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A phase-field model on the hysteretic magneto-mechanical behaviors of ferromagnetic shape memory alloy

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Abstract—A phase-field model with a friction-type resistance in the kinetic equation for the martensite reorientation is proposed to simulate the coupled magneto-mechanical behaviors of ferromagnetic shape memory alloy (FSMA). The phase-field simulation is able to capture the evolution of the microstructures (martensite twins and magnetic domains) and the rate-independent hysteresis in the associated responses under various quasi-static loading paths of controlling a mechanical stress or/and a magnetic field. Phase diagrams are constructed, by summarizing many simulation cases, to demonstrate the dependence of the material state (martensite variant state and the level of magnetization along the external magnetic field) on the magneto-mechanical loading. Particularly, the critical levels of the stress/field to trigger the martensite reorientation in the cases like Magnetic-Field Induced Strain (MFIS) and field-assisted quasi-plasticity/pseudoelasticity (superelasticity) can be predicted, which agree with experimental observations.

Keywords: Phase-field method; Ferromagnetic shape memory alloy; Deformation twinning; Magnetic domains; Rate-independent hysteresis

1. Introduction

There have been intensive researches on magneto-mechanical coupling behaviors of NiMnGa ferromagnetic shape memory alloy (FSMA) since its Magnetic-Field Induced Strain (MFIS) was discovered by Ullakko et al. in 1996 [1]. The material can provide high-frequency responses with a large strain of 6–10% [2–7] which make the material have many potential applications such as actuators and sensors [8,9]. The main physical mechanism underlying the material's large recoverable deformation is the reorientation between the martensite variants (with approximately tetragonal symmetry) whose short- and long-axes have different magnetization susceptibilities [2,3,5,10]. The mechanical and magnetic anisotropy of the variants, correlating the deformation and the magnetization, governs the material's magneto-mechanical coupling behaviors. For different purposes in various situations, the martensite reorientation induced by rotating/non-rotating magnetic fields and/or uniaxial/multi-axial mechanical stresses has been studied [10–18].

One of the key research issues is the driving force for the martensite reorientation or the kinetics of the twin boundary motion by which the martensite reorientation takes place [3,11,12,19–21]. The driving force (also called twinning stress σ_{tw}) means some energy dissipation during the process and leads to rate-independent hysteresis in responses during cyclic martensite reorientation for reversible deformation (The hysteresis is so-called rate-independent because it exists even though the external loading is very slow or quasi-static) [13,14,10,15]. The rate-independent hysteresis (quasi-static hysteresis) in responses implies that there is some heat generated from the dissipated energy during the martensite reorientation, which will increase significantly the material's temperature and change the behaviors of the specimen/system under high-frequency dynamic cyclic loadings [22,23]. Therefore, it is important to understand the effects of the twinning stress and the associated hysteresis on the magneto-mechanical behaviors (particularly the coupled microstructures including the martensite twins and magnetic domains). It has been experimentally observed that the twinning stress is related to microstructures (e.g., $\sigma_{tw} = 1$ MPa and 0.2 MPa for type I and II twin boundaries, respectively) [24–28]. So, models capable of describing/simulating the hysteretic microstructure evolution and the associated magneto-mechanical responses will be helpful for both academic research and engineering applications.

In literature, there are theoretical models focused on different aspects of magneto-mechanical behaviors of FSMA.

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These models can be mainly classified into three categories: (1) Simple energy models [12,17,29,30] with energetic analysis in terms of macroscopic variables can predict the critical stress/field levels triggering martensite reorientation and provide design criteria for obtaining reversible strain. (2) Thermodynamic models [31–35] describing irreversible processes with internal variables are able to capture the dissipative phenomena (rate-independent hysteresis and the loading-path dependence) and to provide detailed predictions about the macroscopic behaviors under various loading conditions. (3) Microstructural models [36–47] with the principle of minimizing system's total free energy are capable of studying the fundamental magneto-mechanical coupling mechanisms at micro- (meso-) scales (coupling martensite twins and magnetic domains) and associating the microstructures with the macroscopic responses.

