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Elastoplastic phase-field simulation of martensitic transformation with plastic deformation in polycrystal

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ABSTRACT

The martensitic transformation with plastic deformation in polycrystal is investigated by the elastoplastic phase-field model. The model can capture not only spatiotemporal change of martensitic microstructure, but also plastic deformation behavior to accommodate transformation-induced stress. In this paper, fcc→bcc martensitic transformation in Fe–Ni polycrystalline alloy is simulated in two-dimensions. The effects of self- and plastic accommodations on the transformation kinetics and morphology of microstructure are studied. The simulation results demonstrate that the martensite phase nucleates near crystal defects and grows into the parent phase. The morphology of the growing martensite phase presents a plate-like shape to minimize the elastic strain energy. The present simulation clearly shows that stress relaxation behavior is dominant factor which characterizes the morphology of martensite phase. The martensitic transformation only with the self-accommodation produces fine multivariant lamellar microstructure which accommodates internal stress-field. The high stress-field in the microstructure prevents completion of the transformation and causes formation of retained parent phase. In the martensitic transformation with the self- and the plastic accommodations, since the plastic deformation largely reduces the elastic strain energy, the self-accommodation driven by reduction of the elastic strain energy is suppressed. As a result, coarse multi-variant microstructure emerges in the grain where large amount of plastic strain is introduced. Furthermore, the parent phase can transform into the martensite phase completely.

1. Introduction

In many metallic and ceramic materials, martensitic transformation can be observed [1]. In particular, the martensitic transformation in steel is one of the most important phenomenon from an engineering viewpoint, because distribution and morphology of the martensite phase in steel play a key role on characterizing mechanical properties of the steel. However, the morphology of martensite phase drastically changes from thin plate, lenticular shape to lath shape depending on transformation temperature and chemical composition [2]. Therefore, it is quite essential for controlling the mechanical properties of steels to predict the transformation kinetics and the morphology of martensitic microstructure by numerical simulation.

Recently, the phase-field (PF) method has been extensively developed as a powerful tool to predict microstructure evolution during solidification, phase transformation and recrystallization [3–10]. Many researchers have proposed PF models of the martensitic transformation [11–13]. Especially, the PF model of the martensitic transformation based on the Khachaturyan and Shatalov theory, which is now called as the phase-field microelasticity theory [14,15], is successfully applied to simulate the evolution of polytwinned martensitic microstructure during cubic→tetragonal [16–19], cubic→trigonal [20] martensitic transformations in alloys.

As suggested in the above studies, the morphology of martensitic microstructure is characterized by accommodation process of transformation-induced stress. The stress-accommodation during the martensitic transformation proceeds by formation of multivariant microstructure and plastic deformation. These accommodation behaviors are called as the self-accommodation and the plastic accommodation [11,21]. In the previous studies, the formation of twinned martensitic microstructure characterized by the self-accommodation has been simulated. However, to the authors knowledge, no PF model which can treat the martensitic transformation with the plastic accommodation has been proposed. In order to predict various morphologies of the martensitic microstructure including lath martensite

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structure, a new PF model which is able to describe the martensitic transformation accompanying with the plastic accommodation should be developed.

In our previous work, we proposed the elastoplastic phase-field model (EP-PFM) describing the martensitic transformation with the plastic deformation [22]. And, we simulated the evolution of the martensite phase and the plastic accommodation behavior during the cubic→tetragonal martensitic transformation in a single crystal.

In this study, the martensitic transformation accompanying with the self- and the plastic accommodations in polycrystalline materials is investigated. First, we reformulate the EP-PFM to simulate the martensitic transformation with the plastic deformation in polycrystals. Then, the PF simulation of isothermal fcc→bcc martensitic transformation in Fe–Ni polycrystalline alloy is conducted. Through the simulation, the effects of the plastic accommodation on the morphology of microstructure are studied.

2. Elastoplastic phase-field model

In our previous study [22], the EP-PFM of the martensitic transformation in a single crystal was developed by combining the PF model of the martensitic transformation proposed by Wang et al. [16] with the kinetic equation of plastic strain proposed by Guo et al. [23]. In this section, we reformulate the EP-PFM to simulate the martensitic transformation in polycrystalline material.

To simulate the martensitic transformation using the PF method, the total free energy of the system, G, is defined as a sum of the chemical free energy, G_{ch}, the gradient energy, G_{gr}, and the elastic strain energy, G_{el}, as

$$G = G_{ch} + G_{gr} + G_{el}. \tag{1}$$

Here, by considering that the chemical free energy is invariant with respect to any rotation and symmetry of the crystal lattice of the parent phase, it can be formulated, using the Landau polynomial expansion [16], as

$$G_{ch} = \int_V \Delta f \left\{ \frac{A}{2}\sum_{i=1}^{3}\phi_i^2 - \frac{B}{3}\sum_{i=1}^{3}\phi_i^3 + \frac{C}{4}\left(\sum_{i=1}^{3}\phi_i^2\right)^2 \right\} dV, \tag{2}$$

where ϕ_i is the order parameter that describes the continuous distribution of the i-th orientation variant of the martensite phase. In the cases of the fcc→bcc martensitic transformation, three orientation variants can be produced as a result of the transformation. Hence, $i = 1$, 2 and 3 correspond to three orientational variants of the martensite phase whose tetragonality axes are along the three $\langle 100 \rangle$ directions in the parent phase. ϕ_i $(0 \le \phi_i \le 1)$ gradually changes from $\phi_i = 1$ in the i-th variant to $\phi_i = 0$ in the other variants of the martensite and parent phases. Δf is the magnitude of the driving force of the transformation, which is equal to the free energy difference between the parent and martensite phases. A, B and C are the expansion coefficients of the Landau polynomial expansion. In this study, these constants are defined as $A = 0.15$, $B = 3A + 12$ and $C = 2A + 12$ [20].

