MONTE CARLO SIMULATION OF STRUCTURAL PHASE TRANSFORMATIONS DURING CRYSTALLIZATION IN TITANIUM-BASED NANOCLUSTERS

D.N. Sokolov, N.Yu. Sdobnyakov, V.S. Myasnichenko, E.M. Davydenkova, A.Yu. Kolosov, P.M. Ershov, S.A. Veresov

Tver State University, Tver, Russia

nsdobnyakov@mail.ru

In this paper, we intend to simulate and analyze changes of the structure of nanosized bimetallic titanium-based clusters (*TiAl* and *TiV*) during cooling. To specify the interatomic interaction, the many-body tight-binding potential was chosen. The known numerical parameters of the potential for titanium, vanadium, and aluminum were used [1, 2]. The simulation was carried out by the Monte Carlo method and using software [3]. The initial configuration of 500 atoms (including 250 *Ti* atoms) was heated to complete disordering. Then the nanoparticle was cooled to 100 K in increments of 10 K. The particles' energy spectrum is shown in Fig. 1 (for intermediate configurations) and was implemented in Ovito [4]. The analysis shows a significant difference both in the range of particle energies and in the average energy, which can affect the stability of such particles.

The thermodynamic and structural characteristics of *TiAl* and *TiV* bimetallic nanoalloys in sequential heating and cooling processes were presented in fig. 2-7.

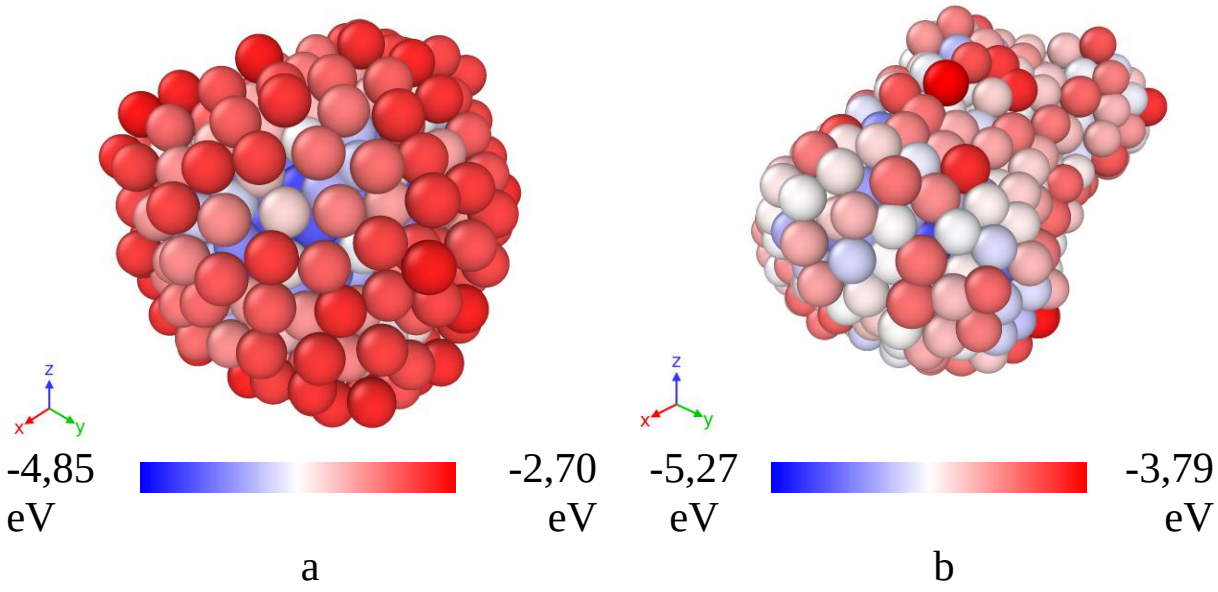

Fig. 1. Energy spectrum of *TiAl* (a) and *TiV* (b) nanoparticles at T=650 K.

