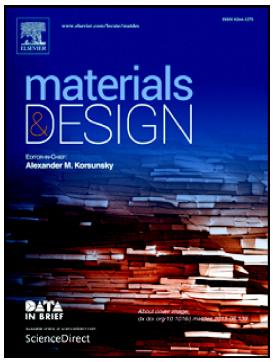

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PII: S0264-1275(17)30080-1
DOI: doi: 10.1016/j.matdes.2017.01.060
Reference: JMADE 2701

To appear in: *Materials & Design*

Received date: 3 August 2016
Revised date: 18 January 2017
Accepted date: 19 January 2017

Please cite this article as: Xueyan Zhu, Xingyu Gao, Haifeng Song, Guomin Han, De-Ye Lin , Effects of vacancies on the mechanical properties of zirconium: An ab initio investigation. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jmade(2017), doi: 10.1016/j.matdes.2017.01.060

Effects of vacancies on the mechanical properties of zirconium: An *ab initio* investigation

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Abstract

The irradiation-induced defects strongly influence the mechanical behaviors of zirconium (Zr) and its alloys in nuclear reactors. In this work, we focus on how the vacancies change the mechanical properties of α-Zr through density functional theory (DFT) calculations. Both uniformly distributed vacancies and vacancy clusters were considered. And a wide range of vacancy concentrations from 0.005 to 0.063 (molar fraction) was modeled. The most stable configurations of di- and trivacancy clusters were predicted, which correspond to the most compact distribution of vacancies. Mechanical properties were explored in terms of single-crystal elastic constants, based on which the polycrystalline elastic moduli, Pugh's ratio for ductility and Vickers hardness were derived. Our results show that the existence of uniformly distributed vacancies can reduce the ductility, while enhance the hardness in general. However, when the vacancy concentration is larger than a critical value, a rise in the ductility and a reduction in the hardness occur, which may contribute to the degeneration of the material. Compared with the uniform distribution of vacancies, clustering of vacancies strengthens the above changes of ductility and hardness. Moreover, it was found that the anisotropy of Young's modulus decreases with increasing vacancy concentration.

Keywords: zirconium; irradiation; vacancy; mechanical property; density functional theory

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