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Computer Simulation of Grain Growth Based on Actual Orientation Data

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The data format of crystallographic orientation obtained from SEM/EBSP analysis system is similar to that of Potts model in Monte Carlo (MC) simulation. In order to predict microstructural evolution, the modified MC simulation of grain growth has been performed in the model applying practical orientation data to an initial microstructure. Moreover, we have discussed changes in microstructure feature and texture between practical and simulated results. Experimental samples used in this study were annealed sheet and foil of pure aluminum (A1N99) after rolling. To apply orientation-mapping data to the simulation, these specimens were analyzed by SEM/EBSP method. The calculation was carried out using modified MC simulation that was considered activated states for grain boundary migration. As a result of SEM/EBSP analysis, it was found that the sheet sample had a typical recrystallization texture in rolled sheet. The texture became sharper with increasing annealing time. Texture development in the simulation was in good agreement with that in the experiment. In addition, grain boundary migration in the foil sample was predicted by using the modified MC technique.
Key words: grain growth, Monte Carlo simulation, SEM/EBSP analysis, aluminum, CSL boundary

1. INTRODUCTION

The Monte Carlo (MC) simulation technique using Potts model has been successfully used to study microstructural evolutions in polycrystalline materials, such as grain growth, recrystallization, sintering, phase transformation and so on. In the evolved microstructure grain boundary features, their topological properties and grain size distribution are reproduced by the MC technique. Recently the scanning electron microscopy / electron backscatter diffraction pattern (SEM/ EBSP) method is noted as an effective technique to get statistical and geographical information of crystallographic orientation [1]. The data format of SEM/EBSP analyzing system is similar to that of the Potts model in MC simulation [2]. In the present study, in order to predict microstructural evolution, the modified MC simulation of grain growth is performed in the model applying practical orientation data to an initial microstructure. Changes in microstructure feature and texture are compared between experimental and simulated results, and moreover, what factor plays an important role during grain growth is discussed.

2. EXPERIMENTAL PROCEDURE AND SIMULATION METHOD

Experimental samples used in this study were annealed sheet and foil of 99.99% pure aluminum (A1N99) after rolling. Small specimens cut from the sheet and the foil were isothermally annealed in salt bath at 673K for 60s ~ 57.6ks and in vacuum at 723K for 3.6ks, respectively. After annealing the specimens were polished mechanically and electrochemically in the rolling direction (RD)-transverse direction (TD) section. Orientation mapping data of them were investigated by SEM/EBSP method in the square area of 2mm × 2mm by a step size of 10 μm.

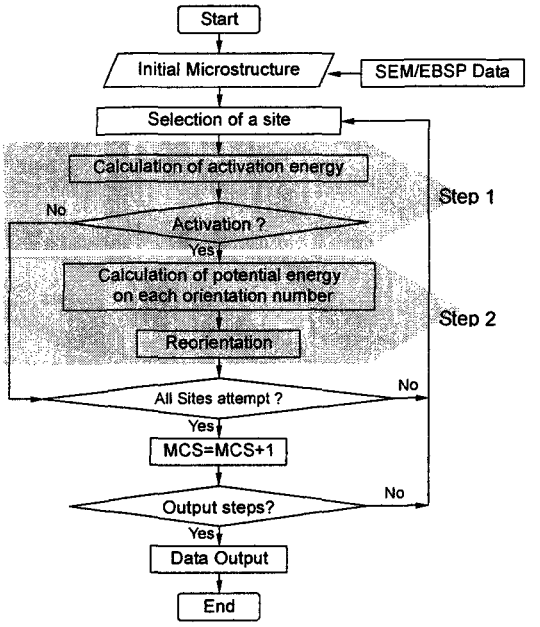

Fig. 1. Flow chart for simulation of grain growth.

