

# Prediction of Microstructure Evolution during Hot Forging using Grain Aggregate Model for Dynamic Recrystallization

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*In this study, dynamic recrystallization during nonisothermal hot compression test was numerically simulated by finite element analysis using new grain aggregate model for dynamic recrystallization. This model was developed based on mean field approach by assuming grain aggregate as representative element. For each grain aggregate, changes of state variables were calculated using three sub-models for work hardening, nucleation, and nucleus growth. A conventional single parameter dislocation density model was used to calculate change of dislocation density in grains. For modeling nucleation, constant nucleation rate and nucleation criterion developed by Roberts and Ahlblom were used. It was assumed that the nucleation occurs when the dislocation density of certain grain reaches a critical nucleation criterion. Conventional rate theory was used to model nucleus growth. The developed dynamic recrystallization model was validated by comparing with isothermal hot compression of pure copper. Then, the finite element analysis was conducted to predict the local changes of microstructure and average grain size by using the grain aggregate model. The predicted results were compared with nonisothermal hot compression results. The simulation results were in reasonably good agreement with experimentally obtained microstructures and the calculation time was much shorter than cellular automata-finite element method.*

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## 1. Introduction

Dynamic recrystallization (DRX) is one of the key processes that governs the final microstructure during hot deformation. Metals with low or medium levels of stacking fault energy such as copper and nickel undergo the DRX while metals with high stacking fault energy undergoes dynamic recovery. During the DRX process, new grains originate at high-angle grain boundaries such as prior grain boundaries, the boundaries of recrystallized grain, and deformation bands and twins. The new grains grow to the high dislocation density of the original grain due to the driving force, which is driven by the difference in the dislocation density. However, recrystallized grains will cease to grow as the material deforms further, resulting in reducing the dislocation density difference. The resulting microstructure and material behavior during the DRX vary with the deformation condition. Differences in grain size, texture, and material behavior affect in final mechanical properties and deformation aspect of final product. Therefore, predicting

the DRX better is essential when attempting to control mechanical properties and deformation process of final product.

Various models have been proposed thus far to predict microstructural changes and material behavior during the DRX. Typically, the Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory<sup>1</sup> was widely used to model homogeneous recrystallization kinetics. This empirical mathematical model was widely used to model the flow behavior and microstructure for industrial applications.<sup>2-4</sup> In these works, microstructure evolution was described as a function of strain, strain rate, temperature, and initial grain size. However, these applications only concentrated on the hot strip and plate rolling processes because of the difficulties that arise in exact thermo-mechanical modeling of bar rolling or hot forging processes.

Therefore, such modeling was extended by integrating with a finite element analysis to provide more realistic description of local process parameters such as strain, strain rate, and temperature.<sup>5-7</sup> However, these methods predicted local microstructure as an average grain size only and local heterogeneity was not considered properly. In addition,

it is not applicable to complex problem because of phenomenological characteristics.

To describe heterogeneous nature of the DRX and predict local microstructure evolution in detail, many mesoscale modeling methods such as the Monte Carlo model,<sup>8,9</sup> the phase field model,<sup>10,11</sup> and the cellular automata model<sup>12-14</sup> have been proposed as well. Although these models successfully described microstructure evolution during the DRX, most studies have focused on the DRX of ideal process like isothermal compression with a constant strain rate because of difficulty in modeling the deformation.

Recently, there have been attempts to combine mesoscale microstructure simulation with macroscale finite element (FE) method for describing deformation during DRX more accurately. Lee et al.<sup>15</sup> combined cellular automata and the finite element (CA-FE) method to predict microstructural changes by DRX during a nonisothermal hot forging process and validated the proposed model by comparing its results with the experimental results obtained by electron backscattered diffraction (EBSD). The proposed model generally predicted microstructural changes accurately. However, industrial application of this multiscale method is difficult owing to the long calculation time due to the large scale of problem.

To overcome the limitation of JMAK model and multiscale model, grain scale model using mean field theory has been proposed recently.<sup>16,17</sup> In these models, the dynamic recrystallization was modeled by using grain as a representative element and mean field theory was used to simulate interaction between grain during dynamic recrystallization.

