Iranian Journal of Physics Research, Vol. 20, No. 1, 2020

The study of the properties of point defects in pure-Zr and Zr-1%Nb alloy using density-functional theory and atomic simulation

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(Received 09 September 2019 ; in final form 11 December 2019)

Abstract

Crystal defects play an important role in the material strength and its mechanical properties. The Zr-1%Nb alloy, because of its low cross-section for thermal-neutron capture, corrosion resistance in water and suitable mechanical properties, is widely used in nuclear reactors. This alloy has an HCP structure at low temperatures and for low concentrations of Nb impurity. In this work, using the first-principles density-functional theory calculations, as well as molecular dynamics calculations with interatomic potentials, we have investigated the properties of vacancy and self-interstitial point defects in pure zirconium. The formation energy and formation volume are calculated; the results show a good agreement with the experimental values. These quantities are calculated for the Zr-1%Nb alloy as well; the results do not show any significant differences with those of the pure Zr. In addition, the interaction between two vacancies is investigated; by the calculation of the binding energies for di-vacancy clusters in different configurations, it is shown that only those clusters are stable for which the vacancies are in the first neighbor positions. Finally, the displacement energy of a vacancy in the basal plane is calculated, showing a good agreement with experiment.

Keywords: nuclear reactor, zirconium-niobium alloy, crystal defect, density-functional theory, molecular dynamics

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