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CRYSTAL PLASTICITY PHASE-FIELD SIMULATION OF DEFORMATION BEHAVIOR AND MICROSTRUCTURE EVOLUTION IN POLYCRYSTALLINE MATERIAL

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Summary. A new crystal plasticity phase-field model is developed to simulate microstructure evolution with elastoplastic deformation. In this paper, three-dimensional simulation of the growth of precipitates during solid phase transformation is performed. And, it is demonstrated that the distribution of stress and dislocation density around the growing precipitates can be predicted by the developed phase-field model.

1 INTRODUCTION

Recently, the phase-field (PF) method has been actively studied as a powerful tool to simulate microstructure evolutions in various materials. In particular, Guo et. al. [1] proposed the elastoplastic PF models to simulate the microstructure evolution with both elastic and plastic deformations. However, since their elastoplastic PF model is based on the J2 flow theory and, therefore, can not describe changes of crystal orientation and dislocation density during the microstructure evolution. In order to conduct precise numerical simulation of the microstructure evolution with the elastoplastic deformation, such as formation of lath martensite structure, using the PF method, it is essential to enable us to evaluate the changes of crystal orientation and dislocation density due to the microstructure evolution in frame of the PF theory.

In this study, a new crystal plasticity phase-field model (CP-PFM) is developed by coupling the phase-field microelasticity (PFM) theory [2] with the crystal plasticity theory. Furthermore, using the developed CP-PFM, the three-dimensional simulation of the growth of precipitates

during solid phase transformation is performed. And, it is demonstrated that the CP-PFM can predict the evolution of the precipitates and investigate the plastic deformation behavior around the precipitates including the change of dislocation density.

2 CRYSTAL PLASTICITY PHASE-FIELD MODEL

The total free energy of the system is defined by the Ginzburg-Landau free energy functional, which is the sum of chemical free energy G_{chem}, elastic strain energy $G_{elastic}$ and gradient energy G_{grad} as, $G_{total} = G_{chem} + G_{elast} + G_{grad}$. Here, the chemical free energy G_{chem} is represented by the Landau polynominal expansion of the phase-field variable ϕ_i. ϕ_i is defined as $\phi_i = 1$ in the i th precipitate and $\phi_i = 0$ in the parent phase and other precipitates. In the interface region, ϕ_i gradually changes from 1 to 0.

In this CP-PFM, the elastic strain energy is evaluated by the PFM theory proposed by Khachaturyan [2]. According to the PFM theory, the elastic strain energy can be described by the following equation.

$$\begin{aligned} G_{elast} &= \frac{1}{2}\int_V C_{ijkl}\epsilon^{el}_{kl}\epsilon^{el}_{ij}dV \\ &= \frac{1}{2}\int_V C_{ijkl}\left(\epsilon^{c}_{kl}-\epsilon^{0}_{kl}\right)\left(\epsilon^{c}_{ij}-\epsilon^{0}_{ij}\right)dV \end{aligned} \tag{1}$$

Here, ϵ^{el}_{ij}, ϵ^{c}_{ij}, ϵ^{0}_{ij} are the elastic strain, the total strain and the eigen strain, respectively. The total strain is defined as the sum of the homogeneous strain $\bar{\epsilon}^{c}_{ij}$ and heterogeneous strain $\delta\epsilon^{c}_{ij}$ as, $\epsilon^{c}_{ij} = \bar{\epsilon}^{c}_{ij} + \delta\epsilon^{c}_{ij}$. The homogeneous strain is determined from the macroscopic boundary condition. On the other hand, the heterogeneous strain is calculated by solving the mechanical equilibrium equation using the Fourier transformation. And, the heterogeneous strain can be obtained by the inverse Fourier transformation of the following heterogeneous strain in the Fourier space.

$$\delta\hat{\epsilon}^{c}_{ij}(\vec{k}) = \frac{1}{2}\left(n_j\Omega_{mi}(\vec{n}) + n_i\Omega_{mj}(\vec{n})\right)n_n\hat{\sigma}^{0}_{mn}(\vec{k}) \tag{2}$$

Here, $\Omega^{-1}_{mi}(\vec{n}) = C_{ijmn}n_n n_j$ and $\vec{n} = \vec{k}/\left|\vec{k}\right|$ is the unit vector in the Fourier space.

