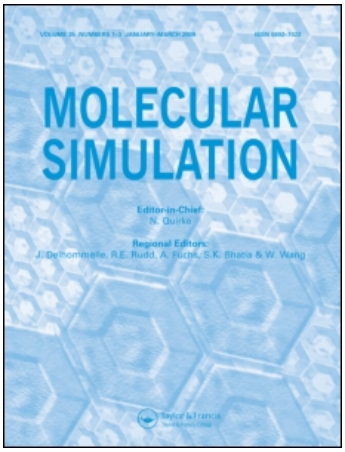

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Atomistic Simulation of a Neighbor-Switching Event in the Deformation of a Model Polycrystal

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ATOMISTIC SIMULATION OF A NEIGHBOR-SWITCHING EVENT IN THE DEFORMATION OF A MODEL POLYCRYSTAL

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This paper describes the simulated atomistic process in a large deformation of polycrystalline matter. Molecular dynamics method was applied to a model polycrystal of yttria-stabilized zirconia composed of eight small grains to investigate the microscopic mechanism of superplastic deformation. During the tensile deformation up to the strain of 0.55, a neighbor-switching event of grains similar to that proposed by Ashby and Verrall was observed in the present simulation. The large strain was accomplished by non-uniform diffusional flows in the polycrystal. By analyzing the diffusive motions of oxide ions, the mass transport during the deformation was found to take place mainly in the boundary layer of about 1 nm thickness, which covers about 0.4 times of the total volume. This result is different from the quasi-uniform flow expected in the classical creep models, but is consistent with the Ashby and Verall's model.

Keywords: Neighbor-switching; polycrystal; deformation; molecular dynamics

1. INTRODUCTION

Polycrystalline materials composed of very fine grains are known to be largely deformed at elevated temperatures. The typical example is the superplasticity of metals or ceramics which show large elongation up to several thousand percent [1]. Such large ductility of bulk materials is difficult to be understood by classical creep models [2], hence many experimental studies have been carried out to investigate the deformation mechanisms.

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Ashby and Verrall [3] proposed a model for superplasticity that large deformation can be attained by the grain boundary sliding accompanied by a switching of grain configuration. A schematic view of a typical neighbor-switching event is shown in Figure 1. Let us consider a group of four grains initially contacting to each other except the B – B′ pair. When a horizontal tensile is loaded to the group (left), the distance of A – A′ pair will increase and that of B – B′ pair will decrease due to the grain boundary sliding. In the intermediate state of the deformation, the boundary between A and A′ will disappear (middle), and then B – B′ becomes a new neighboring pair (right). Because the grains change their shapes during the deformation as we see in the figure, this event is considered to be controlled by mass transports near the grain boundary. This model is accepted as a fundamental mechanism of superplasticity.

In the previous papers [4 – 6], the present author proposed a new method for investigating polycrystalline matters by molecular dynamics, and showed the simulated microscopic processes in the deformation of ceramic polycrystals. These studies, however, were limited to small strains which were not enough to reproduce the neighbor-switching event. In the present paper, the author extended the previous studies by increasing the number of grains and the maximal strain to simulate the rearrangement of grain configuration during large deformation.

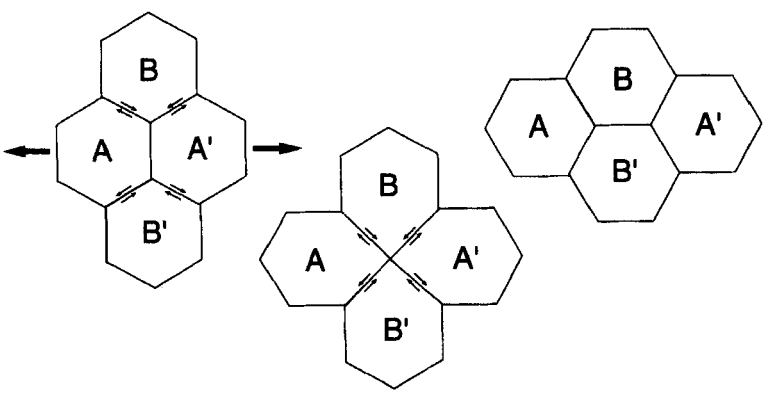

FIGURE 1 Schematic diagram of the neighbor-switching event during the superplastic deformation proposed by Ashby and Verrall [3]. A group of four grains changes the neighboring pair from the initial state (left) *via* the intermediate (middle) to the final states (right). The small arrows denote the directions of grain boundary slidings.

