Effects of subgrain size and static recrystallization on the mechanical performance of polycrystalline material: A microstructure-based crystal plasticity finite element analysis

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Abstract

In this paper, the effects of subgrain size and static recrystallization on the mechanical performance of polycrystalline material were investigated using a microstructure-based crystal plasticity finite element (CPFE) model. Firstly, polycrystalline microstructures with different mean subgrain sizes were prepared using simple assumption based on experimental observations, and intermediate microstructures during static recrystallization (SRX) were simulated by a cellular automata model adopting curvature driven grain/subgrain growth mechanism. Then, CPFE method was applied to perform stress analysis of plane strain tension on these virtual microstructures. The results show that the subgrains inside pre-existing grains have an effect on the heterogeneity of the stress distributions. The average stress decreases with increasing the mean subgrain radius. As grain/subgrain grows during SRX, the average stress also decreases. It can be deduced that well-defined and finer subgrain structure may strengthen the polycrystalline material, while grain/subgrain growth during SRX process will degrade the strength.

Keywords: Static recrystallization; Subgrain growth; Cellular automata; Crystal plasticity finite element; Stress analysis

1. Introduction

It is well known that the mechanical properties are very important when choosing a material for structural use, and microstructure has great effect on the mechanical properties of a material. The microstructure characteristics of the materials, e.g., the grain size, phase morphology, and grain orientation distributions often govern their mechanical properties. In order to obtain ideal microstructure with expected mechanical properties, various methods were usually used in material processing. Understanding of the microstructure evolution during material processing, such as annealing after deformation, is of great importance for optimizing the performance of the materials. Annealing heat treatment is often used for cold deformed materials, during which static recovery and recrystallization are the main restoration phenomena and affect the microstructure evolution greatly. In order to optimize the annealing process, the microstructure evolution during annealing is usually investigated by experimental means such as optical microscope (OM) and scanning electron microscope (SEM), and mechanical tests were carried out to evaluate the properties. However, the experimental measurements require lots of well-prepared material samples and various kinds of equipment, and they are relatively time-consuming.

In the past two decades, great progresses in modeling and simulating microstructure evolution of static recrystallization (SRX) during annealing have been made using various computational approaches, among which the cellular automata (CA) method has been widely used due to its flexibility and ease of use. Hesselbarth and Göbel [1] are commonly considered the first simulated the SRX using two dimension CA method. Thereafter, Davies [2–4] studied simulation of SRX using CA systematically and proposed a new kind of neighborhood. Goetz
and Seetharaman [5] simulated homogeneous and heterogeneous nucleation in two dimension and three dimension space for single-phase materials using a further developed CA method. Marx et al. [6] proposed a modified three dimension CA model and simulated the primary recrystallization. Raabe et al. [7] developed a scalable three dimension CA model with a probabilistic switching rule. In recent years, CA method has been applied to model SRX in varies alloys, such as aluminum [8,9], copper [10] and steel [11–15]. All the aforementioned CA simulations of SRX used a nucleation and growth model, in which the nucleation rate is usually calculated by a phenomenological equation depending on temperature, activation energy and stored energy. Besides, the nucleation site is often set as a cell in the CA model. Recently, Han et al. [16,17] developed a CA model of SRX based on the curvature driven subgrain growth mechanism, in which subgrains after cold deformation were considered, and the effect of subgrains on the SRX were investigated.

A number of computational studies have been done to quantificationally estimate the mechanics of polycrystalline materials at the micro-scale, by analyzing the field variables of materials undertaking loads using the finite element method (FEM). In this way, grain structures must be explicitly modeled by EBSD experiments or other microstructure modeling method, such as MC, PF, vertex, CA and Voronoi method, since micromechanical behavior can be strongly influenced by the grain size, shape, orientation and their distributions. Choi et al. [18] constructed a 3D digital microstructure that matched the EBSD measured grain size distribution and mis-orientation distribution of a polycrystalline AZ31 Mg alloy by using a MC method, and captured the heterogeneity of the stress concentration during in-plane compression by crystal plasticity finite element (CPFE) simulation. Liu et al. [19] simulated polycrystalline microstructures by the CA method and analyzed the stress response of polycrystalline material using FEM. Zhou et al. [20] studied the effects of particle size and volume fraction on the strength, elongation, and toughness of Al alloy by using FEM combined with strain gradient plasticity theory, in which the grain structure is represent by hexagon. Zhang et al. [21,22] generated polycrystalline structure by the Voronoi method and applied it to crystal plasticity analysis. As can be seen, CPFE has been a widely used approach in studying the mechanical behavior of polycrystalline material, and more details about it can be found in [23]. However, there seems to be no numerical study on the mechanical behavior of polycrystalline materials containing subgrains.

