Multi-phase-field Simulations of Dynamic Recrystallization during Transient Deformation

Tomohiro TAKAKI,1) Akinori YAMANAKA2) and Yoshihiro TOMITA3)

1) Graduate School of Science and Technology, Kyoto Institute of Technology, Matsugasaki, Sakyo, Kyoto, 606-8585 Japan. E-mail: takaki@kit.ac.jp 2) Graduate School of Science and Engineering, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo, 145-8552 Japan. E-mail: ayamanaka@mes.titech.ac.jp 3) Department of Mechanical Engineering, Fukui University of Technology, Gakuen, Fukui, 910-8505 Japan. E-mail: tomita@fukui-ut.ac.jp

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To develop a multiscale hot-working model that enables us to simulate macroscopic mechanical behaviors depending on microstructural evolution by the coupling the finite element (FE) method and phase-field (PF) method, the multi-phase-field-dynamic recrystallization (MPF-DRX) model has been applied to transient deformation simulation, where strain rate and temperature rapidly change during deformation. As a result, it has been confirmed that the variations in the macroscopic stress-strain curve and average grain size during deformation are in good agreement with the experimental observation qualitatively.

KEY WORDS: transient deformation; dynamic recrystallization; hot working; multi-phase-field method; multiscale simulation.

1. Introduction

Recrystallization has two types: static recrystallization (SRX) and dynamic recrystallization (DRX).1,2) SRX occurs during annealing after plastic deformation, where recrystallized grains are nucleated in the high-energy region and successively grow into deformed materials. On the other hand, DRX occurs during hot working, where hardening due to dislocation accumulation and softening due to dynamic recovery (DRV) and grain growth occur simultaneously. Although both SRX and DRX have many common points such as the nucleation and growth of recrystallized grains, the different point is that, for DRX, the stored energy or dislocation density in deformed and recrystallized grains continuously increases with deformation; for SRX, that in deformed grains decreases owing to recovery and that in recrystallized grains is constant at almost zero.

The macroscopic mechanical behavior of metallic materials with a low to medium stacking fault energy during hot working is largely affected by microstructural evolution.1–3) Generally, the macroscopic stress-strain curve at a high strain rate, a low temperature or a large initial grain size shows a single peak. On the other hand, a stress-strain curve showing multiple peaks is observed at a low strain rate, a high temperature or a small initial grain size. These transitions from a single peak to multiple peaks in the macroscopic stress-strain curve are caused by the nucleation and growth of DRX grains, or by microstructural evolution. Therefore, to predict and simulate mechanical behavior during hot working with high accuracy, a multiscale model that can simulate macroscopic mechanical behavior and microstructural evolution simultaneously is indispensable.

Some finite element (FE) models taking DRX into account have been developed to simulate mechanical behavior during hot working.4–7) Although such models have enabled us to simulate macroscopic mechanical behavior during hot working, the effects of DRX are incorporated into the constitutive equation using the DRX fraction or Zener-Hollomon parameter; however, we cannot obtain microstructural information from those models.

To enable microstructural evolution simulation during DRX, Ding and Guo8) have developed a cellular automaton DRX (CA-DRX) simulation model, where the evolution of dislocation density is modeled by the Kocks-Mecking (KM) model9) and DRX grain growth is simulated by a cellular automaton (CA) method. The macroscopic stress-strain property is related to the microstructure by the Bailey-Hirsch equation10) using average dislocation density. This model is widely applied to the study of other materials and phenomena.11–16) Takaki et al.21,22) developed the MPF-DRX model, where the multi-phase-field (MPF) method proposed by Steinbach and Pezzolla23) is employed instead of the CA method. They emphasized that the MPF-DRX method can simulate the DRX process with higher accuracy than the CA-DRX method. However, these CA-DRX and MPF-DRX simulations are limited to the uniform deformation problem with constant strain rate and temperature.

The final goal of our study is to develop a multiscale hot working model that enables us to simulate macroscopic mechanical behavior depending on microstructural evolution by coupling the FE and MPF-DRX methods. This method is thought to be a promising approach to simulating actual hot working. Figure 1 shows an image of hot rolling simulation using the model, where the MPF-DRX model is
solved in each representative volume element prepared for each integration point or element of macroscopic finite element simulation. The idea is similar to the homogenization method,\textsuperscript{24,25}) where macroscopic mechanical behavior is simulated on the microscopic mechanical properties. The different point is that, in the simulation shown in Fig. 1, macroscopic mechanical behavior is simulated by microstructural evolution.