The MC simulation using the Potts model has been already performed in consideration of reorientation accompanied with activated state for grain boundary (GB) migration [3]. In the present study, the simulation model with the activated state was also carried out using the practical orientation data not only to predict the microstructural evolution but also to clarify effects of GB energy and mobility. The flow chart of the simulation is shown in Fig. 1. A site is selected at random, and then a reorientation trial of the site is done by two steps. The first step is the activation step of the site, in which whether site is activated is determined

with the following equation.

$$W_a \propto \exp\left(-E_a/\alpha^3 k_B T\right), \quad (1)$$

where W_a is activation probability in the selected site, E_a is activation energy of the site, α is a constant concerned with the ratio of site to atom, k_B is Boltzman constant, and T is absolute temperature. Furthermore, the activation energy E_a is given by

$$E_a = E_{act} - (U - E_m), \quad (2)$$

where E_{act} is potential energy of activated state of the site, which is the maximum value calculated as GB energy for the neighbors shells, U is GB energy of the selected site, and E_m is reduction of the energy for the presence of impurities in boundary, which is defined as sum of interaction factor μ in each site and represents mobility of GB migration. If the selected site is activated according to the probability (1), then it goes on to the next. The second step is a selection of next orientation corresponding to the GB energy on the site. The orientation is changed with the following probability

$$W_i = f_i \Big/ \sum_{n=q} f_n, \quad (3)$$

$$f_i \propto \exp\left(-U_i/\alpha^3 k_B T\right). \quad (4)$$

In practice, the equations (1) and (4) are normalized by probabilities at melting point T_m of a material. The simulation proceeds to repeat the above trial. The unit of time is defined as 1 Monte Carlo step (MCS) per site, which corresponds to trials of a number of sites in the model. In this study, the governing parameter of simulations $J/\alpha^3 k_B T_m$ was appropriately given 0.8 for a pure Al and the temperature of simulations, $T = 0.72T_m$ was selected to be consistent with the experiments, where J is an unit GB energy.

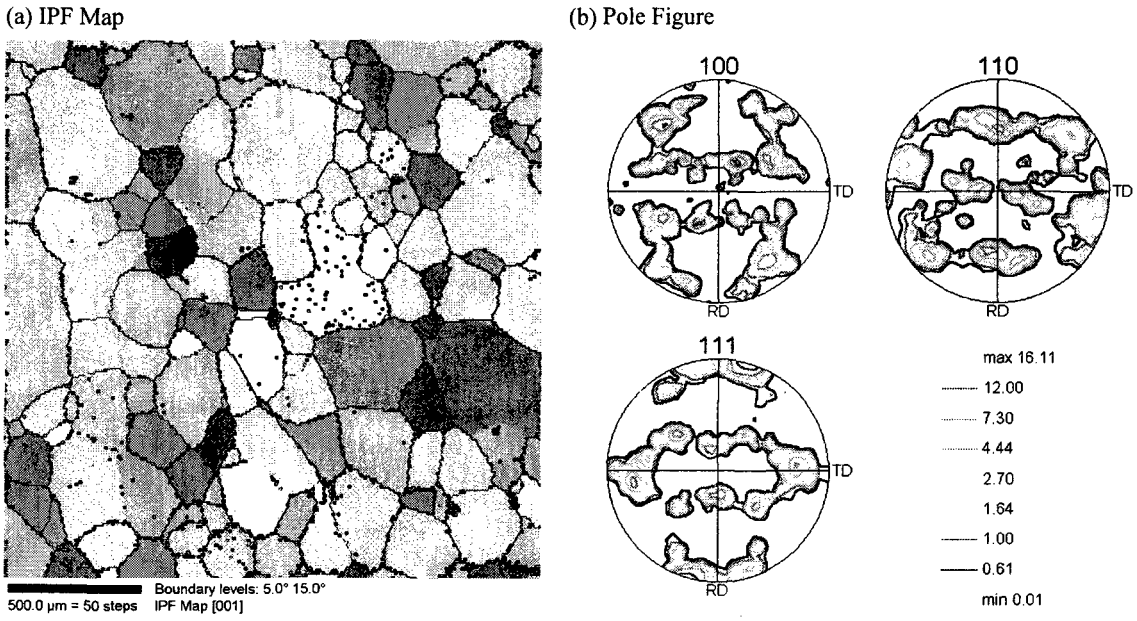

Fig. 2. Results of SEM/EBSP analysis in the specimen annealing for 57.6ks.