In this paper, firstly polycrystalline microstructures with different mean subgrain sizes were prepared using simple assumption based on experimental observations, and intermediate microstructures during static recrystallization (SRX) were simulated by a cellular automata model adopting curvature driven grain/subgrain growth mechanism. Then the simulated initial microstructures consisting of subgrains and the intermediate microstructures during SRX were imported in FEM, and tension load was applied, where the crystal plasticity model was used. Finally, the stress distribution of microstructures with different mean subgrain radiuses and recrystallization states under certain tension load were calculated. And the effects of subgrain size and SRX on the mechanical properties were discussed.

2. Model description and numerical methods

2.1. Cellular automata model

In this model, initial microstructures with large number of subgrains inside every pre-existing grain were generated based on experimental observations [24]. Fig. 1 shows four initial microstructures with different mean subgrain radiuses (\(R_0\)), where there are 12 pre-existing grains, and they are similar to that in Ref. [17,25]. The big pre-existing grains were created by a periodic Voronoi tessellation method and the small subgrains were created by simulating normal grain growth from an initial microstructure with very small grain size. Both the Voronoi tessellation and CA normal grain growth simulation were conducted on the same lattice scale. Then the two were synthesized to one by mapping one to another, just like image processing. The orientation of every grain/subgrain was marked by an integer number, naming orientation number, instead of Euler angles, for it is more convenient for CA simulation. The CA simulation mesh is \(2500 \times 2500\) square lattice and periodic boundary conditions are used.

The curvature driven grain/subgrain growth mechanism was used in the CA simulation model, in which the boundary motion is proportional to the local mean curvature of the interface,

\[
v = M \kappa
\]

where \(v\) is the velocity of the grain/subgrain boundary segment, \(M\) is the grain/subgrain boundary mobility, and \(\kappa\) is the boundary curvature. The mobility \(M\) is dependent on the boundary misorientation angle \(\theta\), and assumed to be as [26]

\[
M(\theta) = M_{HAG} \left(1 - \exp \left(-5 \left(\frac{\theta}{\theta_m}\right)^4\right)\right)
\]

where \(M_{HAG}\) is the mobility of high-angle boundary with misorientation greater than \(\theta_m\), and it is estimated by the following equation:

\[
M_{HAG} = \frac{\delta D_n}{kT} \exp \left(- \frac{Q_n}{RT}\right)
\]

The boundary energy is also dependent on the misorientation angle \(\theta\), and can be calculated by the following equation:

\[
\gamma = \gamma_m \left(\frac{\theta}{\theta_m}\right) \left(1 - \ln \left(\frac{\theta}{\theta_m}\right)\right)
\]

where \(\gamma_m\) is the high-angle boundary energy.

An equivalent approach to calculate the boundary curvature for square lattice known from solidification [27] was adopted...
in the current simulation, which is defined as

\[ \kappa = \frac{A}{C_{cell}} \frac{Kink - N_i}{N+1} \]  

where \( C_{cell} \) is the cell size in the CA model, \( A = 1.28 \) is a topological coefficient, \( N = 24 \) is the total number of the first and second nearest neighbors for a square lattice, \( N_i \) is the number of cells within the neighborhood belonging to grain or subgrain \( i \), and \( Kink = 15 \) is the number of cells within the neighborhood belonging to grain or subgrain \( i \) for a flat interface (\( \kappa = 0 \)). The detail topological considerations of this model can be found in Figs. A1–A3 in Ref [27].

