Nonlinear response of titanium to deformation at high temperature

Sinyakov R I[@] and Belov M P

National University of Science and Technology "MISIS", Leninskiy Avenue 4, Moscow 119049, Russia

[@] sinyakov999@mail.ru

Lattice dynamics and mechanical properties of the bcc titanium (β–phase) at high temperatures were studied using the method of ab initio molecular dynamics. The temperature-dependent effective potential method (TDEP) [1, 2] was used to analyze the anharmonic vibrations of the atoms at 1300 K. This method was utilized to build effective lattice Hamiltonian, which was used to calculate the phonon spectra and the broadening of the dispersion curves. In addition, the stress-strain relation of the bcc titanium at 1500 K were calculated. For a given deformation scheme, analytical expressions for the stress-strain dependence for the cubic lattices with the elastic constants up to 4th order were derived based on the relations from [3]. The elastic constants of the bcc phase of titanium were calculated up to the 4th order at 1500 K. In this work we showed the dynamic stability of the β–phase of titanium at high temperatures. Accounting the anharmonic terms in the lattice Hamiltonian is necessary to reproduce all the features of the phonon spectrum of this system. Remarkably, the response of the titanium β–phase lattice to deformations is nonlinear and considering nonlinear terms makes it possible to achieve better agreement with experimental results.

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[1] Hellman O, Abrikosov I A and Simak S I 2011 *Phys. Rev. B* **84** 180301
[2] Hellman O and Abrikosov I A 2013 *Phys. Rev. B* **88** 144301