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Atomistic Simulation of the Two-Dimensional Grain Growth

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A molecular dynamics simulation of metallic polycrystals was carried out to analyze the two-dimensional grain growth phenomenon. The model structure were initially composed of 64 grain in nanometer sizes with two-dimensional arrangement. In the simulation at an elevated temperature, the grain growth phenomenon was successfully observed. The density of the sample slightly increased during the grain growth due to the decrease of the boundary area. The simulated growth rate was close to the parabolic law. The dominant type of the grain boundary in the simulated sample was random boundary, but a few coincidence boundaries were also observed.

Key words: molecular dynamics, grain growth, parabolic law, coincidence boundary

1. INTRODUCTION

The grain growth phenomenon can be understood as a time evolution of the grain boundary network in polycrystals toward minimizing the boundary energy. In this phenomenon, small grains shrink and disappear, and the mean size of grains increases with time. This process is influenced by not only the temperature or pressure but also the microstructures such as boundary misorientation and dislocation. These microstructures are also important for controlling and improving the material properties of metals and ceramics.[1)]

Various studies have been developed in order to understand the grain growth kinetics for many years. These studies including theories, models and computer simulations before 1980's are summarized in the review by Atkinson.[2)] For example, the mean field approach by Hillert[3)] and Louat,[4)] Monte Carlo method (so called Potts model) by Srolovitz et al.[5)] and Anderson et al,[6)] the vertex model by Nagai et al.[7)] Most of these studies were limited to the two-dimensional grain growth problems. Recently, Wakai et al.[8)] extended the 2D vertex model to the 3D one by expressing the grain boundaries with curved surfaces. These "classical" methods assume the grains as a homogeneous media or a vacant space and the grain boundary as a simple geometrical surface. Such assumptions are not always acceptable in the atomistic level.

In order to overcome the limitation of these methods, the present authors apply the molecular dynamics (MD) method to the grain growth phenomenon.[9)] In the MD simulation, we can deal with all types of microstructure including boundary misorientation and dislocation, curved interface, and triple junctions which are frequently ignored in the classical methods. We can also follow detailed motions of atoms at grain boundaries. In this paper, the present authors outline the MD

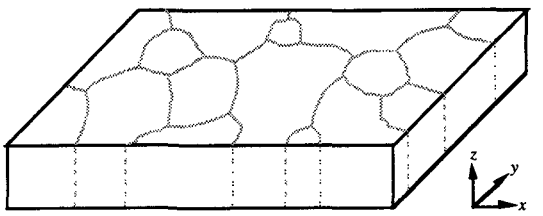

Fig. 1 A schematic diagram of the simulated polycrystalline sample. The curved lines and the outer rectangular box denote the grain boundaries and the basic cell of the MD simulation, respectively. Each grains have infinite lengths and periodic structures toward z axis.

simulation on the grain growth and show several important results.

2. SIMULATION

The polycrystalline model used in this study was initially composed of 64 grains of about 3.5 nm diameter. All grains are two-dimensionally arranged in the rectangular basic cell with applying the three-dimensional periodic boundary conditions, as shown in Fig. 1. Hence, all grains have an infinite length toward one direction (in this case, the z axis). The size of the MD basic cell is $25 \times 25 \times 1.4$ nm^3. The crystallographic orientation of each grain has common rotation axis toward z axis, and the rotational angles in the x–y plane were selected randomly. Such limitation of the orientation is necessary to satisfy the boundary condition toward the z axis.

The target material of the present study is b.c.c. Fe. The interatomic potential proposed by Finnis and Sinclare[10] was used. The MD simulation was started at the room temperature and heated up to 1680 K at the atmospheric pressure. The constant *NPT* simulation using the Nosé thermostat was carried out for more than 500 ps. The parallel calculation system HIT HPC-HP2SC/Myrinet composed of 12 CPUs were used.

3. RESULTS AND DISCUSSION

In fig. 2 we show the time variation of the density of simulated sample. At the beginning of the simulation, the density

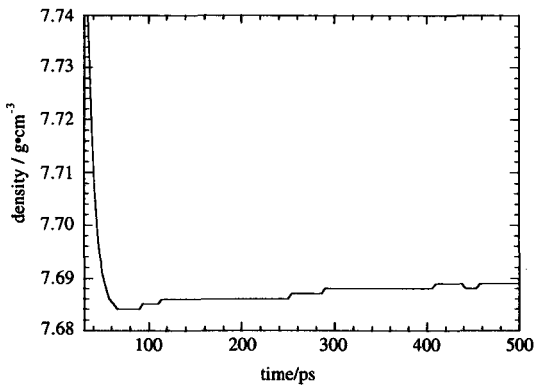

Fig. 2 Time variation of the density of the simulated polycrystalline sample.

