Static Recrystallization Simulation Using Phase-Field Model Based on Crystal Plasticity Theory

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ABSTRACT

A numerical model and computational procedure for static recrystallization are developed using a phase-field model coupled with crystal plasticity theory. The microstructure and accumulated dislocation density during deformation of a polycrystalline metal are simulated using finite element method based on the strain gradient crystal plasticity theory. Phase-field simulation of the nucleation and growth of recrystallized grain is performed using the crystallographic orientation and stored energy calculated by crystal plasticity finite element simulation. Through this computational procedure, we can get the final recrystallization microstructure taking the deformation microstructure into consideration.

1. Introduction

The microstructures formed during annealing are significantly affected by the pre-deformation microstructures, since the recrystallization originates from dislocation cells or subgrains which appear after deformation and subsequently the recrystallized grain growth occurs driven by the stored energy resulted from the dislocation accumulated during deformation. Recently, the numerical studies using Monte Carlo Potts model [1] and cellular automata model [2] based on the data measured by EBSD analysis are made on static recrystallization. However, to enable more systematic investigations for recrystallization texture, it is key to develop the computational procedure without using experimental data.

In this study, we develop a phase-field model which can simulate the nucleation and growth of recrystallized grain. Here, the crystallographic orientation and dislocation density at the deformation of polycrystalline metal are simulated using finite element method based on the strain gradient crystal plasticity theory [3].

2. Numerical Procedure

The numerical procedure developed here consists of following three steps:

< Step. 1> The crystallographic orientation and dislocation density after deformation of polycrystalline metals are calculated by crystal plasticity finite element simulation.

< Step. 2 > The calculated data are mapped onto a regular lattice used in phase-field simulation. The stored energies calculated from dislocation density are smoothed on the lattice, because phase-field method requires the continuous driving forces.

< Step. 3 > Phase-field simulation during recrystallization is performed in which the nucleation and growth of recrystallized grain are reproduced.

3. Models and Results

By following the procedure shown in previous chapter, crystal plasticity theory, data mapping method and phase-field method employed in this study are briefly explained together with numerical results.

3.1 Strain gradient crystal plasticity

The crystal plasticity finite element method based on a strain gradient theory of rate dependent plasticity [3] is used to examine the microstructure and dislocation distribution during deformation of polycrystalline metals. Here, the critical resolved shear stress on slip system (a) is assumed to be a Bailey-Hirsch type function:

$$g^{(a)} = g_0^{(a)} + a\mu\tilde{b}\sum_{(b)}\varpi_{ab}\sqrt{\rho^{(b)}} \tag{1}$$

where, $g_0^{(a)}$ initial value of $g^{(a)}$, a constant, m elastic shear modulus, $\tilde{b}$ the magnitude of Burgers vector, ϖ_{ab} interaction matrix, and $\rho^{(b)}$ accumulated dislocation density. The accumulated dislocation density is the sum of the densities of SSD and GND. The evolution of SSD is expressed by the balance between the production rate of dislocations and the annihilation by dynamic recovery. The density of GND is calculated from the gradient of shear strain on slip system (a). Since the hardening equation, Eqn. 1, includes the strain gradient term through the dislocation density, it is possible to express the grain size effects.

Figure 1(a) shows the polycrystal model with 23 grains where the average grain diameter is 115.5 μm. This model is divided into 64x64 regular crossed-triangle elements and is compressed at a strain rate 10^{-3} s^{-1} as a 2-slip plane strain problem. Figure 1(b) and (c) illustrate the crystallographic orientation and stored energy after 50% compression, respectively. The stored energy E_{store} is calculated by $E_{store} = 0.5\rho\mu\tilde{b}^2$, where ρ is the total dislocation density of all slip systems.

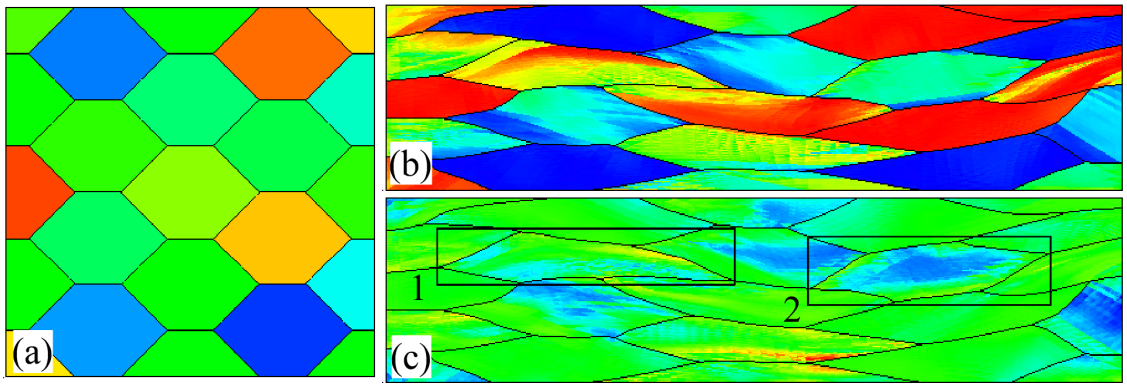

Figure 1. Crystallographic orientation (a) before deformation and (b) at 50% compression, and (c) stored energy. Solid lines indicate initial grain boundaries.

