Multi-scale simulations of metamagnetic martensite transition in NiCoMnIn

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ABSTRACT

A multi-scale theoretical model is performed to investigate magnetic field-induced metamagnetic martensite transition in NiCoMnIn alloys. First, the total energy is calculated to demonstrate antiferromagnetic-ferromagnetic transition from first principle calculation. Second, the transition temperature from antiferromagnetic to ferromagnetic can be tuned by the external magnetic field and hydrostatic pressure in thermodynamic calculation, which is consistent with experimental results. Third, phase field simulation found that martensite variant boundaries are superposed with the 90° antiferromagnetic magnetic domain walls, revealing magneto-structural coupling between structural and magnetic domain structures. It is demonstrated that this multi-scale model is very effective for describing antiferromagnetic-ferromagnetic accompanied with martensite-austenite transitions with magnetostructural coupling.

KEYWORDS

Phase field simulations, Metamagnetic transition, NiCoMnIn, Magnetostructural coupling

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1. Introduction

Heusler alloys NiMnIn have attracted great attention due to their magnetic shape memory and magnetocaloric effects in the past decades¹. In those alloys, the ferroelastic and ferromagnetic orderings are coupled, thus a magnetic field can manipulate the reorientation of ferroelastic domains to obtain giant strain. The strain is one order of magnitude higher than that of the giant magnetostrictive materials². On the other hand, the large entropy change, which is an essential property of magnetic refrigeration material³, can be realized under the driving of an external magnetic field.

The key to finding metamagnetic materials is in search for the materials whose phase transition temperature is sensitive to the external magnetic field. The experiments showed that doping Co in NiMnX alloys (X=Ga, In, Sn, Sb) can improve the response sensitivity of the phase transition temperature⁴. For NiCoMnIn alloy, there are two-phase transitions with the decrease of temperature, from paramagnetic (PM) austenite (Aust) to ferromagnetic (FM) Aust, then to antiferromagnetic (AFM) martensite (Mart). In addition, the phase transition temperatures can be adjusted by the external magnetic field or stress. Consequently, several similar alloys such as NiCoMnSn⁵, NiCoMnSb⁶, NiCoMnGa⁷, and even their Cu-coped counterparts⁸⁻¹⁰ were investigated for the magnetocaloric effect. In addition, Landau phenomenological theory^{11, 12} and the first principle calculation¹³⁻¹⁵ were developed to describe Mart phase transitions. Although several groups have already simulated FM in Mart phase transitions of NiMnGa¹⁶⁻²⁰, they focused on the phase stability and domain orientation without considering the metamagnetic behavior. There is no existing theoretical description of systems with metamagnetic features²¹.

We investigate the magnetic phase transition as a function of temperature, and the saturation magnetization M_s of NiCoMnIn is temperature-dependent. Therefore, we propose to use the

time-dependent Ginzburg-Landau (TDGL) equation to describe the metamagnetic transition^{22, 23}. In this paper, we firstly calculated the total energy as a function of the magnetic unit to indentify the metamagnetic transition temperature by using first principle calculation. Then the metamagnetic transition temperature can be tuned by the external magnetic field and hydrostatic pressure according to the thermodynamic calculations. Furthermore, the phase field simulation is performed to investigate the microstructure of magnetic domain.

2. Theoretical Model

In this work, we performed the calculation based on the density functional theory (DFT) using the Vienna ab initio simulation package (VASP)^{24, 25}. The electronic exchange-correlation were described within a spin polarized generalized-gradient approximation (GGA) using the functional proposed by Perdew et al²⁶. The electron-ion interaction was described with the projector augmented-wave (PAW) formalism²⁷. We use L2₁ cubic structure (*austenite*) which is the conventional 16-atoms cell (Ni₈Mn₆In₂) substituting two In atoms with Mn atoms and L1₀ tetragonal structure (*martensite*) with c/a=1.27 for the calculation. The AFM configuration is that the magnetic moment of Mn atoms at In sites is antiparallel to that at the original sites. Cut-off energy was truncated at 450 eV for the plane wave basis, and a Monkhorst-Pack²⁸ type 11 × 11 × 11 k-point grid was adopted for energy calculation. In the fixed spin moment (FSM)^{29, 30} procedure, we determine the total energy E of a system constrained to have a given magnetic moment M per unit cell.

