Multiscale Hot-working Simulations Using Multi-phase-field and Finite Element Dynamic Recrystallization Model

Chihiro YOSHIMOTO and Tomohiro TAKAKI*

Mechanical and System Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo, Kyoto, 606-8585 Japan.

(Received on July 22, 2013; accepted on October 7, 2013)

In this study, we simulated non-uniform compression of a cylinder under various temperatures and deformation rates using a multi-phase-field and finite element dynamic recrystallization (MPFFE-DRX) model, which couples the multi-phase-field dynamic recrystallization (MPF-DRX) model with a large-deformation elastic-plastic finite element (FE) method using J2 flow theory for DRX microstructure evolution and macroscopic mechanical behavior, respectively. Detailed examination of the results confirmed that microstructure evolution and macroscopic mechanical behavior were accurately coupled over a wide range of temperature and deformation rate conditions. We also concluded that the MPFFE-DRX model can be used with a wide variety of temperatures and deformation rates.

KEY WORDS: multiscale simulation; hot-working; dynamic recrystallization; phase-field method; finite element method.

1. Introduction

In hot-working, metallic materials are plastically worked above their recrystallization temperature. It is widely used since the working force is much lower than that of cold-working, it can increase in ductility of the product, diffusion at high temperature reduces chemical inhomogeneities, etc.1,2) Microstructures greatly change during hot-working. Particularly for low to medium stacking fault energy materials, dynamic recrystallization (DRX)—where recrystallized grain nucleate and grow after the dislocation density reaches a critical value—occurs in addition to dynamic recovery (DRV) and dislocation accumulation due to plastic deformation. For DRX materials, the macroscopic mechanical behavior during hot-working is largely affected by the microstructure evolution due to DRX.3,4) To predict the mechanical behavior and control the microstructure of the final product with high accuracy, constructing a numerical tool that can evaluate the mechanical behavior and microstructure evolution simultaneously is important.

Hot-working simulations are usually performed by employing the finite element (FE) method, where internal state variables such as the DRX volume fraction and average DRX grain diameter are incorporated into the constitutive equation.5–14) Although the FE method is the most powerful tool for evaluating the macroscopic mechanical behavior during hot-working, the microstructure cannot be obtained directly. In addition, predicting the stress–strain curve for a complicated deformation history during working in advance is difficult.

The microstructure evolution during hot-working with the DRX is numerically simulated using grain growth models such as cellular automaton (CA), Monte Carlo (MC), and phase-field (PF) models. Ding and Guo15) developed a cellular automaton dynamic recrystallization (CA-DRX) model. They computed the DRX grain growth, evolutions in dislocation density due to plastic deformation and DRV, and average stress of the entire computational region with the CA method, Kocks–Mecking model,16) and Bailey–Hirsch’s equation,17) respectively. Their pioneering work enabled the prediction of macroscopic mechanical behavior based on microstructure evolution and has been applied to various materials and working conditions.18–23) Takaki et al.24–26) developed a multi-phase-field dynamic recrystallization (MPF-DRX) model where the multi-phase-field (MPF) method,27) which can be used to accurately simulate the microstructure evolution and has been applied to various materials and working conditions,28–31) developed a multi-phase-field dynamic recrystallization (MPF-DRX) model that couples the MPF-DRX model with a large-deformation elastic-plastic FE method using J2 flow theory for DRX microstructure evolution and macroscopic mechanical behavior, respectively. The MPFFE-DRX model was used to successfully simulate the compression of a cyl-
under indicating non-uniform deformation.

In this study, we performed a series of hot-working simulations using the MPFFE-DRX model under a wide variety of temperatures and deformation rates and confirmed the wide applicability of the MPFFE-DRX model. We also investigated the non-uniform compression deformation behavior of a cylinder in detail. This paper is structured as follows. The MPFFE-DRX model is briefly explained in Section 2. Conditions for compression simulation with non-uniform deformation of a cylinder are introduced in Section 3. The numerical results from various temperatures and deformation rates are presented in Section 4 in detail. The conclusions are presented in Section 5.