Therefore, we aim to develop a new dynamic recrystallization model, grain aggregate model, that can predict microstructural changes and to use this model for hot forging applications by combining it with FE analysis. In the current model, the grain aggregate was used as a representative element of mean field theory different with previous grain scale model. This model provided a reduced calculation time as compared to that required for simultaneous analysis by cellular automata and the finite element method. Then, the results based on developed model were compared with cellular automata results and experimental result. Finally, the developed grain aggregate model will be combined with FE analysis to predict microstructure change during nonisothermal hot forging process and compared with CA-FE method.

## 2. Grain Aggregate Model for Dynamic Recrystallization

### 2.1 Model structure

The local microstructure during DRX is extremely heterogeneous. The microstructure has both severely deformed grains and recrystallized grains with different cycles of DRX. In the current model, the microstructure was represented by certain number of representative grain aggregate with different component and different cycle. Each grain aggregate has state variables of the component number, dislocation densities, surface boundary area, sum of grain diameter in the grain aggregate, number of grains in the aggregate and volume fraction of grain aggregate.

The major difference of cellular automata, grain scale model and grain aggregate model is shown in Fig. 1. The cellular automata generally used a cell which is much smaller than grain as a representative

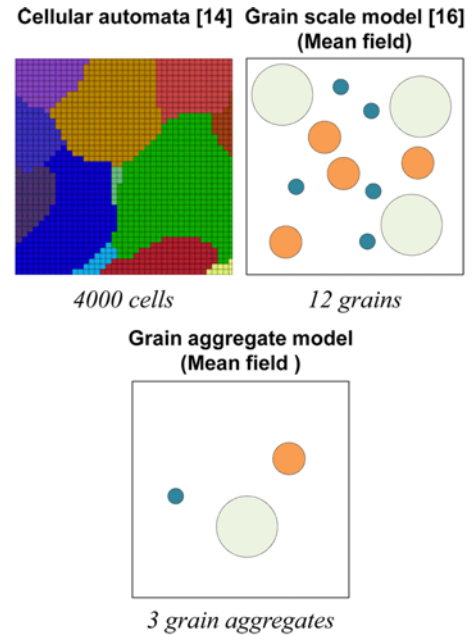


Fig. 1 Schematic illustration of dynamic recrystallization model for comparing representative element of microstructure between three models

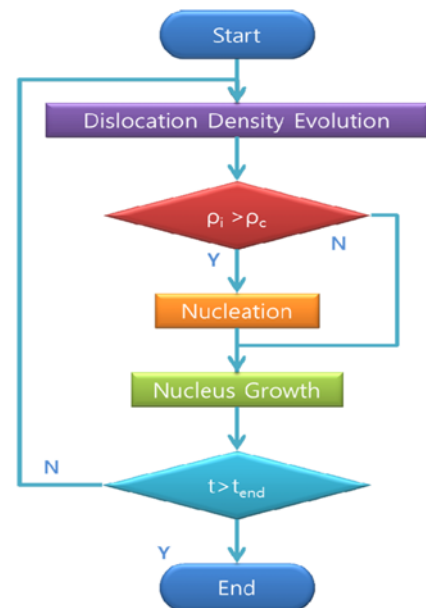


Fig. 2 Flow chart of the current grain aggregate model for calculating dynamic recrystallization process

element of microstructure. The grain scale model and grain aggregate model used a grain and a grain aggregate as a representative element of microstructure, respectively. Therefore, 1600 cells, 12 grains, and 3 grain aggregates are used for cellular automata, grain scale and, grain aggregate models, respectively. The grain scale model and grain aggregate model are based on mean field theory without spatial distribution of grains available in cellular automata model. The metallurgical phenomena between grains considered as an interaction of a grain with mean field. Therefore, spatial distribution of grains was

not considered and actual microstructure is not visible like cellular automata model. These models only calculated the change of other state variables by assuming grain as a sphere.

