NUMERICAL STUDY OF THERMODYNAMICS AND STRUCTURE OF SMALL CLUSTERS IN DENSE GOLD VAPOR USING EAM POTENTIAL

Zhukhovitskii D.I.,* Zhakhovsky V.V.

JIHT RAS, Moscow, Russia

**dmr@ihed.ras.ru*

Clusters containing up to 26 atoms in dense subcritical gold vapor were studied using atomistic modeling. To this end, a new EAM potential for gold has been developed, which is applicable both to the lightest clusters and to solid matter. For the vapor–liquid phase boundary, the ratio of the Tolman length to the radius of the molecular cell in the liquid is found. With the obtained value of 0.16, the classical theory of nucleation with Tolman's correction is almost identical to the two-parameter model of "hot" clusters; i.e., small clusters can be described as macroscopic droplets of liquid metal. Both models are in good agreement with the results of numerical simulations. It was shown that the lightest clusters have a structure close to a freely jointed chain, i.e. they can be considered as quasi-fractals with fractal dimension close to two. The structural transition of a cluster from a compact to a quasi-chain state is a crossover at a characteristic temperature of about 2500 K [1].

The work is supported by the grant in the form of a subsidy for a large scientific project in priority areas of scientific and technological development No. 13.1902.21.0035.

---

1. Zhukhovitskii D.I., Zhakhovsky V.V. // J. Chem. Phys. 2020. V. 152. No. 22. P. 224705.