Irradiation induced Microstructural evolution and Damage Depth of Zr-1%Nb alloy using atomistic simulation

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Introduction

Zirconium-niobium alloy is used as structural materials in reactors. The study of micro-structure evolution of this alloy is, therefore, important when it is subjected to energetic irradiations due to fission in reactors. Zr-1%Nb has the HCP structure at low temperature and Niobium atoms is distributed homogeneously. This study is included in three major sections: At first, lattice structure properties have been reviewed to verify the validity of the calculations. Then, Damage Depth (DD) have been calculated for Zr and Nb as PKA atoms and the results of DD have been compared.

Method

All calculations have been done using atomistic simulation by LAMMPS code packages. Angular Dependent Potential (ADP) is used for simulations. This potential is a new interatomic potential and it has been mostly used for metals and metal alloys. 43008 atoms in 8×8×7 supercell (with 96 atoms) have used for simulation of Zr-1%Nb alloy. There is no any temperature effect on this study, so all calculations have been done at near zero temperature. The structures have been fully optimzed with NPT ensemble and then NVE ensembles have been used to simulate DD process. The 8 Picoseconds have needed for equilibration of the structure DD phenomena when the structure have been subjected to radiation.

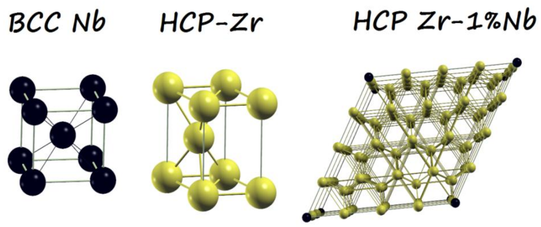

Figure 1
Zirconium, Niobium and Zr-1%Nb alloy structures at low temperatures

	a	c	VFE	SIFE
Pure-Zr-this work	3.188	5.206	1.90	2.76
Pure-Zr-exp	3.232	5.149	1<	2.75
Zr-1%Nb	12.856	15.360	-	-

Table 1
Lattice properties for Zr and Zr-1%Nb

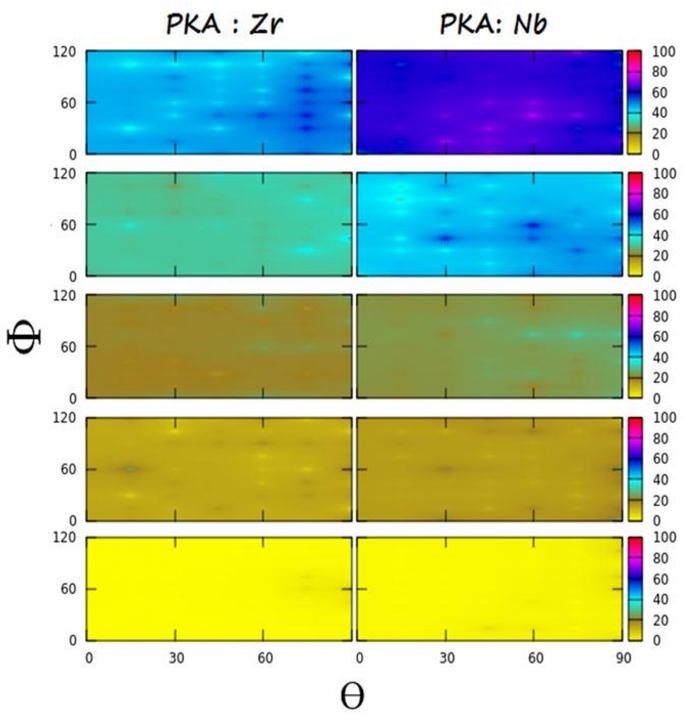

Figure 2
The 2D map dependency of DD to the polar and azimuthal angles of irradiation for different E(PKA): 10, 50, 100, 200 and 300 eV.

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Results & discussion

The damage depth (DD) is the maximum distance of PKA position to the furthest SI namely the maximum length which is affected of the structure by irradiation. On the other hand, this factor is a damage criterion of the structure for each incident energetic particle. The DD of Zr-1%Nb alloy can show the strength of this alloy when it is subjected to irradiation and it is highly dependent to the irradiation with respect to crystalline orientations. When this alloy is subjected to irradiation, PKA atoms can be Zr or Nb atoms. Therefore, the results of damage of the structure can be different for different PKA atom type. In general DD is larger for Nb-PKA atoms in this structure. From experimental data the threshold displacement energy for Zirconium structure to produce a stable Frenkel pair is about 22.5 eV. According to our calculation for PKA energy between 20-30 eV stable Frenkel pair can be seen in most directions.

References

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