In this study, as a preliminary work to develop the multiscale hot-working model shown in Fig. 1, the MPF-DRX model\textsuperscript{21,22}) is extended to transient deformation,\textsuperscript{26,27}) where strain rate and temperature are changed during hot deformation, because, in actual hot working, such parameters change continuously depending on time and position.

2. MPF-DRX Model

We have developed a MPF-DRX model\textsuperscript{21)} in which the grain growth driven by stored energy is simulated by the MPF method\textsuperscript{23)} using an efficient computational algorithm\textsuperscript{28}) and the dislocation density evolution due to plastic deformation and dynamic recovery (DRV) is expressed by the KM model.\textsuperscript{9)} A macroscopic stress-strain curve is obtained from the Bailey-Hirsch equation\textsuperscript{10}) using average dislocation density. In this chapter, the MPF-DRX model is briefly explained.

2.1. Multi-phase-field Model

A polycrystalline system including $N$ grains is indicated by $N$ phase-field variables. The $i$th grain is indicated by the phase field $\phi_i$, where $\phi_i$ takes values of 1 inside the $i$th grain, 0 inside the other grains, and $0 < \phi_i < 1$ at the grain boundary. The evolution equation of $\phi_i$ is expressed by\textsuperscript{23)}

$$
\dot{\phi}_i = \frac{2M_i^2}{n} \left( \sum_{j=1}^{n} \left[ (W_{ij} - W_{ii}) \phi_j + \frac{1}{2} (a_{ij}^2 - a_{ii}^2) \nabla^2 \phi_j \right] - \frac{8}{\pi} \sqrt{\phi_i \phi_j} \Delta \phi \right)
$$

\text{.......................... (1)}

where $n$ is the number of phase-field variables larger than 0 at the lattice point, and $a_{ij}$, $W_{ij}$, and $M_i^2$ are the gradient coefficients, the height of double-well potentials and the phase-field mobilities related to the grain boundary thickness $\delta$, the grain boundary energy $\gamma$ and the grain boundary mobility $M$, respectively, by

$$
a_{ij} = \frac{2}{\pi} \sqrt{2\delta \gamma}, \quad W_{ij} = \frac{4\gamma}{\delta}, \quad M_i^2 = \frac{\pi^2}{8\delta} M \quad \text{......... (2)}
$$

Here, $\delta$, $\gamma$ and $M$ are assumed to be constant at all boundaries. Equation (2) is true only for $i \neq j$ and the diagonal components for $i = j$ are zero. The driving force $\Delta \phi_i$ can be obtained as $\Delta \phi_i = 1/2 \mu b^2 (\rho_i - \rho_j)$, where $\mu$ is the shear modulus, $b$ is the magnitude of the Burgers vector, and $\rho_i$ and $\rho_j$ are the dislocation densities in the $i$th and $j$th adjacent grains, respectively. To solve Eq. (1) efficiently, we introduce the algorithm proposed by Kim et al.\textsuperscript{23}.

2.2. Dislocation Evolution Model

The accumulation of dislocations due to plastic deformation and DRV is expressed by the KM model\textsuperscript{9)} as the relationship between the local dislocation density $\rho_i$ in the $i$th grain and the true strain $\varepsilon$:

$$
d\rho_i = k_1 \sqrt{\rho_i - k_2 \rho_i} \quad \text{.................................. (3)}
$$

Here, the first term on the right-hand side expresses the work hardening, where $k_1$ is a constant that represents hardening. The second term is the DRV term, where $k_2$ is a function of the temperature $T$ and the strain rate $\dot{\varepsilon}$.\textsuperscript{8)} Macroscopic stress is related to the average dislocation density $\overline{\rho}$ as

$$
\sigma = \alpha \mu b \sqrt{\overline{\rho}} \quad \text{.............................. (4)}
$$

where $\alpha$ is the dislocation interaction coefficient of approximately 0.5. From Eqs. (3) and (4), a macroscopic stress-strain curve can be determined. Note that all stresses and strains used in this study are set as $y$-direction components.

