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Molecular dynamics simulations of irradiation cascades in alpha-zirconium under macroscopic strain

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ABSTRACT

Numerous computer simulation studies have been performed on the radiation damage of zirconium. In contrast to most of the work in the literature which has focused on the effects of temperature and recoil energy on defect production and defect clustering, we have developed a computational model to consider the influence of elastic strain field on the formation of defects and their clusters, as strain is commonly present in a real reactor environment. In this work, irradiation induced displacement cascades in alpha-zirconium experiencing a macroscopic strain have been studied by molecular dynamics (MD) simulations using a many-body interatomic potential. The external strain mainly affects the size of defect clusters rather than the total number of defects. The sizes of interstitial and vacancy clusters respond differently to the external strain conditions.

1. Introduction

The CANDU (Canadian Deuterium Uranium) pressurized heavy water nuclear reactor has some distinguishing features compared with the pressurized water reactor (PWR) design. The CANDU reactor uses deuterium-oxide (heavy water) as the moderator and coolant. In contrast to the enriched uranium fuel required for PWRs, natural uranium fuel can be used in the CANDU design. Multiple pressure tubes, together with the calandria tubes, act as the pressure boundaries in the CANDU, compared to the single steel pressure vessel of a PWR. Currently, the pressure tubes are produced from Zr-2.5Nb alloy; calandria tubes are made from Zircaloy-2; and Zircaloy-4 is used for fuel cladding. Zirconium alloys are widely used in the CANDU reactors due to the low neutron absorption cross section of zirconium, the high neutron efficiency of the CANDU design is why natural uranium fuel can be used.

However, the harsh neutron irradiation in the reactor can induce macroscopic deformation and mechanical property degradation of zirconium alloys [1]. Moreover, deuterium ingress due to the corrosion of zirconium alloys can lead to the presence of hydride precipitates, and cracks can also be initiated and propagated in the alloy when those hydrides are large enough by the delayed hydride cracking process [2]. Numerous experimental [3,4] and simulation studies [5–7] have been carried out to investigate the irradiation damage of zirconium alloys.

Previous simulation studies, especially molecular dynamics (MD) simulations of the displacement cascade in zirconium, did not consider the potential effect of strain on the irradiation-induced defects [5–7]. During operation, the pressure tube experiences moderately high tangential and axial stresses. In addition, flaws and stress concentrations exist in the structure, locally raising the stress. Furthermore, the deuterium precipitates have significant strain fields surrounding them (up to 5% in one crystallography direction) due to the associated local volume expansion [8]. Therefore, understanding the impact of strain on irradiation-induced structures has importantly practical consequences. It has been noticed that strain effects have only been studied by MD in bcc alpha iron and fcc copper [9,10]. In this paper, external strains will be applied to investigate the impact of strain on defect production and defect clustering in hcp zirconium.

2. Method

The most important factor in MD simulation is the potential since it determines the interaction of atoms in the MD simulation. There are various methods that have been developed to create a reliable potential, including the embedded atom method (EAM) potential [11], F-S potential [12], Modified-EAM [13], Tersoff potential [14] and lattice inversion methods potential [15,16]. All these potentials are intended to reproduce the physical properties of the system as close as possible to the experimental value or to ab initio results.

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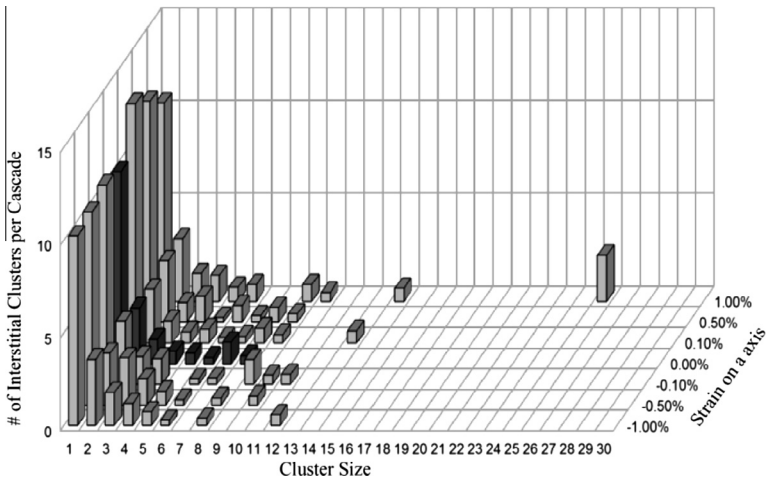

Fig. 1. Interstitial cluster distribution under ⟨a⟩ axial strain conditions (dark column: reference condition; light gray column: with strain applied).

