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A Molecular Dynamics Study of Plastic Deformation of Ceramics Polycrystals at High Temperature

Hiroshi Ogawa*,**, Naoya Sawaguchi* and Fumihiro Wakai***

* National Industrial Research Institute of Nagoya, AIST, 1-1, Hirate-cho, Kita-ku, Nagoya 462-8510, Japan
FAX: 81-52-916-2802, e-mail: ogawa@nirin.go.jp, nasawa@nirin.go.jp

** Atom Technology Group, National Institute for Advanced Interdisciplinary Research, AIST, 1-1-4, Higashi, Tsukuba 305-8562, Japan.
FAX: 81-298-54-2788, e-mail: h-ogawa@jrcat.or.jp

*** Material Structure Laboratory, Tokyo Institute of Technology, 4259, Nagatsuda-cho, Midori-ku, Yokohama, 226-8503 Japan
FAX: 81-45-924-5390, e-mail: wakai@rlem.titech.ac.jp

Molecular dynamics method is applied to a model polycrystals of yttria-stabilized zirconia composed of eight grains to investigate the microscopic mechanism of plastic deformation. During the tensile deformation, a neighbor-switching event of grains similar to the Ashby and Verrall's model is observed. The large strain is accomplished by non-uniform diffusional flows in the polycrystal. By analyzing the time variation of the positions of oxide ions, the mass transport during the plastic deformation is found to take place mainly in the boundary layer of about 1 nm thickness.

Key words: superplasticity, deformation, zirconia, molecular dynamics

1. INTRODUCTION

Superplasticities of metals and ceramics are quite interesting phenomena [1]. The large ductility up to several hundred percent of bulk materials is difficult to be understood by classical creep models [2, 3], and many experimental or theoretical studies have been carried out to investigate the deformation mechanisms. Ashby and Verrall [4] proposed a model for superplasticity that large deformation can be attained by grain boundary slidings accompanied by a switching of grain configuration. They considered a model configuration composed of four grains contacting to each other. When a tensile stress is loaded to the group, the configuration is modified so as to change the neighboring pairs by the grain boundary slidings. Grains should change their shapes during the deformation in order to fill up the space without any cracks, hence the neighbor-switching event is considered to be controlled by mass transports at the interface layer.

In the previous papers [5–8], the present authors investigated polycrystalline matters by molecular dynamics (MD), and showed the microscopic processes in the deformation of ceramic polycrystals. Most of these studies, however, were limited to small number of grains not enough to reproduce the neighbor-switching event. The least number of grains to reproduce a neighbor-switching event similar to the Ashby and Verrall's model is four. However, several additional grains are needed when the periodic boundary conditions were adopted because grains in a polycrystal are surrounded by approximately twelve to fourteen neighbors. In the present paper, the author extended the number of grains in order to simulate the rearrangement of grain configuration during the plastic deformation.

2. MOLECULAR DYNAMICS

The model polycrystalline structure is composed of eight grains of a nanometer size. They were two-dimensionally arranged with the three-dimensional periodic boundary conditions. All grains have the hexagonal shape on xy plane and infinite size toward z direction. Such a polycrystalline structure can be generated by the Laguerre–Voronoi construction as described in the previous paper [5].

The target material is yttria-stabilized zirconia which is the first ceramic material observed the superplasticity [9]. The selected composition is 0.067 Y_2O_3 – 0.933 ZrO_2. The atomic configuration in each grain was constructed by substituting the appropriate

numbers of yttrium ions for zirconium ions in the ZrO_2 structure. The crystal orientations of the grains were selected to be different to each other. Finally, more than 10000 atoms were arranged in the rectangular MD basic cell of approximately $8 \times 12 \times 1.5\ nm^3$.

The interatomic potentials of Born-Mayer type proposed by Catlow and co-workers [10, 11] were adopted in the present simulation. The shell term in the original potential function was neglected. The potential functions concerning the yttrium ion were partially modified so as to reproduce the experimental density values [12]. 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.

