THERMODYNAMIC AND MICROMECHANICAL-BASED MODELLING OF MARTENSITE VARIANTS REORIENTATION IN FSMAS

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Summary Ferromagnetic shape memory alloys (FSMAs) are smart heterogeneous materials with different orientated martensite variants and high magnetic anisotropy properties to produce giant magnetic field-induced strains and high frequency responses. Aim at the magneto-mechanical behaviors during the martensite variants reorientation, we present a thermodynamic and micromechanical-based modelling for FSMAs in this study. The thermodynamic balance between the thermodynamic driving force and the corresponding resistive force is formulated to calculate the volume fraction of the martensite variant during the reorientation process under different given stress and magnetic field. The theoretical results are found to be in good agreements with experimental data.

INTRODUCTION

At room temperature, ferromagnetic shape memory alloys (FSMAs) are always in the martensite states which consist of different variants with dissimilar magnetic and material properties like two-phase materials. Since their larger magnetic field-induced strains (MFIS) of 6%-10% and higher response frequencies, FSMAs have received much attention in the past decade. The origin of the extremely large MIFS is from the reorientation of martensite variants due to an external magnetic field and/or stress [1]. Plenty of theoretical models were proposed for predicting the macroscopic responses and microstructural characteristics of the martensite variants rearrangement process in FSMAs [2-4]. In these models, either the macroscopic responses or domain microstructural formations has been simulated, while the effect of microstructural evolutions on nonlinear magneto-mechanical constitutive behaviors always have not been incorporated. In addition, some theoretical models involve too much modelling parameters and some of them are quite difficultly determined by experimental measurements. In this study, a thermodynamic and micromechanical-based modelling of the martensite variants reorientation for FSMAs is proposed to investigate the magneto-mechanical behaviours. The model follows the well-established Eshelby equivalent inclusion method and the Mori-Tanaka scheme to describe the mechanical potential contribution to the Gibbs free energy in the heterogeneous FSMAs system. The thermodynamic balance between the thermodynamic driving force and the corresponding resistive force is formulated to calculate the volume fraction of the martensite variant during reorientation. The theoretical results are found to be in good agreement with experimental data.

THEORETICAL MODELLING AND FORMULATION

Consider a single-crystal FSMAs sample consisting of two martensite variants V_0 (with the volume fraction 1-ξ) and V_1 (with the volume fraction ξ), respectively denoted as the matrix and inclusion, as shown in Fig. 1. It is placed under external magnetic field and compression stress. Following the Eshelby equivalent inclusion method and the Mori-Tanaka scheme, the average stresses inside the two martensite variants under an applied uniform stress $\bar{s}$, are expressed in the forms

$$\mathbf{s}^{(0)} = \bar{\mathbf{s}} + \tilde{\mathbf{s}}^0 = \mathbf{L}_0(\mathbf{e}^0 + \tilde{\mathbf{e}}^0), \tag{1}$$

$$\mathbf{s}^{(1)} = \bar{\mathbf{s}} + \tilde{\mathbf{s}}^0 + \tilde{\mathbf{s}} = \mathbf{L}_1(\mathbf{e}^0 + \tilde{\mathbf{e}}^0 + \tilde{\mathbf{e}} - \mathbf{e}^p) = \mathbf{L}_0(\mathbf{e}^0 + \tilde{\mathbf{e}}^0 + \tilde{\mathbf{e}} - \mathbf{e}^p - \mathbf{e}^*). \tag{2}$$

Here $\mathbf{L}_0$ and $\mathbf{L}_1$ are respectively the stiffness tensors of the variants V_0 and V_1. $\mathbf{e}^p$ represents the eigenstrain during the martensite variants reorientation process. $\tilde{\mathbf{e}}^0 = -x(\mathbf{S}-\mathbf{I})(\mathbf{e}^p + \mathbf{e}^*)$, $\tilde{\mathbf{e}} = \mathbf{S}(\mathbf{e}^p + \mathbf{e}^*)$ where $\mathbf{e}^*$ is the equivalent eigenstrain given by $\mathbf{e}^* = \{\mathbf{L}_0 + (\mathbf{L}_1 - \mathbf{L}_0)[\mathbf{S} - x(\mathbf{S}-\mathbf{I})]\}^{-1}(\mathbf{L}_0 - \mathbf{L}_1)[\mathbf{e}^0 + (1-x)(\mathbf{S}-\mathbf{I})\mathbf{e}^p]$, and $\mathbf{S}$ is Eshelby tensor. By means of volumetric average, the elastic strain in the FSMAs sample is gained by

$$\bar{\mathbf{e}} = (1-x)\mathbf{e}_e^{(0)} + x\ \mathbf{e}_e^{(0)} = \mathbf{e}_0 + x\ \mathbf{e}^*. \tag{3}$$

