ATOMISTIC STUDY OF SIZE EFFECT IN TORSION TESTS OF NANOWIRE

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Summary   The inelastic deformation of an atomistic model of single crystal and polycrystalline wire under torsion is studied using molecular dynamics. Torsion deformation is incorporated using a twisted periodic boundary condition proposed by the authors. We focus on grain refinement and size effect as they are affected by the combination of two length scales, i.e., radius of specimen and grain size. The result is compared with that from continuum strain-gradient plasticity.

INTRODUCTION

The strength of polycrystalline material is increased with decreasing grain size. This tendency is known as the Hall-Petch relation (HPR). Strengthening through grain refinement of polycrystalline materials is a promising process because it has the advantage of recycling. In particular, a severe plastic deformation (SPD) process using cheap equipment attracts a great deal of attention. On the other hand, there is a trend towards miniaturization. Many small-scale structures are designed. However, the assumption on which conventional continuum theories are based breaks down for them. Many strain gradient theories are proposed to explain the size effect (e.g. [1]). The physical base of the theories is usually backed up by dislocation theory [2, 3]. However, the problem is still unsolved for nanostructured material where the HPR also breaks down, i.e., smaller is softer.

We conduct an atomistic simulation of torsion tests of nanowire. There is some literature on torsion tests (e.g. [4]) but most findings are affected by boundary constraints. In this study, we propose a novel treatment of the boundary condition, a twisted periodic boundary condition (TPBC). Ideally, torsion can give SPD to the specimen without any change of its profile. In particular, the application called high pressure torsion (HPT) is notable for grain refinement. Mechanically, there is interest in the fact that the deformation field in torsion has its gradient along radial coordinates. The specimen size effect is significant in the torsion test, as well as in the bending test [2], and the results are used to verify the validity of strain-gradient theory in the nano-scale region.

FORMULATIONS AND COMPUTATIONAL SETUP

The materials of the nanowire for the torsion problem are single- and polycrystalline iron in which interatomic interaction is introduced by the Finnis-Sinclair type potential [5]. Solid cylindrical wire with a radius R is modeled as shown in Figure 1 and analysis models are listed in Table 1.

A brief summary of TPBC is shown as follows. A coordinate transformation between the natural coordinate's component $(Q^{(\alpha)})^I$ and the twisted coordinate's component $(q^{(\alpha)})^i$ is considered for an atom α. The canonically conjugate moments $(P^{(\alpha)})_I$ and $(p^{(\alpha)})_i$ with coordinates $(Q^{(\alpha)})^I$ and $(q^{(\alpha)})^i$ are introduced as follows:

$$(q^{(\alpha)})^i = h^i{}_J(Q^{(\alpha)})^J, \qquad (p^{(\alpha)})_i = [(\boldsymbol{h}^{-1})^T]^J_i(P^{(\alpha)})_J, \tag{1}$$

When we assume Cartesian coordinates, and $\boldsymbol{Q}^{(\alpha)}$ and a specific twist angle θ along the z axis are taken into account, $\boldsymbol{h}$ is the transformation matrix and the metric $g^I{}_J = (\boldsymbol{h}^T)^I{}_k h^k{}_J$ specifies the macroscopic deformation.
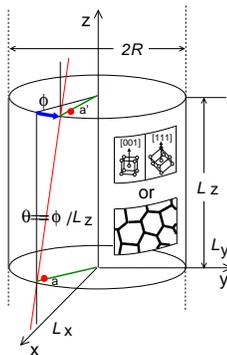

Figure 1. Schematic of test model. TPBC is employed in z direction with dimension L_z of the unit cell. The lateral dimensions L_x and L_y of the unit cell are taken to be sufficiently larger than the diameter $2R$.

Table 1. Material models, specimen geometries, analysis conditions and procedures

Specimen (d: Grain size, R: Radius of specimen)		Height l_z	Number of atoms
Single crystal	in $\langle 001 \rangle$ torsion	20 nm	535 711
	in $\langle 111 \rangle$ torsion	20 nm	544 235
Nanocrystal	$d = $ 5 nm ($R = 10$ nm)	20 nm	511 943
	$d = 10$ nm ($R = 10$ nm)	20 nm	522 607
	$d = $ 5 nm ($R = 20$ nm)	10 nm	994 167
	$d = 10$ nm ($R = 20$ nm)	40 nm	4 026 817