The difference between grain aggregate and grain scale models is representative element. The basic idea of grain aggregate model is to reduce calculation time by combining similar grains into a grain aggregate in average sense.

The current grain aggregate model numerically calculated DRX with the following steps as shown in Fig. 2: Calculation of the minimum time interval to ensure better results; calculation of dislocation density changes by work hardening at each time interval; nucleation of the recrystallization embryo by comparing the dislocation densities in the grain boundaries with the critical dislocation density; simulation of the growth of the nucleus to the high dislocation density area. The details of each process will be given in the following sections.

## 2.2 Dislocation density evolution

To model the dislocation density changes by work hardening, the conventional ‘one-parameter’ model by Kocks and Mecking<sup>18,19</sup> was used in the current study due to its simplicity and applicability in a hot deformation process. The Kocks-Mecking (KM) model is based on the assumption that the average dislocation density determines the kinetics of the plastic flow. In the kinetic equation for hot deformation, the flow stress ( $\sigma_{[j,i]}$ ) is proportional to the square root of the dislocation density as follows:

$$\sigma_{[j,i]} = \alpha \mu b \sqrt{\rho_{[j,i]}} \quad (1)$$

In this equation,  $\alpha$  is a numerical constant,  $\mu$  denotes the shear modulus,  $b$  is the magnitude of Burger’s vector of dislocation, and  $\rho$  is the average dislocation density of grain aggregate  $[j, i]$ . Where,  $i$  and  $j$  represents DRX cycle and component number, respectively.

The change in the dislocation density of a fine-grained material may be considered to consist of two components as follows:

$$\frac{d\rho_{[j,i]}}{d\varepsilon} = k_1 - k_2 \rho_{[j,i]} \quad (2)$$

Here,  $\varepsilon$  represents strain,  $k_1$  is a constant, and  $k_2$  is a function of temperature and strain rate. The  $k_1$  and  $k_2$  values were acquired from the isothermal hot compression results of pure copper available in the literature.<sup>14</sup>

## 2.3 Nucleation

Nucleation can happen when the stored energy due to dislocation accumulation overcomes the boundary energy related to the curvature. In the present investigation, the critical dislocation density proposed by Roberts and Ahlblom<sup>20</sup> was used.

$$\rho_c = \left( \frac{20\gamma\dot{\varepsilon}}{3bIM\tau} \right)^{1/3} \quad (3)$$

In this equation,  $l$  is the dislocation mean free path,  $M$  represents the grain boundary mobility,  $\tau$  is the dislocation line energy,  $\gamma$  is the grain boundary energy, and  $\dot{\varepsilon}$  is the strain rate.

In Eq. (3), the grain boundary mobility is given as follows shown in the literature.<sup>21</sup>

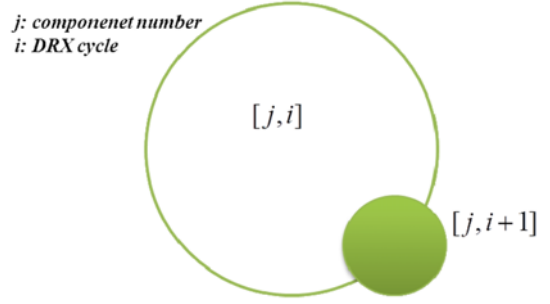


Fig. 3 Schematic illustration of nucleation process in the DRX model

$$M = \frac{\delta D_{ob} b}{kT} \exp\left(-\frac{Q_b}{RT}\right) \quad (4)$$

Here,  $\delta$  is the characteristic grain boundary thickness,  $D_{ob}$  denotes the boundary self-diffusion coefficient,  $Q_b$  is the activation energy for boundary diffusion,  $k$  represents the Boltzmann’s constant,  $R$  is the gas constant, and  $T$  is the absolute temperature.

The nucleation rate was assumed to be constant during the whole DRX process and a function of temperature. Then, number of nuclei for grain aggregate  $[j, i]$  can be defined as follows:

$$N_{[j,i]} = n \dot{\varepsilon}^m \exp\left(\frac{Q_{nuc}}{RT}\right) \cdot f_{[j,i]} \cdot \Delta t \quad (5)$$

where  $n$ ,  $m$ , and  $Q_{nuc}$  are constants,  $f_{[j,i]}$  is the volume fraction of grain aggregate  $[j, i]$ , and  $\Delta t$  is a time interval.

