Molecular dynamics analysis of fcc nanowire under torsional loading†

OGAWA Takaki *, ** and NAKATANI Akihiro***

KEY WORDS: (Molecular dynamics) (Atomic simulation) (FCC crystal)

1. Introduction

The macroscopic mechanical properties of polycrystalline materials strongly depend on their microscopic structure. For example, grain refinement by some severe plastic deformation can improve the tensile strength of industrial pure aluminum from 80 to 350MPa[1]. The knowledge obtained by the study of the mechanism of deformation from a microscopic point of view can be useful for the fundamental principles of the material design. Even if the crystallographic structure is initially perfect, lattice defects such as the dislocation, stacking fault, etc. which occur after the plastic deformation contribute the mechanical properties for inelastic behavior. Therefore the evaluation of an ideal strength of a single crystal including evolution of defect structure is meaningful as the first step.

Nguyen and Ortiz presented two different approaches for coarse-graining interplanar potentials and determining the corresponding macroscopic cohesive laws on the basis of energy relaxation and renormalization group [2]. They show that a universal asymptotic form of macroscopic cohesive law can be derived from the analysis of cohesive behavior of a large, but finite, number of interatomic planes. In our previous study, we analysed fcc Cu and Al nanowires under torsional loading using molecular dynamics and investigated systematically the influence of the stacking-fault energy on defect structures in nanowires[3]. In this study, we conduct a detailed investigation into the localization of deformation and derive a constitutive relation of interplanar tosional deformation from the similar concept to cohesive law of interplanar tensile deformation.

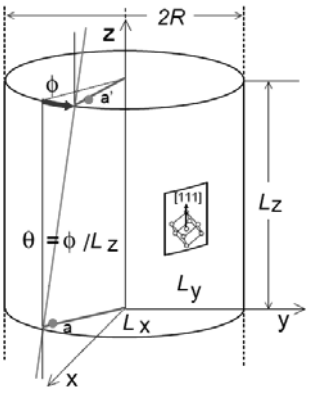


Fig. 1 Schematic of specimen.

2. Model and Simulation Method

We consider the torsional deformation of a single-crystal Cu nanowire having a circular cross section, as shown in **Fig. 1**. Here, the length and radius of specimen is 7.514 nm and 3.615 nm, respectively. The torsion axis is along the crystal orientation 〈111〉. The crystal comprises 36 atomic layers along the z-axis, for a total of 26,076 atoms. We adopt the twisted periodic boundary condition [4] along the z-axis with dimension L_z of the unit cell. θ denotes the twist angle per unit length, ϕ denotes the twist angle for the specimen, and their relation is $\theta = \phi / L_z$.

The interaction between the Cu atoms is analyzed using the embedded-atom method of Mishin et al. [5], which can be used to accurately determine the stacking-fault energy. The time step is set to 2 ps, and the simulation period is up to 350 ps. First, we set atoms with a random initial velocity and calculate the time required under no load to reach a condition of equilibrium. Subsequently, the torsional deformation is determined under repeated cycles comprising a small torsion $\Delta\theta$ = 6.25 × 10.4 rad/nm followed by relaxation for 0.5 ps. On average, there exist a proportional relation between the energy relaxation time and the twist angle per unit length. Temperature is

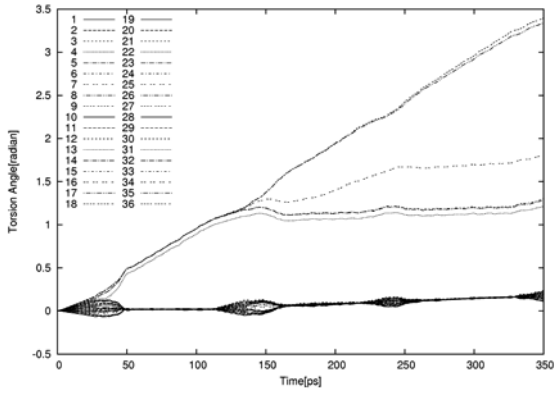
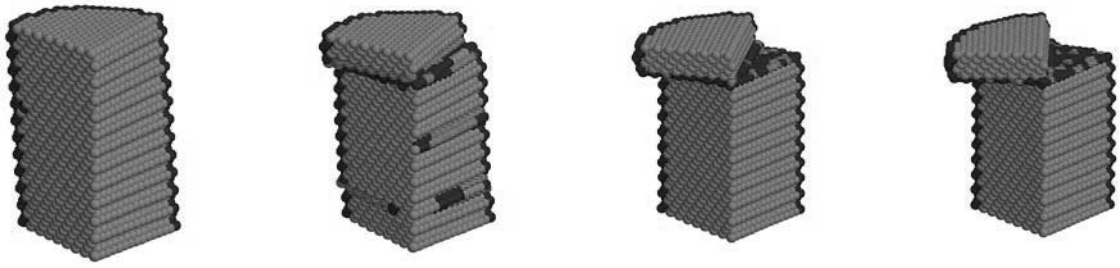


Fig. 2 Time vs torsion angle.

† Received on 30 September 2010
* JSOL Corporation, Osaka, Japan
** Graduate School, OSAKA University, Suita, Osaka, Japan
*** OSAKA University, Suita, Osaka, Japan
Proceedings of the Visual-JW2010 organized by JWRI, Osaka University.



