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Interface stress evolution of martensitic transformation in MnCu alloys: A phase-field study

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H I G H L I G H T S

- Phase-field modeling was applied to obtain the internal stress associated with martensitic transformation.
- The state of interface stress strongly depends on the type of martensite domain.
- The internal stress increases with the growth of martensite when there is macroscopic transformation strain.
- Fluctuant internal stress retains in multi-variant martensite domain.

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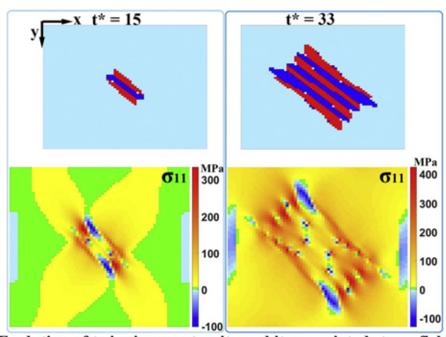

Evolution of twinning martensite and its associated stress field

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Martensitic transformations (MTs) in shape memory alloys (SMAs) usually give rise to internal elastic stress, because of the shape change from austenite to martensite. The stress condition of the interface plays a key role in the thermoelastic transformation behaviour and shape memory effect. In order to investigate the stress field originated from MT, a three-dimensional (3D) phase-field model was applied to the face-centered cubic structure to face-centered tetragonal structure (fcc-to-fct) MT in a MnCu alloy. The following results were obtained: The interface stresses on the invariant habit plane arise with the thickening of martensite plate; When the habit plane is not an invariant plane, the stress state around the interface changes abruptly; The formation of transformation twin is resulted from the fluctuant interface stress, the macroscopic habit plane has not been well obtained, and the elastic strain energy increases with the growth of twinning martensite; Martensitic block containing several twinning domains can be generated from a single-variant embryo, and the fluctuant elastic stresses have retained in the block.

1. Introduction

MnCu shape memory alloys (SMAs) have been commercially used in noise and vibration control fields [1], owing to its interface-type high damping property [2]. The shape memory effect [3] and magnetic induced strain effect [4] were also found in γ-Mn-based SMAs (γ denotes fcc), which were related to the face-centered cubic structure to face-centered tetragonal structure (fcc-to-fct) thermoelastic martensitic transformation (MT) [5]. The distortion degree of the fct phase increases with temperature decreasing [6].Twinning domain is the typical microstructure according to the observations by means of transmission electron microscopy (TEM) [7], and the formation of $\{101\}_{\gamma}$ transformation twins was explained by a double-shear model [8].

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For thermoelastic MT, the shape changes accompanied with MT are constrained by surrounding matrix, thus, internal stresses are generated and elastic strain energy is stored around the phase interface [9]. The increasing elastic energy resists the growth of martensite and a larger chemical driving force is needed, so the martensite plate will grow and shrink upon cooling and heating, respectively [6]. Tang et al. [10] established a modified one-dimensional Landau-Ginzburg model for MT, in which the strain energy in austenite was considered, and the results revealed that the stress field around the austenite-martensite (A-M) interface determined the athermal and autocatalysis features. The relationship between microstructure and macroscopic deformation has been widely studied [11–17]. Nevertheless, there is a growing interest in the microscale heterogeneous deformation [18–23]. The inhomogeneous elastic strain/stress distribution at the micro scale can be precisely measured by means of electron backscatter diffraction (EBSD). For example, Miyamoto et al. [24] investigated the local strain distributions in austenite for lath, lenticular and thin plate martensitic steels. Nakada et al. [25] discovered that the hydrostatic pressure was generated in untransformed austenite during MT in Fe-27%Ni alloy, which was in agreement with the microscopic strain mapping measured by means of EBSD. Zhang et al. [26] observed the heterogeneous distribution of elastic strains near the precipitation due to different thermal expansion rates of different phases.

For computer simulations of microscopic stress caused by phase transformation, an elastic precursor was observed ahead of the transition front, which resulted in the formation of transformation twinned martensite, by molecular dynamics (MD) simulation [27]. Chowdhury et al. [28] obtained the stress distribution around Ni_4Ti_3 precipitate by MD simulation as well. A thermomechanical approach was proposed for modeling the transformation induced elastic/plastic strains [29].The internal stress induced by microstructure change can also be simulated by phase-field method, for example, the stress field around the precipitate [30]. In addition, it was found that the martensitic structure was stabilized by internal stress, investigated by first principles study [31]. The authors proposed that the shape information related to shape memory effect was stored in the stresses. As we know, the 3D microstructure contains more information than that of 2D, as well as the stress state. However, systematic simulation studies being focused on the 3D interface stress states of MT are not abundant. In our opinion, these studies can be easily realized by phase-filed modeling. As a mesoscopic simulation approach, phase-field model has been extensively applied to MT [32]. The model [33] integrates the time dependent Ginzburg-Landau (TDGL) transformation theory [34] and Khachaturyan-Shatalov (KS) microelasticity theory [35], the internal stresses can be obtained by KS theory, and several self-accommodated microstructures can be observed [36].

