1st International & 28th National Conference on Nuclear Science & Technology 2022 (ICNST22)
Nuclear Science & Technology Research Institute

Molecular static simulation of irradiation induced collision cascade and micro-structure evolution in Zr-1%Nb alloy

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Abstract

Because of the stability, corrosion resistance and other good mechanical properties, zirconium and its alloys with niobium have extensive applications in nuclear industry, especially in fuel cladding. In this study, we have considered the micro-structural evolution of this alloy when it is subjected to energetic irradiation. Lattice parameters and other mechanical properties have been calculated and there was a good conformation with experimental results. It has been shown that the maximum damage depth of defect production in this alloy is highly correlated to the direction of irradiation and the average is changed nearly linear with Primary Knocked-on Atom (PKA) energy. Also the collision cascade phenomenon in this alloy has been studied and analyzed to produce defects.

Keywords: Molecular statics, Zr-1%Nb alloy, collision cascade, damage depth, threshold displacement energy.

Introduction

Zirconium, as structural materials in reactors, has special mechanical properties and has a good resistivity against corrosion as well as the low neutron absorption cross section [1]. One of the most important application of this alloy is fuel cladding. It is, therefore, important to study micro-strcure evolution on irradiation due to fission in reactors. According to available data, there are three phases for zirconium crystalline: α-phase (<863 °C), β-phase (> 863°C) and ω-phase (Pressure 2-7 GPa) [2-3]. Zr-1%Nb has the HCP structure at low temperature.

This alloy is under irradiation effects in reactors. Vacancies (V) and Self-Interstitials (SI) (which called Frenkel Pairs [FP] together) can be produced during fission reaction. Some of these defects will be dissappeared because of recombination between V and SI and some others will move through the alloy and make greater defects like voids and other extended defects [4]. All of these phenomenon can be happened in this alloy and can cause to change in mechanical and chemical properties of that. If the incident energetic particles have enough energy they can transfer some energies into the structure and displace atoms from its crystal positions (Primary Knocked-on Atom [PKA]) and produce FPs. Each PKA can also collide to another atoms and produce other knocked-on atoms and the collision cascade (CC) phenomenon can occur.

This article consists of two sections: at first, the lattice parameters of Zr-1%Nb has been calculated and the damage depth of PKA as a function of their energy has been considered for Zr atoms in this alloy. Second, the elastic properties of this micro-structure evolution have been studied. In each part the CC phenomenon have been analyzed carefully.

Methodology and computational details

Molecular Statics (MS) is an effective tools to simulate all phenomena which is happening during CC. In this article the LAMMPS [5] code package has been used to simulate the iraddiation induced defects in Zr-1%Nb alloy. All of the simulations have been done at near zero temperature. The structures have been fully optimzed with NPT ensemble and then NVE ensemble has been used to simulate the CC phenomenon. The recent Zr-Nb interatomic potential [6] has been used in these results.

Results and discussion

Lattice parameters and damage depth of PKA.

At first, the lattice parameters of pure-Zr have been obtained 3.188, 5.206 Å in X- and Z-direction which is in accordance with experiments 3.232, 5.149 Å [7]. Each supercell of Zr-1%Nb has 96 atoms and HCP structure and the lattice parameters for this alloy in X- and Z-directions have been also calculated as 12.856, 15.360 Å. Vacancy and self-interstitial formation energy for Zr-structure have also been obtained as 1.90, 2.76 eV respectively, which can be compared with experiments and DFT (> 1eV) [8], 2.75 eV [9].

The damage depth (DD) is the maximum distance of PKA position to the furthest SI namely the length affected of the structure by irradiation. On the other hand, this factor is a damage criterion of the structure for each incident energetic particles. The DD of Zr-1%Nb alloy is highly dependent to the irradiation with respect to crystalline orientations. This spatial angle dependency is depicted in Figure 1 for different PKA energies. Five direction have been chosen as the 1st Nearest Neighbor (NN), 2nd NN in X-direction, 2nd NN in XY-plane direction, 3rd NN and 4th NN of the HCP structure. It is shwon that the DD for each direction is different and the maximum DD can be found in the 2nd X- and 2nd XY-directions. It has also shown that an increase of the E(PKA) can leads to an increase of DD. Furthermore, The treatment of mean value of all DD in these orientations with respect to the PKA enegy is nearly linear and is shown in table1.