2. MPFFE-DRX Model

In the MPFFE-DRX model, the microstructure evolution is expressed by the micro-model, and the macroscopic mechanical behavior is evaluated by the macro-model. In the simulation using the model, a metallic material worked at an elevated temperature is meshed by finite elements in the micro-field, the grain growths are calculated with the Kocks–Mecking model:16) where $\varepsilon$ is an equivalent strain, $\gamma$ is the mean free path of the mobile dislocation, $\delta$ is the grain boundary energy, $\rho_0$ is the grain boundary mobility, $\rho$ is the dislocation interaction coefficient. The tangent modulus between the micro-field and temperature $T$ calculated in the macro-field.

2.1. Micro-field

In the micro-field, hardening due to dislocation accumulation and softening due to the DRV and DRX are expressed at the same time. At the beginning of the simulation, we prepared a polycrystal with uniform initial dislocation density. The dislocation density $\rho$ in the $i$th grain of the polycrystal with $N$ grains is calculated by the Kocks–Mecking model:16)

$$\frac{d\rho_i}{d\varepsilon} = k_1\sqrt{\rho_i - k_2\rho}, \quad \text{......... (1)}$$

where $\varepsilon$ is an equivalent strain, $k_1$ is a constant, and $k_2$ is a function of $T$ and $\varepsilon$ that represents the DRV. The first term of the right-hand side expresses hardening, and the second term expresses softening by the dislocation dynamics.

The nucleation of the DRX was assumed to occur by bulging of the grain boundary.33,34) Therefore, when the dislocation density on the grain boundary becomes larger than the critical dislocation density $\rho_c$, expressed by

$$\rho_c = \left(\frac{2\pi\sigma_0}{3b\gamma E_d}\right)^{\frac{3}{2}}, \quad \text{......... (2)}$$

the DRX grain with the initial dislocation density is nucleated on the grain boundary at the nucleation speed of

$$n = c\varepsilon^d \exp\left(-\frac{T_0}{T}\right). \quad \text{......... (3)}$$

In Eqs. (2) and (3), $\gamma$ is the grain boundary energy, $b$ is the magnitude of the Burgers vector, $T$ is the mean free path of the mobile dislocation, $\delta$ is the grain boundary mobility, $E_d$ is the elastic strain energy $E_d = 1/2G\delta^2$ caused by one dislocation, $G$ is the shear modulus, and $c$, $d$, and $T_0$ are constants.

The polycrystalline structure and grain growths are expressed by the MPF model. The $i$th grain is indicated by the phase-field variable $\phi_i$. In this simulation, $\phi_i$ is 1 in the $i$th grain and 0 in the other grains. In the grain boundary between the $i$th grain and other grains, $\phi$ changes from 0 to 1 smoothly. The time evolution equation of $\phi$ is expressed as

$$\frac{\partial \phi_i}{\partial t} = -\sum_{j=1}^{n} M_{ij} \left[ \sum_{k=1}^{n} \left( W_{ik} \phi_k + \frac{1}{2} \left( a_{ik}^2 - a_{ik}^1 \right) \right) \right]$$

where

$$\sigma_{ij} = -\frac{8}{\pi} \sqrt{\phi_j} \frac{\Delta \gamma_{ij}^\phi}{\Delta \rho_j} \left[ \begin{array}{c} \phi_j \\ 1 \end{array} \right] \quad \text{......... (4)}$$

where $n$ is the number of phase-field variables, $a_{ij}$ is the gradient coefficient between the $i$th grain and the $j$th grain, $W_{ij}$ is the amount of the energy barrier and $M_{ij}$ is the phase-field mobility. $\rho_j$ is the grain boundary thickness $\delta$, grain boundary energy $\gamma$, and grain boundary mobility $M$ as $a_{ij} = 2\gamma\delta / \pi$, $W_{ij} = 4\gamma\delta$ and $M_{ij} = \pi^2 M / 8\delta$. $\Delta \gamma_{ij}^\phi$ is the stored energy difference between the $i$th and $j$th grains expressed by $\Delta \gamma_{ij} = E_d (\rho_i - \rho_j)$. In order to estimate the mechanical behavior of each micro field, the equivalent stress $\sigma$ is calculated by the average dislocation density $\rho_{ave}$ in the micro-field. It is expressed by the Bailey–Hirsch equation

$$\sigma = \alpha G b \sqrt{\rho_{ave}}, \quad \text{......... (5)}$$

where $\alpha$ is the dislocation interaction coefficient. The tangent modulus of the stress–strain curve by $d\sigma / d\varepsilon$ is delivered to the macro-field.