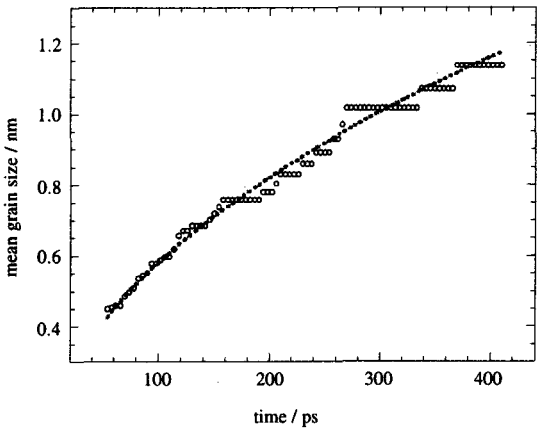

Fig. 3 Time variation of the averaged area of the cross-sections of the grains.

decreased rapidly due to the insufficient relaxation of the initial structure. After about 60 ps, the density gradually increased by the grain growth phenomenon. The higher density by about 0.1 % was observed at 500 ps which was resulted by the decrease of the total area of grain boundaries.

In the first stage of the grain growth, several grains grew by absorbing the neighboring grains, and some of other grains disappeared. The number of grains reduced to 20 at about 150 ps, and to less than 10 at 500 ps. As the result, the mean size of grains increased as shown in Fig. 3. It is known that the experimental grain growth rate frequently follows the parabolic law, $r^2 \propto t$, where r and t are the mean radius of the grains and time, respectively. In fig. 3 we show the fitting curve of the observed value by the parabolic law. The fitting was satisfactory.

During the grain growth phenomenon, the grain boundary network changes its topological form. The elemental processes of such topological change are the grain switching (T1) and the disappearance of a grain (T2) in the case of the 2D grain growth.[2] The T1 process was not frequently observed in the present simulation. The T2 process, on the other hand, was observed whenever any grain disappeared. It should be noted that the driving force of the topological change is the curvature of the grain boundaries. Generally

speaking, large grains have concave boundary shapes and small grains have convex ones. The grain boundary migrates toward concave direction, hence the grain growth occurs. In the present simulation, any consideration was not paid on the grain boundary curvature explicitly, but the mechanism of the grain boundary migration was correctly reproduced.

In the present study, initial orientation of each grain was selected randomly, and most of the simulated grain boundaries are the random (high-energy) boundaries. However, we observe a few low-energy boundaries as shown in fig. 4. By analyzing the misorientation angles of such boundaries, we found some of them are the Σ3 coincident boundaries. A coincidence boundary was created during the grain growth when meet the grains satisfying the special angular relation. In the case of the atomistic simulation, we can analyze all misorientation angles anytime. This is a significant merit because the grain boundary characteristics are quite important for considering the materials properties.

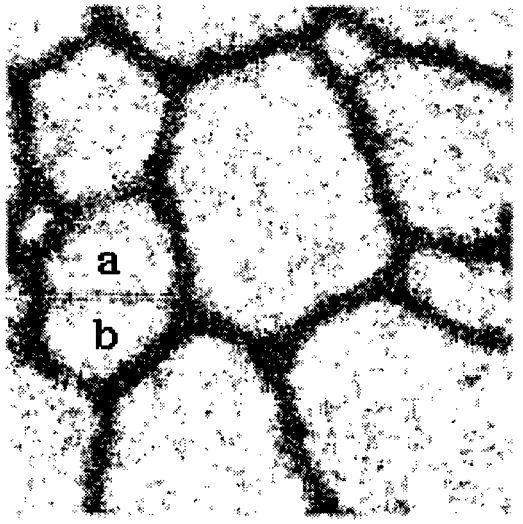

Fig. 4 An example of the low energy boundary (between a and b) observed in the simulation. Only the atoms having higher potential energy were plotted in order to emphasize the grain boundaries.

4. SUMMARY

The present study was successful for reproducing the grain growth phenomenon in the atomic scales. The MD simulation correctly account for the driving forces of grain growth: the grain boundary energy and the boundary curvature. The simulated results are close to the well know parabolic low. In conclusion, the present authors stress that the MD simulation is useful for investigating the dynamics of the polycrystalline structures including the grain growth.

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