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MULTI-PHASE-FIELD MODELING AND SIMULATION FOR STATIC RECRYSTALLIZATION

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Summary. The static recrystallization simulations by driving force model and subgrain growth model are performed and both results are compared in detail. As a result, the similar recrystallized microstructures are observed for both models.

1 INTRODUCTION

It is well known that the static recrystallization (SRX) which occurs during post deformation annealing is largely affected by deformation microstructure formed during cold working. Therefore, to investigate and predict SRX microstructure and texture numerically with high accuracy, it is necessary to simulate SRX process by taking the deformation microstructure into consideration. A coupling of deformation simulation by crystal-plasticity finite element (CP-FE) method and microstructure evolution simulation by phase-field model, Monte Carlo model or cellular automata model is believed to be the most promising approach for SRX microstructure design. In this coupling model, there are two kind of approach in the evolution simulation of recrystallized grain. One is a grain growth model driven by stored energy or elastic energy of dislocation [1, 2]. The other model is subgrain growth model where the microstructure evolves so as to keep the balance of grain boundary energies and the SRX simulation starts from the deformation microstructure predicted from the results of CP-FE simulation [3, 4]. Here, we call the first model "driving force model" and second model "subgrain growth model". Figure 1 schematically shows the growth of recrystallized grain (RG) in deformed grain (DG).

In this study, we compare the recrystallization microstructures calculated by driving force model and subgrain growth model. Although the subgrain growth model enables a spontaneous nucleation of recrystallized grain through abnormal grain growth, the driving force model needs

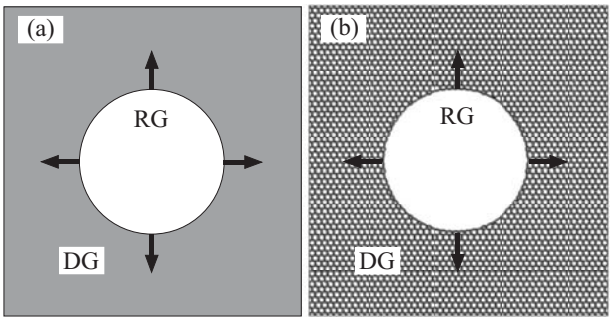

Figure 1: Two recrystallization models: (a) driving force model and (b) subgrain growth model

a nucleation criterion. Therefore, the recrystallization simulations from a shear band are performed, where the shear band is assumed as a region formed by many subgrains with arbitrary crystal orientation.

2 PHASE-FIELD MODEL

A multi-phase-field (MPF) model proposed by Steinbach and Pezzolla is employed here [5]. Let us consider a polycrystalline system including N grains. The ith grain is indicated by the phase field ϕ_i, where ϕ_i takes a value of 1 inside the ith grain, 0 inside the other grains and $0 < \phi_i < 1$ at the grain boundary. The evolution equations of phase field ϕ_i are expressed by

$$\dot{\phi}_i = -\sum_{j=1}^{n} \frac{2M_{ij}^{\phi}}{n} \left[\sum_{k=1}^{n} \left\{ \left(W_{ik} - W_{jk}\right) \phi_k + \frac{1}{2} \left(a_{ik}^2 - a_{jk}^2 \right) \nabla^2 \phi_k \right\} - \frac{8}{\pi} \sqrt{\phi_i \phi_j} \Delta E_{ij} \right], \tag{1}$$

where, n is the number of phase field with a value of $0 < \phi_i \leq 1$ on a grid point and a_{ij}, W_{ij} and M_{ij}^{ϕ}, are respectively related to the grain boundary thickness δ_{ij}, grain boundary energy γ_{ij} and grain boundary mobility M_{ij} by

$$a_{ij} = \frac{2}{\pi} \sqrt{2\delta\gamma_{ij}}, \quad W_{ij} = \frac{4\gamma_{ij}}{\delta}, \quad M_{ij}^{\phi} = \frac{\pi^2}{8\delta} M_{ij}. \tag{2}$$

ΔE_{ij} is the difference in stored energy between grains i and j and $8/\pi$ is obtained from $\int_0^1 \sqrt{\phi_1 \phi_2} d\phi = \int_0^1 \sqrt{\phi\,(1-\phi)} d\phi = \frac{\pi}{8}$.

From a numerical point of view, the MPF model has a high computational cost, because usually N phase fields must be saved and N evolution equations must be solved at all grid points. However, Steinbach and Pezzolla's MPF model has some computational merits that we do not have to solve Eq. (1) at the grid points with $n = 1$ and it is sufficient to save not N but n phase fields at a grid point. To further improve the computational efficiency, we introduce the algorithm proposed by Kim et al. [6] and modify it to achieve more accurate computation.

