Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 82 (2015) 94–99

Acta MATERIALIA

www.elsevier.com/locate/actamat

Dislocation-accelerated void formation under irradiation in zirconium

Sali Di,[a,*] Zhongwen Yao,[a] Mark R. Daymond,[a] Xiaotao Zu,[b] Shuming Peng[c] and Fei Gao[d,*]

[a]*Department of Mechanical and Materials Engineering, Queen's University, Kingston, ON K7L 3N6, Canada*
[b]*School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu 610054, People's Republic of China*
[c]*Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621900, People's Republic of China*
[d]*Department of Nuclear Engineering and Radiological Science, University of Michigan, Ann Arbor, MI 48109, USA*

Received 6 July 2014; accepted 8 September 2014
Available online 3 October 2014

Abstract—Molecular dynamics simulations have been performed to model defect creation in alpha zirconium with tensile strains comparable to the elastic strains near the interfaces between zirconium and hydrides. Irradiation-induced vacancy clusters under the strain field could be initiation sites for dislocation nucleation, and the gliding of these dislocations provides channels for transporting atoms from the cascade core, significantly accelerating the growth of vacancy clusters to form a void. The critical number of vacancies in a cluster that is enhanced to grow by the external stress is estimated. The present results provide an atomic-level mechanism to explain the stress-enhanced void growth under irradiation in zirconium, as observed in experiments. The acceleration of delayed hydride cracking under irradiation might be partially attributed to the formation of these voids.

Keywords: Displacement cascade; Void growth; Dislocations; Zirconium; Molecular dynamics simulations

1. Introduction

In both fission and fusion environments, the basic effects of irradiation damage in solids are the displacement of atoms from their equilibrium positions and the formation of point defects (vacancies and interstitial atoms), as well as defect clustering. These defects can be annihilated by defects of opposite nature or accumulate with defects of the same type to form defect clusters. Due to the surface energy, vacancy clusters tend to agglomerate to vacancy loops unless insoluble gases or sufficiently large net vacancy flux are present to stabilize the formation of voids from vacancy clusters. Voids and bubbles (voids containing gas) have been observed in numerous neutron, heavy ion and high-voltage transmission electron microscopy (TEM) irradiation experiments in metals and alloys [1–13]. The significant contributions of insoluble gases (from pre-implantation or nuclear (n, α) transmutation reactions) to the cavity (voids and bubbles) nucleation and growth have been extensively discussed [1–7]. The formation of voids has also been observed with an increase of the dose by in situ heavy ion irradiation [8]. Without insoluble gases, void growth has been also demonstrated by high-voltage TEM [9] because of the much higher displacement damage rate seen in heavy ion irradiation than observed in neutron irradiations. Furthermore, previous experimental work has also demonstrated that tensile stress can enhance cavity growth during irradiation [1,10–12].

Deuterium ingress due to the corrosion of zirconium alloys can lead to the presence of hydride precipitates, and when those hydrides are sufficiently large cracks can also be initiated and propagate in the alloy via the so-called delayed hydride cracking (DHC) process [14–19]; neutron irradiation can also increase the velocity of DHC in cold-worked Zr–2.5Nb [20]. A recent nano–beam electron diffraction experiment suggests that elastic strain in zirconium close to a hydride could be very high on a local scale, up to 5% in one crystallographic direction, because the hydride is coherent with zirconium matrix. This high strain only extends ~10–20 nm away from the hydride [21]. Strain effects have been studied by molecular dynamics (MD) in body–centred cubic (bcc) alpha iron [22], face–centred cubic (fcc) copper [23] and hexagonal close-packed (hcp) zirconium [24]. In hcp zirconium, the external strain (up to 1%) mainly affects defect clustering. In this paper, we show that the strain field induced by precipitates (hydrides) could have a physical origin giving rise to stress-enhanced void growth during irradiation.

2. Methods

We have used MD simulations in alpha zirconium to study the effect of strain field on irradiation–induced defect

* Corresponding authors; e-mail addresses: dis@me.queensu.ca; gaofeium@umich.edu

http://dx.doi.org/10.1016/j.actamat.2014.09.020
1359-6462/

generation. The zirconium potential selected is the embedded atom method (EAM) potential developed by Mendeleev and Ackland [25]. This potential provides a better description of stacking fault energy than previous potentials [26]. In this zirconium potential, the most stable interstitial defect configuration is the O (octahedral) configuration. However, recent ab initio studies of self-interstitial atoms in hcp zirconium indicated a higher stability of the BO (basal octahedral) configuration than the O position [27–29]. With respect to the small difference in interstitial defect formation energies at different configurations, the 2007 potential is still one of the latest and best available EAM potentials for cascade simulation. The size of the simulation block is either $56 \times 32 \times 35$ unit cells with a total of 250,880 atoms or $72 \times 41 \times 45$ unit cells with a total of 531,360 atoms, depending on the energy of a primary knock-on atom (PKA). In displacement cascade simulation, the PKA energy is given as 5 or 10 keV, and the simulation temperature is set to 100 K. To study the strain effects, a tensile strain is applied along the ⟨c⟩ axis ([0 0 0 1]) to represent the volume expansion (based on Fig. 2b in Ref. [21]), and the selected tensile strains are 3% and 5%. The simulation system is first equilibrated at 100 K for 10 ps to achieve thermal equilibrium, then one PKA is introduced into the system and a production run of duration to 50 ps is followed. For each strain condition, 20 simulations with different PKA positions and recoil directions are carried out. Periodic boundary conditions and various time–step approaches are applied in the MD simulations. Ovito is used to visualize the final results [30].

