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Research paper

Effects of demagnetization on Magnetic-Field-Induced Strain and microstructural evolution in Ni-Mn-Ga Ferromagnetic Shape Memory Alloy by phase-field simulations

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ABSTRACT

Demagnetization effect plays a vital role in ferromagnetic materials. However, its influence on Magnetic-Field-Induced Strain (MFIS) in Ni-Mn-Ga Ferromagnetic Shape Memory Alloy has not yet been fully quantified. This study investigates demagnetization effects on MFIS and microstructural evolution in Ni-Mn-Ga for different demagnetization factors (i.e. vector $\boldsymbol{N}$) by phase-field simulations. The investigation reveals that demagnetization can exert substantial impact on both macroscopic and microscopic behavior of Ni-Mn-Ga through the influence of internal magnetic field on twin boundary movement and domain evolution. The switching field and the saturating field as well as their difference increase with N_f (component of $\boldsymbol{N}$ parallel to easy axis of field-favored martensitic variant). For larger N_f values, the increase of strain appears to be less sharp and more stable (hardening-like). The stable increase of strain is ascribed to the steady movement of twin boundary. The velocity of magnetic domain wall motion during MFIS process decreases as N_u (component of $\boldsymbol{N}$ parallel to easy axis of field-unfavored martensitic variant) increases and their relationship obeys the power law. However, N_u does not seem to affect strain behavior or twin boundary movement. The dependence of switching field and saturating field on N_f is established for application design purposes.

1. Introduction

Ni-Mn-Ga Ferromagnetic Shape Memory Alloys (FSMAs) are ferromagnetic materials that exhibit large Magnetic-Field-Induced Strain (MFIS) and high-frequency response at room temperature as a result of martensitic phase transformation through the imposition of applied magnetic fields. Due to such unique characteristics, Ni-Mn-Ga FSMAs have attracted growing interests in academia and industry and have emerged as promising materials for applications in sensors [1,2], actuators [3,4] and dampers [5]. Typically, Ni-Mn-Ga single crystals have three different martensitic phases, i.e., tetragonal five-layered modulated martensite (5M), orthorhombic seven-layered modulated martensite (7M), and tetragonal non-modulated martensite (NMT) [6], among which 5M martensite has received the most significant research attention in recent years probably because of its high availability and possibilities for applications. For 5M Ni-Mn-Ga, which is studied in the present work, there are three tetragonal martensitic variants, whose short axes (c-axis) of the lattice are also the magnetic easy axes [7]. It has been shown that the underlying physical mechanism for large MFIS of 5M Ni-Mn-Ga is the reorientation of tetragonal martensitic variants under the condition of high magnetocrystalline anisotropy and low twinning stress [7,8]. Under an external magnetic field, the martensitic variant with the magnetic easy axis parallel to the field (i.e., field-favored variant) grows at the expense of another martensitic variant with the magnetic easy axis perpendicular to the field (i.e., field-unfavored variant) through the twin boundary movement, resulting in a macroscopic strain. Moreover, Ni-Mn-Ga FSMAs can actuate at higher frequencies (up to 1 kHz) by magnetic fields as compared to the relatively slow process of shape change by temperature in conventional shape memory alloy [9].

Driven by the increasing demands in academia and industry, MFIS and the underlying microstructural evolution in Ni-Mn-Ga have been extensively studied in the past two decades. For example, Ullakko et al. [10] first observed a field-induced strain of 0.2% in single crystalline Ni-Mn-Ga with a sample measuring a few mm square in cross section by 6 mm long. In a later study, Chopra et al. [11] reported direct microscopic evidence of magnetoelastic coupling between martensite twin domains and magnetic domains by using a Ni-Mn-Ga single crystal with a dimension of 16 mm × 2 mm × 0.4 mm. On the other hand, Heczko et al. [12] discovered a strain of 5.1% under the influence of a magnetic field along the long axis of a sample with a dimension of 5 mm × 5 mm × 9 mm. Similarly, Murray et al. [13] unveiled strains of 6% by applied fields of order 400 KA/m in single crystalline Ni-Mn-Ga samples measuring 6 mm × 6 mm × 20 mm and concurrently captured the martensite twin structural evolution via high-speed camera.

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In a different way, Ge et al. [14] observed broad stripe-like magnetic domains and zig-zag shape of martensite twin domains by means of scanning electron microscope in single crystal specimens with a dimension of 3 mm × 4 mm × 6 mm. From a different perspective, Heczko [15] studied simultaneous responses of magnetization and strain during magnetic field loading-unloading cycles using single crystalline samples with a dimension of 5 mm × 5 mm × 9 mm and proposed a simple energy model to determine the criterion of martensite reorientation. More recently, Faran and Shilo [16] directly measured individual twin boundary velocities as a function of an applied pulsed magnetic field in Ni-Mn-Ga single crystals with a dimension of 3 mm × 2.4 mm × 0.9 mm. It should be noted that most of these above-mentioned studies were carried out by using different sample shapes and applying magnetic fields along different axes of the sample, which will lead to different demagnetization factors and effects [17].