2.2. Macro-field

Macroscopic mechanical behavior during hot-working was evaluated by the large-deformation elastic–plastic FE method.35) In this simulation, we used a constitutive equation where the elastic and plastic strain rates are derived from Hooke’s law and J2 flow theory, respectively. The total strain rate $\dot{\varepsilon}_j$ is a total amount of elastic strain rate $\dot{\varepsilon}_e$ and plastic strain rate $\dot{\varepsilon}_p$:

$$\dot{\varepsilon}_j = \dot{\varepsilon}_e + \dot{\varepsilon}_p \quad \text{......... (6)}$$

Due to Eq. (6), the relation between the Jaumann rate of the Kirchhoff stress $\dot{S}_{ij}$ and strain rate is indicated by

$$\dot{S}_{ij} = \frac{D_{ijkl} \dot{\varepsilon}_{kl} - 2G\sigma_i'\sigma_i'}{g} \dot{\varepsilon}_{ij}, \quad \text{......... (7)}$$

where $D_{ijkl}$ is the elastic tensor, $\sigma_i'$ is the deviatoric stress, and $g$ is calculated by

$$g = \frac{2}{3} \sigma + \left(1 + \frac{h}{2G}\right) (1 - h) \quad \text{......... (8)}$$

where $\sigma$ is the Mises equivalent stress and $h$ is expressed by

$$1 = \frac{3}{2} \left(1 + \frac{1}{E_i} \frac{1}{E_o} \right) \quad \text{......... (9)}$$

where $E$ is the Young’s modulus and $E_i$ is the tangent modulus calculated in the micro-field. In this simulation, the temperature was set to be constant at all times. Therefore, only the equivalent strain rate $\dot{\varepsilon}_{e}$ calculated in the finite elements of the macro-field are delivered to the macro-field.
3. Numerical Conditions

By simulating the inhomogeneous compression of a cylinder, as shown in Fig. 1(a), we confirmed the applicability of the MPFFE-DRX model to a wide range of temperatures and strain rates and estimated the effects of the temperature and deformation rate on hot-working properties. In the macro-field, we considered the cylinder to be an axisymmetric body; the model is shown in Fig. 1(b). Here, the quarter region is meshed into $4 \times 5$ crossed-triangle elements based on the symmetry. The macro-domain size was set to $\Delta R = 8$ mm and $\Delta Z = 10$ mm. The cylinder was compressed at a constant displacement rate $\bar{u}$ under the displacement constraint of the bottom and the $r$-direction for the left and top. We prepared 80 micro-computational domains for the micro-field shown in Fig. 1(c), which has four grains where the initial grain size $d_{ini}$ was $50 \mu m$ under the periodic boundary condition. Table 1 shows the temperature $T$, average strain rate $\bar{u}/\Delta Z$, and size of the FD lattice for the micro-domain. We set the standard conditions as $T = 800$ K and $\bar{u}/\Delta Z = 0.01$ s$^{-1}$, and we changed $\bar{u}$ and $\Delta Z$ in five steps from 700 K to 900 K and from 0.001 s$^{-1}$ to 0.1 s$^{-1}$, respectively. The micro-domain shown in Fig. 1(c) was meshed into 380 $\times$ 329 FD lattices with sizes of $\Delta x = 0.5 \mu m$. For the condition of $T = 800$ K and $\bar{u}/\Delta Z = 0.01$ s$^{-1}$ only, we used 190 $\times$ 164 lattices of $\Delta x = 0.5 \mu m$. The time increment $\Delta t$ was determined by a condition to solve Eq. (4) explicitly or $\Delta t = (\Delta x)^2/(4\alpha^2 M^2)$. When the temperature was changed, the time increment $\Delta t$ changed because the mobility $M^2$ is a function of the temperature. When the average strain rate $\bar{u}/\Delta Z$ was changed, although $\Delta t$ was constant, the computational step number changed due to the change in deformation speed. In the present series of computations, we needed a large number of computational steps for only the condition of $T = 800$ K and $\bar{u}/\Delta Z = 0.001$ s$^{-1}$. Therefore, we used $\Delta x = 0.5 \mu m$ for the condition of $T = 800$ K and $\bar{u}/\Delta Z = 0.001$ s$^{-1}$ only. At low strain rates, because the grain size became large, the size of $\Delta x = 0.5 \mu m$ was sufficient to maintain accuracy.

