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Influence of thermal barrier effect of grain boundaries on bulk cascades in alpha-zirconium revealed by molecular dynamics simulation

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ABSTRACT

The effect of grain boundaries (GBs) on bulk cascades in nano-structured alpha-zirconium has been studied by molecular dynamics (MD) simulations. It turns out that the existence of GBs increases the defect productivity in grains, suggesting that the GBs may act as a thermal barrier and postpone the annihilation of defects within grains. Moreover, it is found that the thermal barrier effect of GBs facilitates the shift of symmetric tilt GBs to the grain with higher temperature, and the smaller the tilt angle is, the easier the boundary shift will be. Thus, the influence of GBs on radiation damage in the nano-structured materials comes from the competition between damage increase in grains and defect annihilation at GBs.

1. Introduction

Nano-structured materials have been developed as a kind of anti-irradiation materials because they possess a large volume fraction of grain boundaries (GBs) which were supposed to serve as effective sinks for irradiation-induced defects. In recent years, the defect-healing effect of GBs has been proven by some simulation or experiment studies [1–5]. X. Bai et al. [1] demonstrated by molecular dynamics (MD) simulations that GBs can absorb interstitials and then emit them to annihilate vacancies in the bulk. Nevertheless, most of the simulation studies have focused on the process of defect annihilation at GBs, but few of them have investigated the influence of GBs on the process of defect production. Recently, our investigations revealed that GBs may serve as the thermal barrier to hinder energy transportation by phonons and affect the temperature distribution in material systems [6,7]. At present, whether the GB-induced obstacle for energy transportation will affect the defect production process of bulk cascades in nano-structured materials is still unclear. Therefore, it is of interest to investigate the influence of the thermal barrier effect of GBs on defect production under irradiation.

MD simulations have demonstrated to be a valuable technique for investigating the primary state of irradiation damage. It can provide information of the actual number and arrangement of the defects produced by displacement cascades, which is critical to predicting and assessing the material performance in power reactor systems. Since alpha-zirconium (α-Zr) and its alloys are widely employed in fuel cladding, calandria tubes and pressure tubes in nuclear reactors, several MD simulations about cascades in α-Zr have been reported in recent years [8–10]. However, none of them have considered the influence of GBs. In the present study, we conduct parallel MD simulations in α-Zr with or without GBs to investigate the comprehensive influence of GBs on defect production of bulk cascades.

2. Simulation methods

In this research we focused on symmetric tilt GBs with a [0001] tilt axis. Three different coincident site lattice (CSL) boundaries of α-Zr [11], listed in Table 1, were studied using an embedded atom method (EAM) potential. To investigate the influence of GBs on cascades, we conducted the parallel studies in two simulation cells with or without GBs. The geometry of the simulation cells is shown in Fig. 1. The simulation cell with GBs was set similarly to that of

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Table 1
The parameters of symmetric tilt GBs and its corresponding simulation cell. $L_x \times L_y \times L_z$ is the actual size of simulation cell. N_{atoms} is the total number of atoms.

Sigma value and GB plane	[0001] tilt angle (θ)	$L_x \times L_y \times L_z$ (Å)	N_{atoms}
$\Sigma = 7/(\bar{1}3\bar{2}0)$	21.8°	85.5 × 177.7 × 92.6	60480
$\Sigma = 13/(\bar{2}7\bar{5}0)$	27.8°	80.7 × 186.5 × 92.6	59904
$\Sigma = 19/(\bar{2}5\bar{3}0)$	13.2°	84.5 × 195.2 × 92.6	65664

adopted for both simulation cell I and II, with the interval of 0.2 (or 0.5) KeV when PKA energy is less (or greater) than 1.0 KeV. In addition, 3.0 and 6.0 KeV cascades are also conducted in simulation cell I to investigate the influence of PKA energy on the stability of Σ13 GB. While for other two GB (Σ7 and Σ19) systems with small titled angles, only 0.6 and 1.0 KeV cascades are conducted in simulation cell I. For each E_P, at least nine cascades were simulated to obtain meaningful statistics.