In the present CA simulation, the square lattice was used. The eight nearest cells were chosen as the neighborhood of a cell and the cell size is 0.04 \( \mu \)m. A deterministic transformation rule used by Zheng et al. [28] was applied to determine the changing state of each CA cell. For the cell \((i, j)\) with positive curvature belonging to the moving boundary, the moving distance of the boundary cell in a single time step, \( \Delta t \), is described as follows:

\[ \ell_{ij} = \int_{t}^{t+\Delta t} \text{v} \text{d}t \]  

The indices \((i, j)\) denote the coordinate of the selected boundary cell. The transformation fraction in cell \((i, j)\), \( f_{ij} \), is then calculated by

\[ f_{ij} = f_{ij} / L_{CA} \]  

where \( L_{CA} \) is the distance between two neighboring cells. If the accumulated value of the transformation fraction variable is greater than 1.0, the boundary cell switches into the new state from the neighboring cells belonging to the corresponding growing grain/subgrain determined previously. The material parameters used in CA simulation are as follows: \( Q_b = 107 \text{ kJ/mol}, \delta D_b = 5.4 \times 10^{-14} \text{ m}^3 \text{s}^{-1}, b = 2.56 \times 10^{-10}, \gamma_m = 0.625 \text{ J m}^2, \theta_m = 15^\circ \).

Fig. 1. Initial microstructures with different mean subgrain radiiuses \( \langle R_0 \rangle \) (a) 0.31 \( \mu \)m (b) 0.39 \( \mu \)m (c) 0.50 \( \mu \)m and (d) 0.58 \( \mu \)m.
2.2. Crystal plasticity finite element method

CPFE has been a fascinating approach to obtain comprehensive mechanical behavior of polycrystalline material at mesoscopic level. In the current work, the CPFE frame and method based on the works of Asaro and Needleman [29] and Peirce et al. [30] was employed. The crystal orientation and the activated slip systems were taken into account in the model. The velocity gradient \( \mathbf{L} \) is decomposed as follows:

\[
\mathbf{L} = \mathbf{D} + \mathbf{\Omega}
\]

where \( \mathbf{D} \) and \( \mathbf{\Omega} \) are the symmetric and the skew parts of the velocity gradient respectively. \( \mathbf{D} \) and \( \mathbf{\Omega} \) can be additively decomposed into elastic parts \( (\mathbf{D}^e, \mathbf{\Omega}^e) \) and plastic parts \( (\mathbf{D}^p, \mathbf{\Omega}^p) \) as:

\[
\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p
\]

\[
\mathbf{\Omega} = \mathbf{\Omega}^e + \mathbf{\Omega}^p
\]

The elastic parts correspond to elastic deformations and lattice rotations. The plastic parts represent the plastic shear slips of the lattice caused by dislocation slip, relating to the plastic shear strain rate on each slip system. Then the plastic part of the velocity gradient \( \mathbf{L}^p \) is written as follows:

\[
\mathbf{L}^p = \mathbf{D}^p + \mathbf{\Omega}^p = \sum_{\alpha=1}^{N} \dot{\gamma}^{(\alpha)} s^{(\alpha)} \otimes n^{(\alpha)}
\]

where \( \dot{\gamma}^{(\alpha)} \), \( s^{(\alpha)} \) and \( n^{(\alpha)} \) are shear strain rate, slip direction vector and the normal vector to the slip plane of any given slip system \( \alpha \), respectively. \( N \) is the number of the active slip systems. The superscript * indicates that the vectors are taken in the deformed configuration following lattice stretching and rotation. The increment of the shear stress \( \tau \) in system \( \alpha \) is then prescribed through:

\[
\dot{\gamma}^{(\alpha)} = \mathbf{n}^{*(\alpha)} \mathbf{C} : \mathbf{D}^p - \mathbf{D}^e \cdot \mathbf{\sigma} + \mathbf{\sigma} \cdot \mathbf{D}^e \mathbf{n}^{*(\alpha)}
\]  

where \( \mathbf{C} \) is the elastic stiffness tensor and \( \mathbf{\sigma} \) is the Cauchy stress tensor.