In the present simulations, we used a copper cylinder, and the material properties$^{24,25}$ are given below: $\delta = 5 \Delta x$, $\gamma = 0.2 J/m^2$, $M = M_0 \exp(-Q_b/R T)$, where the pre-exponential factor $M_0 = 0.139 m^2 K^{-1} J s^{-1}$, the activation energy $Q_b = 110 kJ/mol$, and the gas constant $R = 8.314 J/mol K$. $k_1 = 4.00 \times 10^{-6}$ m$^{-1}$, $k_2 = \alpha G\bar{b}_0^2/\sigma_{ei}$, $\alpha = 0.5$, $G = 42.1$ GPa, $b = 2.56 \times 10^{-10}$ m, $l = 10/(0.5 \sqrt{\rho_b})$, where $\rho_b = 1.7 \times 10^{13}$ m$^{-2}$, $c = 1.125 \times 10^5$, $d = 1$, and $T_b = 2400$ K. In the micro-field, one DRX nucleus was placed every $(\pi \Delta n_{ini}(\Delta x)^2/\delta)^{\frac{1}{2}}$ steps, where $n_{ini}$ is the number of lattice points satisfying $0 < \phi < 1$ and $\rho_i \geq \rho_s$. The initial dislocation density was set to $\rho_{ini} = 10^9$ m$^{-2}$. The Young’s modulus was calculated in the first step. To stabilize of the simulation, we calculated the macro-model every ten calculations of the micro-model.

4. Numerical Results

4.1. Standard Conditions

Before evaluating the effects of temperature $T$ and average strain rate $\bar{u}/\Delta Z$, we considered the simulation results under the standard conditions of $T = 800$ K and $\bar{u}/\Delta Z = 0.01$ s$^{-1}$ in detail. Figure 2 shows the relations between the average stress $F/A_0$ and strain $\bar{u}/\Delta Z$ for changing $T$ and $\bar{u}/\Delta Z$ based on Table 1. In this section, we only focus on the curve calculated under the standard conditions of $T = 800$ K and $\bar{u}/\Delta Z = 0.01$ s$^{-1}$; other curves are considered in the next section. Figure 3 shows the deformations and distributions of the (a) equivalent stress $\bar{\sigma}$, (b) equivalent strain rate $\bar{\varepsilon}$, and (c) average grain size $d_{ave}$ for the micro-field shown in Fig. 1(b) at points A ($\bar{u}/\Delta Z = 0.132$), B ($\bar{u}/\Delta Z = 0.206$), and C ($\bar{u}/\Delta Z = 0.50$) in Fig. 2(a). Figure 4 shows the variations of the (a) equivalent stress $\bar{\sigma}$, (b) equivalent strain rate $\bar{\varepsilon}$, and (c) average grain size $d_{ave}$ for the eight elements 1, 3, 4, 5, 7, 10, 11, and 12 in Fig. 1(b). Points A–C in Fig. 4 are the
same as those in Fig. 2. **Figure 5** shows the microstructure evolutions for the three elements 1, 4, and 12 at points A, B, and C.

