Article ID: 1003－6326(2005)01－0130－05

Simulation and visualization of recrystallization microstructure after solution treatment①

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Abstract: Simulation models for heterogeneous and simultaneous nucleation and random growth of nuclei were developed in terms of the mechanism of recrystallization and Monte Carlo stochastic simulation method. Combining deterministic simulation with stochastic simulation, the simulation and visualization of the recrystallization microstructure of Ti-15-3 alloy after hot compression deformation and solution treatment were realized. Comparison of the simulated results with the experimental ones suggests that the size and distribution of the simulated recrystallized grains agree well with the actual ones. This proves that the obtained statistic equivalent microstructure models are effective. This study is helpful for determining reasonable hot forming process and improving the forming quality.

Key words: nucleation; growth; Ti-15-3 alloy; recrystallization microstructure; simulation; visualization
CLC number: TG 302 **Document code:** A

1 INTRODUCTION

Physical and mechanical properties of metals are determined by their microstructures. Therefore reasonable simulation and visualization of microstructure evolution during hot deformation can show the distribution and evolution of grains intuitively. It has important theoretical significance and practical utility prospect for studying microstructure evolution and determining reasonable hot forming process and ensuring product quality. Because of the complexity of the deformation mechanism, temperature change, nucleation behavior, interaction between grains and the large number of factors influencing the grain boundary mobility, the simulation on microstructure evolution during hot deformation is very difficult[1-5].

In this paper, simulation models for heterogeneous and simultaneous nucleation and random growth of nuclei have been proposed in terms of the mechanism of recrystallization and MC stochastic simulations. Micro-parameter values are used as controls parameters, and simulation and visualization of the recrystallization microstructure of Ti-15-3(Ti-15V-3Cr-3Sn-3Al, metastable β-type) alloy after hot compression and solution treatment have been realized by combining deterministic simulation with stochastic simulation. This study is helpful for determining reasonable hot forming process and improving the forming quality.

2 MONTE CARLO METHOD

Monte Carlo(MC) stochastic simulation method is an effective tool for simulating polycrystal microstructure and can provide kinetic and topological information of microstructure evolution[6-8].

In Monte Carlo stochastic simulation technique which models grain growth, the complexity of the grain structure is approximated by discretizing the continuum microstructure on a two dimensional, square mesh with periodic boundary conditions. Each element of the mesh is called a site. Each site is assigned a random integer between 1 and Q, where Q is the total number of grain orientations introduced in the simulation, representing the orientation of the grain to which it belongs. Define the neighbor of the sites. Neighboring sites with the same orientation belong to the same grain, and those neighboring sites with different orientations form grain boundary sites. For each site, its orientation is changed into the orientation of the neighbor randomly. If the grain boundary energy decreases or maintains the same value, new orientation will be accepted. Otherwise, the reorientation attempt will not succeed. Grain growth occurs as a result of the change in the orientations of individual sites[9, 10].

The energy can be expressed by the formula:

$$E = J \sum_j (1 - \delta_{s_i s_j}) \quad (1)$$

① **Foundation item:** Project(50405020) supported by the National Natural Science Foundation of China; Project supported by the Excellent Youth Fund of Anhui Province
Received date: 2004－02－26; **Accepted date:** 2004－10－18
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where J is the contribution from each elementary boundary between the analyzed site and its neighbors. In the case of isotropic material, $J = 1$. S_i and S_j are the orientation of the analyzed site i and its neighboring site j, respectively, and $\delta_{S_i S_j}$ is the Kronecker delta function

$$\delta_{S_i S_j} = \begin{cases} 1 & (S_i = S_j) \\ 0 & (S_i \neq S_j) \end{cases} \quad (2)$$

3 SIMULATION MODELS

3.1 Nucleation model

Static recrystallization will take place in the deformed specimens after solution treatment. In the classical recrystallization models, the nuclei are assumed to be distributed at random in space. Because of the non-uniform distribution of the stored deformation energy, the recrystallized embryos appear preferentially on the grain boundaries or triple junctions with higher stored energy. The existence of preferential sites and the non-random distribution of these sites suggest a non-random character of the spatial distribution of the nuclei[11, 12]. In this paper, the heterogeneous and simultaneous nucleation model is established.

