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ATOMISTIC SIMULATION OF THE CHANGE IN MICROSTRUCTURE OF A POLYCRYSTALLINE FCC METAL UNDER COMPRESSION

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Abstract. In this study, the change in microstructure during large deformation is simulated using molecular dynamics method. A polycrystalline fcc model consisting of four grains with periodic boundary condition is prepared, and a compressive external force is imposed on the model. The plastic deformation behavior, such as change in grain shape, motion of grain boundary, generation of dislocation and slip, are investigated. Initial orientation of every grain and the combination of the adjacent grains are varied, and the dependency of the crystallographic conditions on the change in microstructure along with the stress-strain relation are investigated. As a result, grain refinement due to generation of grain boundaries revealed to strongly depend on the relation between the original crystal orientation and imposed load direction.

1 INTRODUCTION

Mechanical properties of a material depend strongly on the microstructure, and hence various methods have been developed to improve the microstructure. One of the most simple indicators representing the state of microstructure is grain size, and the strength of the material is generally stronger as the grain size is smaller. This relation is well known as Hall-Petch relation, and to refine the grain size is generally effective to make the material stronger. Therefore, sustained effort have been devoted to refine the crystal grains; some of the successful schemes are equal-channel angular pressing (ECAP)[1], accumulative roll bonding (ARB)[2], and asymmetric rolling[3] methods, and these processes have been applied to industrial purposes. The common condition in these processes is that the material is subjected to severe plastic deformation, and especially compressive load is the key factor. However, the mechanism of the grain refinement is not straightforward, and many kinds of researches have been ongoing. Experimental observation of

the microstructure using electron backscatter diffraction (EBSD) method is quite effective to investigate the change in microstructure, but the dynamic mechanism is not directly observed. Several kinds of electron microscopy have made it possible to observe the atomistic real image, but the dynamic motion is not yet observable. Therefore, computer simulation is indispensable for clarification of the mechanism, and the molecular dynamics (MD) method is the most suitable for the purpose. A great number of researches have been reported on the deformation mechanism of polycrystalline materials based on MD simulations, and various kind of fundamental plastic behaviors such as generation and motion of dislocation, grain-boundary migration, change in crystal orientation, and their relation and interactions [4-8]. The author has demonstrated MD simulations on plastic deformation and related phenomena such as grain-boundary stability and change in shape of a polycrystalline material [9], shape-memory behavior [10], and transformation-induced plasticity [11]. We are now motivated to investigate the mechanism of grain refinement due to large deformation. In our previous report [12], change in microstructure under tensile load was simulated, and grain-boundary migration and change in grain shape were observed. In this study, supposing the grain refinement, a large compression is imposed to the same model, and the change in grain shape and size is investigated.

2 MODEL AND CONDITIONS

2.1 Fundamental equations

In this study, a classical molecular dynamics method is used. The fundamental equation is the following Newton's equation of motion, and the force $\boldsymbol{F}_i$ acting on the i-th atoms is assumed to be represented by a Lennard-Jones-type interatomic potential function ϕ.

$$\frac{\mathrm{d}^2\boldsymbol{r}_i}{\mathrm{d}t^2} = \boldsymbol{F}_i, \quad \boldsymbol{F}_i = -\sum_{j\neq i}^{N} \frac{\mathrm{d}\phi}{\mathrm{d}r}\frac{\boldsymbol{r}_{ij}}{|\boldsymbol{r}_{ij}|}, \tag{1}$$

with

$$\phi = 4\varepsilon\left((\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}\right) \tag{2}$$

Here, $\boldsymbol{r}_i$ is the position vector of the i-th atoms from the origin, and $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$. The variables in LJ potential ε and σ are the material parameters in the dimension of energy and length, respectively. For a generalized analysis, the equations are non-dimensionalized. Then the potential parameters are diminished, and other physical quantities including stress and temperature are all shown in the non-dimensional values in this paper.