According to Fig. 3, the cylinder changes its shape like a barrel during compression due to the constraints in the radial direction of the top surface; the different local deformations in all triangular elements are clearly visible. The macroscopic stress–strain curve shown in Fig. 2(a) shows the characteristic changing that is closely associated with the macro-deformations shown in Fig. 3 and microstructure evolutions shown in Fig. 5. In the macroscopic stress–strain curve shown in Fig. 2(a), \( F/A_0 \) increased with increasing \( \bar{u}/\Delta Z \) until point A. This is because all elements hardened due to dislocation accumulation. \( F/A_0 \) then decreased in the region from A to B, where the dislocation densities reached critical value and softening occurred due to nucleation and growth of recrystallized grains in many elements. After B, the macroscopic stress increased monotonously as shown in Fig. 2(a), due to the displacement constraint in the radial direction of the cylinder. As shown in Fig. 4(a), the equivalent stress \( \bar{\sigma} \) of many elements became almost constant here because they kept a balance between softening and hardening. On the other hand, equivalent stresses \( \bar{\sigma} \) of elements 11 and 12 increased even after point B because those continuously hardened in the region. The same results are shown in Fig. 3(a), where the equivalent stress \( \bar{\sigma} \) of the elements around the top-center of the cylinder (around elements 11 and 12) monotonously increased. This variation was different from those of the other elements.

**Figure 3** shows that \( \sigma \), \( \bar{\varepsilon} \), and \( d_{ave} \) showed similar distributions and variations. Both the equivalent stress \( \bar{\sigma} \) and equivalent strain rate \( \bar{\varepsilon} \) of the elements located on the diagonal line where the deformation was concentrated (e.g., elements 3, 4, and 7) showed higher values, as shown in Figs. 3 and 4. In Fig. 4(a), when the equivalent stresses \( \sigma \) of elements 3 and 4 approached a constant value at around \( \bar{\varepsilon}/\Delta Z = 0.17 \), the increasing rates of the equivalent strain rate \( \bar{\varepsilon} \) decreased. This is because of the balance between softening due to nucleation and growth of recrystallized grains and hardening due to dislocation accumulation as a constant strain rate deformation was approached. Although element 7 was also located on the diagonal line, the equivalent strain rate \( \bar{\varepsilon} \) of element 7 increased monotonously unlike elements 3 and 4. According to Fig. 4(b), when the increasing
rates of equivalent strain rate $\dot{\varepsilon}$ of elements 3 and 4 started to decrease in the region between A and B, those of elements 10–12 started to increase. Because elements located around the top-center were difficult to deform, those equivalent strain rates decreased at the beginning of compression. However, because the cylinder was compressed under a constant displacement rate, the increasing rate of the equivalent strain rate of elements around the top surface increased as those of elements located around the bottom decreased. Figures 3(b) and 4(b) show that the equivalent strain rates $\dot{\varepsilon}$ of elements 1 and 5 stayed almost constant throughout the simulation. This means that the deformation conditions of the outer perimeter of the cylinder were close to those of uniaxial compression. Therefore, at the end of compression, the equivalent strain rates $\dot{\varepsilon}$ of elements 10, 11 and 12 exceeded those of elements 1 and 5.

A comparison of Figs. 4(a) and 4(c) shows that the decreasing rates of the average grain size $d_{ave}$ decreased; $d_{ave}$ then began to approach a constant value when equivalent stresses $\bar{\sigma}$ of elements 1, 3, 4, 5, and 7 approached a constant value at around point B. Figure 4(c) show that the average grain size $d_{ave}$ in element 4 indicated the smallest value throughout the simulation. This is because the nucleation rate was higher in element 4 than in the other elements because of the high strain rate shown in Fig. 4(b). In element 12, where dislocations were difficult to accumulate, nucleation finally occurred at B. This is because the equivalent strain rate $\dot{\varepsilon}$ of element 12 rapidly increased and nucleation became frequent from B to C; the average grain size $d_{ave}$ of element 12 finally became smaller than that of element 1 at C.

The above details on the simulation under standard conditions, confirmed that the MPFFE-DRX model developed in our previous study can estimate both macroscopic mechanical behavior due to microstructure evolution and microstructure evolution due to macroscopic non-uniform deformations.

4.2. Effects of $T$ and $\bar{\sigma}/\Delta Z$ on Hot-working

We performed a series of compression simulations of a cylinder with changing $T$ and $\bar{\sigma}/\Delta Z$ following Table 1 to investigate hot-working properties under different conditions and confirmed the applicability of the MPFFE-DRX model over a wide variety of $T$ and $\bar{\sigma}/\Delta Z$.