(a) 20 ps (b) 40 ps (c) 60 ps (d) 80 ps

Fig. 3 Atomic arrangement of quarter Cu nanowire under 〈111〉 torsion

maintained at a constant 300 K by the velocity scaling method.

3. Results and Discussion

atomic layer of the specimen with respect to time. The atomic layers are sequentially numbered along the z-axis. The rotation angle is evenly distributed until approximately 30 ps. Then they are divided into two.

Next, **Fig. 3** shows the atomic configuration of a quarter of the Cu specimen at 20–80 ps. In order to analyze the defect structure, common neighbor analysis (CNA) is used to classify the structure of the Cu atoms into local face-centered-cubic (fcc), local hexagonal-close-packed (hcp) or the other. In this specimen, it is the hcp atomic structure that makes up the stacking faults. These hcp atoms are named as stacking-faults atoms and represented in red. Other atoms are named as other defects and represented in blue. Fcc atoms are represented in gray. Elastic deformation occurs at 20 ps. The external force causes equal strain along the twist axis. At 40 ps, multiple stacking faults are observed, and at 60 ps, the deformations are found to be concentrated in some of the stacking faults. These concentrations give rise to localization of defect structures. Finally, at 80 ps, the defect structures are almost fully localized. The other stacking faults recover from their deformations. As a result, we conclude that the given load induces only localized defect structures.

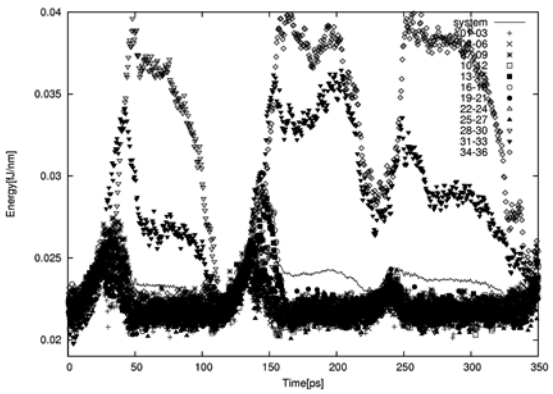


Fig. 4 Potential energy vs time.

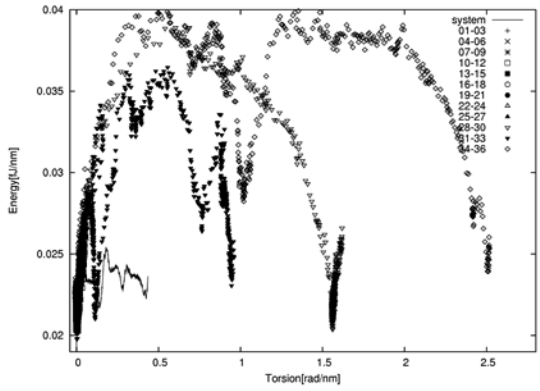


Fig. 5 Potential energy vs torsion angle.

Next, **Fig. 4** and **5** show the change in the potential energy per unit length, along the z-axis. It shows plots for the entire system and for sets of three adjacent atomic layers. Figure 4 shows the change in the potential energy with time. Up to approximately 30 ps, the potential energy increases quadratically with time. That is, the potential energy increase quadratically with the macroscopic torsion, and all atomic layers of the crystal structure exhibit elastic deformation. Then, up to approximately 120 ps, the 34–36 atomic layers show an increase in their twist angle, but the other atomic layers show none. Hence, we can confirm that macroscopically, the nanowire exhibits plastic deformation; however, from the microscopic point of view, the stacking fault elastic recovery is going. Next, Fig. 5 shows the relative twist angle for each set of three adjacent atomic layers. The twist angle of the atomic interplane is represented by δ rad/nm. The relation between the twist angle and the potential energy for atomic layers is obtained. As a result, we are able to define the microscopic interplanar potentials.

4. Conclusions

We analyze fcc Cu nanowires under torsional loading using molecular dynamics analysis. We investigate the mechanism of localization by observing the potential energy of each atomic layer and its twist angle in detail. We obtain the following findings through this study:

(1) We demonstrate that macroscopic plastic deformation occurred in the nanowires, but that from the microscopic

point of view, the stacking fault elastic recovery is going.
(2) We obtain the relation between the twist angle and the potential energy for each of the atomic layers. That helps us define the microscopic interplanar potentials.

References

[1] N. Tsuji, Y. Ito, Y. Saito and Y Minamino: Scripta Materialia, 47 (2002), pp. 893-899.

[2] O. Nguyen and M. Ortiz: Journal of the Mechanics and Physics of Solids, 50 (2002), pp. 1727-1741.

[3] T. Ogawa and A. Nakatani: International Symposium on Structures under Earthquake, Impact, and Blast Loading 2008 (IB2008), (2008), pp. 47-52.

[4] A. Nakatani, T. Shimokawa, R. Matsumoto and H. Kitagawa: Solid Mechanics and Its Applications, 115 (2004), pp. 365-380.

[5] Y. Mishin, M. J. Mehl, D. A. Papaconstantopoulos, A. F. Voter and J. D. Kress: Phys. Rev. B 63 (2001), p. 224106.