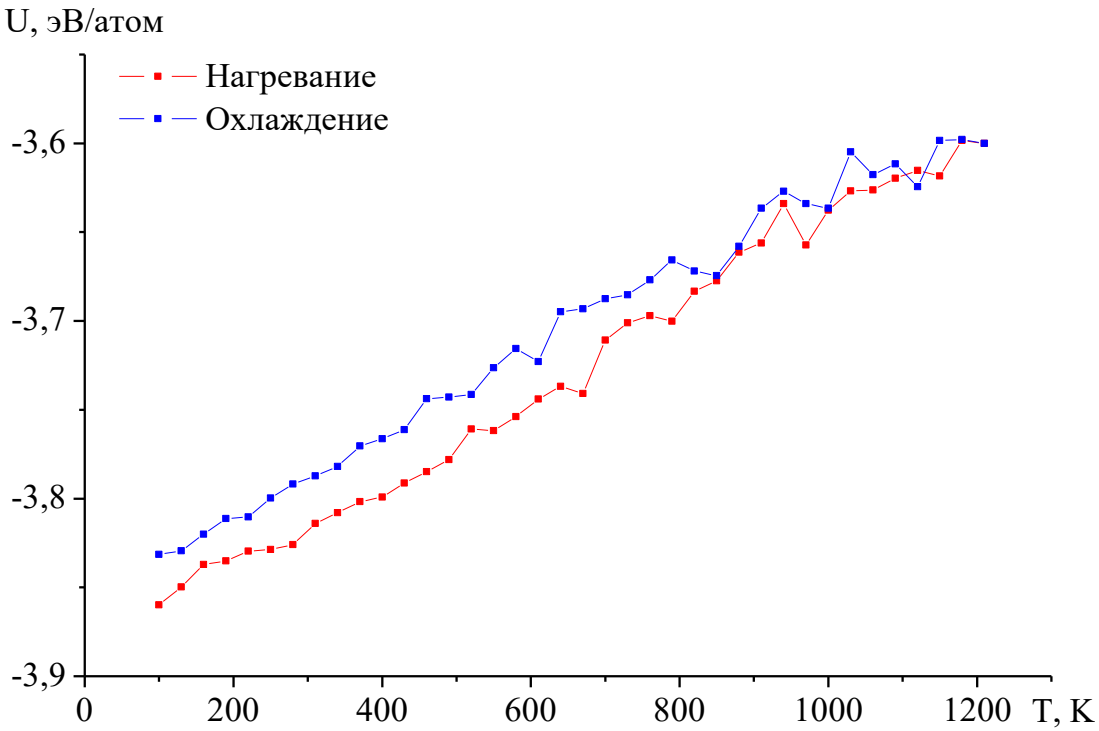

Fig. 2. Caloric dependences of a bimetallic system $Ti_{250} - Al_{250}$.

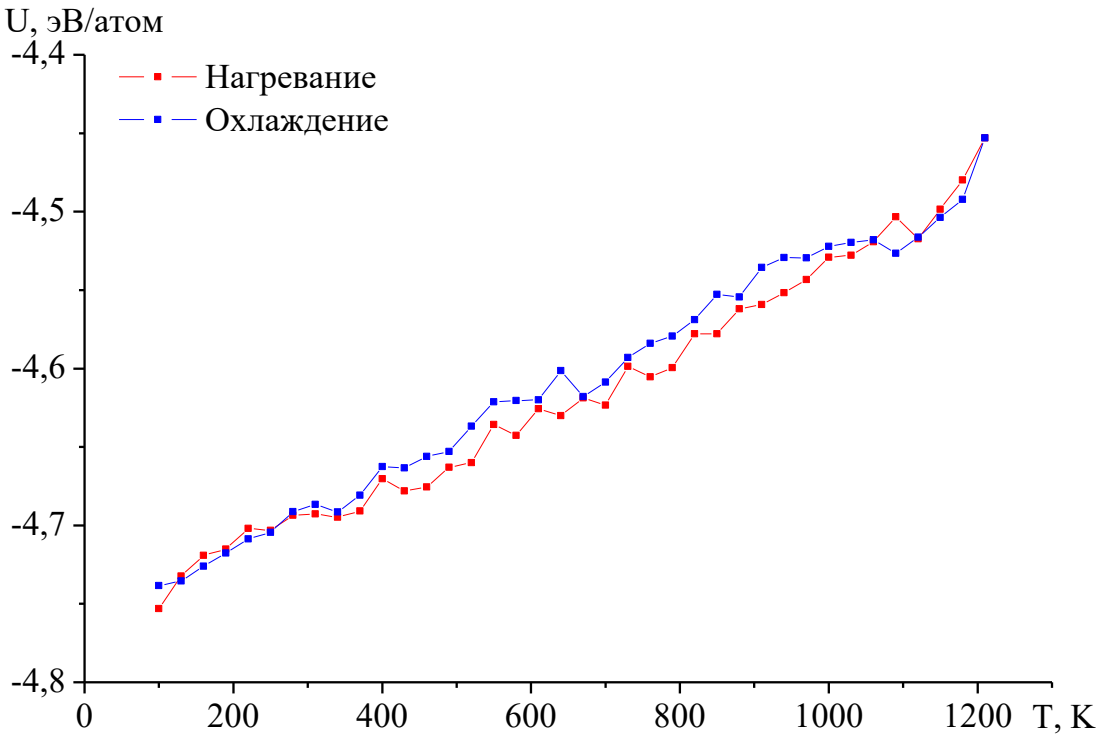

Fig. 3. Caloric dependences of a bimetallic system $Ti_{250} - V_{250}$.