The shear strain rate \( \dot{\gamma}^{(\alpha)} \) of the \( \alpha \)th slip system is determined by a simple rate-dependent power law relation proposed by Hutchinson [31]:

\[
\ddot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{1/m} \text{sgn}(\dot{\tau}^{(\alpha)})
\]

where \( \dot{\gamma}_0^{(\alpha)} \) is the reference strain rate, \( \tau^{(\alpha)} \) is the resolved shear stress, \( g^{(\alpha)} \) is the slip system strength or resistance to shear, and \( m \) is the strain sensitivity exponent. Due to the accumulation of dislocations, strain hardening will occur, and is characterized by the evolution of the strengths \( g^{(\alpha)} \) through the incremental relation:

\[
\ddot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha \beta} \dot{\gamma}^{(\beta)}
\]

where \( h_{\alpha \beta} \) are the slip hardening moduli. The hardening model of Asaro and Needleman [29], and Pierce et al. [30] is used.

Fig. 2. Pole figures of initial microstructure (a) containing 12 pre-existing grains without subgrains and (b) containing large number of subgrains with mean subgrain radius \( \langle R_0 \rangle = 0.31 \, \mu m \).
here, and the self-hardening moduli is expressed as follows:

\[ h_{\alpha\alpha} = h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right) \]  

(15)

where \( h_0 \) is the initial hardening modulus, \( \tau_0 \) is the initial value of current strength \( \dot{\gamma}^{(\alpha)} \), \( \tau_s \) is the saturation value. “sech” is the hyperbolic secant function, and \( \gamma \) is the Taylor cumulative shear strain on all slip systems:

\[ \gamma = \sum_{\alpha} \int_0^\ell |\dot{\gamma}^{(\alpha)}| \, dt \]  

(16)

The latent hardening moduli are given by

\[ h_{\alpha\beta} = q h(\gamma)(\alpha \neq \beta) \]  

(17)

where \( q \) is a constant, and it is chosen as 1 for isotropic hardening.

The employed material parameters for copper are as follows: \([32]\) elastic constant \( C_{11} = 168,400 \) MPa, \( C_{12} = 121,400 \) MPa, \( C_{44} = 75,400 \) MPa; \( h_0 = 541.5 \) MPa, \( \tau_s = 109.5 \) MPa, \( \tau_0 = 60.8 \) MPa, \( \gamma_0 = 0.001 \, \text{s}^{-1}, \, m = 0.1 \). Several typical rectangular domains selected from the CA simulated microstructures are used for CPFE simulation. All the CPFE simulations used the same boundary conditions, the left side of the domain is assigned to be symmetrical boundary, the top and bottom side are free, and the right side is applied a total displacement of 1% in the tensile direction.

3. Results and discussion

3.1. Effect of mean subgrain radius on the stress

The initial microstructures with different mean subgrain radius as shown in Fig. 1 were used to investigate the effect of mean subgrain radius on the stress. As aforementioned, the orientation of every grain/subgrain in CA simulation was marked by an integer number, naming orientation number. It is not enough to use the same method in CPFE calculation, and a more accurate orientation characterization method is needed. In the current work, the Euler angle \( (\varphi_1, \psi, \varphi_2) \) was used in CPFE to characterize the grain/subgrain orientation. The orientations of 12 pre-existing grains are random generated, and we just should make sure that the misorientations between neighboring grains are high angle. The pole figures of planes \{001\}, \{110\} and \{111\} for the 12 pre-existing grains are shown in Fig. 2(a). Subgrains inside each pre-existing grains have low angle misorientation between neighboring subgrains. In order to meet this condition, a rotation angle lower than 10° is randomly generated, and the rotation is made based on the Euler angle of the pre-existing grain, and then the orientation of subgrain was obtained. Fig. 2(b) shows the pole figures of planes \{001\}, \{110\} and \{111\} for all the subgrains. Clearly we can see that there are

Fig. 3. Stress S11 distribution for selected domains (at the top right) of initial microstructures with different mean subgrain radiuses \( \langle R_0 \rangle \) (a) 0.31 \( \mu \)m (b) 0.39 \( \mu \)m (c) 0.50 \( \mu \)m and (d) 0.58 \( \mu \)m.
slightly deflections for the poles of subgrains from the pre-existing grains.