3. RESULTS AND DISCUSSION

3.1 Grain growth experiment in aluminum sheet

Isothermal grain growth in the pure aluminum sheet was investigated by SEM/EBSP. An initial mean grain size was 79.9 μm in equivalent area diameter. Figure 2 shows an inverse pole figure map in the normal direction (IPF Map [ND]) and pole figures in the specimen annealed at 673K for 57.6ks. Grains grow with the increase of annealing time to reach the grain size of 175.4 μm for 57.6ks (Fig. 2 (a)) It is found that the sample has a typical recrystallization texture in rolled sheet as shown in Fig. 2 (b). The texture became sharper than that before annealing. Further, normal grain growth was confirmed by the scaling rule observed in grain size distributions during annealing.

3.2 Simulations based on orientations data of a pure aluminum sheet

The simulations based on orientation mapping data obtained in the specimen annealed for 60s have been performed to compare changes in microstructure feature and texture between practical and simulated results. Following four types of simulations were carried out:

1) Basic model, which has a constant energy for all of the GBs.

2) LAGB/HAGB model, in which dependence of GB energies on crystallographic misorientation is taken into account.

3) LAGB/HAGB & CSL model, in which coincidence site lattice (CSL) boundaries is considered to extend 2).

4) GBE + Mobility model, in which GB mobility is considered, in addition to 3).

The first simulation is a basic model, which has been often seen in early studies of the MC simulation. The grains have grown commonly in the simulation. The grains after simulation are equiaxed and have the same size as shown in Fig. 3. It was found in the model that the texture was randomized.

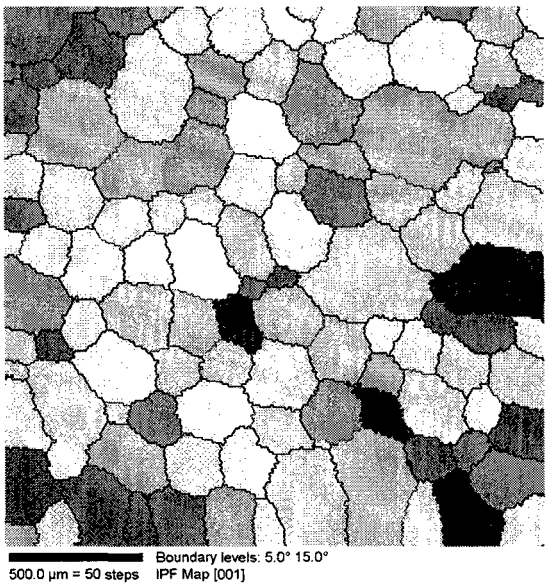

Fig. 3 IPF Map [ND] simulated in a basic model (1000MCS).

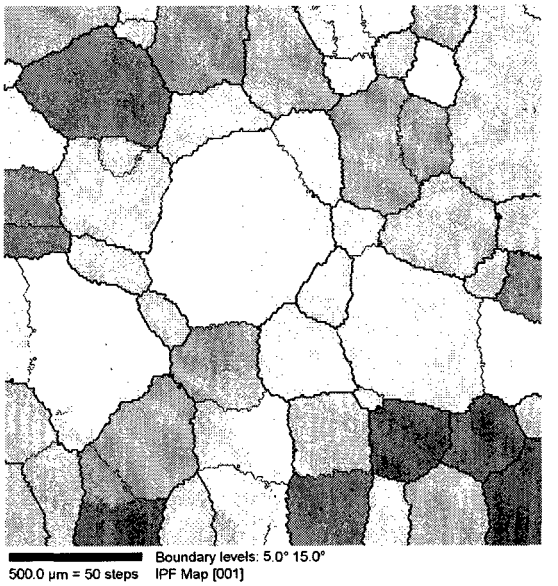

Fig. 4 IPF Map [ND] simulated in a LAGB/HAGB model (5000MCS).

