MULTI-PHASE-FIELD RECRYSTALLIZATION SIMULATION BASED ON DEFORMATION MICROSTRUCTURE

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Summary We developed a static recrystallization model which enables natural nucleation and grain growth from deformation microstructure. In this model, the subgrain microstructure at large deformation is predicted from crystal orientation and stored energy calculated by crystal plasticity finite element simulation. The nucleation and growth of recrystallized grains from the predicted microstructure is simulated by multi-phase-field method with computationally efficient algorism. From the results of simulation employing the developed model, we could confirm that the proposed model can reproduce the plausible recrystallization process.

INTRODUCTION

The development of recrystallization model is essential to predict the recrystallization texture, microstructure and kinetics during annealing. There are two types of recrystallization model: One is the grain growth model driven by the stored energy [1], in which the deformation microstructure is characterized by the crystal orientation and stored energy. Since this model needs nucleation criteria, the calculated recrytallization kinetics and structure change depending on the predefined nucleation conditions. The other model describes grain growth by the balance of grain boundary energies of the subgrain structure [2]. This model enables the natural nucleation of recrystallized grains through the abnormal grain growth by introducing the misorientation dependence of boundary energy and mobility [3], although, in order to express subgrain microstructures, it requires smaller computational grids and much computational cost comparing to the first model.
In this study, we develop a coupled model for static recrystallization of a phase-field (PF) method that describes second model mentioned above and crystal plasticity finite element (CP-FE) method. Since the normal CP-FE simulation never give subgrain microstructures, the subgrain microstructures are predicted from the results calculated by the CP-FE deformation simulation. The multi-phase-field model (MPF) of Steinbach et al. [4] is employed as a grain growth model and the misorientation dependency of grain boundary energies and mobility are introduced into the PF model.

RECRYSTALLIZATION MODEL

The procedure of recrystallization model proposed in this study is as follows:
(1) Crystal orientation and stored energy of deformed polycrystalline metal are calculated through CP-FE simulation.
(2) The crystal orientation and stored energy are mapped onto the regular grids for PF simulation and smoothed, because finite elements used in CP-FE simulation and finite difference grids used in PF simulation are different in shape and size.
(3) The amount of local orientation gradient $|\nabla\theta| = \sqrt{(\partial\theta/\partial x)^2 + (\partial\theta/\partial y)^2}$ is calculated on all grid points.
(4) The misorientation $\Delta\theta$ is calculated by $\Delta\theta = \Delta\theta_m \exp\left[1 - 1\Big/\left\{|\nabla\theta| \frac{K}{E_{stoer}} \frac{\gamma_m}{\Delta\theta_m}\right\}\right]$ using the smoothed stored energy E_{stoer} and local orientation gradient $|\nabla\theta|$. This equation is derived by assuming $\Delta\theta = |\nabla\theta|\, D_s$.
(5) Subgrain size D_s at all grid points is determined using $D_s = \frac{K}{E_{store}}\gamma_s$, where γ_s is misorientation dependent grain boundary energy expressed by $\gamma_s = \gamma_m \frac{\Delta\theta}{\Delta\theta_m}\left(1 - \ln\frac{\Delta\theta}{\Delta\theta_m}\right)$.
(6) Nuclei to generate the subgrain structure are seeded on the regular grids for PF simulation taking into account the calculated subgrain size.
(7) Subgrain structures are prepared by performing a normal grain growth MPF simulation from the nuclei.
(8) Recrystallization PF simulation is carried out from the initial subgrain structure.
In grain growth simulation during recrystallization, the MPF model of Steinbach et al. [4] is employed. The time evolution equation of phase field ϕ_i which indicates i-th grain is obtained as

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

where i, j and k are the local grain number from 1 to n at a numerical grid point. a_{ij}, W_{ij} and M_{ij}^{ϕ} are the gradient coefficient, the height of double well potential and the phase field mobility between i-th and j-th grains and are related to the material parameters as follows : $W_{ij} = \frac{4\gamma_{ij}}{\delta}$, $a_{ij} = \frac{2}{\pi}\sqrt{2\delta\gamma_{ij}}$ and $M_{ij}^{\phi} = \frac{\pi^2}{4\delta}M_{ij}$, where δ is the grain boundary thickness and γ_{ij} and M_{ij} are the grain boundary energy and mobility. To introduce the misorientation dependency of grain boundary energy and mobility, the following equations are used [3].

$$\gamma_{ij}\left(\Delta\theta_{ij}\right) = \gamma_m \frac{\Delta\theta_{ij}}{\Delta\theta_m}\left(1 - \ln\frac{\Delta\theta_{ij}}{\Delta\theta_m}\right), M_{ij}\left(\Delta\theta_{ij}\right) = M_m\left[1 - \exp\left\{-5\left(\frac{\Delta\theta_{ij}}{\Delta\theta_m}\right)^4\right\}\right]. \tag{2}$$

