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Molecular dynamics simulations of the primary irradiation damage in Zirconium

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ABSTRACT

Atom-scale numerical calculations were performed to investigate the damage behavior in close-packed hexagonal zirconium (HCP-Zr) by primary irradiation through a molecular dynamics (MD) study. The influences of Primary Knock-on Atom (PKA) energy (E_{PKA}), the PKA incident direction and the ambient temperature (T) on the cascade collision were studied comprehensively. The results show that the athermal recombination corrected displacements per atom (arc-dpa) model is more accurate in comparison with the Norgett-Robinson-Torrens (NRT) model when predicting the steady vacancy (N_s). It was found that the vacancy peak (N_{peak}), the peak time (t_{peak}), and the steady time (t_s) increase as E_{PKA} and T increase. The steady vacancy also increases with the increase of E_{PKA}. It was also found that N_s increases and subsequently decreases by increasing T, suggesting that there is a suitable temperature to maximize N_s when E_{PKA} is constant. In addition, it was discovered that the PKA incident direction has little effect on vacancy dynamic history. It was proved that E_{PKA} can worsen the irradiation damage in crystal Zr, but T can relieve such damage. In addition, the incident direction was found to have an insignificant effect on the damage. This study highlights that the steady vacancy concentration (C) can characterize the material irradiation damage.

1. Introduction

As a rare metal, zirconium (Zr) has been widely applied in the field of military, aerospace, nuclear reaction, atomic energy, and other industries. Some notable advantages of Zr are strong corrosion resistance, high melting point, ultra-high strength, and superior hardness. In atomic energy and nuclear power, Zr has outstanding properties because of its low absorption cross-section of neutrons. Consequently, it has become an indispensable material in nuclear reactor cores [1,2]. Nuclear reactor materials are usually exposed to various types of irradiation (neutrons, ions, electrons, and γ rays). Generally, the irradiation energy associated with nuclear energy is so high that the neutron ray energy easily reaches the MeV magnitude, leading to abundant micro-defects. These include point defects, dislocations, and voids in Zr-based alloys exposed to high energy irradiation [3,4]. The long-term evolution of these microstructures causes irradiation creep, embrittlement, and expansion in the internal structure of Zr materials. These defects compromise the safety of nuclear reactor structures [5,6]. Therefore, it is important to understand irradiation damage behaviors and mechanisms.

During the nuclear reaction, the working environments include high temperatures, large ray-energy, and random ray incident directions. Thus, the primary knock-on atom (PKA) energy (E_{PKA}), the PKA incident direction, and the ambient temperature (T) are important factors that affect the material properties. Due to experimental conditions and their relative high cost, molecular dynamics (MD) simulations are widely used to simulate irradiation damage at the nanoscale [7–9]. As the simplest type of crystal defect, the point defect is one of the most frequently studied topics of irradiation damage. Gao et al. [10–13] performed an investigation on the cascade collision process in some metals with different crystal structures including α-Fe (BCC), Cu (FCC) and Ti (HCP) through MD simulations, whereby the influences of E_{PKA} and T on self-interstitials and vacancies were analyzed comprehensively. Afterwards, the cascade collisions of alloy Ni_3Al were studied and it was found that when the irradiation temperature increased from 100 to 900 K, the steady vacancy number (N_s) decreased by 30% [14]. Gao et al. [15] and Kuksin et al. [16] studied the cascade collisions of α-Fe and molybdenum (Mo), respectively. Their results demonstrated that an increase in T would decrease N_s. Further, Gao et al. [17] studied the

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vacancy evolution in Zr under irradiation damage, and proved that N_s decreased with increasing T, and increased with increasing E_{PKA}. Wu et al. [18] studied the dependence of the number and type of point defects on T during the cascade collision and found that the increase of temperature caused a slight decrease in N_s. Zhang et al. [19] studied the point defect characteristics of tungsten (W) under primary irradiation damage and concluded that the vacancy number was independent of T. Voskoboinikov et al. [20] found that the point defect number of Zr increased with increasing temperature in cascade collisions, and that the point defect number not only depended on T, but also was related to E_{PKA}. It is interesting that the conclusions about the effect of temperature on the vacancy number made between different studies [14–18] and [19,20] do not agree. Therefore, the temperature effect on N_s during irradiation cascade collisions of metal materials is unclear. In the case of the PKA incident direction, Samolyuk et al. [5] studied the anisotropy of the point defect in Zr under irradiation, and argued that a higher temperature caused a more significant anisotropy in vacancy diffusion and self-interstitials. As well, the irradiation damage of iron and γ uranium were investigated by Stoller et al. [21] and Miao et al. [22], respectively, and it was found that the PKA incident direction had no significant effect on the vacancy.

According to the above literature review, it is evident that very few studies have concentrated on investigation of the effects of the vacancy peak (N_{peak}) and its corresponding peak time (t_{peak}) or the steady vacancy and its corresponding steady time (t_s) during the irradiation cascade collision. The numerical simulation performed by the present study differs from those of other studies. The aim of the present work is to investigate the effects of E_{PKA}, the PKA incident direction, and T on the vacancy in HCP-Zr during the process of cascade collision. The open source software LAMMPS (Large scale Atomic/Molecular Massively Parallel Simulator) is used to conduct MD simulations. This paper is organized as follows: first, the simulation procedure of irradiation cascade collisions and the identification method of vacancies are introduced. Next, a potential function is used to characterize the radiation damage under different PKA energies, incident directions, and temperatures. Consequently, the dependence of the vacancy on these variables is revealed. Finally, the vacancy concentration during the collision is also investigated.

