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 $Ti_{250} - Al_{250}$.
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