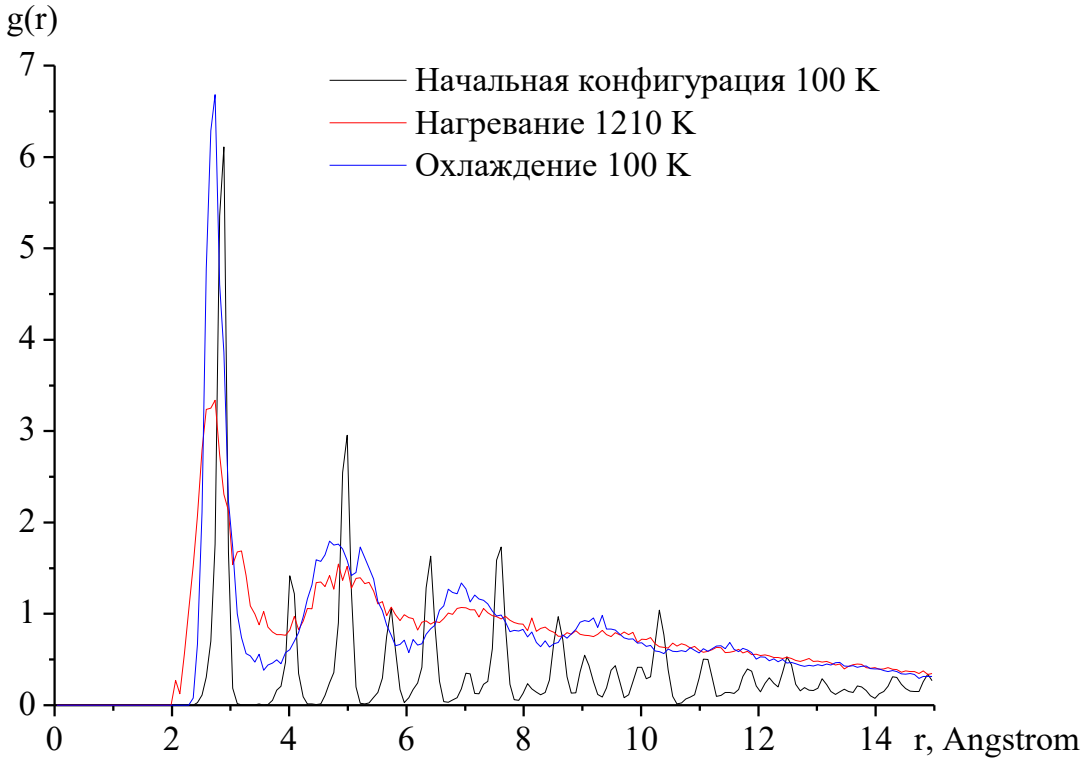

Fig. 4. Radial distribution functions for a bimetallic system $Ti_{250} - Al_{250}$.

Fig. 5. Radial distribution functions for a bimetallic system $Ti_{250} - V_{250}$.