At the beginning of the present simulation, a constant number of nuclei is provided. Thereafter, only the growth of nuclei is admitted during the recrystallization simulation process. The deformed microstructure is discretized into a two dimensional lattice, each site of the lattice is considered as a potential nucleus. The sites are classified into two groups, i. e. the sites situated at the boundaries and those in the interior of the deformed grains. Each site is initially assigned as 0 to represent that nucleation does not occur.

The simulation of nucleation process consists of two stages which proceed one after another, i. e. the nucleation at the boundaries of the deformed grains, and then the nucleation in their interiors. For grain boundary nucleation, we select sites situated at the boundaries of any deformed grains randomly, then examine whether the picked site has already been occupied by other nucleus or not. If nucleation at the site does not take place and the distance between the site with already recrystallized embryos accords with the recrystallized grain size, the nucleation attempt is considered to be successful. The embryo is given a new orientation randomly, so that no two nuclei have the same orientation. If there is already another embryo covering the picked site, then nucleation is neglected. Repeat above procedure till the number of nuclei accords with the recrystallized grain density in the simulating region.

When the nucleation sites situated at the grain boundaries have been covered up with nuclei, the same procedure is performed for nucleation within the deformed grains. In order to make the simulation more time efficient, we select sites within the deformed grains randomly, where the number of nuclei does not satisfy the demand, to carry out the nucleation experiment.

3.2 Growth model

Once a nucleus is formed, it will grow due to the difference between the stored energy of the nucleus and the deformed matrix. The nucleus growth can be modeled using stochastic method and being based on the following assumptions:

1) All nuclei remain fixed in location throughout the growth process;

2) The growth rate of the nuclei is equal, isotropic and independent of time.

The nucleus growth is modeled by capturing the neighboring sites randomly and continuously and orienting the neighbors to the orientation of the analyzed nucleus. If the neighboring site has been captured by other new grain, then the growth of the nucleus stops in this direction. But the nucleus still can grow in other directions. When all the neighboring sites of the new grain are captured by other new grains, or the new grain size satisfies the demand, the nucleus growth terminates.

4 RESULTS AND DISCUSSION

The distribution of the characteristic microparameter values in the samples of Ti-15-3 alloy, which are the control parameters used for this simulation, has been calculated by incorporating the neural network models for predicting microstructure parameters into a coupled thermomechanical rigid-viscoplastic FE model for deformation[13, 14]. In this paper, a three-layer BP neural network is employed for acquiring the prediction models of microstructure of Ti-15-3 alloy. Temperature, effective strain and effective strain rate, which are acquired by simulating hot compression deformation with FEM, are used as the input vectors. The outputs are the average recrystallized grain size and the recrystallized grain density.

The microstructure formed in hot deformation is the microstructural basis for the spatial distribution and growth of nuclei. Analysis shows that dynamic recovery is the main process for Ti-15-3 alloy during hot deformation. The microstructure has been generated by simulating grain structure evolution of Ti-15-3 alloy in hot compression deformation[15]. Static recrystallization microstructure appears after solution treatment at 800 ℃ for 20 min.

The simulation is run by assuming that there is no grain boundary motion between deformed matrix grains. In the present simulation, a grid sys-

tem with a grid spacing of 10 μm is used to discretize the region. Fig. 1 shows the simulated recrystallized microstructures of Ti-15-3 alloy in the center of the samples after solution treatment under different deformation conditions. The simulated results reveal the rules of microstructure evolution intuitively. The recrystallized grain size increases and the recrystallized grain density decreases with deformation temperature increasing. The recrystallized grain size decreases and the recrystallized grain density increases with the strain and strain rate increasing and fine-grain microstructure is obtained. When strain (ε) and strain rate ($\dot{\varepsilon}$) are larger and temperature is lower, the dislocation density in the deformed microstructure increases and the deformation energy stored in the alloy increases also. Moreover, finer grains are obtained during deformation and the grain boundary area per unit volume increases. Hence, the recrystallized grains nucleate and grow more easily during the following solution treatment (the influence on nucleation is more important). The recrystallized grain density increases and the recrystallized grain size decreases.