In this paper, we propose a phase-field model with a friction-type resistance in the kinetic equation for the martensite reorientation in order to describe the hysteretic microstructure evolution and the associated responses under various quasi-static magneto-mechanical loading paths. The remaining parts of this paper are organized as: Section 2 introduces the theoretical framework of the phase-field model while Section 3 reports the results of the phase-field simulation on the microstructure evolutions and response curves for some typical loading paths—MFIS under fixed stress levels and field-assisted quasi-plasticity/pseudoelasticity (superelasticity). In Section 4, the concepts of the loading-path dependence relating to the hysteretic magneto-mechanical behaviors are discussed with some phase diagrams constructed by summarizing our simulation for many cases. Finally, some conclusions are given in Section 5.

In order to simplify the mathematical expressions in the following model, vector and tensor notations are adopted: boldface letters denote vectors or second-order tensors such as $\boldsymbol{\eta}$, $\boldsymbol{m}$, $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$. Symbols such as $\mathbb{C}$, $\mathbb{I}$, denote fourth-order tensors. Direct combination of vectors and tensors such as $\boldsymbol{m\eta}$ and $\boldsymbol{m\varepsilon}$ represents the dot product corresponding to the index notation $m_i\eta_i$ and $m_i\varepsilon_{ij}$ respectively; particularly $\boldsymbol{\eta}^2$ represents $\eta_i\eta_i$. The cross product of two vectors such as $\boldsymbol{m}$ and $\boldsymbol{\eta}$ is denoted by $\boldsymbol{m}\times\boldsymbol{\eta}$. The symbol "$\otimes$" denotes tensor product of tensors. When "$\otimes$" is used with vectors like $\boldsymbol{\eta}\otimes\boldsymbol{\eta}$, the corresponding index notation is $\eta_i\eta_j$. The symbol ":" denotes the double contraction of two tensors, for example $\boldsymbol{\sigma}:\boldsymbol{\varepsilon}$ and $\mathbb{C}:\boldsymbol{\varepsilon}$ correspond to $\sigma_{ij}\varepsilon_{ij}$ and $\mathbb{C}_{ijkl}\varepsilon_{kl}$ respectively. Other notations are: $|\boldsymbol{\eta}|$ represents the norm of the vector $\boldsymbol{\eta}$. $(\text{grad}\boldsymbol{\eta})^2$ corresponds to $\sum_{K=1}^{3}|\nabla\eta_K|^2$ and the nabla symbol "∇" denotes the vector differential operator.

2. Phase-field model

2.1. Phase-field variables and free energy

The state of the microstructure is described by two sets of phase-field variables: (1) long-range order parameters (LRO) for describing the martensite states, $\boldsymbol{\eta}=\boldsymbol{\eta}(\boldsymbol{r},t)=(\eta_1(\boldsymbol{r},t),\eta_2(\boldsymbol{r},t),\eta_3(\boldsymbol{r},t))$; (2) two angles to describe the magnetization direction, polar angle $\theta=\theta(\boldsymbol{r},t)$ and azimuth angle $\varphi=\varphi(\boldsymbol{r},t)$ (with a constant saturation magnetization M_s, the magnetization vector $\boldsymbol{M}(\boldsymbol{r},t)=M_s\boldsymbol{m}(\boldsymbol{r},t)$ where $\boldsymbol{m}$ is determined by the two angles of a spherical coordinate system). The phase field variables are functions of time t and a spatial vector $\boldsymbol{r}$ (containing the three coordinates of a material point). The unit vectors of the magnetization easy directions (short-axes) of the three tetragonal martensite variants ($\boldsymbol{e}_1^{\text{tr}}$, $\boldsymbol{e}_2^{\text{tr}}$ and $\boldsymbol{e}_3^{\text{tr}}$) are mutually orthogonal due to the tetragonal symmetry of the variants; they form a matrix $\boldsymbol{E}=[\,\boldsymbol{e}_1^{\text{tr}}\quad\boldsymbol{e}_2^{\text{tr}}\quad\boldsymbol{e}_3^{\text{tr}}\,]$ which can be used to describe the unit vector of the magnetization easy direction of a material point in a variant state $\boldsymbol{\eta}$ as

$$\boldsymbol{e}^0=\frac{\boldsymbol{E\eta}}{|\boldsymbol{E\eta}|}=\frac{\boldsymbol{E\eta}}{|\boldsymbol{\eta}|} \tag{1}$$

