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Reconstruction of deformed microstructure using cellular automata method

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ABSTRACT

The kinetics of microstructural evolution phenomena like recrystallization, grain growth, and phase transformation of deformed materials is affected by the characteristics of deformed microstructure. In fact, average grain size, grain morphology, texture and grain boundary properties of the deformed material determine the microstructure characteristics. In this paper, the reconstruction of deformed microstructure and changes in the microstructure in mesoscale are studied. Accordingly, the normal growth, topology deformation, and reconstruction of texture and grain boundary misorientation techniques are used to reconstruct the deformed microstructure. Therefore, probabilistic cellular automata method with hexagonal cells is used to create a microstructure with equiaxed grain morphology followed by a new modified topology deformation technique. In this technique, the quality and the quantity of the plastic deformation are considered by applying the deformation gradient tensor to the undeformed microstructure. Finally, a set of crystal orientations is created using a probabilistic algorithm relevant to the real texture of the material and then the crystal orientations are assigned to the deformed grains in such a way that satisfy the misorientation angle distribution. The accuracy of the numerical approaches is verified by comparing the experimental and the simulated results.

1. Introduction

Plastic deformation of metals and alloys increases the density of crystal defects and changes the microstructure of the material. The deformed microstructure after cold work provides the driving force that is needed for annealing phenomena [1]. Different phenomena like recovery, recrystallization, grain growth and phase transformation may occur during annealing processes. These phenomena significantly change the microstructure and mechanical properties of the material. The deformed microstructure totally determines the initial state of the system before annealing and it has an important effect on the kinetics of microstructure evolution phenomena [2]. Generally speaking, the grain size and morphology, grain orientation, grain boundary characteristic and misorientation, and the stored energy level of the material determine the overall state of the system in the deformed microstructure [3]. So, the first step in simulating and modeling of the microstructural evolution during the different thermomechanical processes is the determination of the initial state of the material. Since, in most deformation processes, the deformation is anisotropic, a suitable algorithm is required to reconstruct the microstructural characteristic of the material before simulation. The design of such a simulation tool, which has the ability to account for intrinsic properties like energy and mobility of grain boundaries, microstructure characterizations like grain size distribution, grain morphology, and micro-texture, is attractive.

A vast variety of microstructural simulation methods such as Monte Carlo method, Phase field method, Vertex method and Cellular automata (CA) method have been presented to simulate the microstructure evolution. Today, the CA method is of interest to researchers because the different complicated conditions may be simply and simultaneously applied to the model which is decreasing the calculation time and cost, and simplifying the computing codes from data storing and algorithm points of view [4]. This method was firstly introduced by Neumann [5] in 1966 and Wolfram [6] in 1986. The method was used for simulating static recrystallization by Hesselbarth [7] and then employed for a variety of phenomena. Turk and Kugler [8] corrected the CA model and used it for modeling the effect of the initial microstructure on static recrystallization kinetics and grain size. Xiao et al. [9] considered the effect of deformation topology and the grain deformation procedure on the simulation of dynamic recrystallization by employing the CA method. Also, Chen et al. [10] studied dynamic recrystallization by coupling a CA method with a topology

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deformation technique. The effect of thermomechanical parameters on the recrystallization kinetics and grain size has been evaluated by taking into account the effect of the topology of the deformed grains.

In another work, Chen et al. [11] presented a modified CA model to investigate dynamic recrystallization by using the topology deformation method. In this model, the coordinate systems of the cellular model and the material were separately adopted so that the system would change later during deformation. The grain topology, the recrystallization fraction, and the average grain size of Ni-based superalloy during hot deformation were also predicted by means of the modified model. Recently, dynamic recrystallization has been simulated using CA method coupled with topology deformation technique in order to assess the effect of grain morphology, strain rate and strain [12–14]. Madej et al. [15] proposed a CAFEM model to predict SRX during the cold deformation of the low carbon steel after cold rolling. In this model, the FE results have been considered as input imposed upon the CA model to evaluate the recrystallization kinetics.