For the thermodynamic calculation, the directions of spins do not change significantly from one lattice point to another in the FM materials. However, spins of an AFM phase usually have opposite directions from lattice point to lattice point. As shown in Figure 1, if the AFM is divided

into sublattices³¹, the magnetic moments can be described by two antiparallel FM sublattices of A and B whose magnetizations are expressed by $\mathbf{M}_1$ and $\mathbf{M}_2$. Furthermore, we define $\mathbf{M}=(\mathbf{M}_1+\mathbf{M}_2)/2M_s$ and $\mathbf{L}=(\mathbf{M}_1-\mathbf{M}_2)/2M_s$ as FM and AFM order parameters, respectively, and M_s indicates the constant magnetization at 280 K and zero external magnetic field. If $\mathbf{M}_1$ and $\mathbf{M}_2$ are parallel, $\mathbf{M}\neq 0$, and $\mathbf{L}=0$. Otherwise, if $\mathbf{M}_1$ and $\mathbf{M}_2$ are antiparallel, $\mathbf{M}=0$, and $\mathbf{L}\neq 0$.

It is observed in experiments that NiCoMnIn single crystal stabilizes in three phases, i.e., PM Aust phase above 382K, FM Aust phase between 285K and 380K, AFM Mart phase below 280K. The transition temperatures from PM to FM (Curie temperature T_C), from FM to AFM (T_A), and from Aust to Mart (T_M) can be shifted by applying external stimulus such as magnetic field or stress. Under the external magnetic field or stress, the magnetic domain and Mart variants will evolve to minimize the total free energy.

For phase field model, we focus on the metamagnetic transitions, and the magnetization $\mathbf{M}$ of NiCoMnIn is temperature dependent. Therefore, we use three TDGL equations to evolve the FM magnetization $\mathbf{M}$, AFM magnetization $\mathbf{L}$ and Mart strain ε_{ii}^0 :

$$\frac{\partial \mathbf{M}(\mathbf{r}, t)}{\partial t} = -L^m \frac{\delta E}{\delta \mathbf{M}}, \quad \frac{\partial \mathbf{L}(\mathbf{r}, t)}{\partial t} = -L^l \frac{\delta E}{\delta \mathbf{L}}, \quad \frac{\partial \varepsilon_{ii}^0(\mathbf{r}, t)}{\partial t} = -L^e \frac{\delta E}{\delta \varepsilon_{ii}^0}, \quad (1)$$

where L^m , L^l and L^e are kinetic coefficients relating to the FM, AFM domain evolution and the twin boundary mobility.

The total free energy for NiCoMnIn in the thermodynamic calculation can be expressed by²¹,

