wall motion, magnetization-vector rotation, and magnetic-field-driven martensitic-variant transformation. The first two effects above are present in all ferromagnetic materials. On the contrary, magnetic-field-driven variant transformation is a distinguishing trait of MSMAs. The interest in the possible applications of the unique material behavior of MSMAs is evident and may give some unprecedented possibility of activating devices (sensors, actuators, etc.) *at a distance* by specifically tuning an external magnetic field. Correspondingly, a vast Engineering literature is nowadays available on MSMAs. The reader shall be referred, with no claim of completeness, to DeSimone and James (2002), James and Wuttig (1998), Karaca et al. (2006), Likhachev and Ullakko (2000), O'Handley (1998) and Tickle and James (1999), see also the review in Kiang and Tong (2005).

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http://dx.doi.org/10.1016/j.euromechsol.2014.12.011
0997-7538/

We introduce here a novel modeling of the magneto-mechanical response of MSMAs, already announced in Auricchio et al. (2010, 2011a) and Bessoud and Stefanelli (2011). Moving within the geometrically linear setting, we advance a three-dimensional, phenomenological, internal-variable-type description of MSMAs behavior which is able of replicate pseudo-elasticity, shape-memory, and magnetic shape-memory response as an effect of changes in magnetic field, stress, and absolute temperature. On the thermo-mechanical side, our model reproduces in the single-crystal setting the well-known *Souza-Auricchio* model for SMAs (Auricchio and Petrini, 2002, 2004a, 2004b; Souza et al., 1998), which has been proved to be very effective as well as extremely robust with respect to approximations. The Souza-Auricchio model has been analyzed from the viewpoint of existence and approximation of solutions in Auricchio et al. (2008). Moreover, it has been extended and analyzed in the connection with non-symmetric material behavior (Auricchio and Stefanelli, 2009), residual plasticity (Auricchio and Stefanelli, 2007a, 2007b; Eleuteri et al., 2011), finite strains (Arghavani et al., 2011a, 2011b, 2010a; Evangelista et al., 2009; Evangelista et al., 2010; Frigeri and Stefanelli, 2012), thermal evolution (Mielke et al., 2009a; Mielke and Petrov, 2007) (given temperature) (Krejčí and Stefanelli, 2010, 2011; Paoli and Petrov, 2011; Roubíček and Stefanelli, 2013) (unknown temperature), space discretizations (Mielke et al., 2010, 2009b), beams in bending conditions (Auricchio et al., 2011b), and optimal control (Eleuteri et al., 2013; Stefanelli, 2012).

Despite the effective tridimensionality of the model, we focus here on the assumption that martensites have a single *easy axis* of magnetization (i.e., we focus on the case of uniaxial magnetic materials). This is indeed the case for all known MSMAs which present either a cubic-to-tetragonal ($\nu = 3$ variants) or a cubic-to-orthorombic ($\nu = 6$ variants) systems (or, often a combination of both). Magnetic uniaxiality is deeply exploited in the modeling by choosing as internal variable the microscopic martensitic phase-fraction distribution $\boldsymbol{p} \in \mathbb{R}^\nu$ taking values in the simplex $S := \{p_i \geq 0, p_1 + \ldots + p_\nu \leq 1\}$. In particular, $\boldsymbol{p} = \boldsymbol{0}$ stands for a purely austenitic phase whereas $\boldsymbol{p}/(p_1 + \ldots + p_\nu)$ represents the local distribution of martensitic variants. Within this frame, we shall associate to each proportion $\boldsymbol{p}$ a specific *easy axis* $\boldsymbol{Ap}$ of magnetization, where $\boldsymbol{A}$ is a 3-tensor. Additionally, the *orientation* of the variants with respect to the easy axis will be determined by the scalar (signed) *magnetic-domain proportion* $\alpha \in [-1, 1]$.

The leading *ansatz* of our modeling is that the material presents a very strong magnetic anisotropy so that the actual magnetization of martensites is rigidly attached to the corresponding easy axes and no magnetization rotation actually takes place. In particular, given the phase distribution $\boldsymbol{p} \in S$, we require the magnetization $\boldsymbol{M}$ of the material to be given by

$$\boldsymbol{M} = m_{\text{sat}} \alpha \boldsymbol{Ap} \tag{1.1}$$

where $m_{\text{sat}} > 0$ is the saturation magnetization. This assumption is in large agreement with observations on Ni_2MnGa (O'Handley, 1998; Tickle and James, 1999) in correspondence to the reference experimental (and applicative) situation. Still, the reader is referred to Bessoud et al. (2012) for the mathematical analysis of a more general version of this model including magnetization rotations.

