DEVELOPMENT OF ATOMISTIC MODEL FOR PREDICTION OF PROPERTIES OF BINARY ZR-NB SYSTEM

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Zirconium is a constituent of many alloys, which found their application in substantially different areas: from nuclear engineering to medical prosthetics. As examples, we can mention here corrosion-resistant cladding alloys, namely Zr-2.5%Nb, and a series of Ti-Nb-Zr medical alloys. Characteristics of the given alloy strongly correlate with the properties of zirconium phase on which it is based. Therefore, the determination of the zirconium phase stability conditions is an essential issue for the design of the mentioned materials. At the same time, some controversies exist on the phase transitions in zirconium. The range of questions varies from the uncertainty in the melting line to the disputes about the details of the solid-solid phase transitions and influence of the alloying elements. Here we report a new attempt to study properties of Zr-Nb binary system. For this purpose, we constructed an angular-dependent many-body interatomic potential [1]. The potential functions were fitted towards the *ab initio* data computed for a large set of reference structures. We show that the model reproduces structure and properties of all Nb and Zr phases existing in the Zr-Nb binary system with a good accuracy. Moreover, the model can be applied for prediction of melting and α-Zr $\longleftrightarrow$ β-Zr transition temperatures. The potential provides an opportunity for simulation of Zr-Nb alloys based on α-Zr and β-Zr. This conclusion is illustrated by the results obtained for the alloys with different niobium concentrations: up to 7% in case of hcp alloys and up to 50% for bcc alloys. Besides, we report results of the deformation tests made for the atomistic models of β-Zr-Nb alloys with different niobium content.

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1. Smirnova D.E., Starikov S.V. // An interatomic potential for simulation of Zr-Nb system. Comp. Mater. Sci. 2017 V. 129. P. 259.