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A DYNAMIC RECRYSTALLIZATION SIMULATION BASED ON PHASE-FIELD AND DISLOCATION-CRYSTAL PLASTICITY MODELS

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Key words: Dynamic Recrystallization, Phase-field Model, Dislocation-crystal Plasticity Model, Multiphysics Simulation.

Abstract. In this paper, so as to reproduce the dynamic recrystallization, the dislocation-crystal plasticity model devotes to a deformation analysis and multi-phase-field one to nucleus growth calculation. First, we place a few nuclei on the parent grain boundaries, i.e., high dislocation density site. Next, carrying out the simulation, dislocations start to accumulate in accordance with the deformation. Introducing the energy of dislocations stored locally in the matrix into the phase-field equation, the placed nuclei begin growing. In the region where the phase transitions from the matrix to the recrystallized phase, the values of dislocation density, crystal orientation and slip are reset. Moreover, applying the above information to the hardening modulus and crystal bases of the crystal plasticity model, the deformation is calculated again. With the progress of deformation, the dislocation density increases even inside the growing nuclei. Also, on the basis of the results obtained by the multiphysics simulation, we discuss the microstructure formations dependent on applied deformation.

1 INTRODUCTION

The mechanical properties of metals are significantly affected by microstructures formed during recrystallization in rolling processes. Especially, the nucleus growth that occurs during the warm- or hot-rolling is known as the dynamic recrystallization (See fig. 1). First, applying plastic deformation to materials, cell structure is formed and then, subgrains are formed by pair annihilation and rearrangement of dislocations in the dynamic recovery stage. Next, in the nucleation stage, subgrain groups on the boundaries between parent grains coalesce to nuclei due to grain boundary migration. This mechanism is called bulging. During this process, stress-strain curve describes the hardening because of dislocation accumulation due to plastic deformation shown in fig. 2. However, once nucleus growth starts and recrystallized phase expands, decrease of dislocation density causes softening of materials. If a further deformation is given to the materials, the stress-strain curve sifts to the rehardening due to dislocation accumulation in the recrystallized new phase. With this mechanism, stress-strain curve during dynamic recrystallization is known to have multi-peaks. For control of mechanical properties in materials design, it is industrially important to predict numerically the dynamic recrystallization.

In the previous work [1], the authors developed a simple multiphysics model of the dynamic recrystallization by coupling the KWC type phase-field model and dislocation-crystal plasticity one that can express the dislocation accumulation by calculating GN crystal defects (GN dislocation density and GN incompatibility). Also, we conducted a computation for a single nucleus on the basis of this model. However, it cannot predict the growth of a number of nuclei because the KWC type phase-field model hardly deals with different nuclei. In addition, there still exists a problem about how to update the crystal orientation of the region that change into recrystallized phase from matrix since the initial orientation was given to such area in the previous simulation.

So as to work out the above problems, in this study, we adopt a multi-phase-field model to extend the material model to an enhanced type suitable for a lot of nuclei. Therein, a modification is conducted for the free energy of bulk to be a double well type considering the stored dislocation energy as a driving force of recrystallization. Next, we develop a multiphysics model combining the multi-phase-field model and dislocation-crystal plasticity one through the crystal orientation and the dislocation density. Using the present model, a