It has long been recognized that the sample shape-dependent demagnetization effect plays an important role in ferromagnetic materials. Due to the special ferromagnetic properties of Ni-Mn-Ga FSMAs, the demagnetization effect can also have considerable impact on their behavior. For instance, Heczko et al. [18] showed that the shearing of the magnetization curve during the MFIS process is caused by the demagnetization field. Techapiesancharoenkij et al. [19] pointed out that the switching field (onset of MFIS) and the saturating field (achievement of full MFIS), which determine the device volume and application possibility, depend on the sample shape and the loading conditions. On the other hand, a number of research works focused on the explanation and criterion of MFIS by proposing models without considering magnetic domains and domain walls [8,13,15]. Several other studies placed emphasis on the observation of magnetic domain structure evolution during martensite reorientation or twin boundary movement [11,14,23,24]. However, since the magnetic behavior of Ni-Mn-Ga is highly dependent on the demagnetization effect, in order to comprehend the influence of magnetic domains or domain walls in MFIS, it is necessary to examine the demagnetization effects on the interaction between magnetic domains and martensite twin structure. Moreover, the Ni-Mn-Ga thin film/foil has received considerable research attention due to its potential actuator applications in micro-dimensions [20–22,35,36]. The sudden change of the sample shape from bulk to thin film/foil will lead to a significant variation of the demagnetization effect. In addition, the different sample shape-dependent demagnetization effects on MFIS cannot be eliminated by just excluding demagnetization field, because the process of coupled martensitic and magnetic structure evolution in MFIS is closely related to the loading path. Therefore, it is important to understand and quantify the demagnetization effects on both the macroscopic and microscopic behavior of Ni-Mn-Ga in MFIS. Although there exist experiments (e.g., among others, [7,12,25]) and models (e.g., among others, [23,37–39]) studying on Ni-Mn-Ga by considering the demagnetization field, to the best of our knowledge, the investigation of the demagnetization effects on MFIS and the associated microstructural evolution as well as the fundamental physical mechanism regarding this material has not yet been reported. To develop a more complete understanding of the cause of the problem, further research on both the macroscopic and microscopic behavior of Ni-Mn-Ga in MFIS as well as the utilization of more advanced quantitative analytical techniques is warranted.

Motivated by the aforementioned literature review, this paper examines the effects of demagnetization on MFIS and the associated microstructural evolution in Ni-Mn-Ga by using a phase-field method. Most existing phase-field models on FSMA (e.g. [23,24,26]) have successfully modeled macroscopic responses and microstructural evolution under coupled magneto-mechanical loadings. But the rate-independent hysteresis in macroscopic responses and the full effect of demagnetization (including both the spatially dependent heterogeneous part and the spatially independent average part), which are both important for investigating the demagnetization effect under quasi-static loadings, were only considered in Peng et al. [26] and Zhang and Chen [23], respectively. In this work, the adopted phase-field model is capable of capturing both the rate-independent hysteresis and the full effect of demagnetization in FSMA. Specifically, the field-strain curve, the field-magnetization curve, and the evolution of martensitic/magnetic structure in a Ni-Mn-Ga single crystal are investigated for different demagnetization factors. On the basis of the conducted research investigations, the dependence of switching field, saturating field and domain wall motion on the relevant demagnetization factor is quantified. The physical cause of the demagnetization effects on the behavior of this material is also identified. The results predicted from our simulations are compared with existing experimental observations. The rest of the paper is organized as follows. Section 2 describes the governing equations of the phase-field model. Section 3 reports the phase-field simulation results. Section 4 analyzes the phase-field simulation results and the underlying physical mechanism. Finally, major conclusions obtained from this research work are summarized in Section 5.

2. Governing equations of the phase-field model

Following existing models [23,24,26,27], the phase-field model is adopted in the present study. In addition to its capacity of capturing macroscopic responses and microstructural evolution under quasi-static magnetic/mechanical loads, the main advantage of this model over previous theoretical works is that it considers both the rate-independent resistance in the martensite reorientation and the full effect of demagnetization by incorporating the effects of sample shape on magnetic domain structures. In this model, the microstructure state of Ni-Mn-Ga FSMA is described by two fields: the Long-Range Order (LRO) parameter $\boldsymbol{\eta}(\boldsymbol{r},t)=(\eta_1(\boldsymbol{r},t),\eta_2(\boldsymbol{r},t),\eta_3(\boldsymbol{r},t))$ [24,26,27] that describes the martensite twin structure and the normalized magnetization vector $\boldsymbol{m}(\boldsymbol{r},t)=(m_1(\boldsymbol{r},t),m_2(\boldsymbol{r},t),m_3(\boldsymbol{r},t))$ [23] that represents the magnetic domain structure. Assuming constant saturation magnetization, i.e., $M_s=4.99\times10^5$ A/m [15], the magnetization vectors can then be expressed as $\boldsymbol{M}(\boldsymbol{r},t)=M_s\boldsymbol{m}(\boldsymbol{r},t)$.

