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Prediction Study of the Structural, Elastic and Electronic Properties of the Parent and Martensitic Phases of Nonferrous Ti, Zr, and Hf Pure Metals

Authors : Tayeb Chihi, Messaoud Fatmi

Abstract : We present calculations of the structural, elastic and electronic properties of nonferrous Ti, Zr, and Hf pure metals in both parent and martensite phases in bcc and hcp structures respectively. They are based on the generalized gradient approximation (GGA) within the density functional theory (DFT). The shear modulus, Young's modulus and Poisson's ratio for Ti, Zr, and Hf metals have were calculated and compared with the corresponding experimental values. Using elastic constants obtained from calculations GGA, the bulk modulus along the crystallographic axes of single crystals was calculated. This is in good agreement with experiment for Ti and Zr, whereas the hcp structure for Hf is a prediction. At zero temperature and zero pressure, the bcc crystal structure is found to be mechanically unstable for Ti, Zr, and Hf. In our calculations the hcp structures is correctly found to be stable at the equilibrium volume. In the electronic density of states (DOS), the smaller n(EF) is, the more stable the compound is. Therefore, in agreement with the results obtained from the total energy minimum.

Keywords : Ti, Zr, Hf, pure metals, transformation, energy
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