The eigen strain in Eqn. (1) is assumed to be the sum of the transformation strain ϵ^{trans}_{ij} and the plastic strain ϵ^{p}_{ij} evaluated by the crystal plasticity theory as, $\epsilon^{0}_{ij} = \epsilon^{trans}_{ij} + \epsilon^{p}_{ij}$. The transformation strain is defined as a linear function of the phase field variable and the transformation strain due to formation of m th variant of the precipitates as, $\epsilon^{trans}_{ij} = \sum_{m=1}^{N}\epsilon^{00}_{ij}(m)\phi_m$. The plastic strain is calculated by time integration of the following plastic strain rate; $\dot{\epsilon}^{p}_{ij} = \sum_{a=1}^{n}P^{(a)}_{ij}\dot{\gamma}^{(a)}$. Here, $\dot{\gamma}^{(\alpha)}$ and $P^{(a)}_{ij}$ are shear strain rate and the Schmid tensor on the a th slip plane. In this study, we employ the following equation [3].

$$\dot{\gamma}^{(a)} = \dot{\gamma}^{(a)}_0\frac{\tau^{(a)}}{g^{(a)}}\left|\frac{\tau^{(a)}}{g^{(a)}}\right|^{\frac{1}{m}-1} \tag{3}$$

Here, the evolution of the critical resolved shear stress $g^{(a)}$ is assumed to be the modified Bailey-Harsh equation based on the strain-gradient crystal plasticity theory [4].

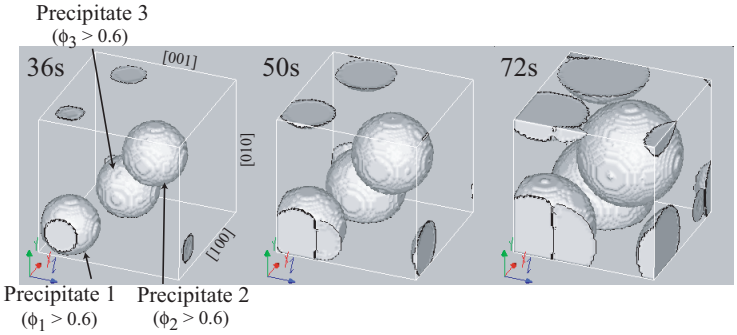

Figure 1: Evolution of the precipitates during phase transformation.

The evolution of the precipitates is described by solving the following time-dependent Ginzburg-Landau (TDGL) equation for the phase field variables.

$$\frac{\partial \phi_i}{\partial t} = -M_\phi \frac{\delta G_{total}}{\delta \phi_i} = -M_\phi \left(\frac{\delta G_{chem}}{\delta \phi_i} + \frac{\delta G_{elast}}{\delta \phi_i} + \frac{\delta G_{grad}}{\delta \phi_i} \right) \tag{4}$$

3 SIMULATION RESULTS

In this study, the three-dimensional simulation of the growth of precipitates with the elasto-plastic deformation is performed. The cubic computational domain of $100 \times 100 \times 100$ μm^3 is meshed with 64^3 regular computational grids. Thus, the mesh size is $\Delta x = 1.56$ μm. Three initial nuclei of the precipitate are set to be formed in the computational domain randomly. It is assumed that the phase transformation induces isotropic dilatational transformation strain. Furthermore, we assume that the precipitate and parent phase have FCC crystal structure and, thus, the twelve slip systems are considered. The TDGL equation is solved with the finite difference method and the fast Fourier transformation under the periodic boundary condition. For the numerical simulation, the following physical values and parameters are used: the mobility of phase field $M_\phi = 1.0$, Young's modulus $E = 77.0$ GPa, Poasson's ratio $\nu = 0.375$, the referencial shear strain rate $\dot{\gamma}_0^{(a)} = 0.1$ s^{-1}, the strain rate sensitivity factor $m = 0.05$, the initial dislocation density $\rho_0 = 10^{10}$ 1/m^{-3} and time increment $\Delta t = 0.002$ s.