Furthermore, the simulation results indicate that the recrystallization microstructure of Ti-15-3 alloy after hot deformation and solution treatment at 800 ℃ for 20 min includes two parts: the initial deformed grains and the recrystallized grains. Under the present deformation conditions, most nucleation occurs heterogeneously at prior grain boundaries. When the new grains increase in size and consume a large portion of the old grain boundaries, clusters of recrystallized grains are visible. The microstructure shows the characteristic "necklace" structure. So the spatial distribution of nuclei is non-random. Moreover, although the grain shape is assumed to be regular and the size is constant, the simulated grains are irregular. It accords with the physical mechanism of recrystallization.

5 TEST TESTIFICATION

Fig. 2 shows the recrystallized microstructures of Ti-15-3 alloy in the center of the specimens after solution treatment for different hot deformation conditions. Fig. 3 shows the comparison between

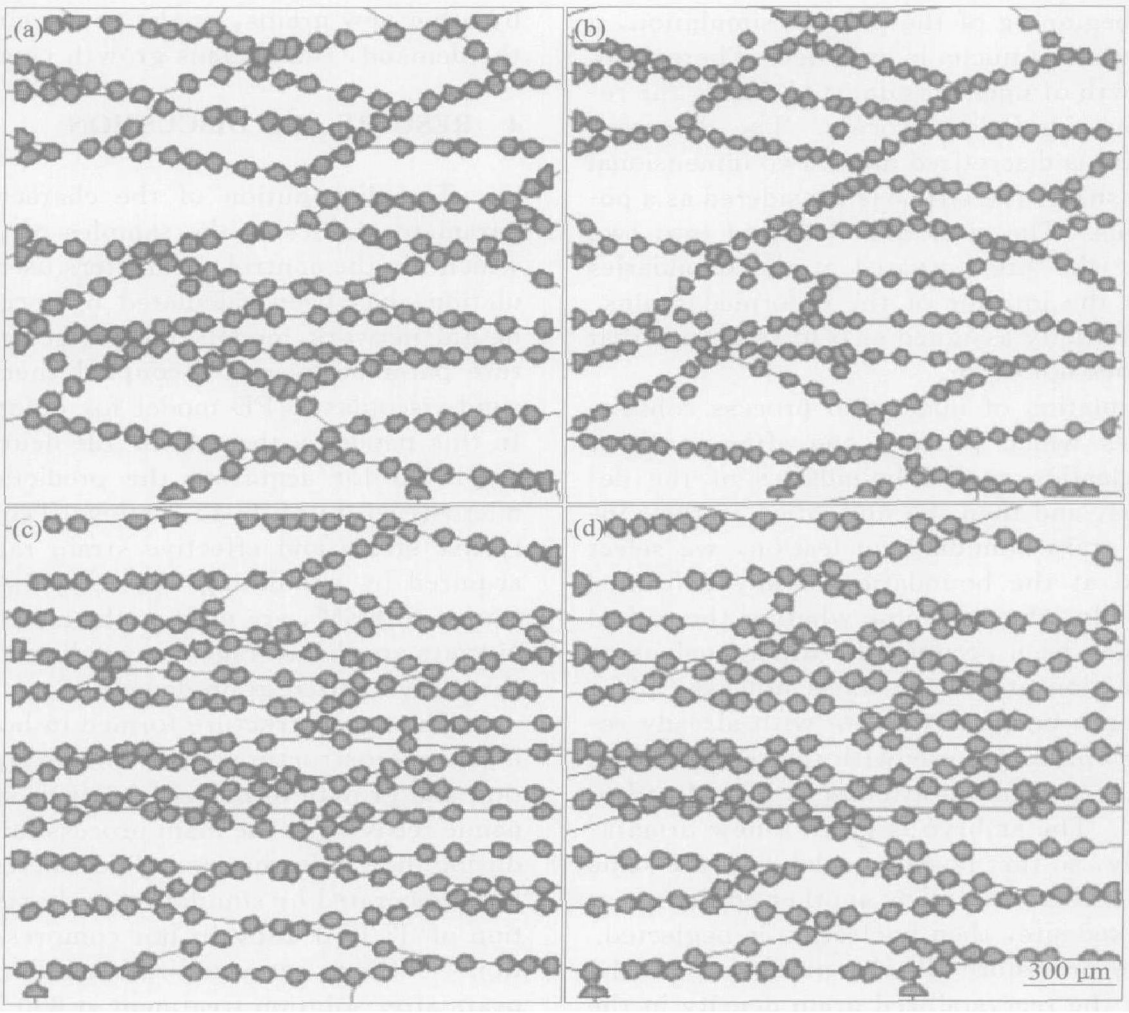

Fig. 1 Simulated recrystallization microstructures of Ti-15-3 alloy after solution treatment
(a) —t= 800 ℃, ε= 0.4, $\dot{\varepsilon}$= 0.01 s^{-1}; (b) —t= 800 ℃, ε= 0.4, $\dot{\varepsilon}$= 1 s^{-1};
(c) —t= 800 ℃, ε= 0.6, $\dot{\varepsilon}$= 0.01 s^{-1}; (d) —t= 900 ℃, ε= 0.6, $\dot{\varepsilon}$= 0.01 s^{-1}

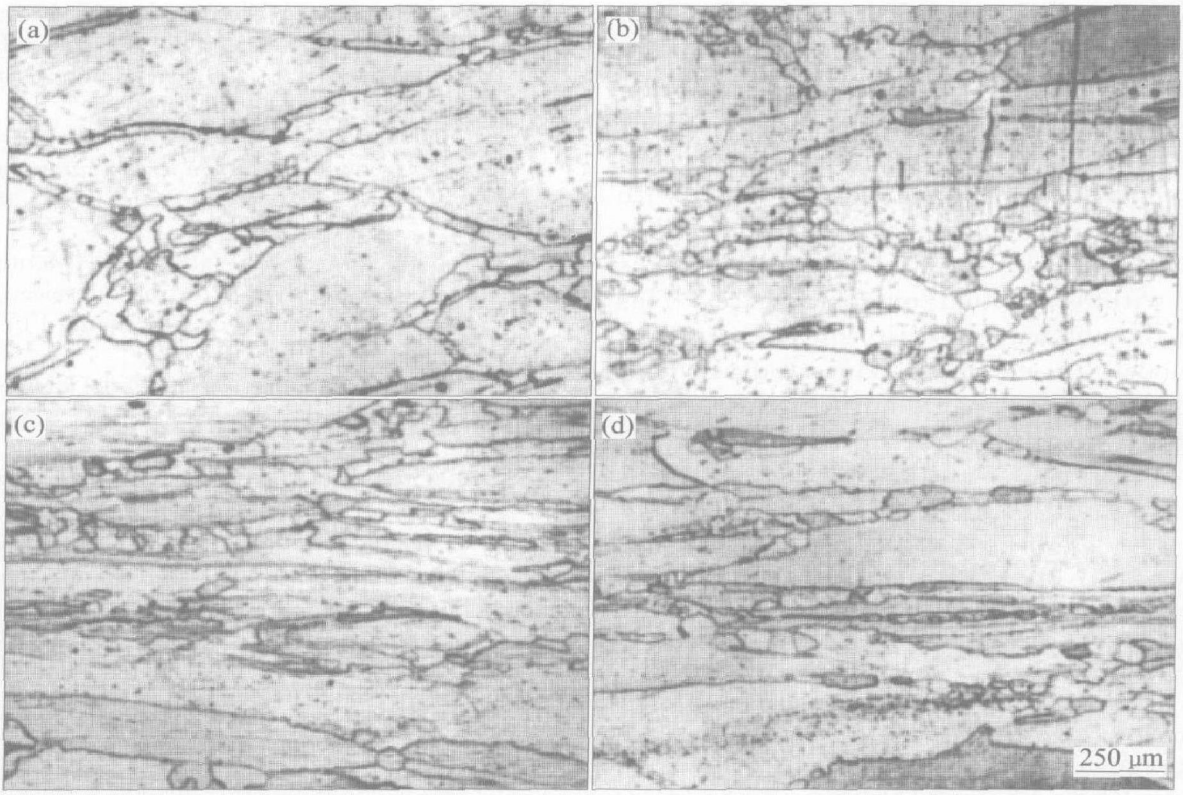

Fig. 2 Microstructures of Ti-15-3 alloy deformed at different parameters after solution treatment
(a) —t= 800 ℃, ε= 0.4, $\dot{\varepsilon}$= 0.01 s^{-1}; (b) —t= 800 ℃, ε= 0.4, $\dot{\varepsilon}$= 1 s^{-1};
(c) —t= 800 ℃, ε= 0.6, $\dot{\varepsilon}$= 0.01 s^{-1}; (d) —t= 900 ℃, ε= 0.6, $\dot{\varepsilon}$= 0.01 s^{-1}