Fig. 3 depicts the distributions of stress along $x$ axis ($S_{11}$) for selected domains of initial microstructures with different mean subgrain radiiues. It is obvious that the stress distributions are heterogeneous due to the presence of grain and subgrain with different orientations. Stress concentrations are observed both at grain boundary and subgrain boundary. As the mean subgrain radius increases, the stress distribution also changes.

The scatter plot of average stress $\langle S_{11} \rangle$ for initial microstructures with different mean subgrain radiuses $\langle R_0 \rangle$ is shown in Fig. 4. It can be seen that the average stress slightly decreases as the mean subgrain radius increases. It should be noted that the average stress is defined as average volume stress over every subgrain.

Fig. 4. Average stress $\langle S_{11} \rangle$ for initial microstructures with different mean subgrain radiiues $\langle R_0 \rangle$.

Fig. 5. Simulated temporal microstructure at different times with annealing temperature $T=973$ K, initial mean subgrain size $\langle R_0 \rangle=0.31$ μm and inter-subgrain misorientation $\theta=5^\circ$ (a) 1 s (b) 2 s (c) 3 s and (d) 6 s.

Fig. 5. Simulated temporal microstructure at different times with annealing temperature $T=973$ K, initial mean subgrain size $\langle R_0 \rangle=0.31$ μm and inter-subgrain misorientation $\theta=5^\circ$ (a) 1 s (b) 2 s (c) 3 s and (d) 6 s.
3.2. Effect of SRX on the stress

Generally, the microstructure of a deformed material will change after annealing treatment, so the mechanical properties will also change. Based on the CA simulated microstructures during SRX and CPFE calculation, the stress responses of intermediate microstructures during annealing are studied. In order to simplify the CA simulation, all the misorientation angles of subgrain boundaries were set to the same in the present study. Fig. 5 depicts the temporal microstructure at different simulation times under the condition of initial mean subgrain radius $\langle R_0 \rangle = 0.31 \, \mu m$ and inter-subgrain misorientation $\theta = 5^\circ$ when the temperature is 973 K. The phenomenon of subgrains at the pre-existing grain boundaries bulging into its neighboring grain as recrystallization nucleus was observed, which shows a better demonstration of the grain boundary bulging nucleation mechanism. Finally all the pre-existing grains are consumed by the recrystallized grains, and the fully recrystallized microstructure is relatively homogeneous. Fig. 6 shows the distributions of stress along $x$ axis ($S_{11}$) for selected domains of microstructures at different simulation times in Fig. 5. The stress distributions are also heterogeneous, and stress concentrations are observed both at grain boundary and subgrain boundary. The scatter plot of average stress ($S_{11}$) for microstructures at different simulation time is depicted in Fig. 7. The average stress decreases as the increase of the simulation time. The misorientation distributions for the four microstructure pictures in Fig. 5 are shown in Fig. 8. Obviously, the fraction of low angle boundaries decreases as the annealing time increases. The degradation of the stress can be ascribed to the decrease of the amount of the subgrain boundaries during SRX. It should also be noted that the orientation Euler angles for calculating the misorientations in Fig. 5 are inherited from the Euler angles that are generated in Fig. 2 for the initial microstructure.

![Fig. 7. Average stress ($S_{11}$) for microstructures at different simulation times.](image)

![Fig. 6. Stress $S_{11}$ distribution for selected domains (at the top right) of microstructures at different simulation times in Fig. 5 (a) 1 s (b) 2 s (c) 3 s and (d) 6 s.](image)
4. Conclusion

The microstructure-based CPFE simulation results show that subgrains inside pre-existing grains have an effect on the heterogeneity of stress distribution. The average stress decreases with increasing the mean subgrain radius. As SRX process continues, the average stress also decreases, due to the reduction of subgrain structure. It can be deduced that well-defined and finer subgrain structure may strengthen the polycrystalline material, while grain/subgrain growth during SRX process will degrade the strength.

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References