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Irradiation-initiated plastic deformation in prestrained single-crystal copper

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ABSTRACT

With large-scale molecular dynamics simulations, we investigate the response of elastically prestrained single-crystal Cu to irradiation as regards the effects of prestrain magnitude and direction, as well as PKA (primary knock-on atom) energy. Under uniaxial tension, irradiation induces such defects as Frenkel pairs, stacking faults, twins, dislocations, and voids. Given the high dislocation concentration, twins and quad-stacking faults form through overlapping of different stacking faults. Voids nucleate via liquid cavitation, and dislocations around void play a lesser role in the void nucleation and growth. Dislocation density increases with increasing prestrain and PKA energy. At a given prestrain, there exists a critical PKA energy for dislocation activation, which decreases with increasing prestrain and depends on crystallographic direction of the applied prestrain.

1. Introduction

Materials used in nuclear engineering have to endure extreme amounts of irradiation, and point defects (interstitials and vacancies) are created as a result [1–4]. Those defects can aggregate to form clusters, stacking fault tetrahedra and voids, causing degradation of materials integrity and performances [5–8]. To ensure long-time and safe service of nuclear reactors, it is necessary to understand microstructure evolution of materials under irradiation in detail. Collision cascade occurs over lengths of nanometers (nm) and times of picoseconds (ps). Computer simulations have the advantage in inquiring irradiation damage evolution in real time and *in situ* with high spatial resolutions. Molecular dynamics simulations is one of the most efficient implements, and has been widely used for studying irradiation damage.

In nuclear engineering, materials often suffer applied strain due to irradiation induced void swelling and transmutation, as well as thermal and mechanical loads. Previous studies found that applied strains have distinct effects on, e.g., Frenkel pair production efficiency, defect cluster size, void density, and size range, under irradiation [9–15]. However, most of them concentrated on low strain (small stress) conditions without extensive structure rearrangement. Local high strains or stresses in materials may also be induced by hydride precipitates, accumulation of He atoms, and so on. Recently, Di et al. [16] and Zolnikov et al. [17] observed that voids and twins formed after irradiation when high prestrains were applied to Zr and Fe. However, it is desirable to examine in detail, and in other types of materials, microstructure evolutions as well as the mechanisms of deformation, and void nucleation and growth under prestrain conditions. In this work, we investigate irradiation induced microstructure evolution in prestrained Cu, a model system for face-centered-cubic metals widely used in fundamental studies of irradiation damage [18–23]. We explore the effects of prestrain magnitude (ε), PKA (primary knock-on atom) energy (E_{PKA}) and prestrain direction on radiation damage. Dislocation emissions and void nucleation are observed, and stacking fault interaction can lead to the formation of twins and quad-stacking faults. Voids nucleate and grow via cavitation of melts induced by thermal spike during cascade. The relation between critical PKA energy (E^c_{PKA}) and prestrain magnitude is established, and depends on crystallographic direction of the applied prestrain.

This article is organized as follows. Section 2 addresses the methodology of MD simulations and data analysis, followed by results and detailed discussions on microstructure evolution in Section 3. Conclusions are presented in Section 4.

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2. Methods

We perform MD simulations using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [24] with an accurate embedded-atom-method (EAM) potential of Cu [25]. This widely used EAM potential has well established accuracy in describing, e.g., defect formation energy, stacking fault energy and melting point [25,26]. When interatomic distance is smaller than 0.5 Å, this EAM potential is smoothly splined to the Ziegler–Biersack–Littmark (ZBL) potential [27].

The coordinate system for irradiation simulations of single crystal Cu is defined in Fig. 1. Since temperature has remarkable effects on irradiation damages [17,22,28,29], sufficiently large system sizes are necessary. In our simulations, the initial configuration dimensions are about 540 Å along *x*-, *y*- and *z*-axes corresponding to ~13 million atoms. The initial configuration is first equilibrated at 300 K and zero pressure with the constant-pressure–temperature ensemble for 50 ps to achieve thermal equilibrium. A tensile strain is then applied along one axis, while the stresses along the other two axes are fixed at zero. The new configuration is then subjected to extra equilibration at 300 K with constant-volume-temperature ensemble for 50 ps. To investigate the effects of prestrain magnitude and direction, prestrain varies from 0% to 5%, and three loading or prestrain directions are explored: $[1\,1\,1]$, $[1\,\bar{1}\,0]$ and $[1\,1\,\bar{2}]$. Since the yield strains along those three directions are about 7.8%, 7.4% [30] and 7.5% at 300 K on MD time and length scales, respectively, the final configurations are in elastically prestrained states. PKA is introduced into the system by assigning an atom specific kinematic energy corresponding to the desired PKA energy. For each prestrain/PKA energy condition, twenty simulations with different recoil directions and random PKA positions are carried out. A total of ~1000 runs are conducted. Microcanonical ensemble (*NVE*) is used during irradiation simulations. The time step is fixed at 0.005 fs within the first 2 ps period of simulation, and then it is increased from 0.005 fs to 1 fs, as long as no atoms are displaced by more than 0.05 Å within a single time step. The total run durations are up to 50 ps. All simulations are conducted under three-dimensional (3D) periodic boundary conditions.