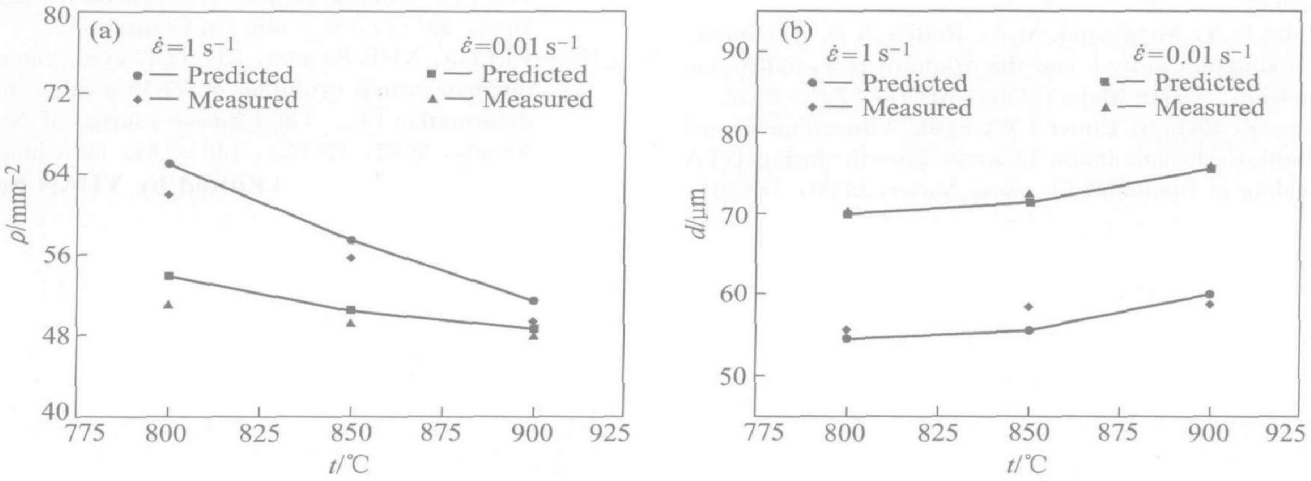

Fig. 3 Comparison between simulated micro-parameters and measured ones
(a) —Recrystallized grain density; (b) —Recrystallized grain size

the simulated recrystallized grain density and the recrystallized grain size with measured ones in the center of the specimens at a deformation degree of 40%. The mean relative error is within 10%. These results indicate that the distribution and size of the simulated recrystallized grains agree well with the actual ones. This proves that the method combining deterministic simulation with stochastic simulation is reasonable and reliable for simulating microstructural evolution. Combining the approach with thermal-mechanical coupled rigid-viscoplastic FE model for deformation and neural network models for predicting microstructure parameters, accurate simulation and visualization of microstructure evolution can be realized in hot deformation. The obtained statistic equivalent microstructure models are effective.

6 CONCLUSIONS

Simulation models for heterogeneous and simultaneous nucleation and random growth of nuclei have been proposed in terms of the mechanism of recrystallization and Monte Carlo stochastic simu-

lation method. The micro-parameter values are used as control parameters and the simulation and visualization of the recrystallization microstructure of Ti-15-3 alloy after hot compression deformation and solution treatment have been realized by combining deterministic simulation with stochastic simulation. Comparison of the simulated results with the experimental ones suggests that the distribution and size of the simulated recrystallized grains agree well with the actual microstructure. This proves that the obtained statistic equivalent microstructure models are effective. This study is helpful for determining reasonable hot forming process and improving the forming quality of Ti-15-3 alloy.

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(Edited by YUAN Sai-qian)