2. MODEL STRUCTURE AND MD SIMULATION

The least number of grains to reproduce the neighbor-switching event is four. However, it is preferable to add several redundant grains for simulating a realistic deformation process. The number of grains used in this study is eight. The model polycrystalline structure is composed of the grains of a nanometer size arranged on the xy plane with three-dimensional periodic boundary conditions, as shown in Figure 2. All grains have the same geometry of hexagonal shape on xy plane and infinite size toward z direction. The crystal orientations of the grains were selected to be different to each other.

The target material of the present simulation is yttria-stabilized zirconia, which is the first ceramic material observed the superplasticity [7]. The selected composition is $0.067\,Y_2O_3 - 0.933\,ZrO_2$. The polycrystalline structure was generated by the weighted Voronoi construction as described in the previous paper [4]. The atomic configuration in each grain was constructed by substituting the appropriate numbers of yttrium ions and oxygen vacancies for zirconium and oxide ions in the ZrO_2 structure, respectively.

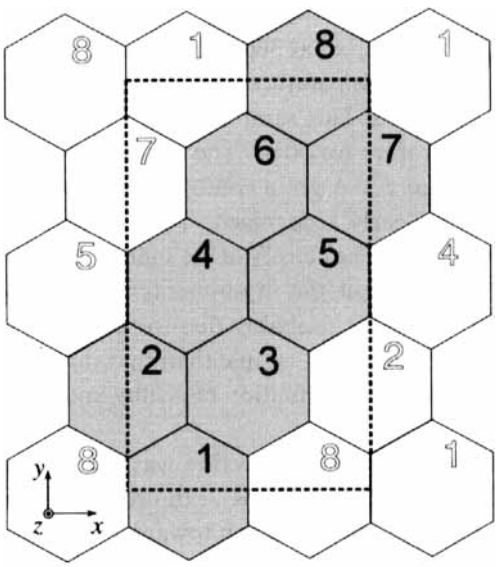

FIGURE 2 The model polycrystalline structure used in this study. The hexagonal regions denote the individual grains, and the hatched and white regions are the original and replica grains, respectively. Grains are numbered for convenience. The dotted rectangle is the MD basic cell.

Finally, 10716 atoms were arranged in the rectangular MD basic cell of approximately $8 \times 12 \times 1.5\,\mathrm{nm}^3$.

In the MD simulation, the equation of motion was integrated by using the Verlet algorithm [8] with a time step of 2 fs. The Coulombic potentials of Born-Mayer type proposed by Dwivedi and Cormack [9] were used. This potential model was constructed based on the energies of cubic, tetragonal, and monoclinic structures of zirconia, and was successful for reproducing fundamental properties of zirconia polycrystals [4–6]. The potential functions concerning the yttrium ion were referred to those by Butler *et al.* [10], but the radius parameter was modified to satisfy the experimental density values of Y_2O_3 single crystals [11, 12]. The shell terms in the original potential functions were neglected in the present simulation due to the limited computer resources. The force calculation was optimized by the neighbors-list and the Ewald-sum methods [8]. Deformation of the model structure was controlled by the scaling of the cell dimensions. During the simulation, temperature of the system was controlled by Nosé's thermostat [8].

3. RESULTS AND DISCUSSION

The MD calculation was started at 300 K and heated up to 2500 K, which is just below the melting temperature (2960 K), in order to obtain the thermally relaxed structure. This sample was then cooled down to 2000 K and held at this temperature for 50 ps. The resulted atomic configuration is shown at the top of Figure 3. A grain configuration similar to that of Ashby and Verrall model is clearly recognized. The simulated crystal structure inside each grain was cubic. The density of the simulated sample is $5.33\,\mathrm{Mg/m}^3$ which is slightly smaller than the experimental one, $5.7\,\mathrm{Mg/m}^3$ [12]. The difference in density values is probably due to the larger fraction of grain boundary region in the simulated sample than that in the experimental one. The grain size according to the definition of Ashby and Verrall [3] is 4.57 nm in this model.

The tensile simulation toward x direction was carried out for this model structure with the strain rate of $0.025\,\mathrm{ps}^{-1}$. In order to avoid an unexpected fracture of the sample, the cell dimension toward y direction, L_y, was scaled so as to maintain the initial density value, and L_z was kept constant. In the first stage of the deformation, an elastic behavior was observed at a strain ε lower than 0.03, and turned to a plastic behavior at $\varepsilon \sim 0.04$. The internal stress reached the maximum, 4.7 GPa at $\varepsilon \sim 0.07$, and then decreased rapidly

