Atomistic Simulations of Small-scale Materials Tests of Nuclear Materials

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1. Introduction

Degradation of materials properties under neutron irradiation is one of the key issues affecting the lifetime of nuclear reactors. Evaluating the property changes of materials due to irradiations and understanding the role of microstructural changes on mechanical properties are required for ensuring reliable and safe operation of a nuclear reactor. However, high dose of neuron irradiation capabilities are rather limited and it is difficult to discriminate various factors affecting the property changes of materials. Ion beam irradiation can be used to investigate radiation damage to materials in a controlled way, but has the main limitation of small penetration depth in the length scale of micro meters.

Over the past decade, the interest in the investigations of size-dependent mechanical properties has promoted the development of various small-scale materials tests, e.g. nanoindentation and micro/nano-pillar compression tests. Small-scale materials tests can address the issue of the limitation of small penetration depth of ion irradiation.

In this paper, we present small-scale materials tests (experiments and simulation) which are applied to study the size and irradiation effects on mechanical properties. We have performed molecular dynamics simulations of nanoindentation and nanopillar compression tests. These atomistic simulations are expected to significantly contribute to the investigation of the fundamental deformation mechanism of small scale irradiated materials.

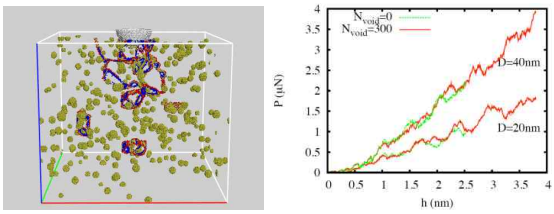
2. Methods and Results

We performed molecular dynamics simulations [1] of the nanoindentation and nano-compression of a Cu (111) single crystal containing voids. We investigated how dislocations interact with voids and what the effects of voids are.

2.1 Nanoindentation

The atomic model used in the nanoindentation simulations comprises a rectangular copper single crystal and a rigid spherical indenter. The dimensions of the copper crystal are 49.4×49.5×44.3 nm^3 containing approximately 8×10^6 atoms. The x, y and z coordinates coincide with the [1-10], [11-2] and [111] directions. Periodic boundary conditions were applied along the x and y coordinates. The atoms in the bottom layer were immobilized, and the top free surface was pushed down by a spherical indenter along the z coordinate. The Cu crystal was thermally equilibrated for 20 ps prior to indentation at a temperature of 300 K. The block of indenter atoms was moved at a constant velocity of 10 m/s, and the motion of the individual indenter atoms relatively to each other was suppressed so as to represent a rigid indenter. The copper atoms in the crystal and its interaction with the indenter atoms were modeled by using an interatomic potential of the Finnis-Sinclair type derived by Ackland et al.[2].

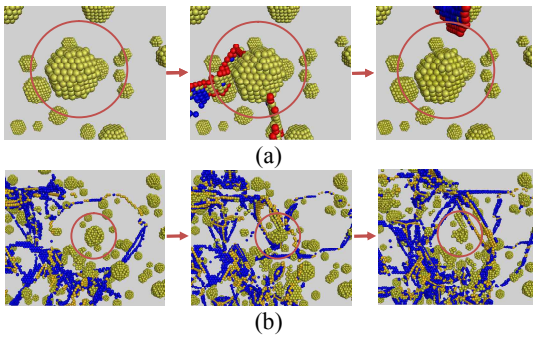
Fig. 1(a) shows that dislocations are generated and propagated into the crystal by the indenter. Dislocations interact with voids and the propagation of dislocations is hindered due to these interactions. As a result, higher loads are required compared with a pure single crystal which contains no voids as shown in Fig. 1(b).



(a) (b)

Fig. 1. (a) Generation of dislocations by an indenter of radius 10 nm on Cu (111) single crystal containing voids, (b) Simulated load-depth curves of Cu crystal with/without voids.

Two possible mechanisms of hardening due to dislocation-void interaction are revealed: shearing and absorption of voids. Fig. 2(a) and (b) shows the shearing and the partial absorption of a void by moving dislocations respectively.