2.2 Simulation model

A simplified polycrystalline model is used to capture the fundamental feature of the grain refinement. Figure 1 represents the schematic illustration of the model; two types are prepared, each of which consists of four grains while the grain arrangement differs from each other: a transversal grain boundary is perpendicular to the loading direction in Type A, while they are parallel in Type B. Periodic boundary conditions are applied in all

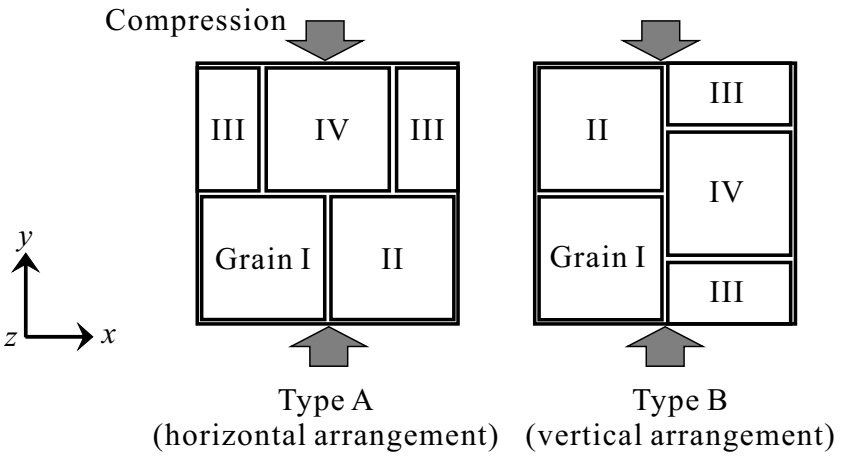

Figure 1: Illustration of the simulation model.

directions. The thickness of the model in the z direction is taken very small; every grain corresponds to infinitely long columnar one. A compressive load is imposed by decreasing the length L_y in the y direction. The lengths L_x and L_z in the x and z directions are adjusted so that the average stress component σ_{xx} and σ_{zz} are kept at zero, while the model retains rectangular parallelepiped.

The atoms are set on the lattice points of fcc crystal so that the (001) plane is on x-y plane and [100] direction is along the x axis, and the number of unit cells are 50×50×5 in the x, y and z directions. Then the atoms are rotated around the z axis by angle θ_k, in which k identify the grain number from I to IV in Fig. 1. The values in the angles are varied, and the results for the combination represented in Table 1 are shown in this paper.

Table 1: Grain angles and their combination for the simulation models presented in this paper.

Model ID \ Grain No.	I	II	III	IV
A1, B1	26.6°	-26.6°	18.4°	-18.4°
A2, B2	26.6°	-18.4°	18.4°	-26.6°
A3, B3	26.6°	18.4°	-26.6°	-18.4°

$26.6^\circ = \tan^{-1}1/2$, $18.4^\circ = \tan^{-1}1/3$

Grain boundaries constructed in Models A1-A3 and B1-B3 are mostly coincident site lattice (CSL) boundaries. For example, in Model A1 and B1, the grain boundaries between Grain I and II, and between III and IV are typical CSL boundaries indicated by low-index sigma values.

2.3 Conditions

The initial configuration of atoms are relaxed for 15000 time steps under constant temperature at T=0.1 and no stress condition. Then compressive load is applied in the y direction by decreasing the edge length L_y in the y diction at a constant decrement $\Delta L_y/t_s$. Here, ΔL_y is the total shrinkage in length and t_s is time steps of the compression period, the these values in this study are taken as ΔL_y=25.0 and t_s=50000. Actually, the initial length L_y^0 at the relaxation period is slightly different for every models, but nearly L_y^0=73.0. Accordingly, the total compressive strain is about 0.34. After the loading period of 50000 time steps, the model is unloaded; the average stress in the y direction is also released, and 5000-step relaxation period is assigned.

3 RESULTS AND DISCUSSION

3.1 Change in microstructure

Simulation results for Model A1 is shown in this section. Figure 2 represents the snapshots of the atomic configuration projected on the x-y plane. The color indicates potential energy of each atom; the atoms in bulk grain have low energy, depicted in blue, whereas the atoms at grain boundaries have higher energy, and depicted in green or yellow.