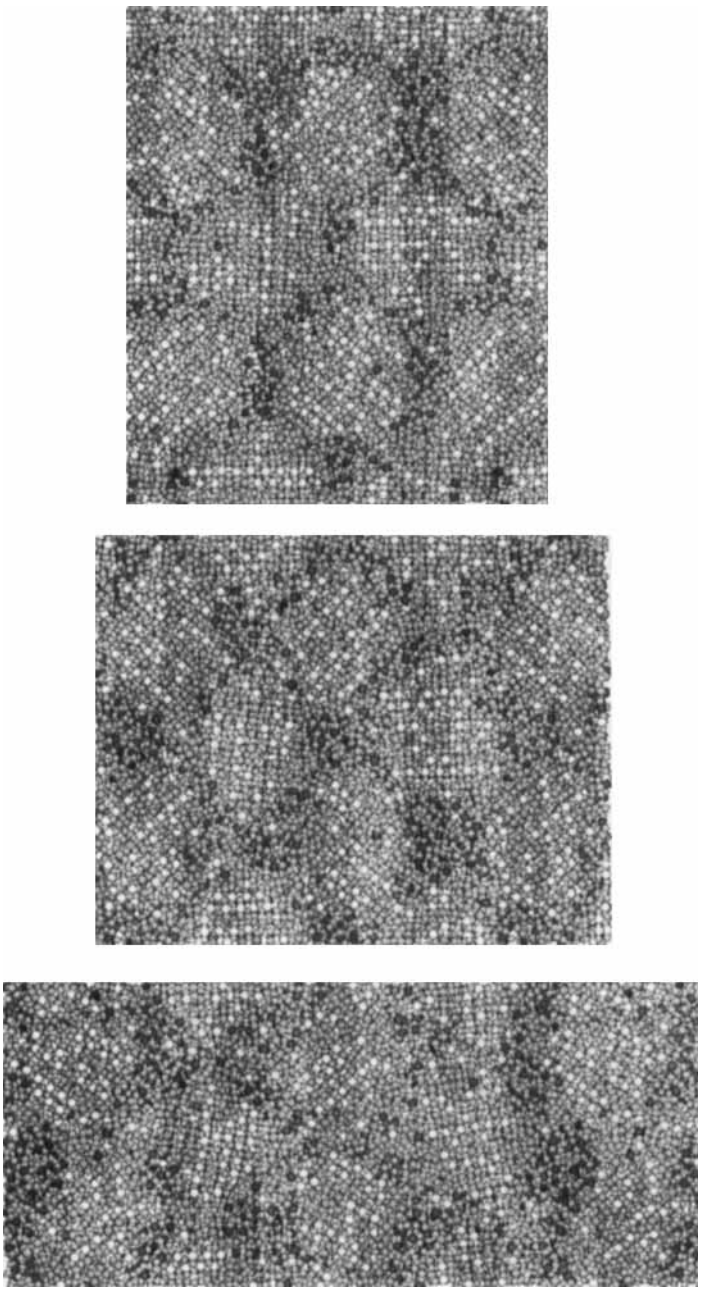

FIGURE 3 Snapshots of the simulated sample at the strains of 0, 0.25 and 0.55 (from top to bottom) with horizontal elongation at 2000 K. Cations which have lower coordination numbers than 8 were painted dark in order to emphasize the position of the grain boundary.

to about 1 GPa at $\varepsilon > 0.12$. The simulated stress–strain relation is a typical one for the plastic deformation of polycrystalline materials.

The time variation of the grain configuration during the deformation is shown in Figure 3 as a series of snapshots at the strains of 0, 0.25 and 0.55. They display the same region of the simulated samples, which covers slightly wider area than the MD basic cell in order to visualize the long-range structures. The positions of grain boundaries are estimated by the coordination number around cations, and are emphasized as dark regions. The neighbor-switching event similar to Figure 1 was successfully reproduced, and the eight original grains can be clearly recognized even at the maximal strain. The shapes of the grains are slightly modified but not elongated extensively. This result is different from those in the classical creep models, but consistent with the Ashby and Verrall model. Small amount of grain rotation is recognized, for example the grain numbered 4 in Figure 2 rotated clockwise by about 5 degrees. The grain boundary layer in the initial structure had a thickness of about 1 nm, and became slightly thicker toward x direction in the course of deformation. Such grain rotation and variation of interface structure were not included in the Ashby and Verrall model, but are considered to take places in an actual deformation process to some extent.

The neighbor-switching model postulates diffusive flow of mass in order to modify the grain shapes properly. In a polycrystalline matter, the diffusive flow is considered to be divided into two independent paths: bulk diffusion inside the grain and diffusion at the grain boundary. In the case of superplastic deformation, the boundary diffusion was considered to be more important. The diffusive motions of oxide ions during the simulation are shown in Figure 4. In order to clarify where the ions in the boundary layer move to, only those closer to the boundary plane than 0.5 nm were displayed. Oxide ions in the boundary layer in the initial state (left) still remained close to the boundary in the final state (right), although the topology of the boundary was modified by the neighbor-switching event. It means that the mass transport occurs mainly in the boundary layer. This result is consistent with the Ashby and Verrall's picture that the grain boundary sliding is accommodated by the diffusional flow at the grain boundary, and is different from the quasi-uniform flow expected in the classical creep models.

