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Original Research

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

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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 MC 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 $\langle R_0 \rangle$, 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 2500×2500 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,

$$v = M\gamma\kappa \tag{1}$$

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

$$M(\theta) = M_{\mathrm{HAG}}\left(1-\exp\left(-5\left(\frac{\theta}{\theta_{\mathrm{m}}}\right)^4\right)\right) \tag{2}$$

where M_{HAG} is the mobility of high-angle boundary with misorientation greater than θ_{m} and it is estimated by the following equation:

$$M_{\mathrm{HAG}} = \frac{\delta D_{\mathrm{b}}}{kT}\exp\left(-\frac{Q_{\mathrm{b}}}{RT}\right) \tag{3}$$

The boundary energy is also dependent on the misorientation angle θ, and can be calculated by the following equation:

$$\gamma = \gamma_m\left(\frac{\theta}{\theta_m}\right)\left(1-\ln\left(\frac{\theta}{\theta_m}\right)\right) \tag{4}$$

where γ_{m} is the high-angle boundary energy.

An equivalent approach to calculate the boundary curvature for square lattice known from solidification [27] was adopted