ELASTOPLASTIC PHASE-FIELD SIMULATION OF CUBIC-TETRAGONAL MARTENSITIC TRANSFORMATION IN POLYCRYSTALS

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Summary We perform an elastoplastic phase-field simulation of the cubic → tetragonal martensitic transformation with plastic deformation in a two-dimensional polycrystal. The results shows that the proposed phase-field model can reproduce the cubic → tetragonal martensitic transformation in the polycrystalline material including not only evolution of stress-accommodating multi-variant martensitic structure from grain boundary of parent phase but also plastic deformation reducing the transformation-induced stress.

INTRODUCTION

Recently, a phase-field (PF) method has been extensively studied as a powerful tool for predicting microstructural evolution [1] and has been applied to martensitic transformation. Khachaturyan and other researchers have proposed the phase field microelasticity (PFM) models of the martensitic transformation [2, 3]. In the previous study [4], we have proposed the elastoplastic phase-field model (EPFM) of cubic → tetragonal (CT) martensitic transformation based on the PFM theory and simulated self- and plastic accommodation behaviors in a single crystal. The results show that plastic deformation during the CT transformation largely accommodates the transformatio-induced stress and arrests growth of the martensite phase. In this study, the CT martensitic transformation in a two-dimensional polycrystal is simulated using the EPFM and study the effects of plastic deformation on the evolution of the martensite phase in the polycrystal.

PHASE-FIELD MODEL

The EPFM of the CT martensitic transformation is constructed by combining the PFM model of the martensitic transformation [3] with the TDGL equation of the plastic strain proposed by Guo et al [5]. To simulate the CT martensitic transformation using the PF theory, the total free energy of the system G is described by the Ginzburg-Landau-type Gibbs free energy functional, which is defined as the sum of chemical free energy, gradient energy and elastic strain energy. The chemical free energy is defined as the Landau polynomial expansion with respect to the order parameters. In this model, the order parameter ϕ_i describes the continuous distribution of the i-th orientation variant of the martensite phase whose tetragonality axes are along the three <100> directions in the cubic phase. ϕ_i gradually changes from ϕ_i = 1 in the i-th variant to ϕ_i = 0 in the other variants of tetragonal and parent phases. The gradient energy is defined as the sum of gradient energies due to the inhomogeneity of order parameters.

The elastic strain energy density of a system with an arbitrary mixture of the cubic and the tetragonal phases can be evaluated using the micromechanical approach proposed by Khachaturyan, i.e., the PFM theory [2] as,

$$g_{el} = \frac{1}{2} C_{ijkl} (\epsilon^c_{ij} - \epsilon^0_{ij})(\epsilon^c_{kl} - \epsilon^0_{kl}), \tag{1}$$

where C_{ijkl}, ϵ^c_{ij} and ϵ^0_{ij} are the elastic coefficient matrix, the total strain tensor and the total eigen strain tensor, respectively. In this study, to simulate the CT martensitic transformation with elastoplastic deformation in two-dimensions, the total eigen strain is defined as [5],

$$\epsilon^0_{ij} = \sum_{m=1}^{2} R_{ik}(\theta) \epsilon^{00}_{kj}(m) + \epsilon^p_{ij}, \tag{2}$$

where the first and second terms are the transformation-induced eigen strain ϵ^t_{ij} and the plastic strain ϵ^p_{ij}, respectively. Here, to describe the CT martensitic transformation in a polycrystalline material, a rotation matrix $R_{ij}(\theta)$ is introduced [3]. $\epsilon^{00}_{ij}(m)$ is the transformation-induced eigen strains of the m-th (m = 1 and 2) tetragonal variants in two-dimensions.

To calculate the distribution and magnitude of plastic strain during the CT martensitic transformation, the evolution of plastic strain is evaluated by the PF methodology. According to the Von Mises yield criterion, because the plastic deformation takes place when the shear strain energy reaches a certain value related to the yield stress σ_y, the yield criterion can be described in energetic form as, $F_y = G^{shear}_{el} - \sigma^2_y/6\mu = 0$, where the shear strain energy, G^{shear}_{el}, is also evaluated by the PFM theory. We assume that the evolution of plastic strain is governed by minimization process of the shear strain energy and can be described with the following TDGL equation [5]:

$$\frac{\partial \epsilon^p_{ij}}{\partial t} = -K_{ijkl} \frac{\delta G^{shear}_{el}}{\delta \epsilon^p_{kl}}, \tag{3}$$

where K_{ijkl} is the fourth-order kinetic coefficient tensor for plastic strain and is assumed to be $K_{ijkl} = (KC_{ijkl})^{-1}$ with constant K for simplicity [5]. Note that since this model does not describe deformation hardening, Eqn. (3) is valid in the case of an elastic-perfectly plastic material. And, the Eqn. (3) is solved only in the region satisfyng the yield criterion.

