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Radiation tolerance of nanotwinned metals – An atomistic perspective

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ABSTRACT

Remarkable properties of ultra-high strength, ductility, and stability have been achieved through the introduction of twin boundaries in nanostructured metals. Here, we report molecular dynamics simulations which elucidate the synergistic role of grain boundaries and twin boundaries in enhancing the radiation tolerance of nanotwinned metals. While grain boundaries are known to be excellent sinks for point defects, coherent twin boundaries do not absorb point defects. A beneficial corollary is that the structural integrity of coherent twin boundaries remains intact as radiation-induced defects pass through them and ultimately get absorbed into grain boundaries. Hence, the twin boundaries can continue to play a role in imparting high strength even after being subjected to irradiation. Thus, nanotwinned structures may indeed be optimal motifs for radiation tolerant materials that preserve high strength and ductility.

1. Introduction

The optimal design of structural materials that can sustain radiation damage while achieving high strength and toughness is an important challenge for future nuclear power systems. Continued exposure to extreme environments due to neutron, proton, and heavy ion irradiation can eventually lead to material degradation thereby raising safety and reliability concerns [1]. The atomistic origin of material damage due to irradiation lies in the formation of vacancies and interstitials. The migration and interaction of these point defects lead to further damage which includes formation of voids, stacking fault tetrahedra (SFTs), and dislocation loops as these vacancies and interstitials coalesce into clusters. Material swelling occurs as interstitials migrate to the surface, while interstitial aggregates act as obstacles to dislocation motion resulting in embrittlement of the material [2,3].

It is well established that grain boundaries (GBs) improve radiation resistance by serving as excellent sinks for radiation-induced point defects [4,5]. Compared to their coarser counterparts, nanocrystalline materials have a much higher volume fraction of GBs which imparts greater strength as well as resistance to radiation. This has led to extensive experimental and computational studies on nanocrystalline materials as radiation-tolerant materials [6–11]. However, the increase in strength and radiation-tolerance of nanocrystalline materials with decreasing grain size comes with severe issues such as loss of ductility, creep, and grain growth which weaken their case for critical structural applications [12]. In contrast, research has provided compelling evidence for the ultra-high strength of nanotwinned metals while preserving ductility, and grain stability [13–19]. These remarkable properties are attributed to twin boundaries that strengthen by arresting dislocation motion and retain ductility by accommodating plastic strain. Naturally then, there is a growing interest in investigating the radiation response of nanotwinned metals. Recent experimental and computational studies have elucidated the interaction of radiation-induced defects with twin boundaries. Demkowicz et al. [20] showed that coherent twin boundaries (CTBs) are poor sinks for point defects through molecular dynamics simulations. They speculated that CTBs could speed up defect recombination and thereby lead to significantly lower number of radiation-induced defects compared to single crystals. Recently, Yu et al. [21] found from experiments that coherent and incoherent TBs in face-centered-cubic (fcc) metals could annihilate radiation-induced SFTs at room temperature. They also reported migration of incoherent TBs under irradiation.

In this paper, we report molecular dynamics simulations which elucidate the complementary role of grain boundaries and twin boundaries in enhancing the radiation tolerance of nanotwinned metals. To this end, we first perform cascade simulations on columnar specimens comprising of both twin boundaries and general grain boundaries. We then perform uniaxial tension simulations to investigate the deformation response of nanotwinned and nanocrystalline specimens subjected to radiation damage. We find that radiation-induced defects can pass through CTBs without distorting the structure of the CTBs and are ultimately absorbed by GBs leaving the intragranular regions with fewer defects. Thus, the results discussed here together with previous

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studies suggest that an optimal volume fraction of GBs and TBs, based on the grain size and twin lamella thickness, could make nanotwinned metals potential candidates as radiation-resistant materials with excellent mechanical properties.

2. Simulation method

Molecular dynamics simulations were performed on columnar specimen of fcc copper consisting of four hexagonal grains. As shown in Fig. 1, the orientation of grain 1 was along the $[1\,1\,\bar{2}]$, $[1\,1\,1]$ and $[1\,\bar{1}\,0]$ crystallographic directions. Grains 2, 3 and 4 were rotated around the $[1\,\bar{1}\,0]$ axis by 30°, 60° and 90° respectively in the X-Y plane. The digital specimens had a size of $35 \times 40 \times 20$ nm, and consisted of about 2,370,000 atoms. The diameter of each grain was about 20 nm. Nanotwinned specimens were constructed by inserting CTBs in each grain. Five different twin spacings were considered, specifically, 0.6 nm, 1.2 nm, 2.5 nm, 5 nm, and 10 nm. The results for these cases were compared with those for the nanocrystalline specimen without CTBs and single crystal specimen. Periodic boundary conditions were specified in all directions. The initial equilibrium structure of each specimen was obtained using conjugate gradient energy minimization. Fig. 1 shows the relaxed atomistic structure of a specimen containing CTBs with a spacing of 5 nm after energy minimization. The atomic interactions were modeled using the embedded atom (EAM) interatomic potential developed by Mishin et al. [22]. The ZBL repulsive potential [23] was splined to the EAM potential for atomic distances smaller than 0.5 Å to prevent atoms from coming unrealistically close during radiation cascades.