3. RESULTS AND DISCUSSION

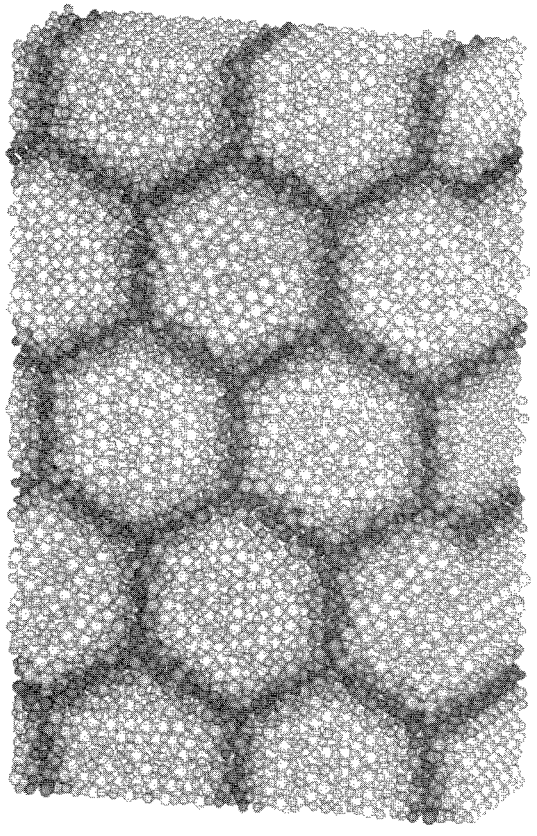

Fig. 1 An example of the simulated polycrystalline sample at 2000 K. The ions are denoted by small spheres, and those having lower coordination numbers are shaded in order to emphasize the grain boundary layers.

3.1. Grain-Switching Event and Variation of the Grain Boundary Structure

The computational sample was firstly heated up to 2500 K in order to obtain the thermally relaxed structure. The sample was then cooled down to 2000 K and held at the same temperature for 50 ps. The resulted atomic configuration is shown in Fig. 1. In the central region of the sample, a group of four grains similar to that of Ashby and Verrall's model is recognized. The simulated crystal structure inside each grain was cubic.

The tensile simulation toward x direction was carried out for this model structure at the strain rate of 0.025 ps^{-1}. In the first stage of the deformation, an elastic behavior was observed at a strain ε lower than 0.03 and then turned to a plastic behavior. The internal stress reached the maximum, 4.7 GPa, at $\varepsilon \sim 0.07$ and decreased rapidly to about 1 GPa at larger strains. The time variation of the grain configuration before and after the deformation is shown in Fig. 2. In the figure, positions of grain boundaries are displayed as bright regions by using the potential energy distribution. The neighbor-switching event similar to the Ashby and Verrall's model was successfully reproduced. The shapes of the grains are not elongated significantly after the deformation, which is different from those expected by the classical creep models. The grain boundary layer seems to become slightly thicker during the deformation. Such variation of grain boundary structure was not included in the Ashby and Verrall's model, but is considered to take place in the actual deformation process.

3.2. Diffusion of Oxide-ions at the Grain Boundary

Mass transports in a polycrystalline matter can be considered to be divided into two parts: bulk diffusion and boundary diffusion. In the case of superplasticity, boundary diffusion is considered to be more important. The diffusive motions of oxide ions at the grain boundary during the tensile simulation are shown in Fig. 3. In the figure, only the oxide ions initially exist in the boundary layer of 1 nm thickness are displayed. In the course of the deformation, such oxide ions remained close to the boundary, even though the boundary topology was changed by the neighbor-switching event. It means that the