2.3. Nucleation of DRX Grains

Nucleation at grain boundaries is the most dominant nucleation mechanism for DRX in single-phase materials.\textsuperscript{17-20}
Therefore, it is assumed that the nucleation of recrystallized grains occurs only with the bulging of a grain boundary in the present model. Therefore, when the dislocation density at a grain boundary exceeds its critical value \( \rho_c \), or
\[
\rho_i = \left( \frac{20\gamma \epsilon}{3bh\mu \tau^2} \right)^{1/3}
\]  
(5) nuclei are placed at a grain boundary by following the nucleation rate per unit area of a grain boundary expressed as
\[
\dot{n} = c\varepsilon^d \exp\left(-\frac{\omega}{T}\right)
\]  
(6) where \( \tau = 0.5\mu b^2 \) is the line energy of a dislocation, \( \varepsilon \) is the mean free path of mobile dislocation expressed by \( \varepsilon = 10/\left(0.5\sqrt{\rho_c}\right) \), and \( c, d, \omega, T \) are constants. The unit of \( \dot{n} \) is \( [1/m^2s] \).

Although the present simulations are performed in two-dimensional space, for the critical dislocation \( \rho_c \) that determines the softening start point, Eq. (5) derived in a three-dimensional problem is required to compare the numerical results with experimental ones using cylindrical compression specimens.

### 2.4. Computational Procedure

The computational procedure of the MPF-DRX model is as follows:

1. The initial polycrystalline structure shown in Fig. 2 is generated by conventional grain growth simulation.
2. The dislocation density at all grid points is set to its initial value \( \rho_{ini} \).
3. The dislocation density and macroscopic stress-strain curve up to the DRX nucleation point are calculated under a constant strain increment \( \Delta \varepsilon = \dot{\varepsilon}\Delta t \) using Eqs. (3) and (4), where \( \Delta t \) is the time increment.
4. If the dislocation density of a finite difference grid point located at a grain boundary exceeds its critical value \( \rho_c \) required to produce nuclei, the grid point is considered a nucleation potential site. Moreover, when the present time step is a step to put one nucleus calculated from a nucleation potential site, one circular nucleus with a dislocation density \( \rho_{nuclei} \) is placed at the grain boundary selected randomly.

\[
\rho_{nuclei} = \frac{20\gamma \varepsilon}{3\mu \varepsilon \tau^2}
\]

(5) The DRX grain growth is simulated by solving Eq. (1).

(6) The dislocation density variables at all grid points and macroscopic stress are calculated by solving Eqs. (3) and (4), respectively.

Steps (4) to (6) are repeated until the prescribed strain is obtained.

### 3. Numerical Conditions

We employ the following material parameters for copper. Almost all numerical conditions are set to be identical to the previous ones. For Eqs. (1) and (2), the grid size \( \Delta x = 0.5 \mu m \), the grain boundary energy \( \gamma = 0.208 \, J/m^2 \), the grain boundary thickness \( \delta = 7\Delta x \) and the grain boundary mobility \( M = M_0 \exp(-Qb/RT) \), where \( M_0 = 0.139 \, m^3KJ/s \), the activation energy \( Q_b = 250 \, KJ/mol \) and \( R = 47 \, KJ/mol K \) is the gas constant. The time increment \( \Delta t \) is set to \( \Delta t = (\Delta x)^2/(4\mu M_0) \), where \( \mu \) and \( M_0 \) are the nondiagonal components of \( a_{ij} \) and \( M_0 \), respectively. For Eqs. (3) and (4), \( k_1 = 4.0 \times 10^{13}/m^2 \) and \( k_2 = 2.56 \times 10^{14}/m^2 \) the shear modulus \( \mu = 42.1 \, KPa \), the magnitude of the Burgers vector \( b = 2.56 \times 10^{-10} \, m \) and the steady-state stress \( \sigma_{ss} = \left\{ A_1 \dot{\varepsilon} \exp(Q_b/RT) \right\}^{1/\beta} \), where \( A_1 = 2.0 \times 10^{44} \), \( A_2 = 7.6 \) and the activation energy \( Q_b = 275 \, KJ/mol \). For Eqs. (5) and (6), \( \rho_0 = 1.7 \times 10^{13}/m^2 \), \( c = 1.125 \times 10^{-7} \), \( d = 1 \) and \( \omega = 2 \times 400 \, K \). Here, one nucleus is created every \( \Delta t \rho_{nuclei} \Delta x^2/\delta \) steps, where unit thickness is taken into account and \( \rho_{nuclei} \) is the number of grid points satisfying both requirements at the grain boundary, or \( 0 < \phi < 1 \), and of which the dislocation density is larger than its critical value by \( \rho_c \). Eq. (5). The initial dislocation density is set to \( \rho_{ini} = 10^{5}/m^2 \).

