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Radiation response of nanotwinned Cu under multiple-collision cascades

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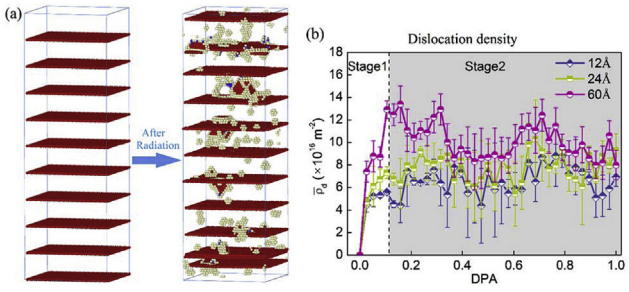
HIGHLIGHTS

- Multiple collision cascades of nt Cu are performed to model the response upon a radiation dose of 1dpa.
- We analyze the microstructural evolution of defect clusters in nt Cu at the different radiation doses.
- Defect clusters could be removed via their frequent interactions with coherent twin boundaries during the MCC process.
- The potential formation and elimination mechanisms of stacking fault during MCC are revealed.

GRAPHICAL ABSTRACT



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ABSTRACT

In this paper, multiple collision cascades (MCC) of nanotwinned (nt) Cu with three different twin spacings are performed to model the response of nt Cu upon a radiation dose of 1 displacements per atom (dpa). Considering the defects developed with high randomness in the material during a MCC process, each MCC in a nt Cu is conducted for eight times. This enables us to analyze some average properties of defect clusters in the radiated nt Cu with different twin spacings at the different radiation doses. We also analyze the microstructural evolution in the nt Cu during the MCC. Smaller size of defect clusters and lower defect density are seen in the nt Cu with smaller twin spacing. In addition, a number of defect clusters could be removed via their frequent interactions with the coherent twin boundaries (CTBs) during the MCC. This induces either the migration of CTBs or the healing of CTBs. Moreover, the potential formation and elimination mechanisms of stacking fault are found to be due to the climb of Frank partial dislocation and glide of Shockley partial dislocations. This study provides further evidence on the irradiation tolerance of CTBs and the self-healing capability of CTBs in response to radiation.

1. Introduction

Irradiation of metallic materials by neutrons or heavy ions leads to a large number of vacancy and interstitial clusters, both produced by direct condensation out of collision cascades [1] and by aggregation of isolated point defects [2]. Radiation induced defect clusters, such as dislocation loops, voids and stacking fault

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tetrahedrons (SFTs), may undermine the mechanical properties of radiated materials in the form of swelling, hardening, embrittlement etc. [3–9]. Therefore, it is highly desirable to suppress the radiation induced defects in structural materials in reactors [10]. One way to achieve this goal is to synthesize materials containing high-density defect sinks that may remove radiation-induced point defects before they aggregate into clusters [11,12].

By far, the effect of various types of defect sinks have been extensively studied. Grain boundaries, as one of the primary defect sinks in the polycrystalline and nanocrystalline materials, have been recognized to be able to reduce the density of radiation induced defects [13–17] and suppress void swelling [18,19]. It has also been found that radiation-induced damage decreases with the decreasing of grain size because of the trapping of defects at more GBs. More recently, heterophase interfaces have shown excellent point defect sinks and drastic impact on defect population in Cu/Nb [20] and Cu/Fe multilayers [21]. Remarkedly fewer defect clusters form in these multilayered composites than that in pure Cu, Nb or Fe under the same ion bombardment conditions.

Coherent twin boundaries (CTBs) are low energy boundaries and are generally anticipated to be less effective in the suppression of radiation damages, comparing to high angle grain boundaries [22–24]. However, nanotwinned (nt) metals have also shown the enhanced irradiation tolerance due to the ability of CTBs to remove SFTs [25], migrate [26] and self-heal [27] during the radiation. CTB affected zones are also discovered wherein time accumulative defect density and defect diffusivity are substantially different from those in twin interior [27]. Moreover, CTBs can provide fast diffusion channels for radiation induced defects, thus deliberately introduced nanovoids shrink by absorbing radiation induced interstitial loops [28].

In fact, radiation damage in Cu has been investigated by both ex situ [29,30], and in situ irradiation experiments [31,32]. SFTs are usually seen in the radiated Cu because of the low stacking fault energy of Cu [33]. Systematic studies are reported on the formation of SFTs [34] and destruction of SFTs by mobile dislocations [35,36] or by CTBs [37,38]. Despite these prior studies, two significant issues remain unaddressed. First, the radiation-induced defects evolution in nt Cu during radiation has not been clearly revealed using atomistic simulation. Second, although experiments show SFT-CTB interactions result in high density SFs [25], the transformation mechanism from SFT to SF during radiation remains a challenge.