3.2 Data mapping

The data computed by crystal plasticity finite element simulation, i.e. crystallographic orientation and stored energy, are mapped onto the regular lattice of phase-field simulation. The relationship between triangle elements used in finite element simulation and lattice used in phase-field simulation is shown in Fig. 2. The regular lattice size is 0.4 μm and triangle elements are a part of Fig. 1 (b). First, the crystallographic orientation and stored energy on lattice are determined as a value inside an element. In other words, the values of lattice located inside a triangle element are all identical. Next, the misorientation on lattice is determined as a maximum value among the four misorientations between the two neighboring lattices, i.e., $\Delta\theta_1$, $\Delta\theta_2$, $\Delta\theta_3$, and $\Delta\theta_4$, represented in Fig.2. Then, the stored energies mapped onto the regular lattice are smoothed using Winslow's smoothing method:

$$E_{store} = \sum_{j=1}^{m} E_j w_j \Big/ \sum_{j=1}^{m} w_j \tag{2}$$

where, E_{store} smoothed stored energy on lattice i, E_j stored energy before smoothing on lattice j, w_j weight represented as an inverse of distance between lattice i and lattice j, and m the number of lattice inside a considering circle with radius r. In this study, $r = 3\Delta x$ is selected where Δx is lattice size. Finally, the crystallographic orientation, misorientation and smoothed stored energies on all regular lattices are determined. Figures 3 (a) and (b) show the distributions of smoothed stored energy and misorientation, respectively, for the regions 1 (332.8 x 64 μm^2) and 2 (268.8 x 76.8 μm^2) illustrated in Fig.1.

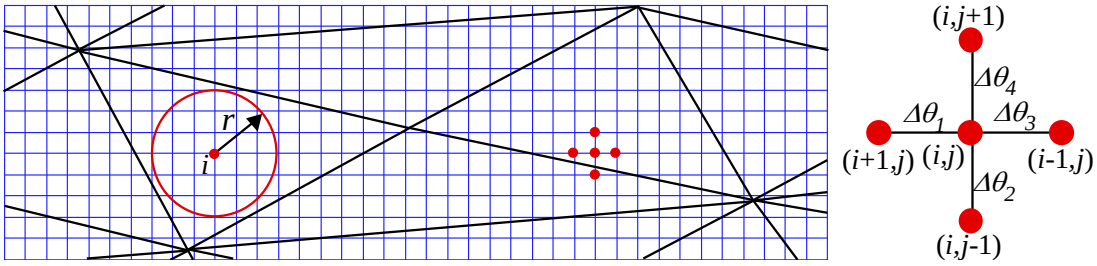

Figure 2. Triangle elements for crystal plasticity finite element simulation and regular lattice for phase-field simulation.

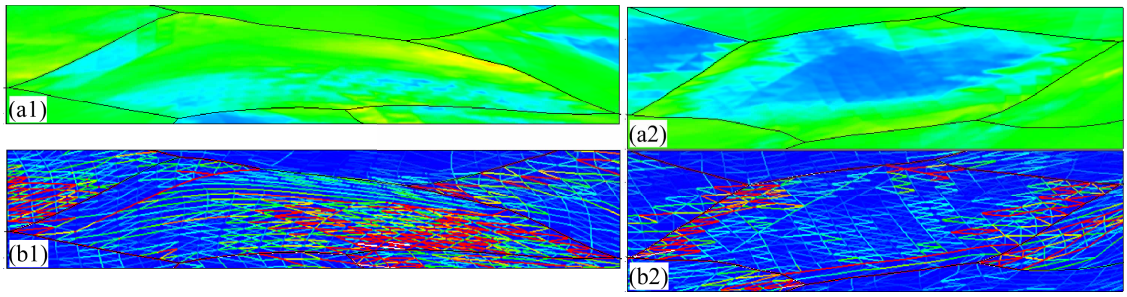

Figure 3. (a) smoothed stored energy and (b) misorientation. 1 and 2 indicates region 1 and 2 of Fig.1, respectively.