Before going on, let us briefly review some literature on MSMA modeling. Early modeling contributions have been mainly focusing on the energy minimization mechanism. Among these, we shall minimally refer to DeSimone and James (2002), Murray et al. (2000a, 2000b), Tickle and James (1999) and Tickle et al. (1999). As for thermodynamically consistent models, one has to mention the contributions by O'Handley (1998), Murray et al. (2001), O'Handley et al. (2000). A completely different perspective exploiting Preisach-type hysteretic relations is presented by Adly et al. (2006). An internal-variable model for MSMAs has been introduced by Hirsinger and Lexcellent (2003), Hirsinger (2004) for two martensitic variants in two space dimensions. This model has then been extended to three variants by Gauthier et al. (2011) where also the magnetic behavior of austenite is considered. Another internal-variable-type model has been proposed by Kiefer (2006) and Kiefer and Lagoudas (2009) again originally in the two-dimensional and two-variants setting (see also Kiefer et al., 2007; Miehe et al., 2011). This very model has been extended in order to encompass some more realistic magnetic response by Wang and Steinmann (2012). A three-dimensional constitutive model with internal variables is proposed in Chen et al. (2014), differing from ours mainly in the description of the magnetic state of the crystal. In particular, the magnetizations of single martensitic variants are there assumed to be collinear with the internal magnetic field whereas here magnetization is determined by $\boldsymbol{p}$ and no magnetization rotation is allowed. Finally, some micro-macro modeling perspective within the realm of irreversible thermodynamical processes is developed by Zhu and Dui (2007, 2008).

Apart from specific modeling choices, the striking distinctive trait of the present model with respect to the above mentioned propositions relies on its sound *variational structure* which in turn entails robustness with respect to approximations and discretizations. In particular, our model is presently the only one allowing a *full mathematical treatment* of the evolutive regime in terms of stability and convergence of time-incremental schemes, existence of solutions, and optimal controllability (Bessoud and Stefanelli, 2011; Bessoud et al., 2012). Moreover, we have been able to establish rigorous Γ-convergence analyses (Mielke et al., 2008) which in turn cross-validate the present model with respect to the original non-magnetic Souza-Auricchio model and to classical magnetoelasticity (Bessoud and Stefanelli, 2011; Bessoud et al., 2012). An additional unique quality of our model is its remarkable simplicity: the knowledge of just 6 material parameters (concretely identifiable from experiments) is sufficient for the description of the full three-dimensional magnetomechanical behavior (see Subsection 2.4).

The paper is organized as follows. We devote Section 2 to the presentation of the model as well as to some discussion on its major features. The existence of *energetic solutions* (Mielke et al., 2005), both at the constitutive equation and at the coupled quasi-static evolution level, are then recalled in Section 3. Algorithmic considerations as well as numerical simulations are reported in Section 4, while conclusions are drawn in Section 5. With respect to our previous contributions on this subject, the present paper brings a number of significant novelties. At the modeling level, we concentrate here on single MSMA crystals instead of polycrystals as the latter present reduced magnetostrictive effects and are hence less interesting for applications. A second novelty resides in the time-discretization scheme, here chosen to be semi-implicit, in consideration of the specific convex–concave structure of the reduced Gibbs energy, see Subsection 2.7. Moreover, we present a novel convergence analysis of a full space–time-discrete scheme by a conformal finite element method. Finally, we also numerically show that the model is able to reproduce standard shape-memory and pseudo-elastic behaviors when no magnetic field is present.

2. The model

2.1. Tensor notation

In the following bold Latin letters stand for vectors in $\mathbb{R}^3$ and bold Greek symbols are for 2-tensors in $\mathbb{R}^3$. Given the 2-tensors $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{R}^{3\times3}$ and a 3-tensor $\boldsymbol{A} \in \mathbb{R}^{3\times3\times3}$, we classically define