Also, in some studies, the reconstruction of crystal orientation of grains and the material texture have been considered and various methods have been proposed for modeling the material texture. Melchior et al. [16] have presented a numerical method to generate a discrete sampling of the crystallographic texture which the orientation samplings statistically represent the given orientation distribution function (ODF). Also, in 2008 a known ODF was reconstructed in discrete EULER space by Eisenlohr et al. [17]. In Eisenlohr's model, the volume fraction of a reconstructed orientation has been approximated by the ratio of each discrete crystal orientation zone to the overall sample space using the discrete ODF representation. For this purpose, the integer approximation and the statistical methods were used. It was shown that by using the correlation factor, the integer approximation method was far better than the statistical one. The correlation factor to assess crystallographic texture for the first time was introduced by Tarasiuk [18] et al. in 1996. Toth et al. [19] also presented two methods for the reconstruction of ODF; these included cumulative ODF or statistical technique and a minimum orientation distance criterion to predict the texture during plastic deformation. Toth et al. showed that statistical approach could be more reliable than other methods of producing the discrete distribution in texture modeling. Ivanova et al.[20] by comparing the two methods (component fit method and orientation grid technique) for the sample of magnesium alloy, illustrated that the first method was more stable and robust. Lobach et al. [21] theoretically analyzed the quantitative texture to reconstruct ODF.

The main purpose of this paper is to present a model for reconstructing the deformed microstructure by considering the initial average grain size, grain morphology, texture and grain orientation, and grain boundary misorientation. To reconstruct the initial microstructure with a suitable initial grain size, the normal growth method is implemented using probabilistic CA coupled with a new topology deformation technique. In this work, by means of a normal growth algorithm, the initial nucleus could be grown according to the real microstructure grain size and the initial microstructure generated with the proposed the growth method. In order to increase the accuracy of the modeling methods in the prediction of the microstructure evolution, it is necessary to consider the distribution of the crystalline orientation and the misorientation of grain boundaries based on the real material microtexture. In this paper, an algorithm is developed for reconstructing the crystalline orientation of grains and also the misorientation of grain boundaries. In order to reconstruct the crystalline orientation of the grains, proportional to the material texture, Euler's angles of the grains are determined in such a way that the discrete ODF has the most consistency with the known texture of the material. Also, the crystal orientation is assigned to the grains to ensure that the misorientation distribution represents the known misorientation distribution of a real material. By using this algorithm for fitting the crystalline orientation and the misorientation, the initial microstructure can be obtained close to the actual state of matter. The details of this model and some possible improvements have also been discussed.

2. Reconstruction of the deformed microstructure

The first step in microstructure simulation of deformed material is the reconstruction of the initial microstructure. The initial general state of the system has an important effect on the kinetics of the microstructural evolution i.e. recrystallization, grain growth and phase transformation. In fact, the initial grain morphology, the crystal orientation of grains, interface characteristics and the energy level of matter determine the general state of the system. The microstructure with a given average grain size and morphology is reconstructed regards to the structure of the real deformed material. So, a variety of algorithms like normal growth based on CA method, topology deformation and crystal orientation reconstruction were used.

2.1. Normal growth

To reconstruct the initial microstructure with a suitable initial average grain size, the normal growth method based on the probabilistic CA method is used. In this method, space is divided into several regular sub-domains are called cells. State variables which are defined the physical states of the cells i.e. the crystal orientation or the state of recrystallization are attributed to the cells. The time is discretized and in every time increment, changing of the cell states are studied according to the overall system state. The state change rule of the cells is determined by the rule of physics governing the grain boundary migration. According to classical theory of boundary migration, the velocity of the grain boundary migration is described by the Turnbull's rate equation as follows [3]

$$v = mp \tag{1}$$

where m is the grain boundary mobility, and p is the driving pressure acting on the grain boundary. The mobility of grain boundary is considered as a function of temperature and grain boundary characteristics, so [22]

$$m = m_0 \exp\left(\frac{-Q_d}{RT}\right) \tag{2}$$

where Q_d is activation energy of grain boundary migration, m_0 is mobility constant, T is the absolute temperature, and R is the gas constant. The driving pressure can be derived by summing the driving pressure due to the grain boundary curvature, driving pressure of stored energy which is related to the difference of Gibbs free energy density of the material located at the two sides of the grain boundary [3]. In this paper, probabilistic cellular automata algorithm was used for determining the state change rule. In this algorithm, the state of cell i in the time step of $k+1$ "ξ_i^{k+1}" is determined by neighbors state at time step k [23], so

$$\xi_i^{k+1} \triangleq \xi_i(t_{k+1}) = \begin{cases} \xi_i^k & \text{if } W_i^k \leqslant 0 \\ \xi & \text{if } W_i^k > (\mathcal{R}|\mathcal{R}\epsilon[01]) \end{cases} \tag{3}$$

where $\mathcal{R}$ is a random number between zero to one, ξ is the new state of the cell and may be derived using the state of the transformed neighbors and W_i^k is the local probability of state change and it's calculated as