The phenomenological theory of martensitic crystallography (PTMC) is a classic method for martensite morphology prediction. According to the lattice parameters of austenite and martensite, the crystallographic orientation relationships, habit plane and variant ratio of twinning martensite can be predicted. An important hypothesis of PTMC is that the transformation strain is an invariant plane strain (IPS), leaving the habit plane invariant, which is equivalent to elastic strain energy vanishing [37]. Actually, the invariant habit plane can also be obtained by minimizing the $B_{pq}(\boldsymbol{n})$ according to KS theory [35]. $B_{pq}(\boldsymbol{n})$ is a function of the vector in the reciprocal space and relates to the elastic constants and transformation strain, the detailed formula can be seen in Ref. [36]. Although the assumption of IPS is reasonable in PTMC, internal elastic strain/stress is usually produced during MT, especially the thermoelastic MT, because of finite thickness of martensite plate, constrained deformation of martensite front from the matrix [38] etc. For the phase-field modeling, the decrease of chemical energy could promote MT even though strain energy increasing, thus the internal stress distribution and interface stress characteristics can be obtained, which is more realistic than theory prediction.

In this paper, the 3D phase-field simulations of fcc-to-fct MT in MnCu alloys were performed so as to display the evolution processes of microstructure and interface stress distribution. In order to study different interface stress features corresponding to different typical microstructures, the formations of single-variant martensite plate, twinning martensite and martensite block containing three variants were simulated, respectively. The strain/stress relaxation mechanism is discussed, and the simulation results are compared with PTMC.

2. Phase-field model

In the phase-field model of fcc-to-fct MT, three order parameters, η_p ($p = 1, 2, 3$), are used to describe the three orientation variants. The evolution of order parameters represents the process of MT, and the time evolution is governed by the following TDGL equation:

$$\frac{\partial \eta_p}{\partial t} = -L\frac{\delta G}{\delta \eta_p} \tag{1}$$

where L is the kinetic coefficient. G is the Gibbs free energy of the system and is the sum of chemical free energy, G_{ch}, gradient energy, G_{gr}, and elastic strain energy, G_{el}, as:

$$G = G_{ch} + G_{gr} + G_{el} \tag{2}$$

The chemical energy, expressed as a Landau polynomial, is given by:

$$G_{ch} = \int_V \left[\frac{A}{2}\left(\eta_1^2+\eta_2^2+\eta_3^2\right) - \frac{B}{3}\left(\eta_1^3+\eta_2^3+\eta_3^3\right) + \frac{C}{4}\left(\eta_1^2+\eta_2^2+\eta_3^2\right)^2\right] dV \tag{3}$$

where the coefficients are expressed as $A = 32\Delta G^*$, $B = 3A - 12\Delta G_m$ and $C = 2A - 12\Delta G_m$. ΔG^* is the Gibbs energy barrier. ΔG_m is the free energy difference between austenite and martensite and its temperature dependence is given by:

$$\Delta G_m = Q(T - T_0)/T_0 \tag{4}$$

where Q is the transformation latent heat, T_0 the thermodynamic equilibrium temperature of austenite and martensite, and T the transformation temperature.

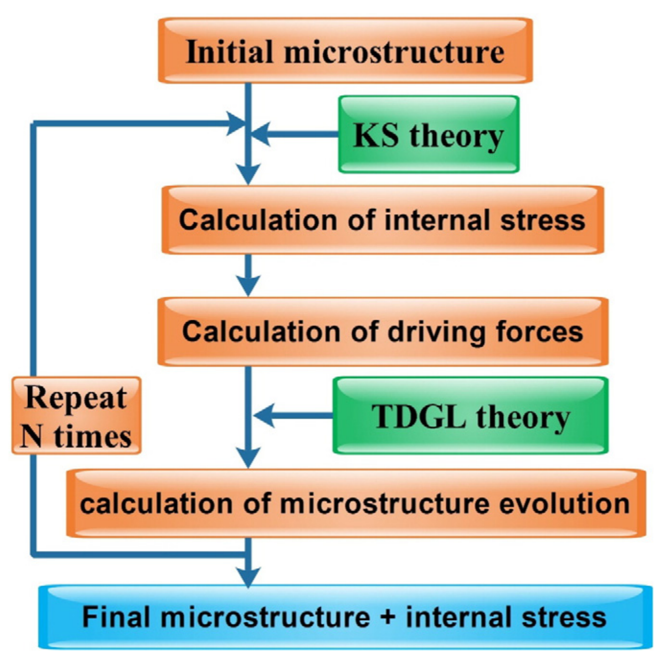

Fig. 1. Flow chart of the phase-field modeling algorithm used in this paper.