### 4. Numerical Results

#### 4.1. Effects of Initial Grain Size, Strain Rate and Temperature

The macroscopic stress-strain curve and microstructural evolution are largely affected by initial grain size, strain rate and temperature. Before transient deformation simulation, therefore, we perform a series of DRX simulations under constant strain rate and temperature. Here, the standard conditions are set as follows: initial grain diameter \( D_{ini} = 50 \mu m \), strain rate \( \dot{\varepsilon} = 0.01/s \) and temperature \( T = 800 \, K \). Figure 2 shows the computational model with \( 476 \times 492 \) grids and an initial polycrystalline structure for the \( D_{ini} = 50 \mu m \) model. 30 regular hexagonal grains exist under the periodic boundary condition.

**Figure 3** shows the macroscopic stress-strain curves (upper figure) and variations in average grain diameter (lower figure) when changing the initial grain diameter to \( D_{ini} = 12.5, 25, 50, 100 \) and \( 150 \mu m \). The following computational domains are employed for each grain size in addition to \( D_{ini} = 50 \mu m \).

- **250 \mu m**: 504 \times 492 grids (252 \mu m \times 249 \mu m), 511 grains
- **25.0 \mu m**: 480 \times 498 grids (240 \mu m \times 249 \mu m), 122 grains
- **100. \mu m**: 470 \times 658 grids (235 \mu m \times 329 \mu m),
12 grains
$D_{\text{ini}} = 150. \mu\text{m}$, 572 $\times$ 495 grids ($286 \mu\text{m} \times 247.5 \mu\text{m}$), 4 grains

From Fig. 3, we can see typical initial grain size dependences: (1) The amount of peak stress $\sigma_p$ increases with increasing $D_{\text{ini}}$. (2) The transition from a single-peak curve to multiple-peak curve occurs with decreasing $D_{\text{ini}}$. (3) Stress and average grain diameter reach their steady-state constant values $\sigma_s$ and $D_s$, respectively; they are independent of initial grain size.

Figure 4 shows the variations in stress and average grain diameter with increasing strain at strain rates $\dot{\varepsilon} = 0.1$, 0.03, 0.01, 0.003 and 0.001/s. With increasing strain rate, it is observed that the peak stress $\sigma_p$ and the steady-state stress $\sigma_s$ increase. On the other hand, the steady-state average grain diameter $D_s$ increases with decreasing strain rate. The transition from a single-peak curve to a multiple-peak curve is also observed with decreasing strain rate. The $D_s$ for $\dot{\varepsilon} = 0.1$/s is 5.8 $\mu$m, which is the smallest among all the sizes obtained in the simulations in this study. Although it is smaller than $2\delta$, the accuracy is maintained because of the presence of too many small grains, such as nuclei and almost disappearing grains. Figure 5 shows the effects of temperature on the stress-strain curves and the variations in average grain diameter, where the temperatures are 700, 750, 800, 850 and 900 K. Comparing Figs. 4 and 5, it is observed that the results obtained with decreasing temperature correspond to those obtained with increasing strain rate. The results in Figs. 4 and 5 are in good agreement with the experimental observations.\textsuperscript{30,31}

4.2. Transient Deformation

Here, we simulate the transient deformation processes

where strain rate or temperature is changed rapidly at a true strain $\varepsilon = 0.5$ during DRX. The standard conditions are set as follows: strain rate $\dot{\varepsilon} = 0.01$, temperature $T = 800$ K and initial grain diameter $D_{\text{ini}} = 50 \mu$m.