$$\begin{aligned}
E = & \int \{ \alpha_1 (M_x^2 + M_y^2 + M_z^2) + \alpha_{11} (M_x^4 + M_y^4 + M_z^4) + \alpha_{111} (M_x^6 + M_y^6 + M_z^6) \\
& + \alpha_{12} (M_x^2 M_y^2 + M_x^2 M_z^2 + M_y^2 M_z^2) + \alpha_{123} M_x^2 M_y^2 M_z^2 \\
& + \alpha_{112} [M_x^2 (M_y^2 + M_z^2) + M_y^2 (M_x^2 + M_z^2) + M_z^2 (M_x^2 + M_y^2)] \\
& + \beta_1 (L_x^2 + L_y^2 + L_z^2) + \beta_{11} (L_x^4 + L_y^4 + L_z^4) + \beta_{111} (L_x^6 + L_y^6 + L_z^6) \\
& + \beta_{12} (L_x^2 L_y^2 + L_x^2 L_z^2 + L_y^2 L_z^2) + \beta_{123} L_x^2 L_y^2 L_z^2 \\
& + \beta_{112} [L_x^2 (L_y^2 + L_z^2) + L_y^2 (L_x^2 + L_z^2) + L_z^2 (L_x^2 + L_y^2)] \\
& + \mu_{11} (M_x L_x + M_y L_y + M_z L_z)^2 + \mu_{12} (M_x^2 + M_y^2 + M_z^2) (L_x^2 + L_y^2 + L_z^2) \\
& - \mathbf{H}_d \cdot \mathbf{M} + Q_1 e_1^2 + Q_2 (e_2^2 + e_3^2) + Q_3 (e_4^2 + e_5^2 + e_6^2) \\
& + Q_4 e_1 (e_2^2 + e_3^2) + Q_5 e_3 (e_3^2 - 3e_2^2) + Q_6 (e_2^2 + e_3^2)^2 + \frac{1}{2} c_{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) \\
& + \gamma_0 e_1 (M_x^2 + M_y^2 + M_z^2) + \gamma_1 [e_2 (M_x^2 - M_y^2) / 2 + e_3 (3M_z^2 - \mathbf{M}^2) / \sqrt{6}] \\
& + \gamma_2 (e_4 M_x M_y + e_5 M_y M_z + e_6 M_x M_z) \\
& + \lambda_0 e_1 (L_x^2 + L_y^2 + L_z^2) + \lambda_1 [e_2 (L_x^2 - L_y^2) / 2 + e_3 (3L_z^2 - \mathbf{L}^2) / \sqrt{6}] \\
& + \lambda_2 (e_4 L_x L_y + e_5 L_y L_z + e_6 L_x L_z) - (H_x M_x + H_y M_y + H_z M_z) - \sigma e_1 \} dV
\end{aligned} \tag{2}$$

where $\alpha_1, \alpha_{11}, \alpha_{111}, \alpha_{12}, \alpha_{123}, \alpha_{112}, \beta_1, \beta_{11}, \beta_{111}, \beta_{12}, \beta_{123}, \beta_{112}, \mu_{11}, \mu_{12}$ are exchange-interaction coefficients, $\mathbf{H}_d$ is the demagnetization field that arises from the long-range interactions among the magnetic moments in the system. The linear combination of the deformation tensor components e_i can be defined in terms of the transformation strains, $e_1 = (\varepsilon_{11}^0 + \varepsilon_{22}^0 + \varepsilon_{33}^0) / \sqrt{3}$, $e_2 = (\varepsilon_{11}^0 - \varepsilon_{22}^0) / \sqrt{2}$, $e_3 = (2\varepsilon_{33}^0 - \varepsilon_{11}^0 - \varepsilon_{22}^0) / \sqrt{6}$, $e_4 = \varepsilon_{23}^0$, $e_5 = \varepsilon_{13}^0$, $e_6 = \varepsilon_{12}^0$. Additionally, $Q_1, Q_2, Q_3, Q_4, Q_5, Q_6$ are the linear combinations of the second-, third-, and fourth-order elastic moduli, respectively; $Q_1 = (C_{11} + 2C_{12}) / 2\sqrt{3}$, $Q_2 = (C_{11} - C_{12}) / 2$, $Q_3 = C_{44}$, $Q_4 = (C_{111} - C_{123}) / 2\sqrt{3}$, $Q_5 = (C_{111} - 3C_{112} + 2C_{123}) / 18\sqrt{6}$, $Q_6 = (C_{1111} + C_{1112} - 3C_{1122} - 8C_{1123}) / 192$. ε_{ij} is the total strain, and ε_{ij}^0 is the stress-free eigenstrain. c_{ijkl} represents the components of the second-order elastic stiffness tensor, and C_{ij} are the elastic constants in Voigt notation, i.e., $C_{11} = C_{1111}$, $C_{12} = C_{1122}$,