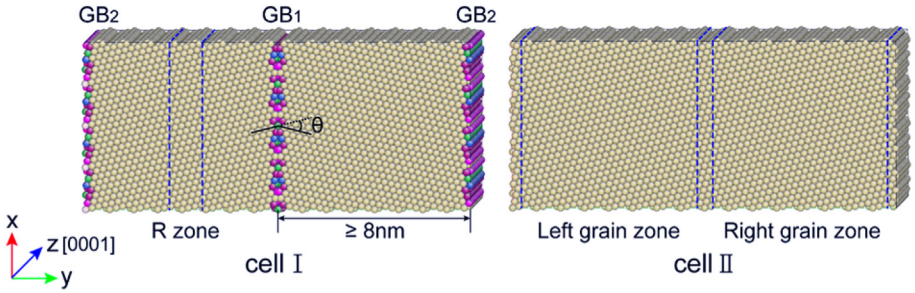

Fig. 1. The two types of simulation cells with or without GBs. Atoms are colored by coordination number where GBs are clearly visible in cell I. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Rittner and Seidman [12]. Atomic positions in the cell I were generated from geometrical CSL constructions, while the cell II was constructed by expanding the lattice of left grain in cell I to form a perfect crystal for comparative study. Born-von Karman (3D) periodic border conditions were employed to avoid surface effects. The periodic borders generated a second GB (GB_2) at the left and right border of the cell I, which was crystallographically similar to the grain boundary in the middle of the cell I (GB_1). The distance between GB_1 and GB_2 was set large enough (≥8 nm) to prevent interactions between them and other finite-size effect.

To improve the chance of finding the correct equilibrium GB structures, rigid body translations (RBT) of one grain with respect to the other was firstly used to generate a number of different initial configurations [12]. The RBT vectors consist of two components parallel to x and z axis, as GBs are located in the x-z plane. The translational components were divided into a grid of points to sample the in-plane translations uniformly [13]. In the present study, the grid spacing in x or z directions was taken to be one fourth of the length of corresponding constructing unit in GB plane. Then, all these 16 initial configurations would be fully relaxed at 300 K and then quenched to 0 K to obtain the equilibrium GB structure. Finally, the one with lowest GB energy was selected to be the correct equilibrium GB structure for latter cascade studies.

The vectorized MOLDY code [14] modified for the HCP structure [15] was used in the present study. The interatomic potential employed was empirical embedded atom method (EAM) potential for α-Zr (#3) [16]. Except for general physical properties, this potential also provided a reasonable description of the defect properties, including interstitial and stacking fault energy (SFE), which was not only crucial to simulating radiation damages but also important to finding the correct GB structure. Each simulation cell was equilibrated for 70 ps at 100 K to establish the equilibrium phonon mode before the cascade happened. A cascade was started by imparting a kinetic energy E_P to one atom, i.e. the primary-knock-on atom (PKA), and then the simulation cell was allowed to evolve for 60 ps. In simulation cell I, the PKA was located at the center of the left grain, and for comparison, the same location was also selected in cell II. All PKA directions were parallel to the Y axis (i.e. perpendicular to the GBs). For the Σ13 GB system with large titled angle, PKA energies ranging from 0.6 KeV to 2.5 KeV are

The effective sphere criterion for identifying the defects in cascade simulations [8] is adopted, i.e. a site is 'vacant' if no atom is found within $0.32a_0$ (a_0 is one of the lattice parameter of Zirconium) of it and a displaced atom is an 'interstitial' if it does not lie within $0.32a_0$ of an atomic site of the perfect crystal. This identification is faster computationally, and using this visualization has the advantage of giving a better indication of the local defect geometry, particularly for defect clusters. However, the number of defects identified by this algorithm must be corrected to account for the nature of the interstitial defect that is formed [17]. For instance, a single interstitial may appear to be two interstitials separated by a vacancy as a dumbbell or may be visualized as three interstitials and two vacancies as a crowdion, depending on the size of the effective sphere for visualization, but the number of apparent interstitials is always one more than the number of apparent vacancies. Therefore, the number of real interstitials should be corrected as the number of apparent interstitials minus the number of apparent vacancies for dumbbells, crowdions and interstitial clusters. In this study, we adopt this method to count the number of defects at the end of cascade simulations (≥30 ps).

3. Results and discussion

3.1. Grain boundary shift

The stable GB structure is essential for investigating its influence on bulk cascades. However, we have found that the bulk cascades in α-Zr will somehow weaken the stability of GB structure. The final states of Σ7, Σ13 and Σ19 GB after cascade simulations with different E_p are shown and compared with their initial states in Fig. 2(a–c, f–h, k–m). It can be seen from Fig. 2(b, g, l) that, for 1.0 KeV cascade, the Σ7 and Σ19 GB have shifted to the left grain while the Σ13 GB is stable (no GB drift) at the end of the simulation. We have further checked the stability of Σ7 and Σ19 GB by reducing E_p from 1.0 to 0.6 KeV, the results showed that the Σ7 GB is stable during 0.6 KeV cascade simulation, but the Σ19 GB is still unstable and shifts to the left grain, as observed in Fig. 2(c, m). For the Σ13 GB, it's stable when $E_p \leq 3.0$ KeV (see Fig. 2(h)), while GB shift has been observed when $E_p = 6.0$ KeV. The above results indicate that the stable sequence of GB structure is Σ13, Σ7 and Σ19 GB.