(a)

(b)

Fig. 2. (a) Shear of a void by a moving dislocation, (b) Partial absorption of void by moving dislocations.

An atomic ledge has formed on the surface of a void once an intact void is sheared by a moving dislocation as is shown in Fig. 2(a). Fig. 2(b) shows that

the size of a void is decreased due to the absorption of vacancies into dislocations during the interaction between a void and moving dislocations.

2.2 Nanocompression

Fig. 3(a) shows a nanopillar compressed by a flat punch indenter. Fib. 3(b)-(f) show deformed shapes after compression test of 5.8, 10, 15.7, 25 and 30 nm diameter pillars respectively. Since pillars were deformed along (111) direction, three other {111} slip planes were activated and resulted in the observed shapes.

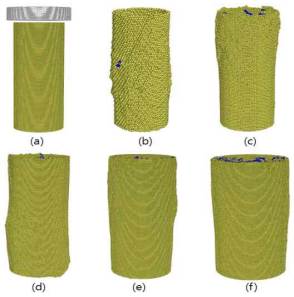


Fig. 3. Geometry of Cu nano-pillar before compression (a), and after compression with a diameter of 5.8 (b), 10 (c), 15.7 (d), 25 (e), and 30 nm (f).

Fig. 4 shows simulated stress-strain curves of nano-pillars. After initial elastic deformation, which shows the elastic modulus of 190.3 GPa, the stress-strain curves show yielding. Yield strength shows size-dependency, i.e. the strength increases with a decrease in diameter. Small pillars shows several elastic deformation after yielding because nucleated dislocations disappear through surface and pillars become dislocation-free crystals.

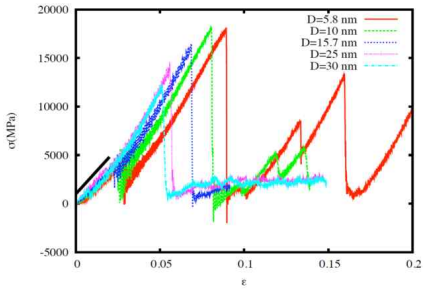


Fig. 4. Stress-strain curves of compression tests of nano-pillars

Fig. 5 shows the stress-strain curves of the compression tests of pillars with a diameter of 15.6 and 25 nm containing voids with a number density of $2\sim3\times10^{24}/m^3$. Initial yielding occurs at a lower strength than defect-free single crystals. This is because dislocations nucleate heterogeneously at a lower strength around voids. After yielding, higher stresses were observed, which is due to the interaction of dislocations with voids. This is radiation hardening.

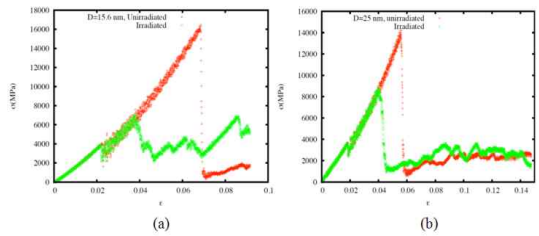


Fig. 5. Stress-strain curves of pillars with and without voids of (a) 15.6 nm diameter, (b) 25 nm diameter.

Fig. 6 shows a detailed interaction and pinning of moving dislocations by voids. The pinning of moving dislocations induces hardening, i.e. increase of stress for further deformation. Voids are sheared or absorbed by dislocations.

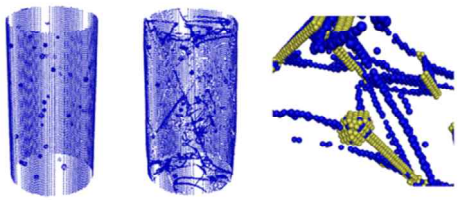


Fig. 6. Nanopillar of 30 nm diameter containing voids (a) before and (b) after compression, (c) the interaction of void and dislocations.

3. Conclusions

Radiation effect was observed which is found to be due to the interaction of dislocations nucleated by spherical indenter with pre-existing radiation defects (voids). Atomistic simulations showed that voids are sheared or partially absorbed by the emitted glissile dislocation loops from the surface.

REFERENCES

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