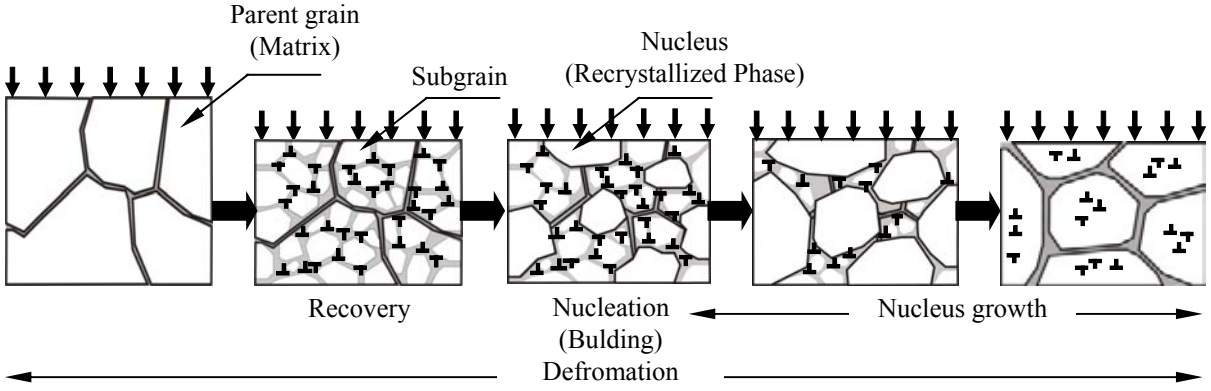


Figure 1 Illustration of dynamic recrystallization

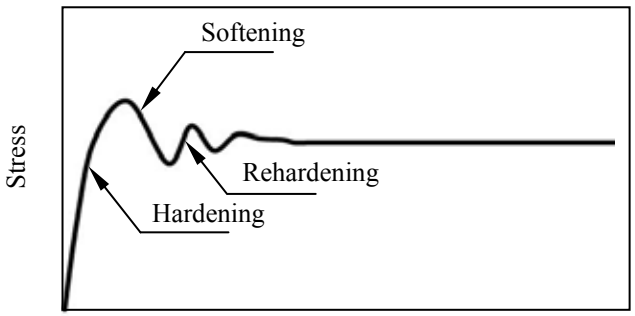


Figure 2 Illustration of stress-strain curve during dynamic recrystallization

numerical simulation is carried out assuming a FCC polycrystal with a few nuclei on the parent boundaries subject to a compressive load in hot-rolling. In this calculation, the current orientation considering deformation is given to the region where the phase changes into recrystallized phase from matrix.

2 MATERIAL MODELS

2.1 Phase-field model

In order to express the growth of a number of nuclei, the multi-phase-field model is adopted in this study. By use of the model, it is possible to calculate growth of a lot of grains simultaneously. Setting the order parameter for grain α as $\phi^\alpha (0 \le \phi^\alpha \le 1)$, and considering the interface field [2] defined as $\psi^{\alpha\beta} \equiv \phi^\alpha - \phi^\beta$ and sum of ϕ^α all over the phases, such as $\sum_\alpha \phi^\alpha = 1$, the evolution equation of ϕ^α is obtained as

$$\frac{\partial \phi^\alpha}{\partial t} = -\sum_{\beta=1}^{N} \frac{M_\phi^{\alpha\beta}}{N} \sum_{\gamma=1(\gamma\neq\alpha)}^{N} \{\frac{1}{2}(\alpha^{\alpha\gamma^2} - \alpha^{\beta\gamma^2})\nabla^2\phi^\gamma + \frac{\partial f(\phi^\alpha,\phi^\gamma)}{\partial \phi^\alpha} - \frac{\partial f(\phi^\beta,\phi^\gamma)}{\partial \phi^\beta}\} \tag{1}$$

where N is the total number of the grains, $M_\phi^{\alpha\beta}$ the mobility of the interface between grains α and β and $\alpha^{\alpha\beta}$ the diffusion constant of the interface between grains α and β. For the free energy of bulk $f(\phi^\alpha,\phi^\beta)$, the function is employed such that

$$f(\phi^\alpha,\phi^\beta) = p(\phi^\alpha,\phi^\beta) f_r(\rho) + \{1 - p(\phi^\alpha,\phi^\beta)\} f_m(\rho) + W^{\alpha\beta} q(\phi^\alpha,\phi^\beta) \tag{2}$$

where $W^{\alpha\beta}$ is the energy barrier between grains α and β. In addition, $f_r(\rho)$ and $f_m(\rho)$ are stored dislocation energies in recrystallized grain and matrix, respectively. Because of $f_r(\rho) \ll f_m(\rho)$, Eq. (2) can rewritten in the form

$$f(\phi^\alpha,\phi^\beta) = \{1 - p(\phi^\alpha,\phi^\beta)\} f(\rho) + W^{\alpha\beta} q(\phi^\alpha,\phi^\beta) \tag{3}$$

where $f(\rho)$ is the difference between stored dislocation energies in recrystallized phase and matrix defined as $f(\rho) \equiv f_m(\rho) - f_r(\rho)$. Using the local stored energy of dislocations $E_s^{\alpha\beta}$, $f(\rho)$ can be represented as $f(\rho) = E_s^{\alpha\beta} = E_s^\alpha - E_s^\beta$. For simplify, we set $E_s^{\alpha\beta} = E_s$ when the phase α is the recrystallized grain and β the matrix, and $E_s^{\alpha\beta} = -E_s$ when the phase α is the matrix and β the recrystallized phase, where E_s is the local energy of stored dislocation

calculated by

$$E_s = \sum_{\alpha} E_s^{\alpha} = \sum_{\alpha^*} \frac{1}{2} \mu \rho^{(\alpha^*)} \tilde{b}^2 \tag{4}$$