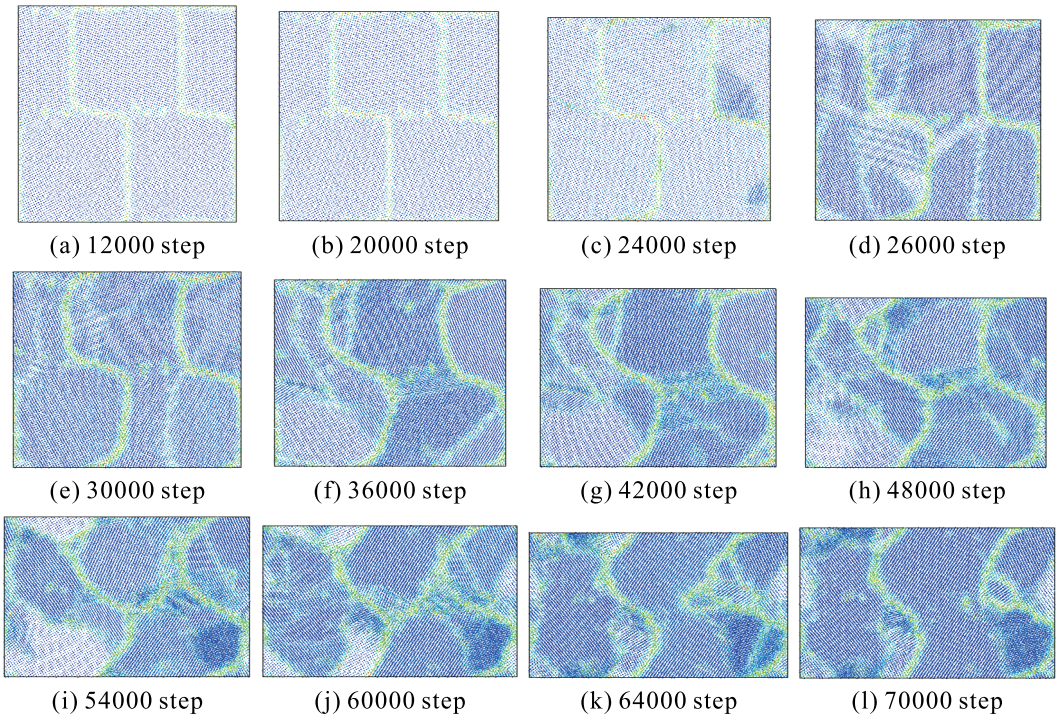

Figure 2: Configuration of atoms for Model A1, in which the color indicates the potential energy of every atom; green and yellow show grain-boundary region.

Figure 2(a) shows a stabilized state by the relaxation period, which represents all grains mostly retain square shape.

Then the compressive load is imposed from the 15000th time step. No specific change is observed at the 20000th time step, but an apparent change is observed at the 24000th time step at the left bottom corner in Grain III; The color is the same in blue but looks denser. This is due to the projection angel on the x-y plane; i.e. initially the z direction is exactly [001] in all grain and all atoms align straight, but the alignment changed when rotation or change in orientation change occurs. Therefore, Figure 2(c) indicates that orientation change is initiated in Grain III. A small change is also observed in right bottom corner in Grain II. These orientation change spread inward grain quickly by the 26000th time step as shown in Fig. 2(d). Simultaneously various changes are observed in other grains; New grain boundaries depicted in green color, are generated. In all of the four grains, a vertical boundary at the middle is observed, while some of which are temporally appeared, and are not observed at the 30000th time step, as shown in Fig. 2(e).

The initial grain shape and grain boundaries are mostly maintained at the 30000th time step, but extreme deformation occurs thereafter: the original square shapes are almost completely unobservable at the 36000th time step shown in Fig. 2(f), and small grains surrounded by the new boundaries is generated.

The main grain boundaries which originate from the initial ones retain even though the grain shapes changed, and depicted in clear and relatively wide lines at the 48000th time step. However, as further compression is imposed, some of them become apparent, and the Grain II and IV is finally unified at the central domain in the model at the 64000th time step. The reason is, however, not only the large strain but may be the influence of the periodic boundary condition. The model height becomes smaller and periodic boundary makes one grain sandwich another, and strong restriction may affect too much. Final unloading makes overall slight recovery in model height in the y direction, but apparent change in microstructure is not observed.