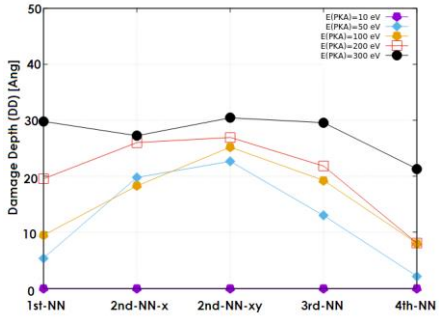

Figure 1. DD dependence to five nearest-neighbors in Å.

Table.1: The average DD for different E(PKA) in Å.

E(PKA)	50	100	200	300
AvgDD	12.59	16.04	20.46	27.66

Elastic properties and collision cascade.

The local elastic moduli of Zr-1%Nb structures have been calculated for different PKA energies and they have been shown in Figure 2. Despite this fact that there is no huge amount of change in elastic moduli, it is clear that the growth in PKA energy have led to: increase in relative bulk modulus (B) and Poison ratio (v) (~1%) and decrease in young (E) and shear (G) modulus (~4%). As it is known in literatures, "E" is the stiffness of the material (how easily the material bended or stretched), "B" is the resistance of material to compression, "G" is the response of material in shear forces and "v" is the behavior of material in vertical plane, when it is subjected to lenghwise stretching. From our results, it has been shown that the stiffness and resistance of Zr-1%Nb to shear force have been decreased because these parameters can be meaningfully affected by distortion of structure symmetry and the resistance of this alloy to compression and fracture have been increased because this parameters are related to stress tensor. In other words, adding some energy to the system will cause to increase in local stress tensor.

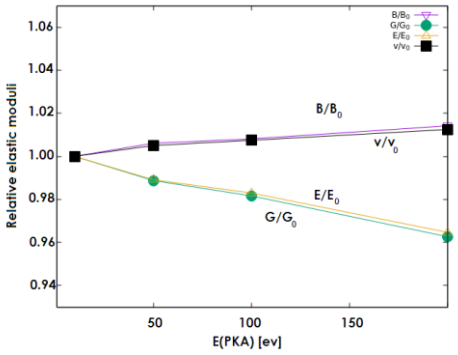

Figure 2. The effect of low PKA energy on local relative elastic moduli.

Finally, we have monitored the collision cascade phenomenon in Zr-1%Nb. The typical CC phenomenon for this alloy have been depicted in Figure 3. The most disturbed is in 0.5 Ps and at the end of the simulation (15 Picoseconds). As it can be seen, there is no any point defect cluster and SIs (Vs) have been detected individually.

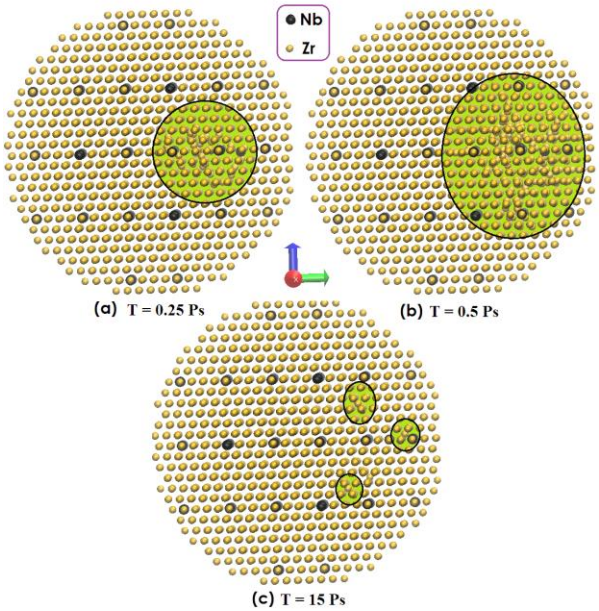

Figure 3. collision cascade for E(PKA) = 200 eV.

Conclusions

In this study we have calculated the DD for Zr-1%Nb alloy and the results showed that the rise in PKA energy will caused to increase in DD. Futhermore, DD is meaningfully dependent on the direction of irradiation. Four nearest neighbor have been chosen for the verification of this topic. At last, it was shown that the local elastic moduli have changed as changing the PKA energy and typical CC phenomenon and the formation of defects have been considered during the irradiation.

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