After energy minimization, each specimen was equilibrated at 300 K under the NPT ensemble for 100 ps. The radiation simulation was started by selecting four primary knock-on atoms (PKA) and giving certain amount of kinetic energy to each of them in order to initiate radiation cascades in the system. Simulations were performed for two different PKA energies, namely, 10 keV and 20 keV. Since the results for both cases are qualitatively similar, we discuss the 10 keV simulations in the main text of the paper and defer the 20 keV results to the Supplementary Material [24]. As shown in Fig. 1, PKA 1 and 3 were located about 48 Å away from the nearest GBs, and PKA 2 and 4 were located about 25 Å away from the nearest GBs. The specific positions of the PKA were chosen such that PKA 1 and 3 impinged on the CTBs first, whereas PKA 2 and 4 impinged directly on the GBs. The velocity for each PKA was chosen to be perpendicular and directed toward its nearest interface. The cascades were equilibrated in the NVE ensemble for 2 ps using a timestep of 0.1 fs and for another 1000 ps using a timestep of 2 fs. Steady state was observed to have reached after about 562 ps when the defect structure appeared stable with no significant changes on the time-scale of molecular dynamics. During the simulation, the outermost layers of atoms of the three-dimensional simulation box were fixed to rescale their velocities for dissipating the energy and maintaining the temperature of the system at 300 K. After irradiation, the irradiated and pristine specimens were subjected to tensile loading. To this end, each system was relaxed for 100 ps at 300 K under the NPT ensemble. Then, the structure was subjected to a tensile deformation along the X direction with a strain rate of $4 \times 10^8\ s^{-1}$ for 300 ps under the NVT ensemble. All simulations were performed using the molecular dynamics code, LAMMPS [25]. Defects were visualized using common neighbor analysis [26] in OVITO [27] and AtomEye [28].

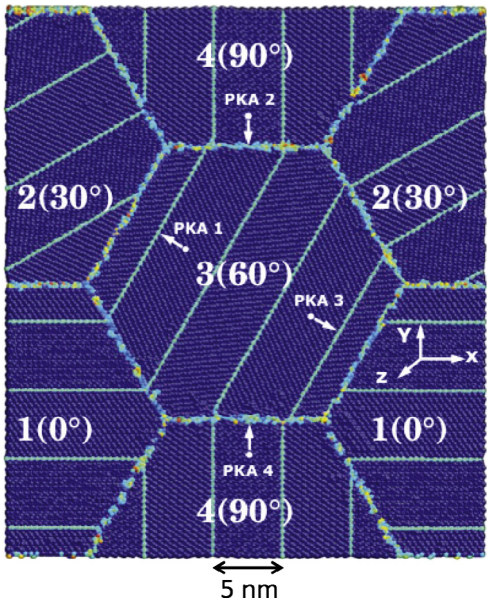

Fig. 1. Equilibrium configuration of columnar nanotwinned Cu with grain size of 20 nm and CTB spacing of 5 nm.

3. Results and discussion

3.1. Radiation response of nanotwinned copper

Fig. 2 shows radiation cascades generated in two representative specimens, specifically, nanocrystalline Cu and nanotwinned Cu with a CTB spacing of 1.2 nm. The kinetic energy imparted to each PKA is 10 keV. The fcc atoms in perfect crystal structure are not shown in order to identify the defects. A large number of atoms are displaced from their initial lattice positions leading to four displacement cascade events due to the four PKAs. Comparing Fig 2a and b, it is interesting to note that most of the twin boundary structure (shown by the rows of red atoms) is still maintained even during the cascade event.

Fig. 3 shows equilibrated structures of the single crystalline, nanocrystalline and nanotwinned specimens using common neighbor analysis. The snapshots are taken at 562 ps after cascade initiation. Blue atoms are in body-centered cubic (bcc) configuration, red atoms are in hexagonal-closed-packed (hcp) configuration and cyan atoms cannot be in classified as fcc, bcc, or hcp. Fcc atoms are not shown. Compared to Fig. 2, most of the displaced atoms recover their perfect lattice positions during equilibration leaving behind various defects that include single vacancies (identified as 12-neighbor clusters), small vacancy clusters, stacking faults, and SFTs. ⟨0 0 1⟩ dumbbells characterized by two interstitials and one vacancy are also observed in all specimens. The dumbbells are stable defects and are seen to move freely within the intragranular regions. Some of these defects are marked in Fig. 3(b) for further clarity. Looking at Fig. 3(a)–(f), we note that the precise defect structures after relaxation are governed by the shape and spread of the radiation cascade which in turn are quite sensitive to a number of factors including PKA direction and energy, the specimen microstructure, as well as the initial velocity distribution of the atoms corresponding to the prescribed temperature. Thus, comparing the specific distribution of radiation-induced defects in different cases is not quite useful. Nevertheless, the simulations furnish two interesting (and related) insights about CTBs. Consistent with prior studies [20], we find that CTBs are indeed poor sinks for radiation-induced defects. In fact, these defects are able to pass through the CTBs without causing any significant distortion. Many of these defects, especially interstitials, ultimately get absorbed by the GBs which are known to be excellent sinks for point defects. A rather unexpected consequence of this property