The transformation strain of each tetragonal martensite variant can be described by

$$\boldsymbol{\varepsilon}_K^{\text{tr}}=\frac{a_t-a_c}{a_c}\boldsymbol{I}+\frac{c_t-a_t}{a_c}\boldsymbol{e}_K^{\text{tr}}\otimes\boldsymbol{e}_K^{\text{tr}},\quad (K=1,2,3) \tag{2}$$

where $\boldsymbol{I}$ is the second order identity tensor and a_c, a_t, c_t are the lattice parameters for the cubic parent phase, the long axis and short axis of tetragonal martensite phases, respectively. The total free energy $F=F(\boldsymbol{r},t)$ includes the following terms:

$$F=F_{\text{chemical}}+F_{\text{gradient}}+F_{\text{elastic}}+F_{\text{ex-mechanical}}+F_{\text{anisotropy}}+F_{\text{magnetostatic}}+F_{\text{exchange}}+F_{\text{Zeeman}} \tag{3}$$

where only $F_{\text{anisotropy}}$ is a functional of all the phase-field variables (LRO parameters and the magnetization angles), coupling the magnetic and mechanical properties.

(i) The chemical energy with the symmetry of the parent cubic phase [42,48] is given as

$$F_{\text{chemical}}=\int_{R^3}\left[\frac{a}{2}\boldsymbol{\eta}^2-\frac{b}{3}\boldsymbol{\eta\eta}^{\text{square}}+\frac{c}{4}(\boldsymbol{\eta}^2)^2\right]d\boldsymbol{r} \tag{4}$$

where a, b, c are coefficients which are chosen to provide the energy minima corresponding to the three tetragonal martensite variants, and $\boldsymbol{\eta}^{\text{square}}=\boldsymbol{\eta}^{\text{square}}(\boldsymbol{r},t)=(\eta_1^2(\boldsymbol{r},t),\eta_2^2(\boldsymbol{r},t),\eta_3^2(\boldsymbol{r},t))$.

(ii) The gradient energy is formulated as

$$F_{\text{gradient}}=B\int_{R^3}(\text{grad}\boldsymbol{\eta})^2d\boldsymbol{r} \tag{5}$$

where B is the gradient coefficient for the LRO parameters.

(iii) The elastic energy is obtained based on Khachaturyan's theory [49] for the strain energy of multiphase alloys as

$$F_{\text{elastic}}=\frac{1}{2}\frac{1}{(2\pi)^3}\int_{R^3}\left(\tilde{\boldsymbol{\varepsilon}}^0:\tilde{\boldsymbol{\sigma}}^{0*}-\boldsymbol{n}\tilde{\boldsymbol{\sigma}}^0\boldsymbol{\Omega}\tilde{\boldsymbol{\sigma}}^{0*}\boldsymbol{n}\right)d\boldsymbol{k},\quad(\boldsymbol{k}\neq 0) \tag{6}$$

where $\boldsymbol{k}$ is a reciprocal spatial vector and $\boldsymbol{n}=\boldsymbol{k}/|\boldsymbol{k}|$; $\tilde{\boldsymbol{\varepsilon}}^0=\tilde{\boldsymbol{\varepsilon}}^0(\boldsymbol{k},t)=\int_{R^3}\boldsymbol{\varepsilon}^0(\boldsymbol{r},t)e^{-i\boldsymbol{kr}}d\boldsymbol{r}$ is the Fourier transform of the strain tensor of a stress-free state $\boldsymbol{\varepsilon}^0(\boldsymbol{r},t)=\sum_{K=1}^{3}\boldsymbol{\varepsilon}_K^{\text{tr}}\eta_K(\boldsymbol{r},t)$; $\tilde{\boldsymbol{\sigma}}^0=\mathbb{C}:\tilde{\boldsymbol{\varepsilon}}^0$, $\boldsymbol{\Omega}=I/G-n\otimes n/[2G(1-v)]$, $\mathbb{C}=[2vG/(1-2v)]I\otimes\mathbb{I}+2G$ is the elastic modulus tensor, $\mathbb{I}$ is the fourth order identity tensor, G is the shear modulus and v is Poisson's ratio; The asterisk indicates the complex conjugate.

(iv) The external mechanical energy (mechanical potential) is given as

$$F_{\text{ex-mechanical}}=-\int_{R^3}\boldsymbol{\sigma}^{\text{ex}}:\boldsymbol{\varepsilon}d\boldsymbol{r} \tag{7}$$