In order to further elucidate radiation response of nt Cu during multiple collision cascades (MCC), we use classical potential molecular dynamics (MD) to model the radiation by sequentially simulating the MCC in the nt Cu. Three different twin spacings (12 Å, 24 Å and 60 Å) have been considered. The microstructural examination of nt Cu with different twin spacings during the MCC are analyzed. Besides, the average properties of defect clusters in the radiated nt Cu with three different twin spacings at the different radiation doses, such as the average value of the SFT size, the number of SFTs, the number of dislocation loop, dislocation density and the CTB migration distance, are compared. Significant findings include twin spacing-dependent reduction of the number of SFTs, SFT size and dislocation density. Our studies also provide evidence for defect-CTB interactions, including the destruction of SFT, the self-healing and migration of CTBs. Besides, two different formation mechanisms and elimination mechanisms of SF during the MCC are analyzed. Our findings about irradiation tolerance of CTBs have important implication for the design of materials under extreme radiation environment.

2. Methodology

We carry out our investigation in atomic models of nt Cu shown in Fig. 1(a). The nt Cu with three different twin spacings, i.e., 12 Å, 24 Å and 60 Å hereafter denoted as 12 Å nt Cu, 24 Å nt Cu and 60 Å nt Cu, respectively, are investigated. The simulation cell is a square cube with 80 Å edge lengths in the x and z directions, 250 Å edge lengths in the y direction, containing around 138,000 atoms. Periodic boundary conditions (PBCs) are applied in all directions. The simulation cell size is large enough so that CC initiated by primary knock-on atoms (PKAs) with the recoil energy chosen for this study (10 KeV) does not interact with their periodic images. Embedded atom method (EAM) interatomic potential for Cu developed by Mishin et al. is used to describe the interatomic interaction [39], splined to the Ziegler-Biersack-Littmark (ZBL) [40] repulsive potential for interatomic distances less than 0.5 Å. All simulations are performed using the software LAMMPS [41].

We accomplish a MCC of nt Cu with identical spacing (12 Å, 24 Å or 60 Å) by successively performing 760 single CC. A single CC is initiated by equilibrating the structure at 300 K and zero pressure for 10 ps? After the equilibration, we assign a kinetic energy of 10 keV to a randomly selected atom (primary knock-on atom-PKA) by rescaling its instantaneous velocity. The system is then allowed to evolve under constant energy and fixed volume for 20ps with dynamically varying time steps using NVE ensemble. After that, we bring the temperature of the model back to initial temperature (300 K) using atomic velocity rescaling for about 10ps and then the model is ready for the next single CC. The change of the temperature in the simulation model in between two successive CC processes is shown in Section 1 and Fig. S1 in the supplementary materials. Considering the great randomness of the defects developed in the material during the MCC, a MCC for each nt Cu with different twin spacings is conducted for 8 times.

Here, we convert the number of PKAs (namely the times of single CC) to displacements per atom (dpa) by the modified Kinchin-Pease formula [42] with a displacement threshold energy of 23eV for Cu [43]. 760 single CC processes in the simulated model achieve a radiation dose of ~1.0 dpa. Microstructure evolutions are studied at atomic scale with the adaptive common neighbor

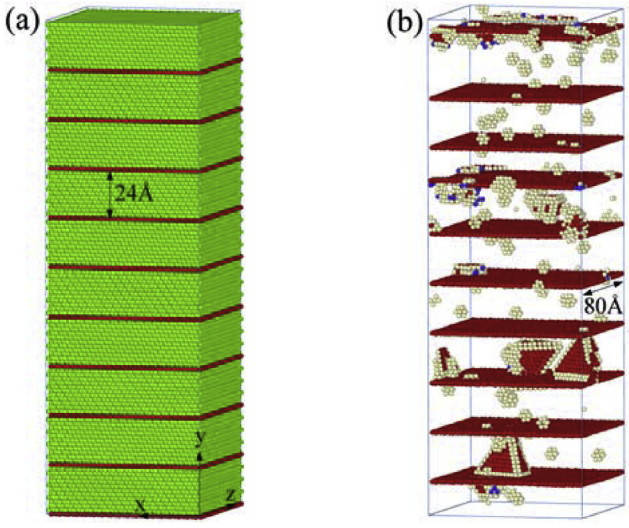

Fig. 1. Schematic simulation cell of (a) an atomic model of the 24 Å nt Cu and (b) the 24 Å nt Cu at radiation doses of 0.8dpa. Atoms in green, red, blue and yellow correspond to the FCC, HCP, BCC and other structures. Note that all perfect FCC atoms are suppressed for clarity in (b). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)