As shown in Fig. 3, it was assumed that new grain of grain aggregate  $[j, i+1]$  is nucleated at the prior grain of grain aggregate  $[j, i]$ .

Therefore, the changes of volume fraction in the grain aggregate  $[j, i]$  during nucleation can be described as multiplication of number of nuclei and ratio of volume of nuclei to the total volume as follows:

$$\Delta f_{[j,i]} = -N_{[j,i]} \cdot \frac{V_0}{V_{tot}} \quad (6)$$

where  $V_0$  is the volume of nucleus and  $V_{tot}$  is the total volume of domain.

The sum of grain diameter ( $D'_{[j,i]}$ ) and surface boundary area ( $S_{[j,i]}$ ) changes according to the volume fraction during nucleation while dislocation density of deformed aggregate did not change as follows.

$$\Delta D'_{[j,i]} = D'_{[j,i]} \cdot \Delta f_{[j,i]} \quad (7)$$

$$\Delta S_{[j,i]} = \frac{\Delta f_{[j,i]}}{f_{[j,i]}} \cdot S_{[j,i]} \quad (8)$$

$$\rho_{[j,i]}^{t+\Delta t} = \rho_{[j,i]}^t \quad (9)$$

The dislocation density of newly formed nucleus ( $\rho_0$ ) is almost zero although it will change during further deformation. Therefore, the dislocation density at the time  $t+\Delta t$  can be described as follows.

$$\rho_{[j,i+1]}^{t+\Delta t} = \frac{\rho_{[j,i+1]}^t \cdot f_{[j,i+1]}^t + \rho_0 \cdot \Delta f_{[j,i+1]}^t}{f_{[j,i+1]}^t + \Delta f_{[j,i+1]}^t} \quad (10)$$

The sum of grain diameter and surface boundary area was calculated using following equation by assuming the spherical grain shape.

$$\Delta D'_{[j,i+1]} = N \cdot D_0 \quad (11)$$

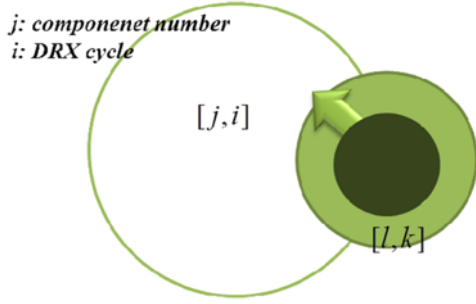


Fig. 4 Schematic illustration of growth process during dynamic recrystallization

$$\Delta S_{[j,i+1]} = N \cdot \pi D_0^2 \cdot V_{tot} \quad (12)$$

where  $D_0$  represents the diameter of nucleus.

## 2.4 Nucleus growth

The driving force for nucleus growth of dynamically recrystallized grains is the difference of stored strain energy between recrystallized grains and prior deformed grains as shown in Fig. 4.

A grain boundary moves with a velocity ( $v$ ) in response to the net pressure ( $P$ ) on the boundary. It is generally assumed that the velocity is directly proportional to the pressure, the constant of proportionality being the mobility ( $M$ ) of the boundary as follows:<sup>1</sup>

$$v = MP \quad (13)$$

$$P = \tau(\rho_{[j,i]} - \rho_{[l,k]}) - \frac{2\gamma}{r} \quad (14)$$

where  $r$  denotes radius for grain.

However, the second term in Eq. (14) is omitted in the current model because it is negligible compare to the first term.

During nucleus growth, the volume fraction of grain aggregate changes as follows by considering volume swept by nucleus surface boundary ( $S_{[l,k]}v\Delta t$ ):

$$\Delta f_{[j,i]} = -\Delta f_{[l,k]} = \frac{S_{[l,k]}v\Delta t}{V_{tot}} f_{[l,k]} \quad (15)$$

In this equation, the changes of volume fraction between aggregate  $[j, i]$  and  $[l, k]$  are only considered by multiplying volume fraction of aggregate  $[l, k]$  to avoid duplication of calculation.