Most previous MD work on displacement cascades in zirconium employed the EAM potential developed in 1995 [17]. Recent ab initio calculations on zirconium indicated that the stacking fault energy predicated by the 1995 potential is lower than the ab initio value. In the 1995 potential, the I_2 basal stacking fault defect energy is 3.3 meV/Å^2 and the prism stacking fault defect is unstable. However, the ab initio calculated values are 12.5 meV/Å^2 and 9.1 meV/Å^2 respectively [18,19], which means that more basal plane stacking faults will be created using the 1995 potential in the cascade simulations than expected based on ab initio calculations. More recently, in 2007, Mendelev and Ackland updated the previous alpha-zirconium potential by fitting using the ab initio data [20]. There have already been a few papers discussing the differences between the 1995 potential and 2007 potential on point defect and cluster structures [21,22]. In this 2007 zirconium potential, the most stable interstitial defect configuration is the O (octahedral) configuration; however in 2012, ab initio studies of the self-interstitial atoms in HCP zirconium indicated that higher stability of BO (basal octahedral) configuration than the O position [23,24]. With respect to the small difference of interstitial defect formation energies at different configurations, the 2007 potential is still one of the latest and best available potentials for cascade simulation. In this paper, the 2007 potential is used in the following MD simulations.

In displacement cascade simulations, the PKA (primary knock-on atoms) energy is given to be 10 keV and the temperature is 100 K. The size of the simulation block is around $18 \times 18 \times 18$ nm^3, with a total of 250,800 atoms inside. The simulation duration lasts 30–45 ps depending on the stability of irradiation induced clusters. Periodic boundary conditions, predictor–corrector algorithms and various time-step approaches are used in the MD simulations. The Wigner–Seize method and common-neighbor analysis are employed to analyze the defects.

To study the strain effects on the hcp structure of alpha-zirconium, strain is applied along either ⟨*a*⟩ axis ([10 − 10]) or ⟨*c*⟩ axis ([0002]). Both tensile and compressive strains are investigated with strains of 0.1–1.0%. It should be noticed that 1.0% elastic strain is associated with a stress beyond yield, but it is still worthwhile considering it along with lower strain conditions in order to highlight potential stress effects. For each strain condition, 20 simulations with different PKA positions and recoil directions were carried out.

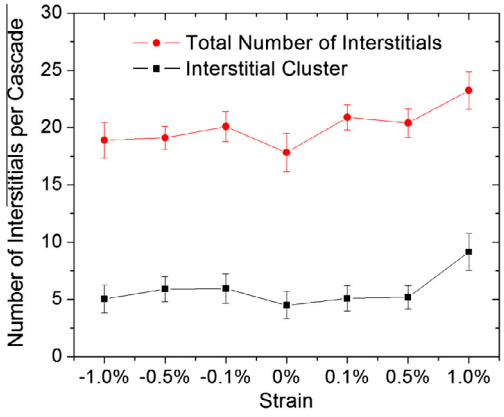

Fig. 2. Average number of interstitial defects under different ⟨a⟩ strain conditions.

3. Results

3.1. Defect configurations

The point defect clusters produced in the current displacement cascades simulations were recognized into different categories according to Ref. [7]. Most common interstitial clusters consist of a set of parallel crowdions in the basal plane and approximate to dislocation loops with Burgers vector ⟨11−20⟩ [5–7]; the second type of interstitial cluster extends along ⟨0002⟩ direction with an irregular structure [5,7]; the third type arranges on one basal plane in a triangle shape, common-neighbor analysis shows this displaced atoms layer is bound by two FCC layers. Regarding the vacancy cluster, the first type consists of three {1−100} faces as a triangular prism structure and lays on the basal plane; the second type has a pyramidal structure with {10−11} faces and a basal plane base, it is created from the collapse of accumulated vacancies on the basal plane and an embryo of c-type vacancy dislocation loop [7,25]; the third type is a mixture structure with components of the former two types of vacancy clusters.

3.2. Strain effects

3.2.1. ⟨a⟩ axial strain

As shown in Fig. 1, the interstitial defects' sizes increase at large tensile strain conditions compared with the results from the reference condition with no strain. The largest interstitial cluster