where $\rho^{(\alpha^*)}$ is the dislocation density for the slip system α^* (explained later.), μ the shear modulus and $\tilde{b}$ the magnitude of burgers vector. First, we consider a bi-phase problem to obtain $p(\phi)$ and $q(\phi)$. The conditions that $f(\phi)$ is the double well function with the driving force of $E_s^{\alpha\beta}$ are $f(0) = E_s^{\alpha\beta}$, $f(1) = 0$, $f'(0) = 0$ and $f'(1) = 0$. On the above conditions, $q(\phi)$ is determined as $q(\phi) = \phi^2 (1-\phi)^2$. While, we choose $p(\phi)$ as $p(\phi) = \{(2\phi e^{\phi} e^{1-\phi} / e) - (2e^{\phi} e^{1-\phi} / e) + 3\}(1-\phi)^2$. Moreover, replacing ϕ and $1-\phi$ with ϕ^{α} and ϕ^{β} respectively to extend these functions to suitable forms for a multi phases problem, $p(\phi^{\alpha}, \phi^{\beta})$ and $q(\phi^{\alpha}, \phi^{\beta})$ are obtained as follows.

$$\{1 - p(\phi^{\alpha}, \phi^{\beta})\} = (\frac{2}{e} \phi^{\alpha} e^{\phi^{\alpha}} e^{\phi^{\beta}} - \frac{2}{e} e^{\phi^{\alpha}} e^{\phi^{\beta}} + 3) \phi^{\beta 2} \tag{5}$$

$$q(\phi^{\alpha}, \phi^{\beta}) = \phi^{\alpha 2} \phi^{\beta 2} \tag{6}$$

2.2 Dislocation-crystal plasticity model

The elastic-viscoplastic constitutive equation of crystal plasticity model is given by

$$\overset{\nabla}{\boldsymbol{T}} = \boldsymbol{C}^e : (\boldsymbol{D} - \sum_{\alpha^*} \boldsymbol{P}_s^{(\alpha^*)} \dot{\gamma}^{(\alpha^*)}) \tag{7}$$

where $\overset{\nabla}{\boldsymbol{T}}$, $\boldsymbol{C}^e$, $\boldsymbol{D}$, $\boldsymbol{P}_s^{(\alpha^*)}$ and $\gamma^{(\alpha^*)}$ denotes the Mandel-Kratochvil rate of Cauchy stress, the anisotropic elastic modulus tensor, deformation rate tensor, Schmid tensor and the slip for slip system α^*, respectively. The evolution equation of flow stress $g^{(\alpha^*)}$ and the hardening modulus $h^{(\alpha^*\beta^*)}$ dependent on dislocation density are written in the forms

$$\dot{g}^{(\alpha^*)} = \sum_{\beta^*} h^{(\alpha^*\beta^*)} \| \dot{\gamma}^{(\beta^*)} \| \tag{8}$$

$$h^{(\alpha^*\beta^*)} = \frac{1}{2} \frac{ac\mu \Omega^{(\alpha^*\beta^*)}}{L^{(\beta^*)} \sqrt{\rho^{(\beta^*)}}} \dot{\gamma}^{(\beta^*)} \tag{9}$$

where $\Omega^{(\alpha^*\beta^*)}$ is the interaction matrix, $L^{(\beta^*)}$ the dislocation mean free path, and a and c the numerical parameters. A model depending on dislocation density is adopted for $L^{(\beta^*)}$. The dislocation density $\rho^{(\alpha^*)}$ is defined by $\rho^{(\alpha^*)} = \rho_0^{(\alpha^*)} + \rho_G^{(\alpha^*)} + \rho_{\eta}^{(\alpha^*)} + \rho_R^{(\alpha^*)}$, where $\rho_0^{(\alpha^*)}$ is the initial dislocation density, $\rho_G^{(\alpha^*)}$ and $\rho_{\eta}^{(\alpha^*)}$ the norms of GN dislocation density tensor and GN incompatibility tensor, respectively and $\rho_R^{(\alpha^*)}$ the density of annihilated dislocations [3].

3 SIMULATION METHOD

In the multiphysics simulation, crystal deformation and nucleus growth are taken into account simultaneously. First, the dislocation-crystal plasticity simulation is conducted for

prediction of formation of subdivisions and micro shear bands induced by plastic compression. On the basis of the information of nucleation obtained by the above calculation, it is reproduced that the nuclei generated at a nucleation site start to grow by the driving force, i.e., the stored dislocation energy, through the phase-field simulation. The evolution of order parameter due to nucleus growth can be obtained. During this process, in the area where the phase transition from matrix to new phase, the dislocation density should be initialized so as to be the value of sufficiently annealed metal. The information of nucleus growth such as the dislocation density is introduced into the dislocation-crystal plasticity simulation again. The dislocation density and the crystal orientation are changed by deformation. Giving the updated information back to Eq. (1), the nucleus growth simulation can be carried out. The information of dislocation density is introduced into Eq. (1) through the stored dislocation energy expressed by Eq. (4). Same operations are repeated, and dynamic recrystallization simulation is conducted.