In the Ashby and Verrall model, volume fraction of matter moved during the neighbor-switching event was estimated to be about 0.12 times of the grain volume [3]. In the present simulation, the boundary layer of 1 nm thickness covers about 0.4 times of the total volume. This result is

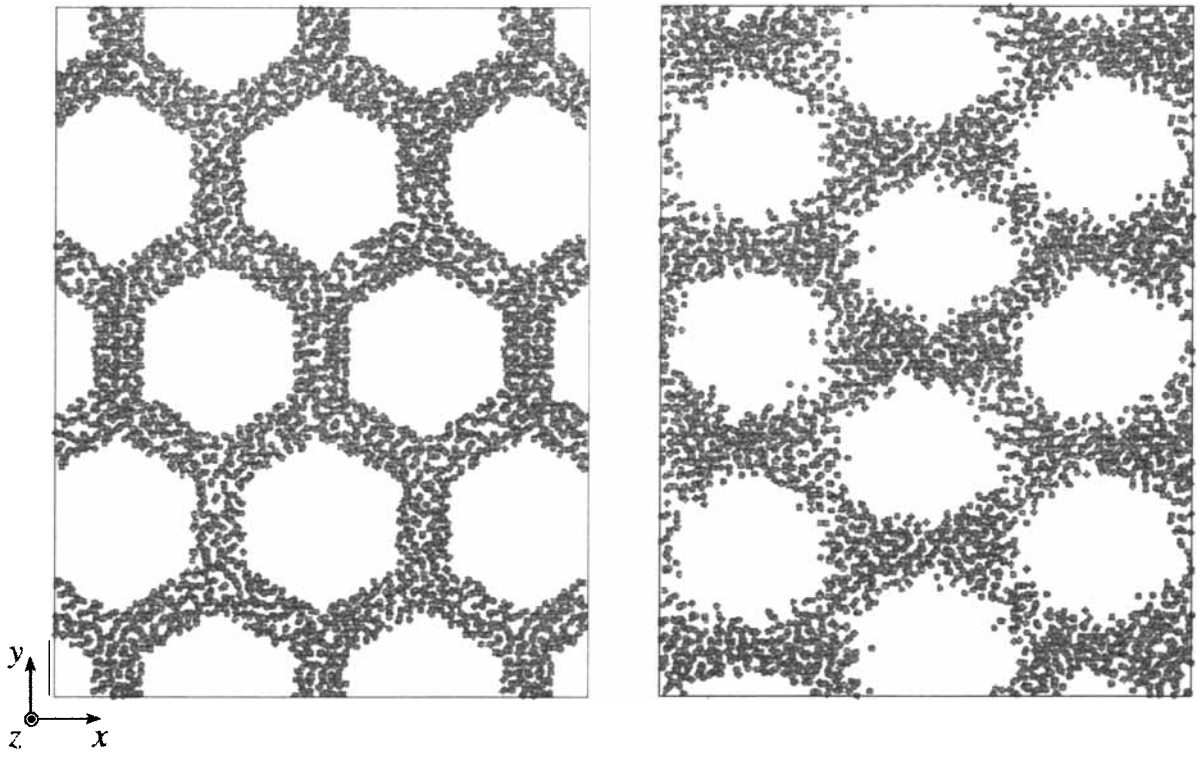

FIGURE 4 Time variation of the positions of oxide ions before (left) and after (right) the deformation. Only the ions within the boundary layer of 1 nm thickness in the initial state are displayed.

reasonable, because the former value was estimated by the simple comparison of the initial and the final grain shapes and neglects the variations in the transient states. Although a more precise analysis must be made based on the individual diffusion paths of ions, it is sure that a non-uniform diffusional flow takes place exceeding the framework of classical creep models.

4. CONCLUSION

The present MD simulation was successful for visualizing what happens during large deformation of a polycrystalline matter. The model polycrystal showed a similar neighbor-switching event to that originally proposed by Ashby and Verrall for the superplastic deformation. Although the adopted grain configuration is much simpler than the actual polycrystalline materials, simulated properties are informative for verifying the theoretical models. In conclusion, the present author stresses that the MD simulation appears to be useful for investigating the deformation phenomena of polycrystalline materials at high temperatures.

Acknowledgment

The MD simulation was carried out by CRAY-C90 of RIPS center, AIST, Tsukuba, and the supercomputer system of JRCAT, Tsukuba.

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