The sum of grain diameter in the aggregate was calculated using following equations.

$$\Delta D'_{[j,i]} = 2v \cdot \Delta t \cdot n_{[j,i]} \cdot f_{[l,k]} \quad (16)$$

$$\Delta D'_{[l,k]} = \frac{D'_{[l,k]} \cdot S_{[j,i]} \cdot v \cdot \Delta t}{V_{tot}} f_{[l,k]} \quad (17)$$

The change of surface boundary area during nucleus growth was calculated as follows:

$$\Delta S_{[j,i]} = 4\pi \cdot D'_{[j,i]} \cdot f_{[l,k]} \cdot v \cdot \Delta t \quad (18)$$

$$\Delta S_{[l,k]} = \frac{\Delta V \cdot S_{[l,k]}}{f_{[l,k]}} \quad (19)$$

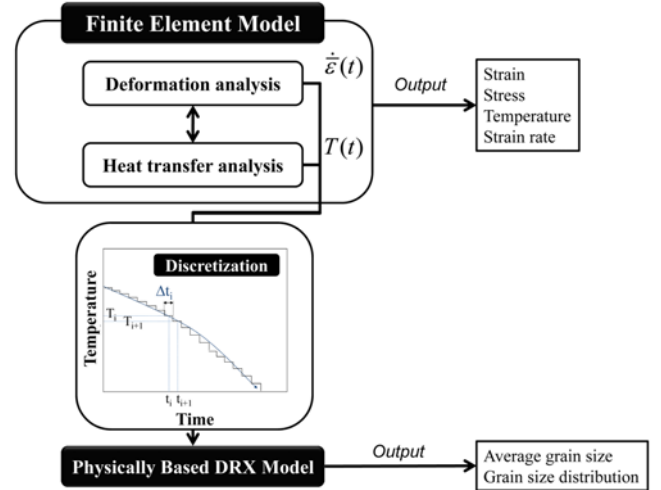


Fig. 5 Numerical procedures for predicting microstructure evolution by DRX during hot forging

## 3. Numerical Prediction

In the current study, the microstructure evolution by dynamic recrystallization during hot forging was analyzed with the aid of a numerical analysis by combining physically based dynamic recrystallization model with FE model as shown in Fig. 5. The thermomechanical modeling was conducted with a two-dimensional FE analysis to predict the thermal and deformation history accurately.

Then, the microstructure simulation based on grain aggregate model was conducted to calculate the microstructural changes using the calculated strain rate and temperature histories from the FE analysis. The temperature and strain rate were discretized with time so that the DRX model could be applied to the nonisothermal process.

The current FE analysis was conducted with *CAMPform-2D*,<sup>22</sup> which was developed based on the rigid thermoviscoplastic FE formulation proposed by Lee and Kobayashi.<sup>23</sup> An axisymmetric condition was assigned to simulate nonisothermal hot forging process. The workpiece has a radius of 20 mm and a height of 40 mm. The total number of quadrilateral elements used was 800. The radius and height of the dies was the same as 50 mm, and the number of quadrilateral elements used was 2116 for the upper and lower dies, respectively. The elements for the dies were used only for the temperature analysis. A constant shear friction model with a friction factor of 0.3 was used for the friction modeling.<sup>23</sup> The ram speed was 4 mm/s and the total stroke was 21.2 mm. For the nonisothermal FE analysis, the flow stress of pure copper and the interface heat transfer coefficient between dies and workpiece was acquired from the literature.<sup>15</sup>

## 4. Results and Discussion

### 4.1 Validation of developed DRX model

To verify the developed physically based model, flow stress curves and final grain sizes at various temperatures and strain rates were compared with the experimental results and cellular automata results in the literature,<sup>14</sup> as shown in Figs. 6 and 7, respectively. The proposed