The total free energy $F=F(\boldsymbol{r},t)$ includes the following eight terms that are written in tensorial notation as:

$$
\begin{aligned}
F = & \int_{\boldsymbol{R}^3}\left[\frac{a}{2}\boldsymbol{\eta}^2-\frac{b}{3}\boldsymbol{\eta}\boldsymbol{\eta}^{\text{square}}+\frac{c}{4}\left(\boldsymbol{\eta}^2\right)^2\right]d\boldsymbol{r}+B\int_{\boldsymbol{R}^3}(\text{grad}\boldsymbol{\eta})^2d\boldsymbol{r} \\
& +\frac{1}{2}\frac{1}{(2\pi)^3}\int_{\boldsymbol{R}^3}\left(\widetilde{\boldsymbol{\varepsilon}}^0:\widetilde{\boldsymbol{\sigma}}^{0*}-\boldsymbol{n}\widetilde{\boldsymbol{\sigma}}^0\boldsymbol{\Omega}\widetilde{\boldsymbol{\sigma}}^{0*}\boldsymbol{n}\right)d\boldsymbol{k}-\int_{\boldsymbol{R}^3}\boldsymbol{\sigma}^{\text{ex}}:\boldsymbol{\varepsilon}^0d\boldsymbol{r} \\
& +K_u\int_{\boldsymbol{R}^3}\left[1-\left(\boldsymbol{m}\boldsymbol{e}^0\right)^2\right]d\boldsymbol{r}+\mu_0M_s^2\left[\frac{1}{2}\frac{1}{(2\pi)^3}\int_{\boldsymbol{R}^3}\left|\boldsymbol{n}\widetilde{\boldsymbol{m}}\right|^2d\boldsymbol{k}-\int_{\boldsymbol{R}^3}\bar{\boldsymbol{h}}_d\boldsymbol{m}d\boldsymbol{r}\right] \\
& +A\int_{\boldsymbol{R}^3}(\text{grad}\boldsymbol{m})^2d\boldsymbol{r}-\mu_0M_s^2\int_{\boldsymbol{R}^3}\boldsymbol{h}_{\text{ex}}\boldsymbol{m}d\boldsymbol{r} \qquad (\boldsymbol{k}\neq0)
\end{aligned}
\tag{1}
$$

where the energy terms are chemical energy [24,27], gradient energy [24,26], elastic energy [27,28], external mechanical energy [24], magnetocrystalline anisotropy energy [29], magnetostatic energy [23,26], exchange energy [23,24], and external field (Zeeman) energy [29], respectively. In the equation, the chemical energy is formulated by Landau polynomial, which is able to reflect the symmetry of the austenite cubic phase, and a, b, c are coefficients to provide the chemical energy minima corresponding to the three tetragonal martensitic variants [24]. $\boldsymbol{\eta}^{\text{square}}(\boldsymbol{r},t)=(\eta_1^2(\boldsymbol{r},t),\eta_2^2(\boldsymbol{r},t),\eta_3^2(\boldsymbol{r},t))$. The gradient energy characterizing twin boundary behavior is simply defined in a phenomenological way and B is the gradient coefficient for LRO parameters [26]. The elastic energy is obtained by Khachaturyan's structural transformation theory, which is capable of describing the elastic strain caused by crystal lattice rearrangement and incorporating the Fourier transform. $\boldsymbol{k}$ is the reciprocal spatial vector such that $\boldsymbol{n}=\boldsymbol{k}/|\boldsymbol{k}|$. $\widetilde{\boldsymbol{\varepsilon}}^0(\boldsymbol{k},t)=\int_{\boldsymbol{R}^3}\boldsymbol{\varepsilon}^0(\boldsymbol{r},t)e^{-i\boldsymbol{k}\boldsymbol{r}}d\boldsymbol{r}$ is the Fourier transform of the stress-free state strain $\boldsymbol{\varepsilon}^0(\boldsymbol{r},t)=\sum_{K=1}^{3}\boldsymbol{\varepsilon}_K^{\text{tr}}\eta_K(\boldsymbol{r},t)$, where $\boldsymbol{\varepsilon}_K^{\text{tr}}$ is the transformation strain of Kth martensitic variant