MULTYSCALE SIMULTATIONSD OF THE FORMATION OF COPPER NANOPARTICLES IN THE DIRECT-CURRENT MICRODISCHARGE

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The search for new ways to synthesize metal nanoparticles is an actual task for modern science. First of all, this is due to the widespread use of them in various fields of human activity. A special place is occupied by biomedical applications of copper nanoparticles [1].

This work is devoted to the modeling of processes leading to the formation of copper nanoparticles in a dc electric microdischarge. The possibility of the formation of conditions for the formation of metal nanoclusters in a gas discharge is due to the bombardment of the electrode surface with high-energy particles and knocking out individual atoms into the interelectrode space. Two main stages of the simulation differing by space-time scales realized. The first stage is based on the extended hydrodynamic model [2], which describes a DC arc discharge in a wide range of currents. It includes the continuity equations for the concentrations of charged (electrons, ions) and excited particles, the continuity equation for the electron energy density, the heat equation for determining the temperature of heavy plasma particles (ions and neutrals). The self-consistent electric field is determined from the Poisson equation for the potential. At the cathode, both the secondary electron emission of electrons and the thermionic emission from its surface were taken into account according to the Richardson-Dashman formula [3, 4]. As a result of modeling, spatial distributions of plasma parameters were obtained in a wide range of discharge currents: from 1A to 15 A.

Then, at the second stage, molecular dynamic (MD) modeling of the nucleation process of copper vapor in argon was carried out in a wide range of parameters (temperature, pressure, particle concentration), which were taken from the data obtained at the first "hydrodynamic" stage. MD calculation was performed using the freely distributed software package LAMMPS [5]. The simulation was carried out with 10,000 particles (atoms) of argon and copper in different ratios. The interparticle interaction of argon-argon and argon-copper was set by the Lennard-Jones potential with parameters for argon [6], the interaction of copper-copper was set by the potential of an embeded atom (EAM-potential) [7]. Information was obtained on the conditions for the formation of copper nanoclusters, their lifetime, growth rate, temperature, phase states, and structural features.

References

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