$C_{44}=C_{2323}$. γ_0 , λ_0 are the volume magnetostriction constants, and $\gamma_{1,2}$, $\lambda_{1,2}$ are the anisotropic magnetostriction constants of the FM and AFM phases, $\mathbf{H}$ and σ are the external magnetic field and stress. In addition, the total energy in the phase-field simulations also includes the gradient and exchange energy densities which can be calculated by,

$$f_{\text{grad}} = g[(\epsilon_{11,1}^0)^2 + (\epsilon_{11,2}^0)^2 + (\epsilon_{11,3}^0)^2 + (\epsilon_{22,1}^0)^2 + (\epsilon_{22,2}^0)^2 + (\epsilon_{22,3}^0)^2 + (\epsilon_{33,1}^0)^2 + (\epsilon_{33,2}^0)^2 + (\epsilon_{33,3}^0)^2] \quad (3)$$

$$f_{\text{exch}} = A_M \left[(\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2 \right] + A_L \left[(\nabla L_x)^2 + (\nabla L_y)^2 + (\nabla L_z)^2 \right] \quad (4)$$

where g is the isotropic gradient energy coefficient, and A_M and A_L are the exchange constants of FM and AFM. The model size of $64 \times 64 \times 1$ is employed. The coefficients are obtained from the thermodynamic simulations²² and can be found in our previous paper²³.

3. Results and Discussions

As shown in Figure 2, we use first principle calculation to obtain the total energy as a function of the total magnetic moment of the unit cell. Our results show that there is a tetragonal phase (Mart) at the small magnetic moment (7.98 μ_B), and a cubic phase (Aust) at the large magnetic moment (25.6 μ_B). According to the curve, the total energy of the tetragonal phase with small magnetic moment is lower than that of cubic phase with high magnetic moment. It means that the tetragonal structure (Mart) is more stable than the cubic phase (Aust) at zero Kelvin.

Using the fitted coefficients, we calculated the metamagnetic transition of NiCoMnIn alloy single crystalline from Eq. (2) by minimizing the total free energy from thermodynamic calculation. Figure 3 shows the total free energy as a function of temperature with different external magnetic fields. For the black line, the free energy of AFM Mart increases with the temperature and becomes zero at around 300K. The free energy of FM Aust under different external magnetic fields also increases with the temperature. The total free energy for AFM Mart

and FM Aust show independent and dependent on the magnetic field, respectively. The external magnetic field will reduce the total free energy of FM at the same temperature. The intersections of AFM and FM free energies curves are the transition temperatures from AFM Mart to FM Aust. If the temperature is lower than that of the intersection, the material is AFM Mart. Otherwise, the material is FM Aust. We observe that the transition temperature (T_A or T_M) is decreasing with the increase of external magnetic fields.

Under a hydrostatic pressure, the applied stress tensors satisfy $\sigma = -p$, where p is the hydrostatic pressure. As shown in Figure 4, the AFM-FM transition temperature as a function of magnetic field and hydrostatic pressure were calculated from thermodynamic simulation. Figure 4 (a) shows the AFM-FM transition temperature decrease with the increase of magnetic field, and FM-PM transition temperature is increasing with the magnetic field, which are consistent with the experimental data. The external magnetic field will favor FM state, which results to the decrease of AFM-FM and the FM-PM transition temperatures. As shown in Figure 4(b), both AFM-FM transition temperature is increasing with the hydrostatic pressure, however FM-PM transition temperature is independent on the hydrostatic pressure.

As shown in Figures 5 (a) and (b), we calculated the FM, AFM magnetizations $\mathbf{M}$, $\mathbf{L}$ and Mart strain ε_{ii}^0 at the temperature of 200 K from the initial random distribution from phase-field simulations. We observed that the FM magnetization $\mathbf{M}$ is zero, and the AFM magnetization $\mathbf{L}$ and Mart strain are increasing with the evolution. It indicates that the metamagnetic transition can be described by our model. Figures 5 (c), (d) and (e) show FM domains, AFM domains and Mart variants at the low temperature. The arrows of figure 5 (d) represents the directions of $\mathbf{L}$ which is along $-x$, $+x$, $-y$ and $+y$ axes. In figure 5 (e), yellow, and purple areas represent Mart variant A, and Mart variant B, respectively. We clearly observed the AFM domains coupled to