Figure 6 shows the variations in equivalent stress $\bar{\sigma}$ and average grain size $d_{ave}$ for average strain $\bar{\varepsilon}/\Delta Z$ for changing $T$. Figures 6(a) and 6(c) show the results of element 4 and Figs. 6(b) and 6(d) show the results of element 12. Figure 7 shows the variations in equivalent strain rate $\dot{\varepsilon}$ for $\bar{\varepsilon}/\Delta Z$ of elements 4 and 12 for changing $T$. Similar to Fig. 6, Fig. 8 shows the variations in equivalent stress $\bar{\sigma}$ and average grain size $d_{ave}$ of $\bar{\varepsilon}/\Delta Z$ for changing $\bar{\varepsilon}/\Delta Z$. Figures 9 and 10 show the microstructures of elements 4 and 12 at the end of the simulation ($\bar{\varepsilon}/\Delta Z = 0.5$). Figures 9(a) and 10(a) show the results for changing $T$, and Figs. 9(b) and 10(b) show the results for changing $\bar{\varepsilon}/\Delta Z$.

First, we considered the difference in macro-deformations under different conditions. According to Fig. 2, the average stress $F/A_0$ increased with decreasing $T$ and increasing $\bar{\varepsilon}/\Delta Z$. Similar to the standard conditions of $T = 800$ K and $\bar{\varepsilon}/\Delta Z = 0.01$ s$^{-1}$, $F/A_0$ decreased after it reached the peak of the $F/A_0$ curve and increased again from the minimum value under all conditions. However, there was no minimum...
value under the conditions of $\bar{u}/\Delta Z = 0.05$ and 0.1 s$^{-1}$. These curves largely reflected the stress–strain curves of uniaxial compressions.26) The macro-deformations shown in Fig. 3 demonstrated that radial deformations of the bottom surface tended to become slightly smaller under the conditions of lower $T$ and higher $\bar{u}/\Delta Z$; the overall macro-deformations and distributions of the equivalent stress $\bar{\sigma}$, equivalent strain rate $\bar{\varepsilon}$, and average grain size $d_{\text{ave}}$ were almost the same qualitatively even if $T$ or $\bar{u}/\Delta Z$ were changed.

Next, we considered micro-deformations and microstructures. Based on the considerations in section 3.1, here we focused on element 4, where deformation was concentrated, and element 12, which deformed with more difficulty than any other element. Figures 6(a) and 8(a) show that the maximum and convergence values of the equivalent stress $\bar{\sigma}$ of element 4 increased, and the number of peaks of the curves decreased at lower $T$ or higher $\bar{u}/\Delta Z$. At low temperatures, the nucleation rate calculated by Eq. (3) and the grain boundary mobility were small. Therefore, a long time was needed to achieve a balanced condition between softening due to nucleation and growth of recrystallization grains and hardening due to dislocation accumulation. As a result, the equivalent stress $\bar{\sigma}$ became higher, and the number of peaks of the curves became fewer. Similar results were confirmed from the changes in equivalent strain rate $\bar{\varepsilon}$ shown in Fig. 7. The equivalent strain rates $\bar{\varepsilon}$ in Fig. 7 showed similar variations under all temperatures corresponding to the hardening, softening, and constant regions of the equivalent stress $\bar{\sigma}$ shown in Fig. 6(a). The inflection points of $\bar{\varepsilon}$–$\bar{\rho}$/$\Delta Z$ curves moved to the higher $\bar{\rho}$/$\Delta Z$ side with increasing $T$. For a large deformation rate $\bar{\rho}$/$\Delta Z$, nucleation occurred easily because the equivalent strain rate $\bar{\varepsilon}$ became larger and the dislocation density reached the critical value according to Eq. (1) faster. Therefore, when $\bar{\rho}$/$\Delta Z = 0.1$ s$^{-1}$, nucleation repeated around the initial grain boundaries, as shown in Fig. 9(b), and the dislocation density in the remaining initial grain increased continuously. Then, the equivalent stress $\bar{\sigma}$ calculated by Eq. (5) became larger due to the high average dislocation density in the micro-field. When $\bar{\rho}$/$\Delta Z = 0.1$ s$^{-1}$, a $\bar{\sigma}$–$\bar{\rho}$/$\Delta Z$ curve with a gentle slope and single peak due to the typical necklace structure26) shown in Fig. 9(b) was observed. As shown in Figs. 6(c) and 8(c), the average grain size $d_{\text{ave}}$ of element 4 converged faster to a higher value with increasing temperature and decreasing deformation rate. This was also confirmed by the results shown in Fig. 9. The above results for element 4 were the same as those of uniaxial compression under a constant strain rate.26)