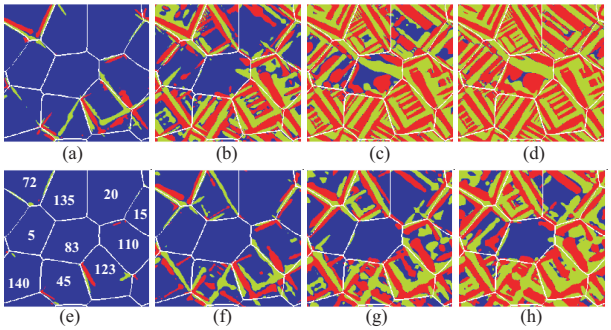

Figure 1. Evolution of tetragonal phase in elastic material ((a)-(d)) and elastoplastic material ((e)-(h)) at different dimensionless times t = 30, 40, 48 and 56.

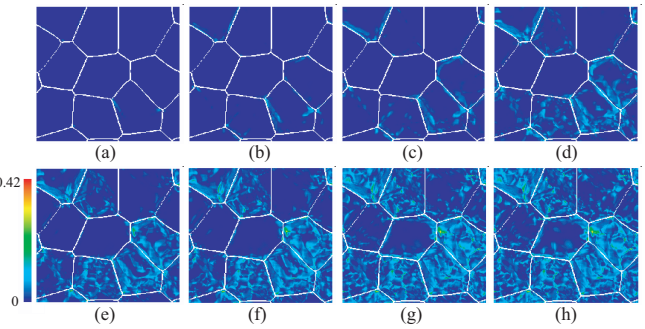

Figure 2. Evolution of equivalent plastic strain in elastoplastic material. Figures (a)-(h) correspond to different dimensionless times t = 24, 30, 34, 40, 44, 48, 56 and 60.

With the above equations, the time evolution of the tetragonal phase, i.e., the order parameters, is described by the following TDGL equation:

$$\frac{\partial \phi_i}{\partial t} = -L' \frac{\delta G}{\delta \phi_i} = -L' \left(\frac{\partial g_{ch}}{\partial \phi_i} + \frac{\partial g_{el}}{\partial \phi_i} - \kappa \nabla^2 \phi_i \right), \tag{4}$$

where L' and κ are the kinetic parameter for the phase field and the gradient energy coefficient, respectively.

RESULTS AND CONCLUSIONS

The CT martensitic transformation in elastically isotropic polycrystal is simulated in two dimensions. The polycrystalline structure with seven parent phase grains is produced by an ordinary multi-phase-field simulation of grain growth. We use a square 256 $\times$ 256 nm^2 computational domain and apply periodic boundary conditions. Equations (3) and (4) are solved by the finite difference method and the fast fourier transformation with the plane strain condition. The magnitude of chemical driving force is set to be constant at Δf = 321 J/mol. The transformation-induced eigen strains are given by $\epsilon^{00}_{22}(1) = \epsilon^{00}_{11}(2)$ = 0.1 and $\epsilon^{00}_{11}(1) = \epsilon^{00}_{22}(2) = -0.1$. The i-th variant of tetragonal phase is defined as the domain of $\phi_i \geq 0.6$, and the yield stress is chosen as σ_y = 250 MPa for the cubic matrix and σ_y = 800 MPa for the tetragonal phase, respectively. It is well known that the martensite phase often nucleates on the grain boundary of the parent phase by local elastic stress due to crystal defect and dislocation. Therefore, to simulate the evolution of the tetragonal phase from the grain boundary, we distribute random shear plastic strain around the grain boundary as a potential nucleation site.

Figure 1 shows the evolution of the tetragonal phase in the elastic and elastoplastic materials. In Fig. 1(e), the number in the grain indicates the crystal orientation of parent phase grain, which is defined as a rotation degree between the [100] axis of each parent phase grain and the horizontal direction. Blue, red and yellow domains correspond to the parent phase, the first and variant second variant of the tetragonal phases, respectively. The randomly distributed plastic strain generates local stress-field in the polycrystal. The distribution of the stress is inhomogeneous and concentrated around the grain boundary of the parent phase by the elastic coupling between different parent grains [6]. Thus, as shown in Fig. 1 (a) and (e), it can be observed that the tetragonal phase preferentially starts to develop around the grain boundary of the parent phase so as to reduce the transformation-induced stress. Furthermore, as shown in Figs. 1 and 2, we can find that in the elastoplastic material the growth of the tetragonal phase is suppressed by the plastic deformation accompanying the martensitic transformation and thus larger fractions of the parent phase is retained.

From above results, we conclude that the present EPFM can describe the CT martensitic transformation in the polycrystalline material including the evolution of multi-variant martensitic structure from the grain boundary of the parent phase and the plastic deformation to reduce the transformation-induced stress. In future work, the extention of this EPFM will be a useful tool predinting for the formation of the martensitic microstructure affected by self- and plastic accommodations, such as lath martensite.

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