4 SIMULATION RESULTS AND DISCUSSIONS

In this simulation, 10% compressive deformation is applied to 80μm×80μm polycrystal aluminum plate under plane strain condition. Considering hot worming process, 2 nuclei are placed on the parent grain boundaries in the initial condition (See figs. 3). The Asaro's 2-slip model is employed and the values of the initial dislocation densities in the matrix and the nuclei are $\rho_0 = 1\mu\,\mathrm{m}^{-2}$ and $\rho_0 = 0.001\mu\,\mathrm{m}^{-2}$, respectively (See fig. 4). In this study, the dislocation-crystal plasticity simulation is carried out by FEM and multi-phase-field model by FDM so that the developed dynamic recrystallization model is calculated by the FEM-FDM hybrid analysis. The number of the finite elements is 2682 and the number of the finite difference grid 40401. In this paper, following 2 cases of simulations are performed: (a) the case that the recrystallization area has the initial crystal orientation and (b) the case that the recrystallization area has the current crystal orientation, i.e., the crystal orientation averaged among the values of neighbor elements.

Figure 5 depicts stress-strain curve obtained by this simulation. In the both cases of simulations, stress-strain curves with oscillations are observed, in which the hardening and softening occur by deformation and by grain growth, respectively. In fig. 5, the arrow of (a) shows the result of the simulation in the case that the recrystallization area has the initial

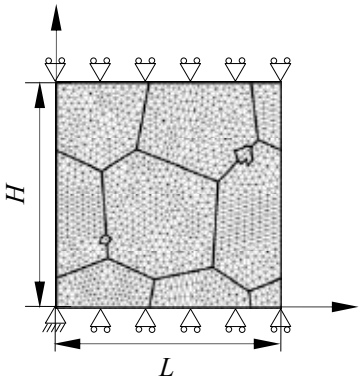


Figure 3 Analysis model

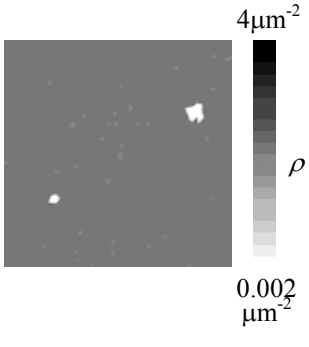


Figure 4 Initial distribution of dislocation density

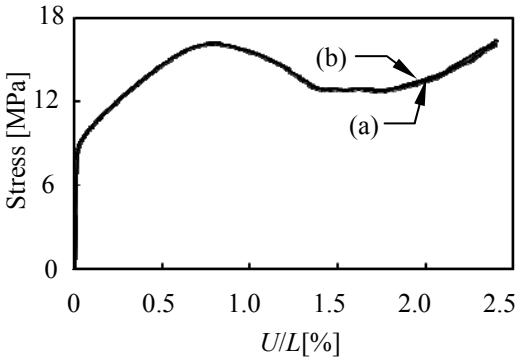
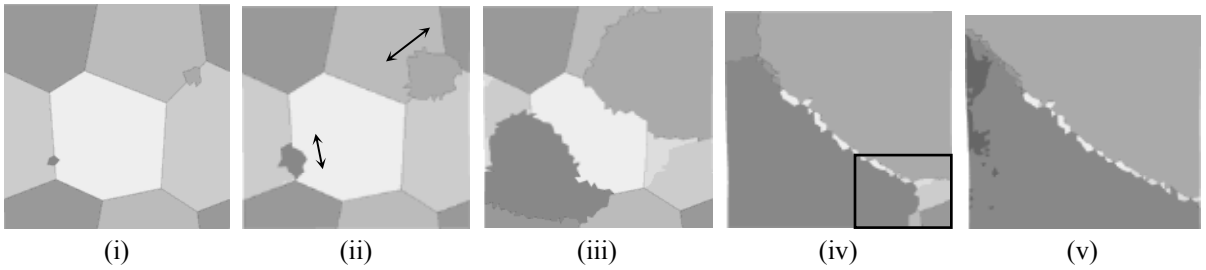
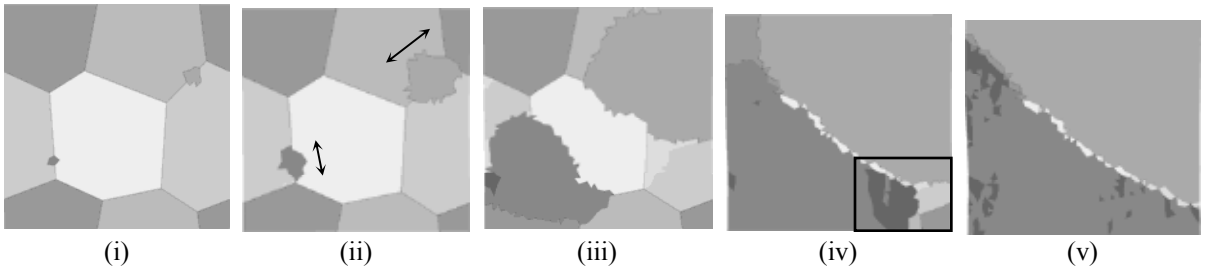