In element 12, where deformation was difficult, Figs. 6(d) and 8(d) show that the average grain size $d_{\text{ave}}$ did not decrease monotonously under the conditions of high $T$ and small $\bar{u}/\Delta Z$. In particular, under the conditions of $T = 900$ K and $\bar{u}/\Delta Z = 0.001$ s$^{-1}$, these phenomena were remarkable. As a result, there were fluctuations in the changes of equivalent stresses $\bar{\sigma}$, as shown in Figs. 6(b) and 8(b). Considering the change in equivalent strain rate $\bar{\varepsilon}$ of element 12 in Fig. 7,
the decreasing rate at the beginning of the simulation and increasing rate after the minimum points were higher when $T$ was higher. These were caused by macro-deformation as described in the previous section; the changes in equivalent strain rate $\dot{\varepsilon}$ of element 12 were also observed to strongly correlate with those of element 4, as shown in Fig. 7. According to this figure, since the equivalent strain rate $\dot{\varepsilon}$ of element 12 increased monotonously after the point where it changed from decreasing to increasing, the equivalent stress $\sigma$ of element 12 increased monotonously, as shown in Fig. 6(b).

Finally, we estimated the average grain size $d_{ave}$ depending on the temperature and deformation rate. Figure 11 shows the average grain sizes $d_{ave}$ for different (a) $T$ and (b) $\dot{u}/\Delta Z$ of elements 1, 4, and 12 at the end of the simulation ($\pi/\Delta Z = 0.5$). The average grain size $d_{ave}$ of element 4, where deformation was concentrated, decreased with decreasing $T$ and increasing $\dot{u}/\Delta Z$. These were the typical results in DRX corresponding to the initial condition of $T$ and $\pi/\Delta Z$ and were similar to those of element 1, which deformed at an almost constant strain rate. However, the average grain size $d_{ave}$ of element 12 did not always change...
monotonously for $T$ and $\bar{\gamma}/\Delta Z$ because element 12 was largely affected by the deformations of other elements.

Based on the above results, the compression of a cylinder under temperatures of 700–900 K and average strain rates of 0.001–0.1 s$^{-1}$. These simulations confirmed that microstructure evolutions and macroscopic mechanical behavior were coupled accurately in the model and that we can use the MPFFE-DRX model under a wide range of $T$ and $\bar{\gamma}/\Delta Z$.

5. Conclusions

In this study, we simulated the non-uniform compression of a cylinder under temperatures of 700–900 K and average strain rates of 0.001–0.1 s$^{-1}$ using the MPFFE-DRX model to consider the hot-working properties in detail and confirmed the wide applicability of the MPFFE-DRX model. The results confirmed that microstructure evolutions and macroscopic mechanical behavior were coupled accurately and that we can use the MPFFE-DRX model under a wide range of temperatures and deformation rates. For temperatures lower than 700 K, average strain rates larger than 0.1 s$^{-1}$, or no DRX condition, we believe that the normal constitutive equation independent of the microstructure can be used. In the present MPFFE-DRX simulations, DRX did not occur when the temperature was higher than 900 K and the average strain rate was smaller than 0.001 s$^{-1}$. Therefore, we need to reconsider the nucleation conditions if we want to simulate such conditions of high temperature and low strain rate.

Acknowledgements

This work was supported by JSPS KAKENHI Grant Number 25630011.

REFERENCES