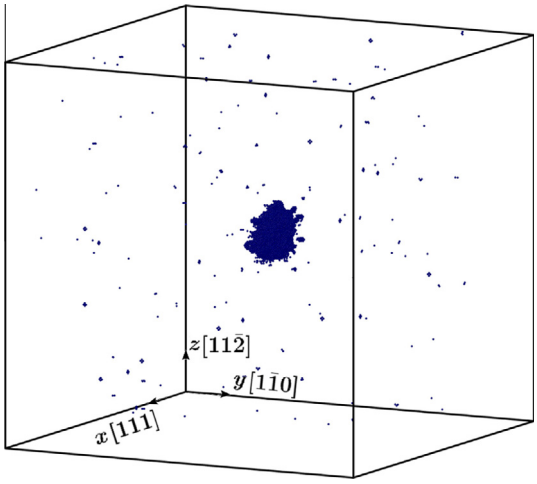

Fig. 1. Coordinate system for simulations of prestrained single crystal Cu. The cluster in the center denotes cascade region.

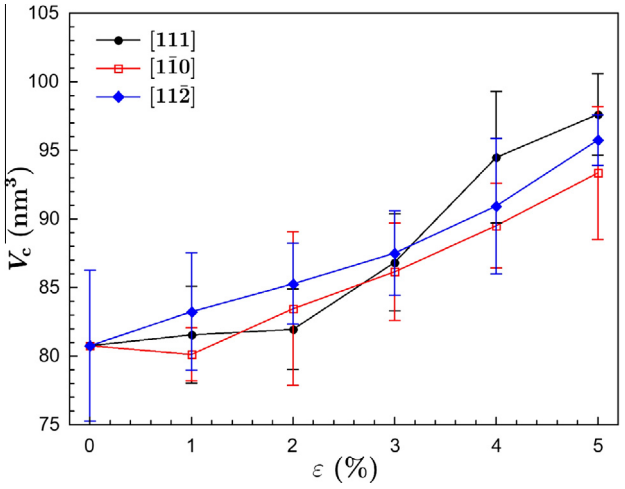

Fig. 2. Cascade volume vs. prestrain for different prestrain directions. PKA energy: 5 keV.

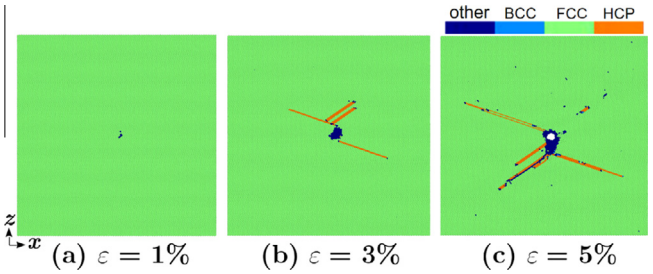

Fig. 3. Radiation-induced damage for different prestrains at $t = 50$ ps (a), 7 ps (b) and 7 ps (c). Color-coding of atoms is based on their local structures. FCC: face-centered cubic; BCC: body-centered cubic; HCP: hexagonal close-packed. Prestrain direction: [1 1 1]; PKA energy: 5 keV. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

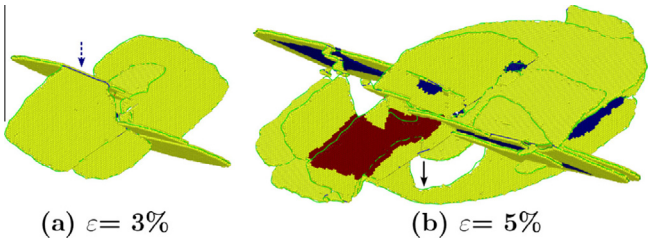

Fig. 4. Radiation-induced defects for different prestrains after collision cascading ($t = 7$ ps). Prestrain direction: [1 1 1]; PKA energy: 5 keV.

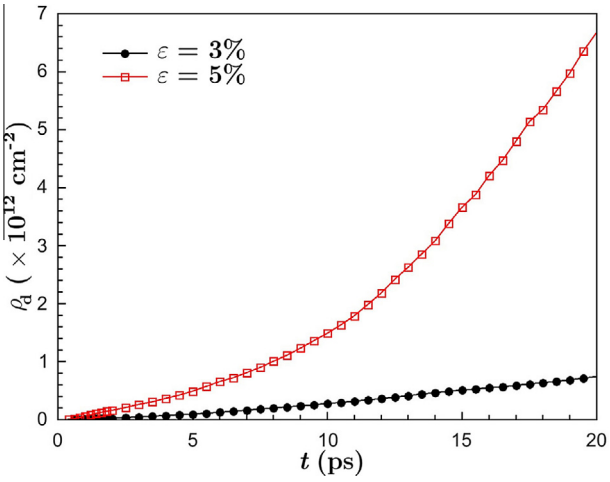

Fig. 5. Time evolutions of dislocation densities for different prestrains. Prestrain direction: [1 1 1]; PKA energy: 5 keV.