Figure 5 Nominal stress-strain curve



(i) (ii) (iii) (iv) (v)

(a) Case that t the recrystallized area has initial crystal orientation

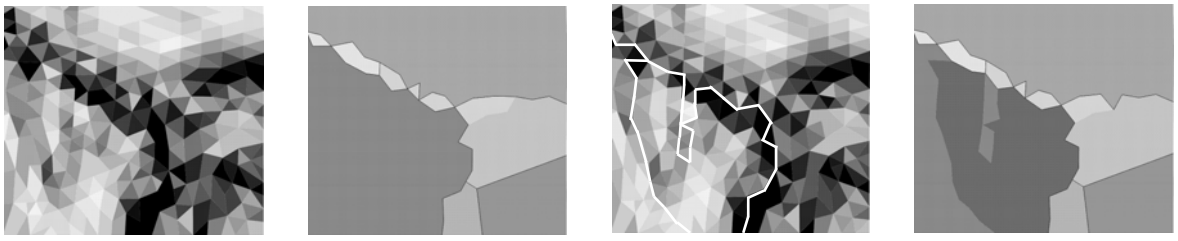


(i) (ii) (iii) (iv) (v)

(b) Case that the recrystallized area has current crystal orientation

Figure 6 Distributions of crystal orientation
(U/L[%]: (i) 0.0, (ii) 0.6, (iii) 1.3, (iv) 2.1, (v) 4.2)

crystal orientation while (b) the result of the simulation in the case that the recrystallization area has the current crystal orientation. It can be seen that the case (b) describe slightly higher rate of hardening than the case (a). The above difference might be explained that the simulation (b) shows higher rehardening rate than (a) because the deformation is taken into account in the simulation (b) more than (a). Also, fig. 6 describes the temporal distributions of crystal orientation. In the both results from the simulations (a) and (b), the nuclei grow along the parent grain boundaries where the dislocations store significantly, shown as the arrows in figs. 6 (a) (ii) and (b) (ii). Furthermore, figs. 7 are the enlarged figures of the rectangulars in figs. 6 (a) (iv) and (b) (iv). Figures 7 (i) and (ii) denote the distributions of dislocation density and crystal orientation, respectively. From figs. 7 (a) (i) and (b) (i), it is noted that the distributions of dislocation density are similar to each other. On the other hand, from the



(i) (ii) (i) (ii)

(a) Case that the recrystallized area has initial crystal orientation

(b) Case that the recrystallized area has current crystal orientation

Figure 7 Distributions of (i) dislocation density and (ii) crystal orientation at U/L=2.1%

distributions of crystal orientation in figs. 7 (a) (ii) and (b) (ii), the growing nucleus at the lower left is not affected by deformation while the one in fig. 7 (b) is affected by deformation. Here, the white lines in fig. 7 (b) (i) mean nucleus-matrix boundaries and the boundaries between the recrystallized area whose crystal orientation does not change from its initial crystal orientation and the one whose crystal orientation does change from its initial crystal orientation. The area surrounded by white lines would be a nucleation site if the grain boundary misorientation were higher than 15˚.

5 CONCLUSIONS

- Simulating dynamic recrystallization by coupling the multi-phase-field model and the dislocation-crystal plasticity model, it can be reproduced that a few nuclei grow responding to the distribution of dislocation density and crystal orientation.
- Givining the averaged value of neighbor elements to the region that transitions to recrystallized phase from matrix, it can be possible to calculate considering the change of crystal orientation due to deformation.

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