3 NUMERICAL CONDITIONS

Figure 2 shows the initial structures for (a) driving force model and (b) subgrain growth model. The computational domain with 150 μm $\times$ 150 μm is divided into 1500 $\times$ 1500 finite

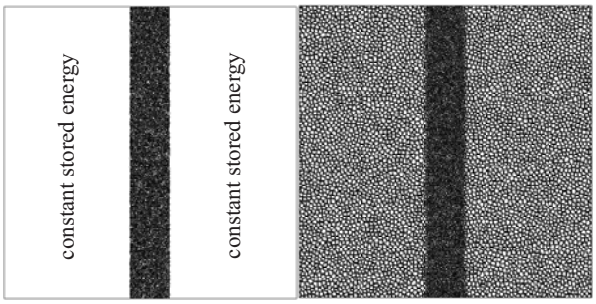

Figure 2: Initial structures

difference grids. The central region consisting of small subgrain with crystal orientation of 0∼90° is shear band and the both sides of shear band are deformed grains. The deformed grain is modeled by subgrains with misorientation of 50±10° for subgrain growth model and a grain with crystal orientation of 50° and stored energy of 0.5 MPa for driving force model. For high angle grain boundary of more than 15°, grain boundary energy γ and grain boundary mobility M are set to $\gamma = \gamma_0 = 0.6$ J/m^2 and $M = M_0 = 4.0741\times10^{-14}$ m^4/Js, respectively. For low angle grain boundary, those are set to $\gamma = \gamma_0 (\Delta\theta/15) \{1 - ln (\Delta\theta/15)\}$ and $M = M_0 \left[1 - \exp\left\{-5 (\Delta\theta/15)^4\right\}\right]$ where $\Delta\theta$ is misorientation of 0∼45°. By setting above condition, spontaneous nucleation from shear band occurs through abnormal grain growth.

4 NUMERICAL RESULTS

Figures 3 and 4 show the microstructure evolutions during static recrystallization simulation for driving force model and subgrain growth model, respectively. Here, the low angle and high angle grain boundaries are indicated by white and black lines, respectively. At the beginning of simulation, the grain growth inside shear band is observed and the size of subgrains in shear band increases. After a period of time, some grains surrounded by high angle grain boundary with high mobility grow abnormally into the deformed grain. Comparing driving force model and subgrain growth model, the size of recrystallized grain of driving force model is relatively smaller than that of subgrain growth model. This is thought to be caused by the difference of the amount of energy stored in the deformed grain. In the driving force model, because the stored energy inside deformed grain is constant, almost flat grain boundaries in front of recrystallized grain are observed. However, because we can see similar nucleation and growth of recrystallized grain for both models, it is concluded that the both model can be used in the coupling SRX model with CP-FE method and phase-field method.

Although we need much more numerical experiments and discussions, it may be said that the driving force model and subgrain growth model can be replaced each other when the nucleation site is clear as a shear band. This brings us computational benefits, because the computational cost needed in driving force model is lower than that of subgrain growth model. These are achieved by employing Steinbach's MPF model, because this MPF model enables the simulations by driving force model and subgrain growth model.

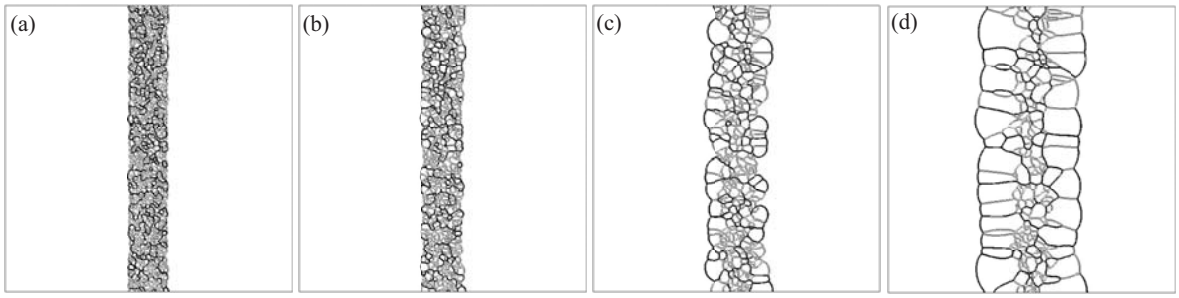

Figure 3: Microstructure evolutions during SRX for driving force model: (a) 10000, (b) 20000, (c) 50000 and (d) 100000 steps

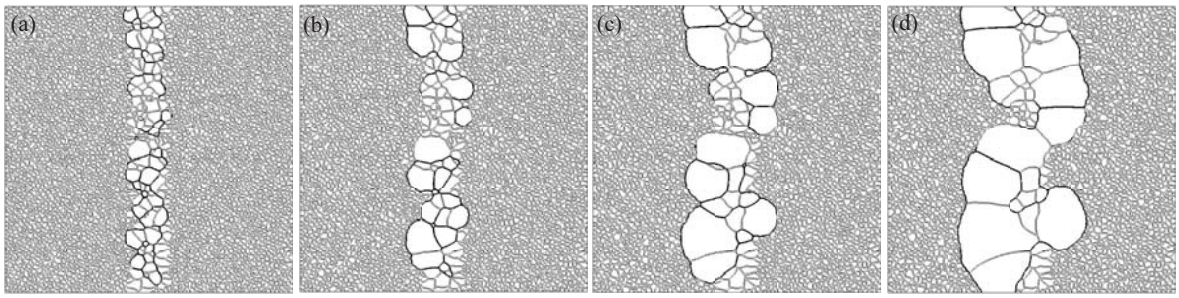

Figure 4: Microstructure evolutions during SRX for subgrain growth model: (a) 100000, (b) 200000, (c) 300000 and (d) 400000 steps

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