Figure 1 shows the growth of the precipitates during the phase transformation. The precipitate i is visualized by the profile of $\phi_i \geq 0.6$ ($i = 1, 2, 3$). All precipitates grow with time and the grain boundary is formed between different precipitates. Figure 2 indicates the evolution of equivalent stress with the growth of the precipitates on the $\{100\}$ cross-section for $x = 40\Delta x$. It is shown that the stress concentrates in the parent phase near the interface and the high stress region migrates with the growth of the precipitates. Furthermore, since we employ the strain-gradient crystal plasticity theory, the changes of SS and GN dislocation densities in the microstructure can be evaluated. The evolution of the dislocation density $\rho_a = \sum_{n=1}^{12} \rho^{(n)}$ around the precipitates is shown in Fig. 3. Here, $\rho^{(n)}$ is calculated by the sum of the SS dislocation density and the GN dislocation density as, $\rho^{(n)} = \rho_{SS}^{(n)} + \|\rho_{GN}^{(n)}\|$. From the Fig. 3, the plastic deformation occurs in the high stress region between the precipitates. Thus, it can be observed that the high dislocation density is exhibited in the vicinity of the grain boundary.

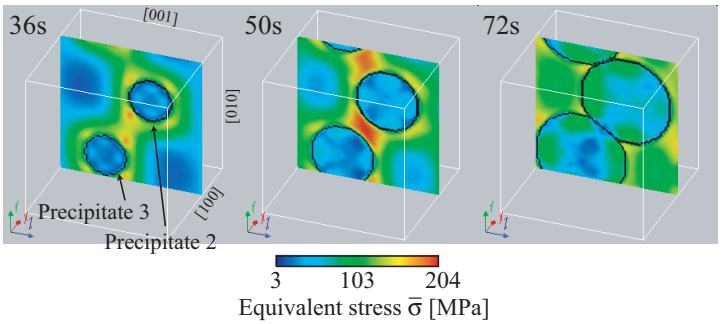

Figure 2: Evolution of equivalent stress on the {100} cross-section for $x = 40\Delta x$.

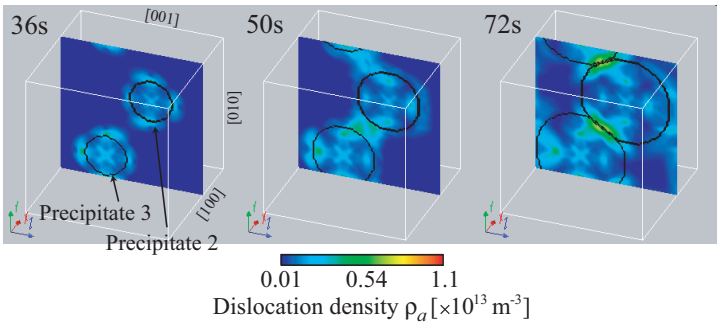

Figure 3: Evolution of dislocation density on the {100} cross-sections for $x = 40\Delta x$.

4 CONCLUSIONS

In this study, a new CP-PFM was developed by coupling the PFM theory with the crystal plasticity theory to simulate the microstructure evolution with the elastoplastic deformations. And, the three-dimensional simulation of the growth of the precipitates was performed by using the developed CP-PFM. The simulation results demonstrated that the high stress region is formed around the precipitates due to the dilatational transformation strain. And, the high dislocatin density was exhibited near the grain boundary. From these results, it can be concluded that the developed phase-field model can simulate not only the microstructure evolution during the phase transformation, but also the plastic deformation behavior during the microstructure evolution including the changes of the crystal orientation and the dislocation density.

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