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Influence of self-interstitial mobility on damage accumulation in zirconium under fission irradiation conditions

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Abstract

Irradiation of zirconium is studied using a kinetic Monte Carlo model. The initial cascade damage produced by 25 keV recoils at a temperature of 600 K obtained from molecular dynamics simulations is used in the calculations. The evolution of the microstructure under fission irradiation conditions has been followed for a number of displacements per atom (dpa) up to 0.5. In particular, the influence of self-interstitial cluster migration on the total defect concentration and size is analyzed. Results are compared with available experimental data.

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1. Introduction

Advanced Zr alloys are proposed to be used for high burnup applications in current light water reactors as well as for cladding and internal components in future Generation IV reactors. Consequently, understanding the effect of irradiation on the mechanical properties of these alloys is crucial for safe operation of these reactors. However, knowledge of basic irradiation effects in Zr is very scarce in particular at a microscopic level. This work focuses on the description of microscopic effects of irradiation using computer simulations in a multiscale approach.

Molecular dynamics (MD) simulations performed by Voskoboinikov and Bacon [1,2] have provided information about the damage produced by displacement cascades in α-Zr with recoil energies up to 25 keV and different temperatures. These calculations show that point defect clusters created in simulations of displacement cascades in zirconium can be classified in three typical self-interstitial atoms (SIA) categories: SIA dislocation loops with Burgers vector 1/3 ⟨1120⟩, triangular arrangement of SIAs within one basal plane, and three-dimensional irregular. Only the first one of these SIA-clusters is glissile while the other two types are sessile. There are also three typical vacancy categories, all of them sessile: triangular prism shape, pyramidal shape and the third type is best described as two components joined together.

On the other hand, MD simulations have also been used to study the mobility of defects in α-Zr

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[3]. These simulations show that single interstitials move in one dimension in the basal plane. Some of the self-interstitial clusters also move in one dimension while others remain immobile. Monovacancies move in three dimensions in the crystal and vacancy clusters are immobile. The mobility of these self-interstitial clusters is a key parameter for developing damage evolution models in metals through either rate theory or kinetic Monte Carlo simulations. In particular, the work of Soneda [4] and of Domain et al. [5] in Fe have shown that the mobility of these clusters is crucial to be able to reproduce the experimental measurements in this material. However, there are still many unknowns mostly regarding the effect of impurities.

The damage accumulation in h.c.p. Zr under irradiation has been studied using a kinetic Monte Carlo (kMC) approach with information provided by MD calculations. We have considered fission reactor conditions, that is, damage (dpa) rate of $10^{-6}\,s^{-1}$ and a temperature of 600 K. The defect concentration as a function of displacements per atom as well as the cluster size distributions has been obtained from these calculations. In particular the influence of self-interstitial cluster migration on the final defect concentration and size is analyzed.

2. Simulation model

An object kinetic Monte Carlo model is used to study the evolution in time of those defects produced during irradiation. The database of displacement cascades produced by Bacon et al. [1,2] using MD is used as initial defect configuration. Cascades were produced by recoils from 10 to 25 keV in steps of 5 keV at 600 K. Information about migration and binding energies of different cluster types and sizes have also been obtained using MD [6,7] and used as input in the kMC [8]. In this model defects are allowed to execute random diffusion jumps (in one, two or three dimensions depending on the nature of the defect) with a probability proportional to their diffusivity. During the simulation, various kinetic processes (events) are allowed to take place: dissociation of a particle from a cluster, diffusive jump of a particle, recombination, association of two defects of the same type, annihilation of a defect at a sink, trapping or de-trapping of a defect at an impurity and introduction of a new cascade.

In order to understand the behavior of the microstructure for Zr, the study initially focused on the evolution of single cascades, and the diffusion and stability of clusters for long times (h), as well as the possibility of formation of clusters. The number of defects escaping recombination was obtained from these calculations, and therefore the number of defects that would interact with the microstructure [9]. These cascade aging simulations followed the same methodology than previous work for Fe [4]. Our simulations showed that dissolution of small vacancy clusters at 600 K is expected as well as migration of single vacancies. 1D migration of interstitials results in small recombination between interstitials and vacancies. The number of vacancies that move to the surface increases when PKA energy decreases because of vacancy clusters are small at low energy and dissolve. However, the number of interstitials that diffuse to the surface is constant with PKA energy.

Using 25 keV cascades, the evolution of the microstructure during irradiation under fission environment conditions has been studied. Periodic boundary conditions were used in this case. The size of the computational box was $100 \times 100 \times 100\ nm^3$. A database of 25 different cascades placed in random locations in the simulation box was repeated in order to simulate the damage accumulation until the total dose was reached. One-dimensional (1D) migration was considered for single interstitial atoms (SIAs) and mobile interstitial clusters, while three-dimensional (3D) motion was used for monovacancies. Vacancy clusters and several interstitial clusters (depending on the initial cascade configuration) are assumed to be immobile. In order to improve the simulation time a grain boundary approximation has been introduced: grain size of 1 μm. That is, if one defect moving in 1D makes 10^6 jumps without finding another one it disappears in a sink.

3. Results

Fig. 1 shows the concentration of visible clusters as a function of displacements per atom for vacancies (triangles) and for self-interstitials (circles). Those clusters that have more than 50 defects, which correspond to loops of about 2 nm, are considered as visible under TEM. In this way, the results of the simulations can be compared to experimental measurements as done earlier in [5,10]. At this temperature, 600 K, the concentration of visible interstitial clusters is very low, approximately $1 \times 10^{15}\ cm^{-3}$ for a dpa dose of 0.5, while the concentration of visible vacancy clusters is three orders of magnitude higher. Therefore, under these condi-