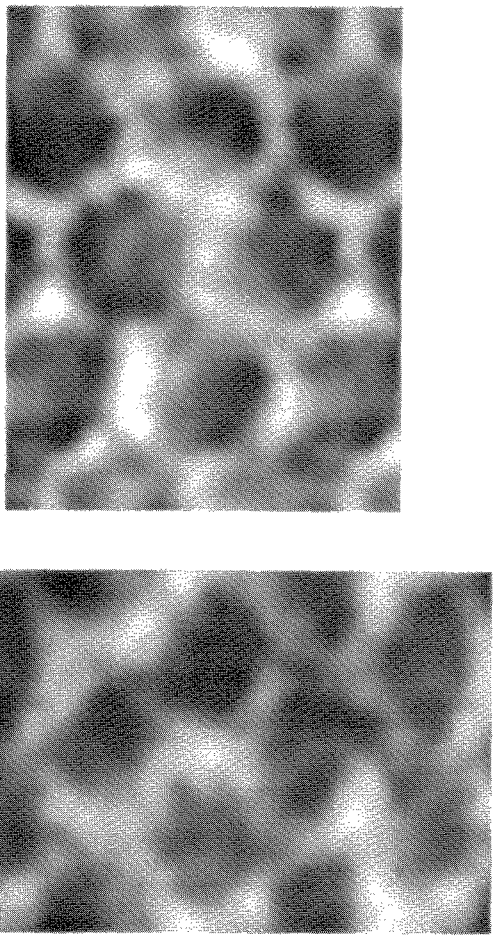

Fig. 2 Snapshots of the simulated sample during horizontal elongation at 2000 K (from top to bottom). Two-dimensional distribution of short-range potential energy is mapped by the brightness. The white area corresponds to the grain boundary region.

mass transport occurs mainly at the grain boundary, which is consistent with the Ashby and Verrall's model.

Trajectory of the grain center does not seem to follow the uniform paths. Non-uniform flows can be recognized in the figure especially at the larger strain. Most of the grains show fairly round shapes, but some of them were horizontally elongated. Such variation of the grain shape is not always consistent with the result of local structural analysis. If we define the grain shape by using the short-range atomic configuration, several grains show more round shapes due to the re-crystallization at the grain boundary. Superplastic deformation is considered to be attained by such re-crystallization at the boundary region and non-uniform flows in polycrystals.

4. SUMMARY

By using the MD simulation, a neighbor-switching event similar to the Ashby and Verrall's model was successfully reproduced. This method may be useful for investigating what happens in a superplastic ceramics during the deformation. Although the adopted grain configuration is much simpler than the actual materials, MD simulation appears to be informative especially on the microscopic dynamics at high temperatures.

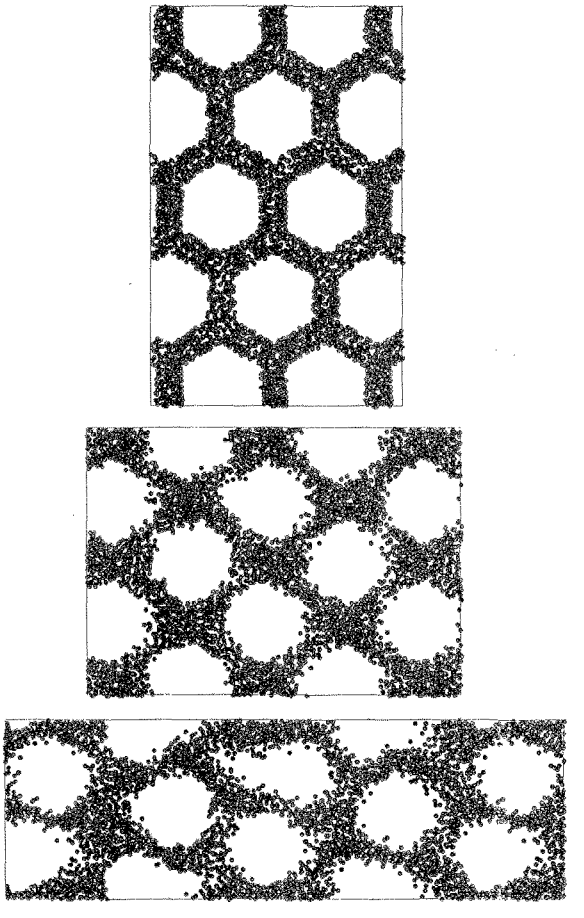

Fig. 3 Time variation of the positions of oxide during deformation (from top to bottom). Only the ions within the boundary layer of 1 nm thickness in the initial state are followed.

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