Analysis conditions and Procedures
* The wire is twisted monotonically by the increment of specific twist angle $\Delta\theta = 1.25 \times 10^6$ rad/m, which is added to the specific twist angle θ every 0.5 ps.
* The nominal surface shear strain $\gamma_0 = R\theta$ is used to express the strain level.
* The system temperature is set as 300 K during the calculation.
* Defect atom is defined as the atomic site at which less than 10 bcc-characteristic atoms are found among the 8 first neighbors and the 6 second neighbors by using common neighbor analysis (CNA).
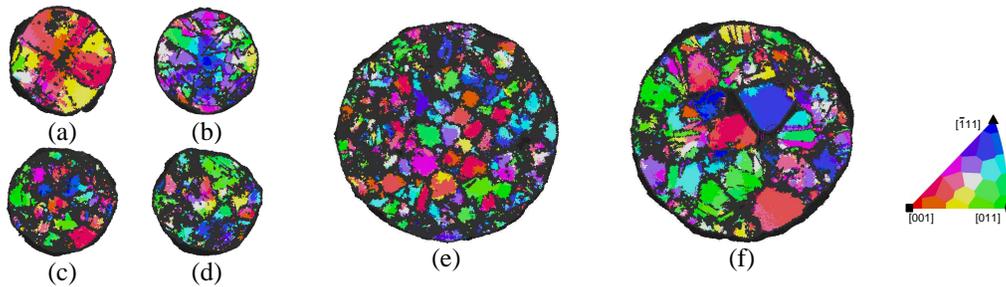
Figure 2. Cross-section views after deformation: (a) single crystal in $\langle 001 \rangle$ torsion. (b) single crystal in $\langle 111 \rangle$ torsion. (c) nanocrystal with $d = 5$ nm ($R = 10$ nm). (d) nanocrystal with $d = 10$ nm ($R = 10$ nm). (e) nanocrystal with $d = 5$ nm ($R = 20$ nm). (f) nanocrystal with $d = 10$ nm ($R = 20$ nm). Defect atoms are colored in black. Colors correspond to the crystallographic orientation of the twist axis in the unit triangle of the reverse stereographic pole figure.
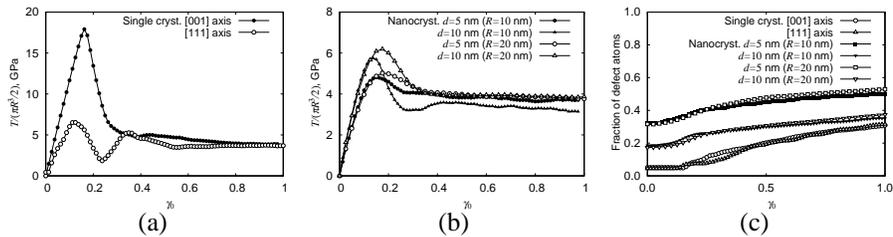

Figure 3. Torque versus twist curves for (a) single crystals and (b) nanocrystals: (c) Fraction of defect atoms as a function of twist. Torque value is converted to a representative value having the dimension of stress with multiplication by a factor of $2/\pi R^3$; twist is expressed by nominal surface strain $\gamma_0 \equiv R\theta$.

RESULTS AND DISCUSSION

Figure 2 shows cross-section views after the deformation. It is observed that a polycrystal structure is developed near the surface in the cases of the twisted single crystals (Figures 2 (a) and (b)). In the polycrystalline case (Figures 2 (c), (d), (e) and (f)), no significant difference between the surface and the interior is recognized in small specimens (Figures 2 (c) and (d); however, grain refinement proceeds more severely near the surface in large specimens (Figures 2 (e) and (f)).

Figures 3 (a) and (b) show the torque versus twist curves for single crystals and for nanocrystals respectively. Anisotropy in the maximum torque is significant in the single crystal cases and the maximum torque in $\langle 001 \rangle$ torsion is two and half times as large as in $\langle 111 \rangle$ torsion. In the polycrystal cases, it is clear that the elastic modulus of nanocrystals with $d = 5$ nm is less than $d = 10$ nm. Comparison between radius $R = 10$ nm models shows that the peak value of torque in the $d = 5$ nm model is about 80 percent of that in the $d = 10$ nm model. Comparison of the peak stress between different radius R models for the same grain size models shows that the peak stress in the $R = 20$ nm model is slightly higher than that in the $R = 10$ nm model. This is a discrepancy with the well known size effect observed by experiment and explained by the strain gradient theory [1]. One reason for the strain rate effect is that the deformation behavior of nanocrystals with small grain size is mainly caused by the deformation on the grain boundary rather than by dislocation behavior; the latter is important in the coarse grain polycrystals [2].

Figure 3(c) denotes the fraction of defect atoms as a function of twist. There is no significant difference between different values of R. The number of defect atoms increases with increase of strain, but the rate gradually becomes low.

CONCLUSIONS

The twisted periodic boundary condition is newly proposed. Its efficiency is confirmed through the analysis of the torsion problem of nanowire. Polycrystallization is observed in single crystal cases. The tendency that smaller is softer is a discrepancy with continuum predictions from dislocation theory. We conclude that the deformation at the grain boundary is significant in nano-scale deformation.

References

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