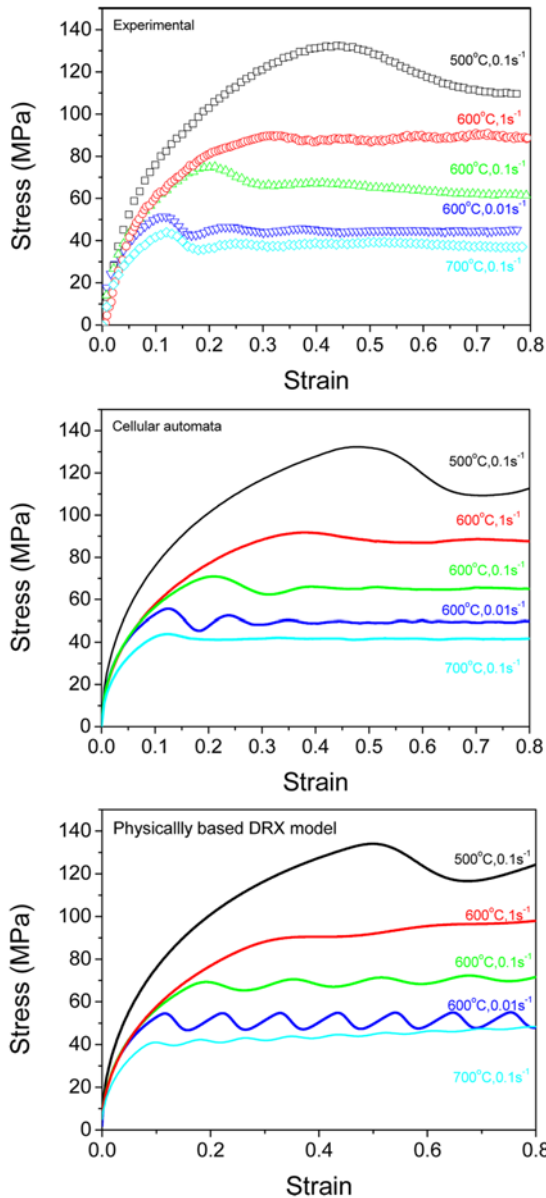


Fig. 6 Comparison of flow stress curves between the experiments,<sup>14</sup> cellular automata model,<sup>14</sup> and grain aggregate model

grain aggregate model predicted the flow stress generally well, although it exaggerated the oscillating flow curves at 600°C and 0.01 s<sup>-1</sup>.

A cellular automata model generally shows better accuracy compared to the current physically based DRX model for the all conditions. This is due to assumption of grain aggregate model such as representative element of microstructure and mean field.

The error in current grain aggregate model occurred because the characteristics of dynamic recrystallization in the single- and multi-peak curves were rather different from each other. To represent both curves accurately, the model should be considered differently in some manner. However, the predicted grain sizes were generally in good agreement with the experimental results, although some error existed in the results.

The majority of current grain aggregate model is short calculation time. The CPU time of grain aggregate model is compared with cellular automata model as shown in Table 1. The calculation time of grain

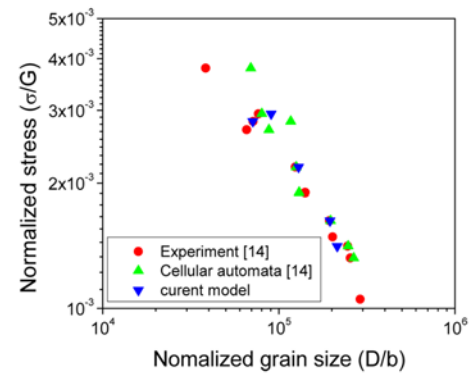


Fig. 7 Comparison of average recrystallized grain sizes obtained from the experiments,<sup>14</sup> Cellular automata,<sup>14</sup> and grain aggregate model

Table 1 CPU time required for simulations based on cellular automata model and grain aggregate model and information on simulation system

Simulation conditions	Temperature (°C)	500	600	600	600	700
	Strain rate (s <sup>-1</sup> )	0.1	0.01	0.1	1	0.1
CPU time (s)	Grain aggregate	0.125	0.905	0.140	0.078	0.187
	Cellular automata	2160	17640	10920	4320	18240

Tested system: 2cpu (Intel Xeon E5-2680v2), 64GB RAM, Windows 7 x64

aggregate model was extremely short and the difference in order of magnitude was more than 4. This time efficiency of grain aggregate model is high enough to compensate the low accuracy compared to the cellular automata model.