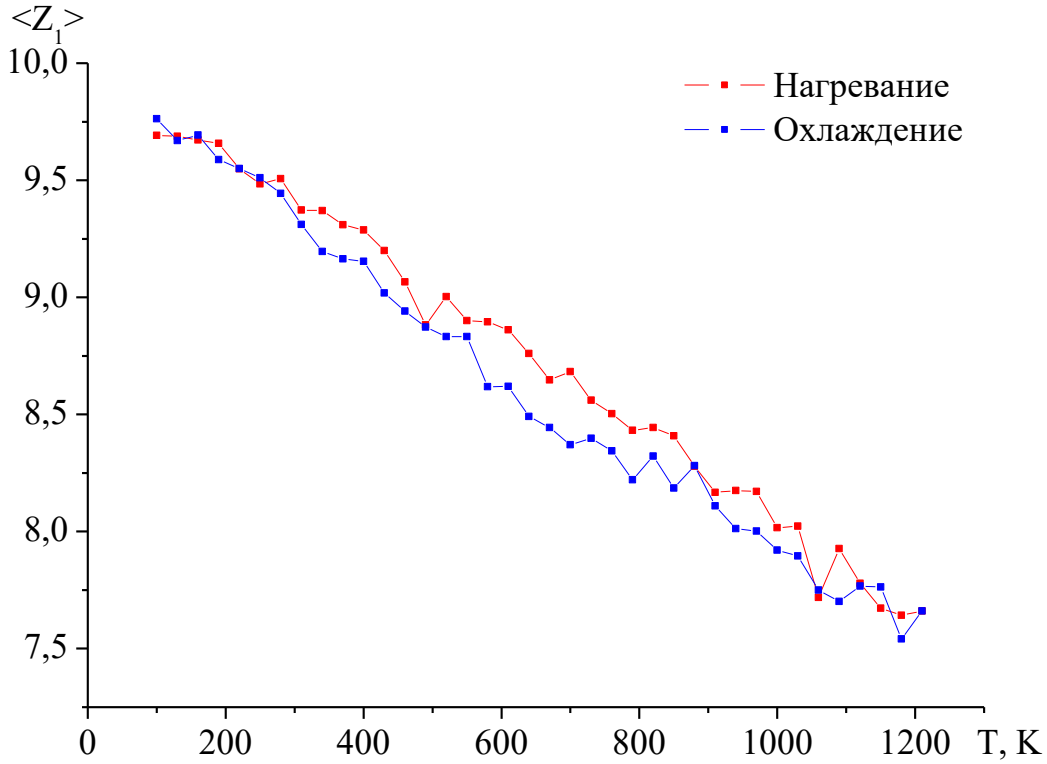

Fig. 6. Temperature dependences of the average value of the first coordination number for a bimetallic system $Ti_{250} - Al_{250}$.

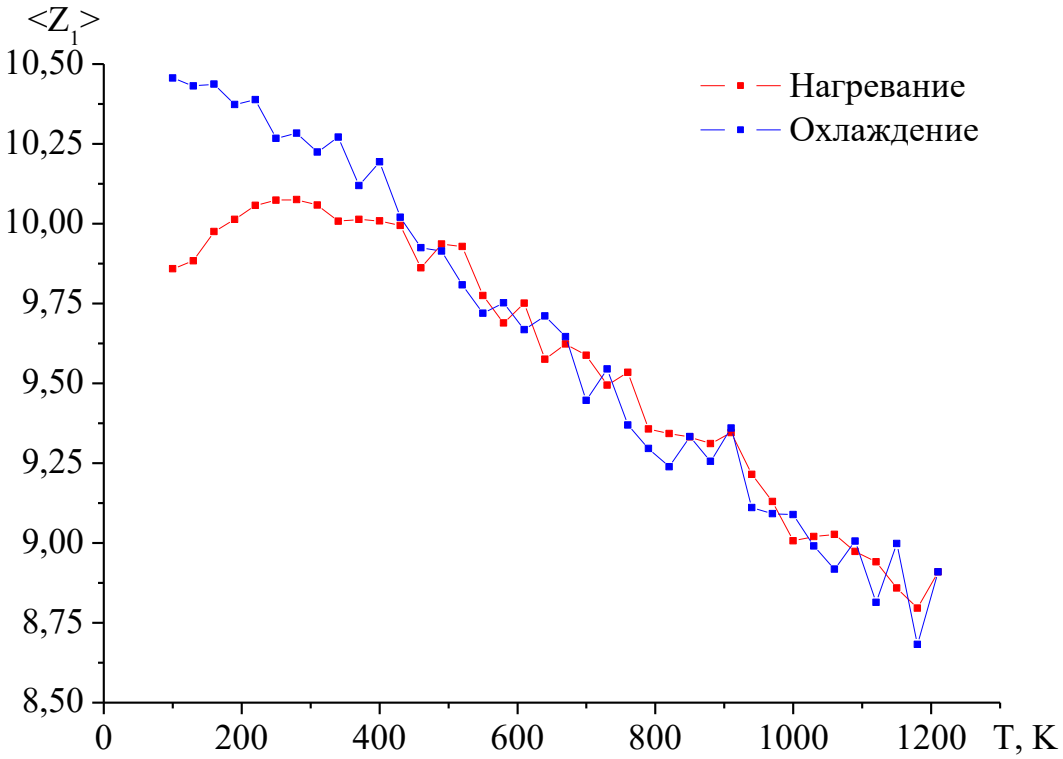

Fig. 7. Temperature dependences of the average value of the first coordination number for a bimetallic system $Ti_{250} - V_{250}$.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation in the framework of the State Program in the Field of the Research Activity and was funded by RFBR, project numbers (№ 18-03-00132, № 20-37-70007).

1. Karolewski M.A. Tight-binding potentials for sputtering simulations with fcc and bcc metals // Radiation Effects and Defects in Solids. 2001. V. 153. I. 3. P. 239-255.
2. Cleri F., Rosato V. Tight-binding potentials for transition metals and alloys // Physical Review B. – 1993. – V. 48. – I. 1. – P. 22-33.
3. Computer Registration Certificate No. 2019661915 Russian Federation. Metropolis. 09/11/2019. Metropolis. 11.09.2019.
4. Stukowski A. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool // Modelling and Simulation in Materials Science and Engineering. 2010. V. 18. № 1. P. 015012-1-015012-7.