THERMODYNAMIC PROPERTIES OF Pd_3Fe ALLOY WITHIN THE QUASIHARMONIC APPROXIMATION*

Y.A. ABZAEV[1], A.A. GUDA [2,3], S.A. GUDA [2,3], V.I. KOLESNIKOV[3]

[1]*Tomsk State University of Architecture and Building, Tomsk, 634009 Russia*
[2]*International Research Institute of Smart Materials, Southern Federal University, Rostov-on-Don, 344090 Russia*
[3]*Rostov State Transport University, Rostov-on-Don, 344038 Russia*
*e-mail: Abzaev2010@yandex.ru
[2]*Affiliation, City, Country*

The ordered alloy Pd_3Fe with the superstructure $L1_2$ was chosen as the object of study. Ab initio calculations of thermodynamic and mechanical properties of Pd_3Fe in the temperature range T = 0 ... 1000K were performed in Phonopy code with VASP interface on the supercomputer "Blokhin" of the International Research Institute of Smart Materials of the Southern Federal University. Fig.1 shows the temperature dependences of the bulk modulus of elasticity, free energy, entropy, specific heat capacity, and lattice volume. The Pd_3Fe lattice was optimized beforehand. An extended Debye model was considered, in which the temperature dependence of the lattice volume was taken into account.

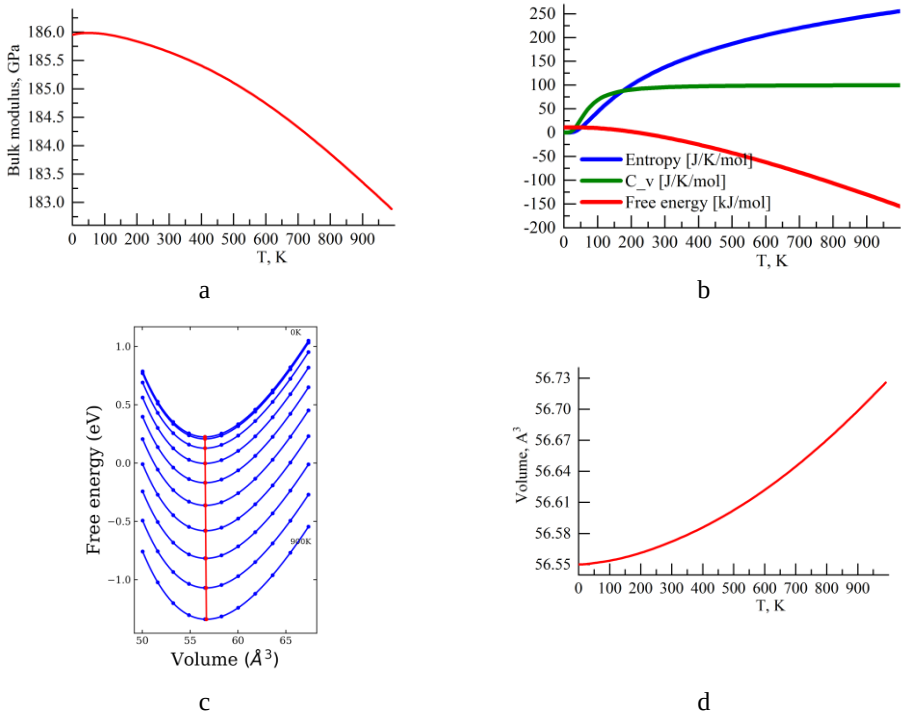

Fig.1. Thermodynamic properties of Pd3Fe alloy: (a) bulk modulus of elasticity; (b) entropy, free energy, specific heat capacity; (c) free energy as a function of volume at different temperatures; (d) lattice volume.

It follows from the analysis of the results that the lattice volume growth by 0.19 A^3 is accompanied by a noticeable change in the thermodynamic and mechanical properties of Pd_3Fe. The bulk modulus monotonically decreases the lattice free energy of the Pd_3Fe alloy also decreases significantly. A significant increase of heat capacity in the low-temperature region is observed, and in the high-temperature region the heat capacity C_p comes to saturation. The results of modeling of thermodynamic and mechanical properties considered in this work can be applied to the evaluation of tribological characteristics for both Pd_3Fe and multicomponent alloys.

* The work was supported by the Russian Science Foundation (project No 21–79–30007).