#### 4.2 Characteristics of flow curves predicted by DRX model

The shape of the flow stress curves is related to the ratio of the prior and recrystallized grain sizes. The flow stress curve at high Zener-Hollomon parameter ( $Z$ ) showed a broad single peak (e.g., 500°C and 0.1 s<sup>-1</sup> in Fig. 6). On the other hand, the flow stress curves at low  $Z$  values showed multi-peak curves under low strain and steady curves under high strain (e.g., 700°C and 0.1 s<sup>-1</sup> in Fig. 6).

It is known that if the prior grain size is greater than two times the recrystallized grain size, a single-peak curve may occur.<sup>24</sup> Therefore, the characteristics of the flow curves were investigated in detail in this study.

The flow curves and recrystallized fraction curves during DRX for the single-peak and multi-peak curves are represented in Figs. 8 and 9 respectively. In Fig. 8, the slope of the flow stress was changed past the critical strain (about 0.47) and reached its peak at a strain of about 0.5. The flow curves then softened and hardened again from the strain value of 0.65 and recrystallized fraction of 0.7.

This re-hardening is related to low nucleation rate due to the small grain boundary area at the higher recrystallized fraction. The average grain size curve changed rapidly due to the DRX process as shown in Fig. 10. The average grain size was held constant up to the critical



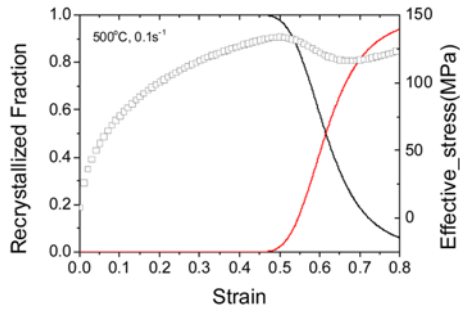


Fig. 8 Flow curve (dot) and recrystallized fraction (line) at the high Zener-Hollomon parameter

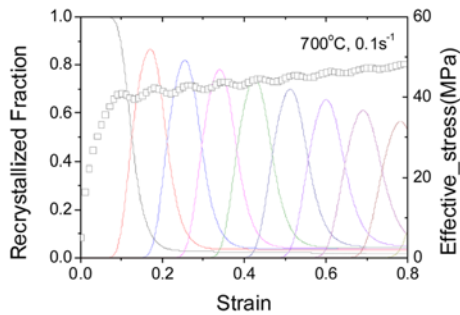


Fig. 9 Flow curve (dot) and recrystallized fraction (line) at the low Zener-Hollomon parameter

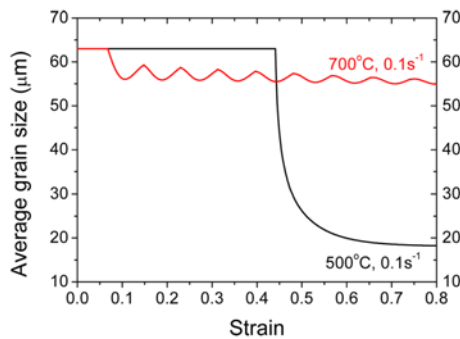


Fig. 10 Changes of average grain size during dynamic recrystallization for the single- and multi-peak flow curves

strain, decreased rapidly directly past the critical strain, and then became saturated. The rapid decrease in the average grain size is due to the difference between recrystallized and initial grain sizes.

In Fig. 9, the multi-peaks flow stress also showed a curve similar to that of the single-peak DRX up to a strain of 0.1. However, the flow stress increased again past a strain value of 0.12 owing to the lack of nucleation between the DRX cycles. The next DRX cycle was then initiated past a certain deformation, and the stress decreased again by further nucleation. The average grain size also oscillated owing to the several cycles of the DRX that were run as shown in Fig. 10.