3.2 Stress-strain curve

The variation of the overall stress is shown in Fig. 3 (a), in which the length in the y direction is also drawn. As the compression starts at the 15000th time step, compressive stress increases monotonously by the 24000th time step. Along with the result shown in Fig. 2 that no specific change in the configuration of atoms is observed, the deformation is elastic region, and the gradient corresponds to the elastic coefficient.

The stress drops drastically between the 24000th and 26000th time steps. This is the initiation of the plasticity, as crystallographic irregularity is observed in Figs. 2(c) and (d). Then the stress starts increasing again, and a similar behavior as the initial elastic region is exhibited by the second peak in stress at the 3000th time step. After the following stress drop, the stress increase and drastic drop are not clearly appeared, whereas gradual increase by the 45000th time step, and mostly flatten at the about σ_y=2.0. The compression is stopped at the 65000th time step, and stress is released. In the stress-strain curve shown in Fig. 3(b), elastic recovery by the unload process is clearly represented.

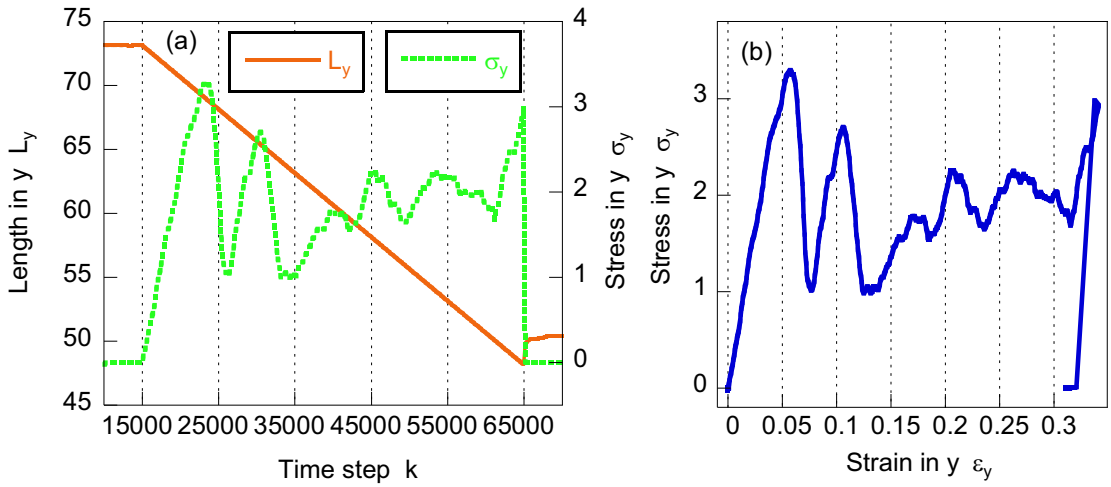

Figure 3: Simulation result for Model A1. Variation of the length in the y direction and stress in y (a), and stress-strain curve (b) .

3.3 All results

The results for the other models are summarized in Figs. 4 and 5. Figure 4 shows the snapshots at the 48000th time step, and Fig. 5 shows stress-strain curves. Grain refinement is observed for every case, and the original square grain shape has disappeared. Only the retained feature of the initial grain feature is a straight grain boundary which transects the model in Models A3 and B3. These boundaries are both constructed by two CSL boundaries between $\pm 26.5^\circ$ and $\pm 18.4^\circ$ which are very stable and seems unaffected by the large straining.