3.3 Phase-field simulation

By using the data mapped onto regular lattice, the nucleation and growth of recrystallized grain are simulated using phase-field method. In the present phase-field model, two order parameters, i.e., phase field ϕ which equals zero in the deformed matrix and unity in recrystallized grain and crystallographic orientation θ, are employed. The time evolved equations for the order parameters are as following:

$$\frac{\partial \phi}{\partial t} = M_\phi \left[\alpha^2 \nabla^2 \phi - \frac{\partial f(\phi)}{\partial \phi} - 2\phi s |\nabla \theta| \right] \quad (3) \qquad \frac{\partial \theta}{\partial t} = M_\theta \frac{1}{\phi^2} \nabla \cdot \left(\phi^2 s \frac{\nabla \theta}{|\nabla \theta|} \right) \quad (4)$$

where, $f(\phi)$ a free energy density expressed by double well type function: $f(\phi) = (1 - p(\phi))E_{store} + Wq(\phi)$ with $p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$ and $q(\phi) = \phi^2(1-\phi)^2$, $W = 6\sigma/\delta$ energy wall height related to interface energy σ and interface thickness δ, $\alpha = \sqrt{3\delta\sigma}$ gradient coefficient, $s = \alpha\sqrt{2W}/\pi$, $M_\phi = m\sqrt{2W}/6\alpha$ mobility for ϕ where m is a mobility of grain boundary migration, and $M_\theta = (1 - p(\phi))M_\phi$ mobility for θ. Equations (3) and (4) are solved by an adaptive finite element method [4].

Figure 4 shows the initial nucleus sits, the growth process, and final recrystallization microstructure. The site saturated nucleation model is used, in which the following nucleation criteria are assumed: (1) the high angle grain boundary of more than 15 degree, (2) the stored energy of more than 0.6 MPa, (3) the orientation of the nucleus is presented in the deformed structure, and (4) the minimum distance between the two neighboring nuclei is $10\Delta x$. The initial radius of nucleus is set to $3\Delta x$. From Fig.4, it is observed that, in region 1, the nucleation and growth of recrystallized grains occur inside the grain before deformation, while, in region 2, the recrystallized grains originate only from grain boundary.

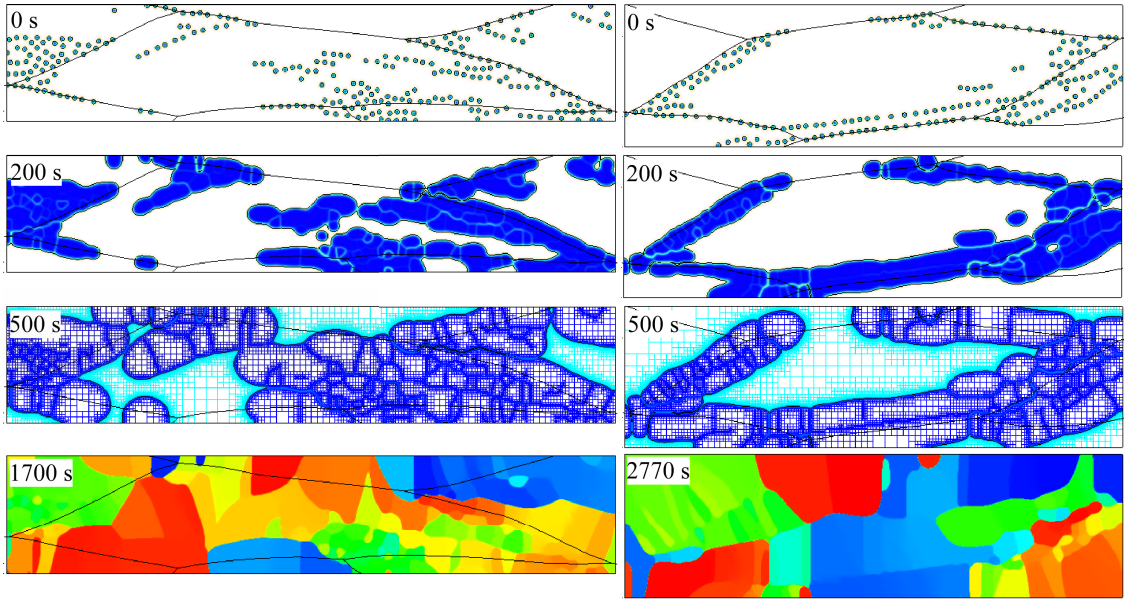

Figure 4. Time evolutions of recrystallized grain growth and final recrystallization microstructures. Adaptive meshes are illustrated only for results at 500s.

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