The average grain size initially decreased immediately after the initiation of the current cycle of the DRX as a consequence of the nucleation stage. It then increased rapidly due to the growth and decreased again by the next DRX cycle.

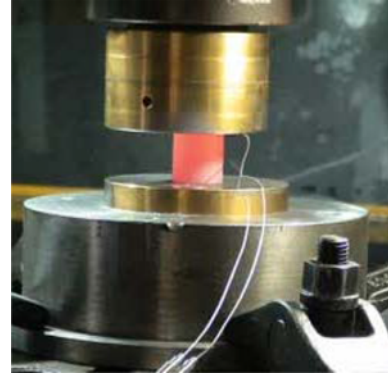


Fig. 11 Experimental set-up of simulated nonisothermal hot forging process

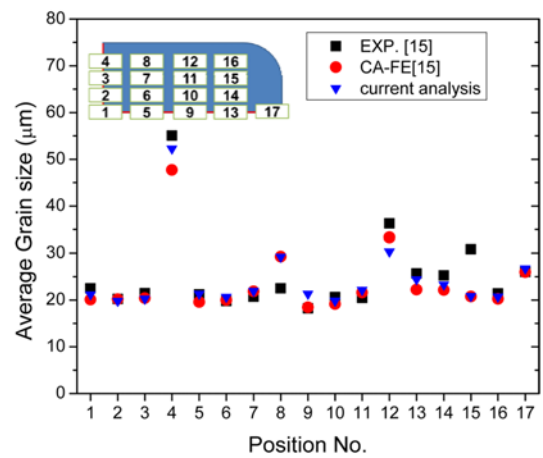


Fig. 12 Comparison of average grain size distribution during hot forging of pure copper acquired by experiment,<sup>15</sup> predicted by CA-FE<sup>15</sup> and current grain aggregate model

### 4.3 Numerical prediction of microstructure during hot forging

The numerical prediction of nonisothermal hot forging test was conducted by combining grain aggregate model with FE analysis and compared with experimental average grain size results and simulated result by CA-FE method.<sup>15</sup>

The nonisothermal hot forging test as shown in Fig. 11 was conducted with a varying strain rate using a hydraulic press. The cylindrical specimen had a height of 40 mm and a diameter of 40 mm. The specimen was heated to about 850°C in a furnace and then moved to a lower die. The specimen was deformed up to a stroke of about 22 mm after a period of dwelling until the temperature reached 700°C. The deformed specimen was water-quenched after about three seconds for further microstructural investigation. The quenched specimens were cut in parallel to the compression axis and polished for further EBSD measurements.

Fig. 12 shows comparison of the average grain sizes at the quarter of section parallel to compression axis after nonisothermal hot forging test. The average grain size is generally in good agreement with the experimental data for both CA-FE and current method, though the grain sizes have some discrepancies at points 8 and 15 in the current analysis and at points 4, 8 and 15 in the CA-FE analysis in the

literature.<sup>15</sup> The current simulation scheme predicted the microstructural change by the DRX in average sense well although it takes much less time compared to CA-FE method. Therefore, current numerical method will be beneficial for predict microstructural change during industrial process to save simulation time.

## 5. Conclusion

In the present study, the grain aggregate model for dynamic recrystallization was successfully developed using mean field approximation. It predicted general tendency of dynamic recrystallization in flow stress and average grain size although it showed some errors in specific conditions. The single-peak and multi-peaks flow curves due to grain refinement and coarsening phenomena were also investigated. In terms of grain refinement, the flow stress curves showed both a single peak and multi-peak, although a multi-peak curve was also noted during the grain coarsening phenomena.

The developed grain aggregate model is also combined with finite element method and applied to nonisothermal hot forging test to predict microstructure in an average sense. The predicted results are in good agreement with experimental results. This physically based dynamic recrystallization model will be very useful to combine with finite element analysis for simulating industrial process compared to the cellular automata-finite element model because of its fast calculation speed and less memory use.

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