Table 1 Grain growth exponents, n in the experiment and the simulations.

Experimental (673K)	0.119
Basic Simulation (a constant GB energy)	0.327
LAGB/HAGB model	0.320
LAGB/HAGB & CSL model	0.362
GBE + Mobility with μ_{HAGB}=0.5 model	0.128

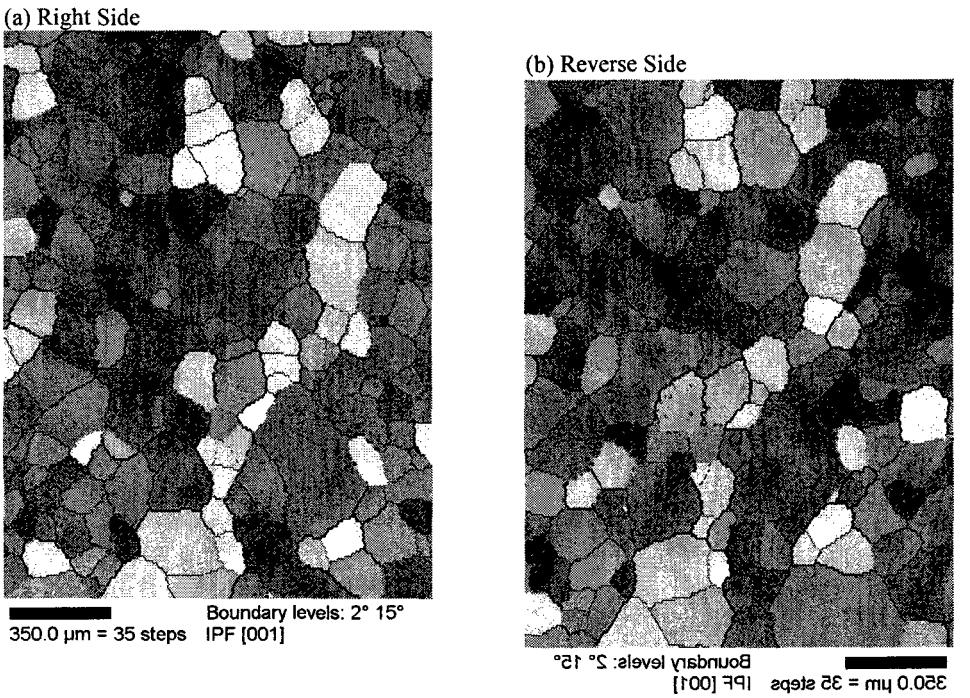

Fig. 5 IPF Maps on (a) right and (b) reverse sides in the annealed foil.

In actual microstructure, GBs have various energies depending on crystallographic misorientation [5]. Figure 4 shows the microstructure evolved in the LAGB/HAGB model assuming low and high angle GBs with low and high energies, respectively. Much-curved and broken-off boundaries are observed in the microstructure. Some grains are colored or oriented with a little difference, which are regard as consisting of subgrains. The simulated microstructure is analogous to experimental one. It was also found the texture was sharpened as corresponding to the experiment.

In the LAGB/HAGB & CSL model, energy cusps are considered for coincidence site lattice (CSL) boundaries of $\Sigma \leq 21$. It was confirmed that fraction of CSL boundaries in the microstructure was almost equivalent to that of experiment. Slow microstructural evolution was observed owing to low mobility set for HAGB.

Grain growth exponents, n in the experiment and the simulations performed in the present study are listed in Table 1. The exponent in the experiment is 0.119 and then that of the three simulations without mobility are more than 0.3. The grain growth exponent, n of 0.128 in the GBE + Mobility model with $\mu_{HAGB} = 0.5$ is in the best agreement with the experimental value.