3. Results

Fig. 1 illustrates several snapshots of the zirconium atomic positions at different times within a cascade with 10 keV PKA energy and 5% ⟨c⟩-axial tensile strain. The red and gray spheres in Fig. 1 represent the atoms in an hcp structure and a deformed structure, respectively, where common neighbor analysis (CNA) is used to identify the structure. Immediately after the collision stage, the temperature at the cascade core is very high, exceeding the melting temperature, and persists for hundreds of femto seconds. As shown in the snapshot at 1 ps in Fig. 1, the atoms near the cascade core become disordered and a large number of them are ejected from the core, several small voids being formed at the centre of the cascade; this atomic configuration is commonly observed during the initiation stage of irradiation cascade simulations. Normally, soon after the cascade, the heated zone will cool down to a relative stable status from 1 to 10 ps, and vacancies and interstitials can annihilate with each other or agglomerate to form defect clusters. Thus, these large empty spaces can also be recovered by the displaced atoms, and the remaining defects in the lattice are the material response to the irradiation damage. However, in our results (Fig. 1, Supplementary Movies 1 and 2 [31]) it is of great interest to note that the voids keep growing, which leads to the formation of a stable void at the cascade core. In the current simulations, external strains have been applied, as compared to the aforementioned normal simulations [32,33], and thus could play a key role in enhancing void growth. CNA in Fig. 1 indicates that starting from 2.0 ps, the ⟨c + a⟩-type dislocations initiate near the edges of the voids in the system. Thereafter (from 5.0 to 20.0 ps), the ⟨c + a⟩ dislocations start to slip on the pyramidal plane along the ⟨1 1 −2 3⟩directions, transporting atoms out from the cascade core, and thus the voids grow into a large void with the increase in deformation. Due to the size limitation and periodic boundary conditions, some dislocations cross boundaries and dislocation slips are pinned by other dislocations (as shown at 30.0 and 50.0 ps in Fig. 1).

Fig. 2 shows the detailed analysis of the final atomic configuration (at 50.0 ps in Fig. 1). Fig. 2a shows the cross-section of the upper-left area of the central void, where the gray and black spheres indicate atomic positions along the ⟨0 1 −1 0⟩ direction at two adjacent prism planes. The broken line in Fig. 2a illustrates the position of the stacking fault plane [34] and the slip direction ⟨2 −1 −1 3⟩, and three-dimensional analysis indicates that the slip system is active on the {1 0 −1 1} plane. The stacking fault and atomic configurations suggest that the ⟨c + a⟩ dislocation on the pyramidal planes dissociates into two partial dislocations, as demonstrated in the following equation and Fig. 3 [35,36]:

$$\frac{1}{3}[2\bar{1}\bar{1}3] \rightarrow \frac{1}{6}[20\bar{2}3] + \frac{1}{6}[2\bar{2}03] \quad (1)$$

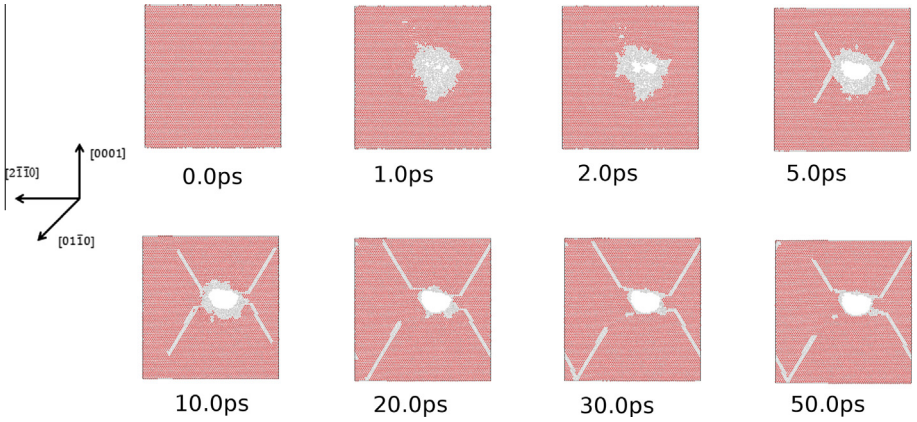

Fig. 1. A series of snapshots of Zr atoms in a 10 keV cascade evolution within a cross-section thickness of a0, viewed along the [0 1 −1 0] direction. Red spheres represent atoms in an hcp structure and gray spheres atoms in a deformed structure, where the atoms are identified based on common neighbor analysis. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)