The Gibbs free energy in the FSMAs system can be written as

$$G = G_{me} + G_z + G_{an} + G_d \ . \tag{4}$$

The contributions are from the mechanical potential energy G_{me}, Zeeman energy G_z, magnetocrystalline anisotropy energy G_{an} and demagnetization energy G_d, which are expressed by

$$G_{me} = -\tfrac{1}{2}\bar{\mathbf{s}} : \bar{\mathbf{e}} = -\tfrac{1}{2}\bar{\mathbf{s}} : (\mathbf{e}_0 + x\mathbf{e}^*),\ \ G_{ze} = -m_0 H M_s[x(2a_1 - 1) - (1-x)(a_2 \sin q_2 + (1-a_2)\sin q_4],$$

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$$G_{an}=(1-x)K[a_2\sin^2 q_2+(1-a_2)\sin^2 q_4],\ \ G_d=\tfrac{1}{2}m_0 NM_s^2[x(2a_1-1)^2+(1-x)(a_2\sin q_2+(1-a_2)\sin q_2)^2]. \quad (5)$$

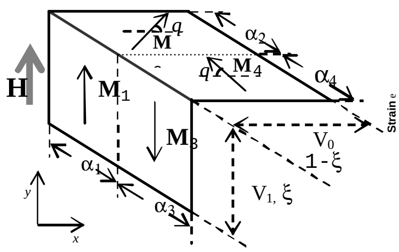
Here, q_i, a_i respectively are the magnetization rotation angles and volume fractions of magnetic domains, K, M_s respectively denote the anisotropy constant and the saturation magnetization. During the martensite variants reorientation, from physical observation, the processes associated with the magnetization rotation and magnetic domain motion are reversible. As a result, the corresponding thermodynamic driving forces are zeros, i.e. $\partial G/\partial q_i=0$, $\partial G/\partial a_i=0$. Furthermore the reduction of Gibbs free energy gives rise to a thermodynamic force that drives the martensite variants reorientation based on the second law of thermodynamics. The driving force is countered by the resistance force from the thermodynamic equilibrium point of view so that a thermodynamic balance is obtained by

$$-\partial G/\partial x=p_{res}, \quad (6)$$

where the resistance force is expressed by $p_{res}=s_{eff}e_r^{\max}=(s_{tw}+\bar{s})e_r^{\max}$, with s_{tw} and $e_r^{\max}$ respectively denoting the de-twinning stress and the maximum reorientation strain. The above thermodynamic balance equation gives the volume fraction of the product (or inclusion) phase V_1 for given external stress and magnetic field. Then the overall strain behavior and magnetization profile of the FSMAs sample can be obtained.

APPLICATION OF MODLE AND RESULTS

The developed thermodynamic and micromechanical-based model is applied to simulate the magneto-mechanical behaviors and the martensite variants reorientation of a single-crystal Ni-Mn-Ga sample under external magnetic field and stress. The applied magnetic field to the sample is oriented in the *y* direction, and the applied compressive stress is oriented in the *x* direction. For validation of the presented model, firstly, the effect of the applied magnetic field on the martensite variants reorientation behavior of FSMA is characterized. The material parameters used for the simulations are chosen from the experimental data [5,6]. The responses of magnetic field-induced strain versus magnetic field during martensite variants reorientation for different compression stress are plotted in Fig. 2(a). The predictions are much closer to the experimental measurements except for the case of compression stress 1.4MPa where the predicted critical magnetic field of the reorientation startup is smaller than the measured one. However, when the applied compression stress is quite large the martensite variants reorientation cannot occur. The present model also gives the good prediction on this feature as shown in Fig. 2(a). And then the corresponding magnetization characteristics are depicted in Fig. 2(b), to compare with the experiment observations. Fig. 2(c) plots the strain-stress responses of the FSMAs sample during the martensite variants reorientation at the different applied magnetic field. There shows that the predictions are in better agreements with the experimental data.



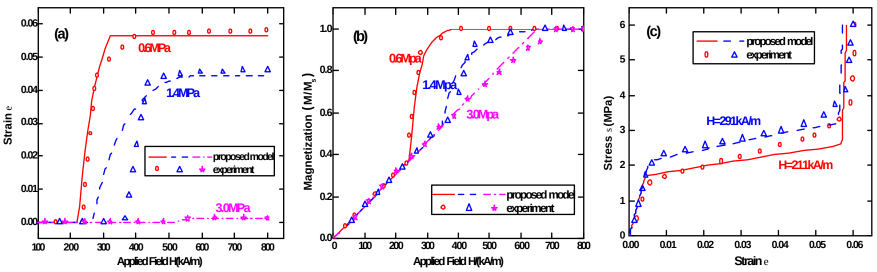


Fig.1 Simplified microstructure. Fig.2 Magneto-mechanical behavior: (a)strain vs. field, (b)magnetization, (c)stress vs. strain

CONCLUSIONS

The micromechanical-based thermodynamic formulation on magneto-mechanical behaviors of FSMAs during the process of martensite variants reorientation has been developed. The microstructural profiles of the magnetization and martensite variants have taken into account for the modelling of FSMAs. The magnetic field-induced strain and nonlinear constitutive response have been predicted to show a good agreement with the experimental data.

Acknowledgmetns: The authors acknowledge the support by the NNSF of China (10872081).

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