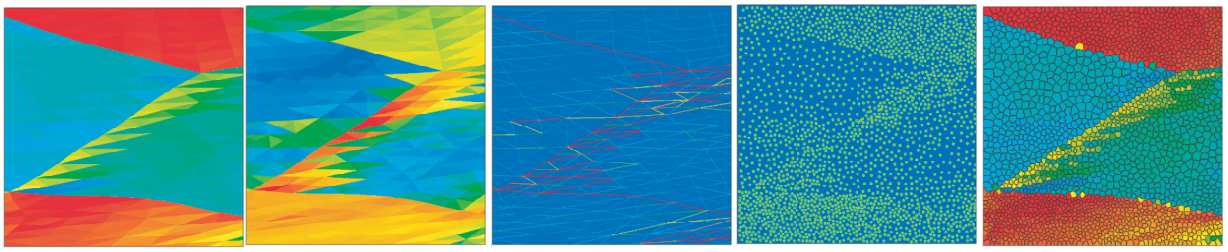

Figure 1. Resutls of CP-FE simulation: (a) crystal orientation θ, (b) stored energy E_{store} and (c) misorientation $\Delta\theta$. (d) Nuclei sowed randomly to generate deformation subgrain microstructure and (e) predicted subgrain microstructures

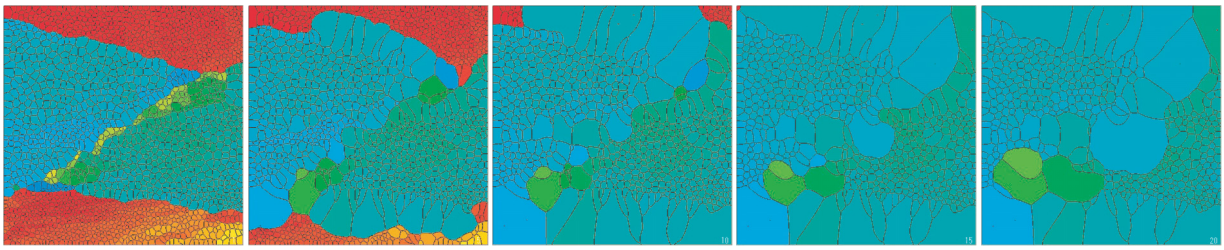

Figure 2. Time evolution during static recrystallization simulation at (a) 300, (b) 1500, (c) 3000, (d) 4500 and (e) 6000 s

Here, $\Delta\theta_{ij}$ is the misorientation between i-th and j-th grains, γ_m and M_m are respectively the boundary energy and mobility at $\Delta\theta_{ij} = \Delta\theta_m$ which is the misorientation when the boundary becomes a high angle boundary. The computational difficulties caused by using many phase field variables are overcome by employing an efficient algorism of Kim et al. [5].

NUMERICAL RESULTS

Figures 1 (a-c) show a part of results calculated by CP-FE simulation, in which the polycrystal metal is compressed until 50%. The created 2229 nuclei determined from the results is shown in Fig. 1 (d). From these nuclei, the normal grain growth is simulated to obtain the subgrain structures. Figures 1 (e) is the predicted subgrain structures. From Fig.1 (e), the crystal orientations are almost same with Fig. 1 (a). The small subgrains are observed at the area where the stored energy is high. Therefore, it is confirmed that the plausible subgrain structures can be predicted by the proposed model.

Figure 2 show the time evolution of subgrain structures and the growth of recrystallized grains during annealing. At the beginning of simulation, the high-angle grain boundaries become smooth owing to their curvature, as can be seen in Fig. 2 (a) with comparing to Fig. 1 (e). After then, some grains with high-angle boundaries grow abnormally and become recrystallized grains. In particular, large recrystallized grains grow into upper and lower grains, because their two grains are deformed intensely and have small subgrain structures. The large deformation area on the diagonal line of computational domain is also preferred nucleation site. However, since the deformation is localized around the diagonal line, the growth rate of recrystallized grains is slower than those of upper and lower regions. In the large initial subgrain regions in Fig. 2 (d), no recrystallization occurs in this simulation period. As a result, the spontaneous nucleation by abnormal grain growth and the recrystallized grain growth depending on the deformation structures are observed in the model developed here.

CONCLUSIONS

We developed a coupled model for static recrystallization with the MPF and CP-FE methods. In this model, the subgrain structures are predicted from the results calculated by CP-FE simulation, and the MPF model is employed as a grain growth model. By performing a series of procedure, we could confirm the plausible recrystallization process.

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