UDC 538.971
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KINETICS OF JANUS-LIKE ATOMIC CLUSTERS UNDER LOW ENERGY BOMBARDMENT

The evolution of free 390-atom Janus-like Ni-Al clusters along 100 and 500 ps under the bombardment by Ar_1 and Ar_{13} particles with energies up to 1.0 keV is simulated by the classical method of molecular dynamics. The initial metastable Janus-like clusters have two monocomponent parts, equal in number of atoms, with a small spatial overlap. After the impact of projectiles and rapid expansion, accompanied by spraying, the observed kinetics of Ar_1 and Ar_{13} cases are critically different; Ni-Al clusters gradually evolve due to exothermic mixing of components, with a tendency to surface segregation of Al atoms.

The melting points of metal nanoclusters are usually lower than the melting points of the same macroscopic materials, moreover, they can change nonmonotonically with decreasing of cluster size, especially below two hundred atoms [1]. The values of AEI (atomic equivalence indices), which are the sums of the modulus of difference of atomic radii-vectors, were calculated in our study using the Berendsen method depending on the temperature of the cluster. As expected, the results show that the melting process, that destroys the atomic structure of the cluster, begins at its surface at lower temperatures and reaches the inner regions at about 870 and 550 K for monocomponent Ni and Al clusters consisting of 195 atoms each.

The difference in the melting points of the surface and inner layers in our calculations reaches more than 200 K, especially for the Ni cluster. Simulation of Ar_1 particle bombardment showed that the temperatures of the Ni-Al cluster after 100 ps of evolution are higher than the melting points of the corresponding monocomponent Al and Ni clusters. Moreover, the temperature of the cluster is higher than the melting points of the clusters Al and Ni after 5 and 15 ps at all impact energies. Therefore, in many cases of bombardment, the aluminum part of the Janus-like cluster demonstrates faster transition to a disordered state. In these cases, over a period of time, part of the nickel is partially covered by more mobile aluminum atoms. Thus, for some period of time there is an unstable for this atomic system form of distribution of components "ball-and-cup" [2].

In addition, the interaction of the target cluster with the Ar projectile leads to the generation of radiation defects and the destruction of the ordered atomic structure in the cluster under strong nonequilibrium conditions for several initial picoseconds, which also contributes to the formation of the melt. Thus, in these simulations, an unstructured form was predicted, which can be interpreted as an

almost liquid state of the Ni-Al cluster after interaction with the Ar_1 projectile. Note, that the transition to an unstructured form of a cluster also leads to an increase in its potential energy.

The cases with Ar_{13} particles are dramatically different. The effects caused by the atomization of most of the atoms lead to a significant gradual increase in potential energy over about 10 ps, excluding the case of Ar_{13} with an energy of 100 eV. Also, a pronounced effect of increasing the temperature of the cluster with the size of the bombardment particle was observed throughout the simulation time. It also helps to increase potential energy. In the case of Ar_{13} bombardment, the cluster temperatures after 15 ps evolution are higher than the boiling points of the Al cluster, and comparable to the boiling point of the Ni cluster (~ 2520 K and 3200 K, respectively), except for low energies.

This is the main reason for the long high sputtering yield after the end of the collision stage, especially for the component Al. This can be interpreted as intense evaporation, which slightly lowers the temperature of the cluster for long periods and is accompanied by a slow increase in potential energy. It is obvious, that under such conditions the substance of the clusters is in a liquid state with an intense transition to the gaseous state. In the case of low energy effects, the sputtering yield and cluster temperature are minimal. As a result, in this case, the potential energy of the cluster after the evolution of 100 ps is lower than the initial one, similarly to the cases of Ar_1 bombardment.

REFERENCES

1. Hamid, I. Molecular dynamical simulations of melting behaviors of metal clusters [Текст] / I. Hamid, M. Fang, H. Duan // AIP Adv. – 2015. – Vol. 5. – p. 047129. doi:10.1063/1.4918770.

2. Ferrando, R. Symmetry breaking and morphological instabilities in core-shell metallic nanoparticles [Текст] / R. Ferrando // J. Phys. Condens. Matter. – 2015. – Vol. 27. – p. 13003. doi:10.1088/0953-8984/27/1/013003.