the Mart variants at low temperatures. The weak magnetic domain can be described at the low temperature of Mart phase in which the Mart variant boundaries are superposed with the 90° magnetic domain wall as an evidence of magnetostructural coupling. The magnetic domains and martensite variants are coupled together due to the magnetoelastic energy. The magnetoelastic energy density can be calculated by,

$$f_{coup} = \gamma_0 e_1 (M_x^2 + M_y^2 + M_z^2) + \gamma_1 \left[e_2 (M_x^2 - M_y^2) / 2 + e_3 (3M_z^2 - \mathbf{M}^2) / \sqrt{6} \right] + \lambda_0 e_1 (L_x^2 + L_y^2 + L_z^2) + \lambda_1 \left[e_2 (L_x^2 - L_y^2) / 2 + e_3 (3L_z^2 - \mathbf{L}^2) / \sqrt{6} \right] \quad (5)$$

It is noticed that the magnetoelastic energy is proportional to two times order of M_i and L_i ($i=x, y$, and z). For the 180° domain wall, M_i or $-M_i$ (L_i or $-L_i$) will not change the magnetoelastic energy. However, M_i or $-M_i$ (L_i or $-L_i$) will change in the 90° domain wall. Therefore, the martensite variant boundaries are coupled with 90° domain walls. Furthermore, FM domain almost equals to zero at the low temperature. However, we can observe the maximum at the 90° domain wall which indicates the metamagnetic transition will happen in this area.

As shown in Figures 6 (a) and (b), we calculated the magnetization $\mathbf{M}$ as a function of external magnetic field $\mathbf{H}$ with different temperatures [from phase-field simulations](#). The curves in Figure 6 (a) at 190 and 320 K exhibit typical AFM and FM M-H behavior, respectively. The curves with the temperature from 250 to 290 K exhibit metamagnetic behavior. The applied magnetic field induces a reversal transformation from AFM to FM. During transformation, a mixed structure containing AFM and FM phases exists at 250~290 K. The hysteresis loops display sigmoid shapes, in which the magnetization rapidly increases and then slowly increases with increasing applied magnetic field strength. The magnetization does not saturate, even at 10 T [5]. If the temperature continues to increase, the magnetic transition from FM to PM phase would occur at T_C . Figure 6 (b) shows that the magnetization is low when the temperature

increases to 490 K, and that the $M(H)$ curves are linear at each temperature. Therefore, there are three types of magnetic field-induced magnetization curves, and these exhibit $M(H)$ typical behaviors of AFM, FM and PM, as a function of temperature. From the magnetization curves, we observe the magnetic field-induced metamagnetic transition, which is coupled to the Mart structural transformation.

4. Conclusions

We developed a multi-scale model to study the metamagnetic transition and domain structure. The metamagnetic transition from AFM to FM was obtained from DFT calculation. The transition temperature from AFM to FM can be tuned by the external magnetic field and hydrostatic pressure in thermodynamic calculation, which is consistent with the experimental results. It is found that the Mart variant boundaries are superposed with 90° AFM magnetic domain walls, revealing magneto-structural coupling between the structural and the magnetic domain structures. Thus, this method can be effectively used to describe the magnetic field induced metamagnetic transition, and explain the mechanism of magnetostructural coupling as well as facilitate applications in a Mart transition system.

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Figure Captions

Figure 1 (a) Schematic diagram of an AFM divided into two sublattices, and (b) schematic diagrams of the magnetic and structure transitions with the decrease of the temperature.

Figure 2 The total energy as a function of total magnetic moment of the unit cell from DFT calculation.

Figure 3 The total free energy as a function of temperature with different external magnetic fields from thermodynamic calculation.

Figure 4 The AFM-FM transition temperatures as a function of magnetic field and hystrostatic

pressure from thermodynamic calculation.

Figure 5 (a) (b) FM and AFM magnetizations and Mart strain average magnitude evolution (c)~(e) FM, AFM domains and Mart variants spatial distribution evolution from phase-field simulation.

Figure 6 (a) (b) Magnetization loops at different temperatures from phase-field simulation.

Figure

(a) Antiferromagnetics

(b)

Figure

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