Figure 6 shows the stress-strain curves and the variations in average grain diameter when changing strain rate from
0.01/s to 0.1, 0.03, 0.003 and 0.001/s at $\varepsilon = 0.5$. The gray lines are the results in Fig. 4 or the constant strain rates. When strain rate increases from $\dot{\varepsilon} = 0.01$/s, true stress increases after the transition of $\varepsilon = 0.5$ and peak stress exceeds the curve of constant strain rate, or an overshooting of true stress can be observed.\textsuperscript{26,27} The peak stress after the transition point is smaller than that corresponding to the constant strain rate. This is caused by the smaller grain size at the transition point than the initial grain diameter, $D_{ini} = 50 \mu$m, as shown in Fig. 3. Average grain diameter gradually decreases with increasing true strain after the transition point. With further deformation, true stress and average grain diameter reach steady-state values that are the same as those in the case of a constant strain rate. On the other hand, by reducing strain rate at $\varepsilon = 0.5$, true stress rapidly decreases and average grain diameter rapidly increases with the growth of recrystallized grains. True stress reaches its steady-state value $\sigma$ after an undershooting and some perturbations of the curve. Figure 7 shows the microstructural evolutions during the transient deformation from $\dot{\varepsilon} = 0.01$/s (a–d) to 0.1 (e1-h1) and 0.001/s (e2-h2). The gray scale indicates the number of DRX cycles defined in Ref. 22). In the cases from (e1) to (h1), a gradual decrease in grain size can be observed. On the other hand, in the case of strain rate reduction, a rapid increase in grain size from (d) to (e2) occurs immediately after a transient is observed and grain size becomes less variable during (e2) to (h2).

Figure 8 shows the macroscopic stress-strain curves and the variations in average grain diameter with changes in temperature from $T = 800$ K to 700, 750, 850 and 900 K at $\varepsilon = 0.5$. Phenomena similar to those in Fig. 6 can be observed. By reducing temperature at $\varepsilon = 0.5$, an overshoot of true stress is observed, the amount of peak stress decreases.
es compared with the constant temperature drawn by gray lines and average grain diameter gradually decreases with increasing true strain. By increasing temperature at \( \varepsilon = 0.5 \), true stress and average grain diameter rapidly change after the transition point, an undershooting of true stress is observed, and some perturbations are observed for both true stress and average grain diameter. Finally, true stress and grain diameter reach their steady-state values, and these values decrease to those in the constant-temperature cases. Compared with the experimental results reported in Ref. 27), no undershooting or perturbation after increasing temperature is observed in the experiment. However, experiments in which the temperature inside the material is suddenly but uniformly changed are impossible, and, in a previous experiment,\(^\text{27}^\) temperature changes occurred not rapidly but within a finite time. The present simulation and the previous experiment\(^\text{27}^\) both showed that the steady-state stresses after changing temperature agree with those at a constant temperature.

Furthermore, we perform multitransient deformation simulation. Figure 9 shows the macroscopic stress-strain curves and the variations in average grain diameter when the strain rate changes in the order of 0.1, 0.01 and 0.001/s and 0.001, 0.01 and 0.1/s at \( \varepsilon = 0.4 \) and 0.8. These strains at transient point are chosen so as to achieve the steady-state condition before and after the transient point by following Refs. \( 26, 27^\). The phenomena observed in Fig. 6 can also be observed after the second transition. The same phenomena can be observed from Fig. 10 where the temperature changes in the order of 900, 800 and 700 K and 700, 800 and 900 K. From Figs. 9 and 10, we can see that, by changing strain rate and temperature, true stress and average grain diameter after transition approach their steady-state values at constant strain-rate and temperature. From these results, it is concluded that the MPF-DRX method can be applied to the
study of an actual hot working process where strain rate and temperature change arbitrarily and continuously.

5. Conclusions

As a preliminary study to develop a multiscale hot working model that will enable us to simulate macroscopic mechanical behavior depending on microstructural evolution by coupling the FE method and the MPF-DRX model, in this study, transient deformation simulation using the MPF-DRX method has been performed. As a result, typical phenomena, such as the overshooting and undershooting of stress after the transitions of strain rate and temperature and the steady-state values of true stress and average grain diameter with transient deformation becoming the same at constant strain rate and temperature, have been observed. Therefore, it has been confirmed that the MPF-DRX model can be applied to the study of an actual hot working process where strain rate and temperature change continuously in time and space.

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