2. Methodology

MD simulations are carried out using LAMMPS to study the effects of E_{PKA}, the incident direction, and T on the point defects induced by primary irradiation damage in Zr. The visual viewer OVITO is utilized to analyze microstructural evolutions during the cascade collision. The simulation procedure is divided into two steps as follows: first, the simulated model has a dimension of 30 × 30 × 20 cells, a total of 72,000 atoms. The x, y and z directions correspond to the [1 0 0], [0 1 0], [0 0 1] crystal axes of the HCP-Zr, respectively. Three-dimensional periodic boundary conditions are used. The simulated system was simulated for 20 ps with a time step 1 fs using an isobaric-isothermal ensemble (NPT). During the process of relaxation, each atom automatically assumes the minimum state of stress and energy to obtain a stable equilibrium structure. This structure is output as a reference for identifying point defects after the irradiation damage. The second step is to select an atom as the PKA in the reference structure and give it an initial energy (the initial energy is converted into a velocity to apply on the PKA) and an incident direction. To facilitate the observation of the vacancy evolution, an atom in the model center is chosen as the PKA. After the PKA is set, the irradiation damage cascade is applied by canonical ensemble (NVT) lasting 20 ps with a time step of 0.1 fs. In order to produce meaningful statistics, ten cascades are performed at each E_{PKA}, PKA incident direction, and T.

After a simulation, the new position of each lattice atom is obtained, and the new structure is compared with the reference structure. Some identification methods of point defects include Wigner-Seitz (W-S) cell method, common neighbor analysis (CNA), and lattice matching method (LMA). The W-S method is used in this work. The advantage of the W-S method is its convenience for identifying defects (vacancies and interstitial atoms) [23]. Therefore, it is included in the OVITO software, and is employed to identify the point defects in this study. The detailed procedure is outlined as follows: the atom lattice position in the stable equilibrium structure after relaxation is taken as the reference structure. If there is no atom in the W-S cell, the lattice position in the cell is defined as a vacancy. In contrast, if a cell contains more than one atom, the atom closest to the original lattice position is defined as the central atom, and the other atoms are defined as interstitial atoms.

3. Potential validation

The interatomic potential plays an important role in MD simulations. In this work, a potential of HCP-Zr is derived from the 2# EAM (Embedded Atom Method) potential proposed by Mendelev et al. [24]. This potential has been proved to be capable of providing a reliable description of primary collision cascades in HCP-Zr [25].

In order to validate the accuracy of the 2# EAM potential, the atomic volumes for a cell are calculated. Fig. 1 shows the temperature dependence of atomic volumes. It is shown that as the temperature increases, the average volume increases gradually. After the temperature reaches about 2266 K, the volume exhibits a jump, which indicates that HCP-Zr has been converted from solid to liquid phase. In other words, 2266 K is the estimated melting point of HCP-Zr. This is close to the standard melting point of 2125 K [26], with an error of 6.6%. Thus, it is demonstrated that this potential can be used in the present simulations.

4. Results and discussion

4.1. Evolution of primary damage

The point defects of Zr contain self-interstitials and vacancies induced by primary irradiation. Fig. 2 shows the dynamic evolution of these vacancies. Between 0 and 0.65 ps, the lattice atoms are knocked out quickly, which can be attributed to the larger E_{PKA}. The lattice atoms with sufficient energies obtained from PKA move by a large displacement, and subsequently collide with other lattice atoms, leading to the cascade collision. Afterwards, many vacancies pile up, and a displacement spike occurs at 0.65 ps (marked with the red circle). This is called the ballistic phase, as shown in Fig. 2a, b. During the period of 0.65–13 ps, the vacancies decrease quickly due to the rapid

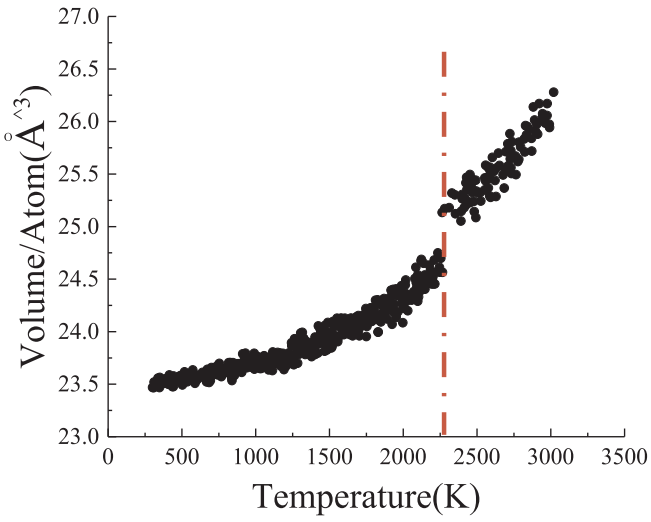

Fig. 1. Influence of T on the average volume per atom.