The gradient energy, which is defined as the sum of gradient energies due to the inhomogeneity of order parameters, is given as

$$G_{gr} = \int_V \frac{\kappa}{2}\sum_{i=1}^{3} |\nabla \phi_i|^2 \, dV, \tag{3}$$

where κ is the gradient energy coefficient.

The elastic strain energy of a system including an arbitrary mixture of the parent phase and the martensite phase is evaluated by the micromechanical approach as [15,24]

$$G_{el} = \int_V \frac{1}{2} C_{ijkl}\varepsilon_{ij}^{el}\varepsilon_{kl}^{el} \, dV, \tag{4}$$

where C_{ijkl} is the elastic coefficient tensor. The elastic strain tensor, ε_{ij}^{el}, is defined as the difference between the total strain tensor, ε_{ij}^{c}, and the total eigen strain tensor, ε_{ij}^{0}, as

$$\varepsilon_{ij}^{el} = \varepsilon_{ij}^{c} - \varepsilon_{ij}^{0}. \tag{5}$$

The total strain, ε_{ij}^{c}, is defined as the sum of the homogeneous strain, $\overline{\varepsilon}_{ij}^{c}$, and the heterogeneous strain, $\delta\varepsilon_{ij}^{c}$, as

$$\varepsilon_{ij}^{c} = \overline{\varepsilon}_{ij}^{c} + \delta\varepsilon_{ij}^{c}. \tag{6}$$

The homogeneous strain, $\overline{\varepsilon}_{ij}^{c}$, is a uniform macroscopic strain and describes the macroscopic shape change of the system. When the system is not constrained during the transformation, the homogeneous strain is given as

$$\overline{\varepsilon}_{ij}^{c} = \frac{1}{V}\int_V \varepsilon_{ij}^{0} \, dV. \tag{7}$$

The heterogeneous strain, $\delta\varepsilon_{ij}^{c}$, is defined as the deviation from the homogeneous strain and does not affect the macroscopic deformation. Therefore, $\delta\varepsilon_{ij}^{c}$ is defined such that $\int_V \delta\varepsilon_{ij}^{c} \, dV = 0$. And, this strain is given by solving the mechanical equilibrium equation, $\sigma_{ij,j} = 0$, with the Fourier spectral method [15,25], as

$$\delta\varepsilon_{ij}^{c} = \frac{1}{(2\pi)^3}\int_k \frac{1}{2}\{n_i\Omega_{mj}(\boldsymbol{n}) + n_j\Omega_{mi}(\boldsymbol{n})\} \cdot \hat{\sigma}_{mn}^{0}(\boldsymbol{k}) n_n \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \, d\boldsymbol{k}. \tag{8}$$

Here, $\Omega_{ik}(\boldsymbol{n})$ is the Green function tensor inverse to $\Omega_{ik}(\boldsymbol{n})^{-1} = C_{ijkl}n_j n_l$ [15,26]. $\boldsymbol{k}$ indicates the reciprocal space vector and $\boldsymbol{n} = \boldsymbol{k}/|k|$ is the unit vector along the $\boldsymbol{k}$ direction. $\hat{\sigma}_{ij}^{0}(\boldsymbol{k}) = C_{ijkl}\hat{\varepsilon}_{kl}^{0}(\boldsymbol{k})$ is the Fourier transformation of $\sigma_{ij}^{0} = C_{ijkl}\varepsilon_{kl}^{0}$. Here, $\hat{\varepsilon}_{kl}^{0}(\boldsymbol{k})$ is the Fourier transformation of the total eigen strain.

In order to simulate the martensitic transformation accompanying with the self-accommodation and the plastic accommodation, we describe the evolutions of the transformation strain and the plastic strain during the transformation. Therefore, the total eigen strain, ε_{ij}^{0}, is defined as a sum of the transformation strain, ε_{ij}^{t}, and the plastic strain, ε_{ij}^{p}, as [23]

$$\varepsilon_{ij}^{0} = \varepsilon_{ij}^{t} + \varepsilon_{ij}^{p}. \tag{9}$$

Furthermore, to describe the martensitic transformation in polycrystalline material, global and local coordinate systems are considered. As shown in Fig. 1, the global coordinate system, x_i $(i = 1$, 2 and 3), is set to be parallel to the three directions of the computational domain. The local coordinate system, y_i $(i = 1$, 2 and 3), are defined in each parent grain. The rotation angle between x_i axis and y_i axis represents the crystal orientation of the parent grain, θ. In order to evaluate the transformation strain

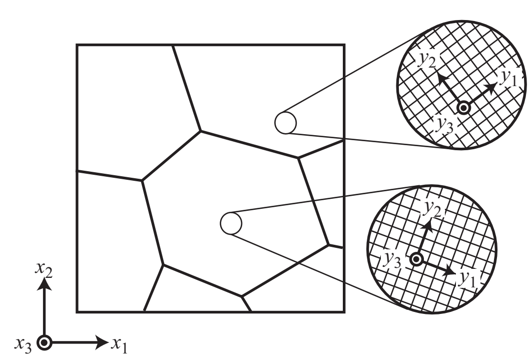

Fig. 1. Schematic illustration of global and local coordinate systems for polycrystalline material.