CHANGE IN THE PHASE DIAGRAM OF A SIMPLE MATTER WITH A DECREASE IN THE SIZE OF THE NANOSYSTEM

Magomedov M. N.

IPG DSC RAS, Makhachkala, Russia
mahmag4@mail.ru

The statistical three-phase model of a simple matter developed earlier in [1] is generalized to the case of a nano-system. Analytic expressions for the Helmholtz free energy and the state equation, which are valid for arbitrary values of the density, temperature, and number of atoms in the system are obtained on the basis of the Mie-Lennard-Jones paired potential of the interatomic interaction.

Calculations of the argon state equation showed that, when the number of atoms in the system decreases, the S-loop on the isotherm of the state equation for the phase transition (PT) of crystal-liquid (C-L) decreases, and at a certain number of atoms (N_0), the PTC-L S-loop disappears. It is shown that the value of N_0 increases when the shape of the nano-system deviates from the most energetically optimal shape. The value of N_0 increases with increasing temperature on the isotherm. In a cluster of $N < N_0$ atoms the PTCL already no.

As the number of atoms decreases, the liquid-gas phase transition (PTL-G) S-loop also decreases. The critical point parameters for PTL-G at decreasing number of atoms vary: the critical temperature and pressure decrease, and the critical specific volume increases.

Earlier, both in experiments and in computer modeling, it was noted that with a decrease in the nano-system size, both a convergence of the size dependences of the melting and crystallization temperatures is observed, as well as a decrease in the latent heat and in the specific volume jump at melting. Proceeding from these facts, and studying the extrapolation of size dependencies to the small dimensions, in [2] pointed out the possible disappearance of the PTC-L with a decrease in the number of atoms in the nano-system. In this work, it is shown that this disappearance of the S-loop of the PTC-L is due to an increase in the fraction of delocalized atoms at a decrease in the size of the nano-system.

This work has been supported by the Russian Foundation for Basic Research (grant No. 16-03-00041_a) and the program of the Presidium of the Russian Academy of Sciences (project No. I.13).

---

1. M.N. Magomedov. Vestnik Moskovskogo Tekhnichsskogo Universiteta im. N.E. Baumana, Ser.: Estestvennie Nauki, 2013, 2, 28-42.
2. M.N. Magomedov. Technical Physics, 2014, 59, 5, 675-681.