3.3 Grain boundary migration in aluminum foil

Typical two-dimensional columnar structure was obtained in aluminum foil 132 μm thick after annealing at 723K for 3.6ks. Figure 5 shows IPF maps on right and reverse sides in the annealed foil. The reverse side map is turned over for the sake of convenience in comparison. It is confirmed that most of grains lie through foil thickness. For this microstructure prediction of grain boundary migration was carried out by using the modified MC technique with and without low mobility in high angle grain boundaries. Grain boundary misorientation distributions are compared between experimental and simulated results in Fig. 6. Experimental results show slight increase in frequency for low angle boundaries after annealing. Frequency for LAGB rises up considerably in the simulation without low mobility in HAGB. The simulated distribution with low mobility in HAGB is similar in shape to the experiment. This suggests that the grain boundary migration in the foil is affected by impurities in HAGB.

4. CONCLUSIONS

In the present study, the Monte Carlo simulation using the Potts model has been performed in consideration of reorientation accompanied with activation state for GB migration, and moreover, using actual orientation data for the sheet and the foil of pure aluminum. The simulation based on practical orientation data has reproduced microstructural features and textural evolution under consideration of dependence of GB energy on misorientation. Therefore, the GB energy is understood to play the most important role in the evolution of actual microstructure and texture, although the GB mobility should be also noted. The MC simulation has the excellent possibility to predict actual microstructural evolution.

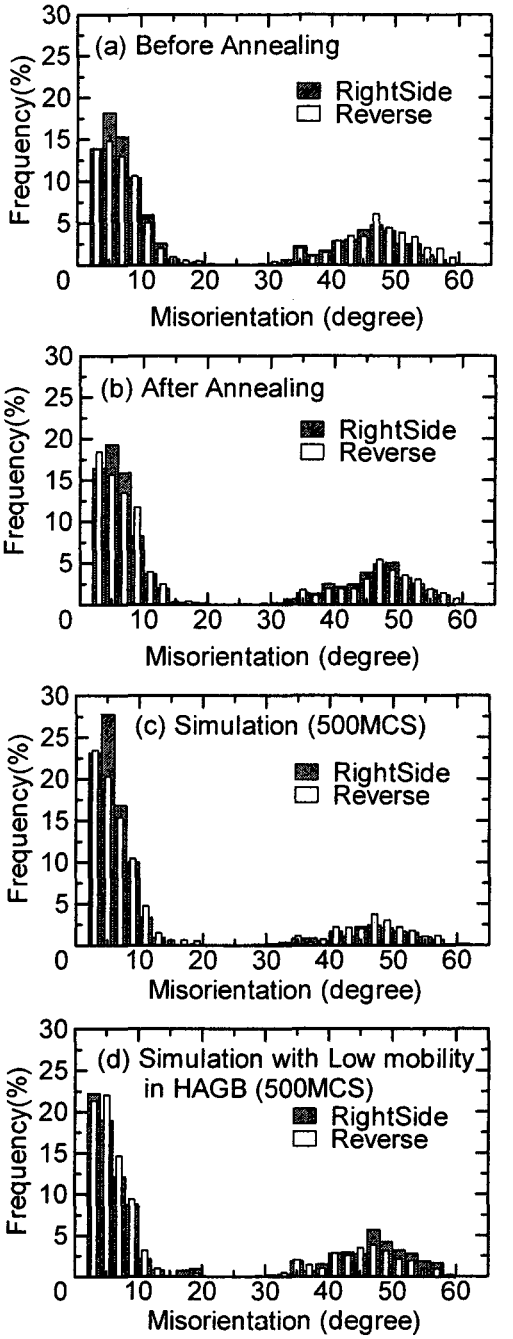

Fig. 6 Grain boundary misorientation distributions of experimental and simulated results.

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