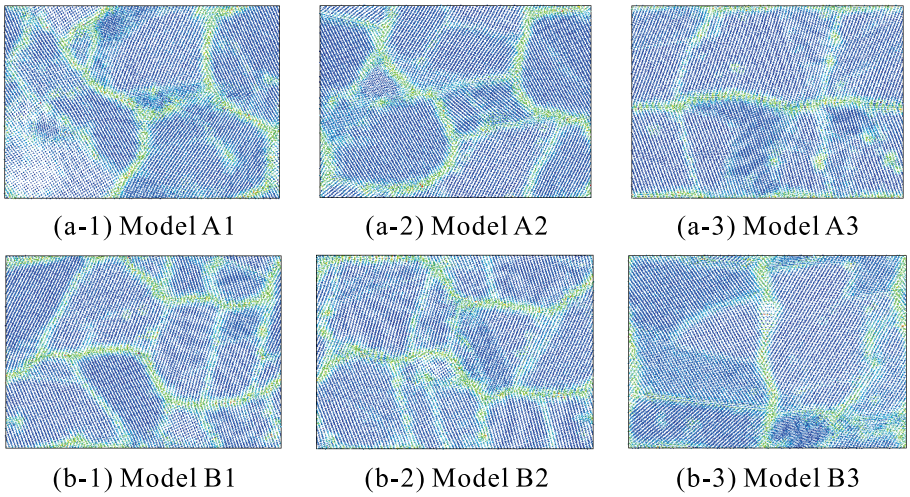

Figure 4: Configuration of atoms at the 48000th time step for all models, in which the color indicates the potential energy of every atom.

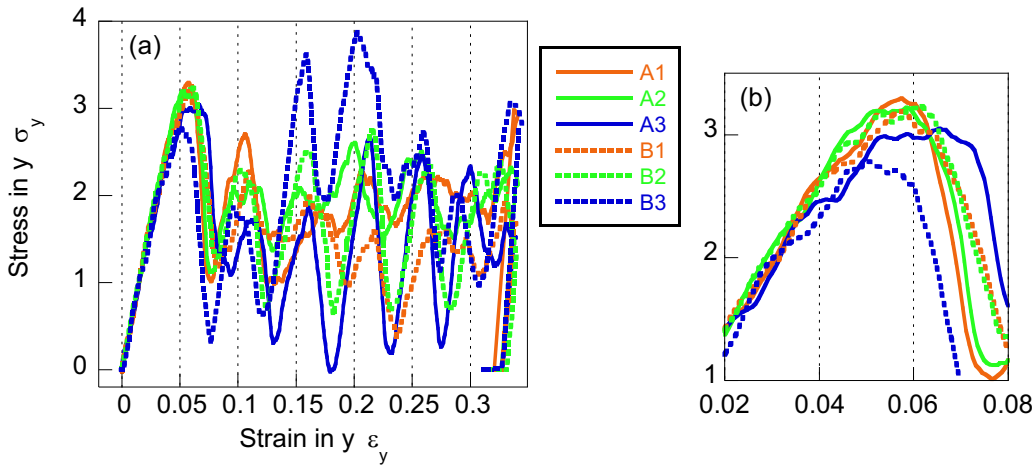

Figure 5: Stress-strain curves for all models (a) and the magnified plots around the first peaks around between ε=0.02 to 0.08 (b).

Stress-strain relation is overall common to all cases; the stress increases monotonically at first, drastically drops following the first peak, and thereafter, gradual increase and drastic drop are intermittently repeated. However, the peak values and the event interval are not identical. For example, the first peak, which is assumed to be the yielding stress, differs as shown in the magnified diagram in Fig. 5(b). Models A1, A2, B1 and B2 have almost identical peak value of σ_y=3.1, while Models A3 and B3 show lower value. The former 4 models commonly exhibit continuously smooth round peak from mostly linear elastic region to the stress drop. In Models A3 and B3, on the contrary, the curve deviate from the elastic curve once at $sigma_y$=2.1 for B3 and 2.4 for A3, and increase again till the peak values of $sigma_y$=2.8 for B3 and 3.0 for A3. In the configuration of atoms, specific features are observed for these two models, as discussed above, and such features may affect the overall stress-strain relation. Detailed investigation on the bases of atomic arrangement, crystal orientation, and grain-boundary structures will be discussed in our future work.

4 CONCLUSIONS

In this study, molecular dynamics simulations were carried out on the atomistic behavior of a polycrystalline fcc material under large compressive deformation. A simplified model with four grains is prepared, and six models which are different in grain arrangement and crystal orientation. All the model consist of typical CSL grain boundaries, while some are different. As a result, change in microstructure is observed for all models when a large compressive strain is imposed. Some of the grains are divided into two or more subgrains, and grain refinement was observed for all cases. The dependence of the grain boundary structure was inferred by a specific behavior found for two models which commonly have straight CSL boundary traversing the model. Further investigation including much more variation of grain arrangement, structure of grain boundaries, and

combination of crystal orientations is necessary to clarify the mechanism of the grain refinement. This study, nevertheless, revealed the effectiveness of the model for the purpose, and hence we will continue the research using the present model.

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