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Objet: Review on the thesis:

"Modeling of the processes of formation and growth of nanoscale clusters in rarefied jet flows" by Nikolay Yurievich BYKOV



The thesis "Modeling of the processes of formation and growth of nanoscale clusters in rarefied jet flows" by Bykov Nikolay Yurievich is devoted to the development of mathematical models of condensation processes in a rarefied vapor. The manuscript includes a numerical study of gasdynamics of rarefied jets, including processes of cluster formation and decay, based on the developed models.

The relevance of the study connected in the first place with applications in vacuum technologies of cluster beams and nanostructured films synthesis, and secondly with a necessity in such kind of models for the description of natural processes of condensation in jets that from the rarefied atmosphere of comets and planets.



Currently the Direct Simulation Monte Carlo method (DSMC) is the main method for simulations of the rarefied flows. Despite the existence of methods and techniques for computations of chemical reactions in the DSMC, an established approach to the simulation of condensation processes does not exist so far. The present manuscript considers various approaches to the construction of the models of cluster formation and growth: the kinetic approach and the one based on the classical theory of nucleation. The models developed by N.Yu.Bykov could be used for calculating the generation of both atomic and molecular clusters. In the frame of the kinetic approach, the author has developed an extension of Bird's the total collisional energy model (TCE). He complemented the TCE model with a model of monomolecular evaporation of clusters, and a model of dimer formation at triple collision of molecular monomers. These models of condensation were implemented in a numerical code for the rarefied gas flows simulations developed by the author. It is worth noting the considerable contribution of N.Yu.Bykov not only in the development of the mathematical models, but in optimization of numerical algorithms for supercomputers as well.



Using the developed numerical code (with new models), the author has undertaken a study of the process of cluster formation in jets of metal and water vapors. This study has established a set of principles, extremely important for understanding the physics of phenomena. It was demonstrated that clusters of subnanometer size range are generated in the rarefied jets expanding into vacuum with characteristic Knudsen numbers greater than 10⁻³. It was revealed that the influence

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of condensation on the flow parameters (density, velocity, temperature) starts to be essential when the volume fraction of clusters in a jet is more than 1%, and it leads to increase of velocity and translational temperature, and decrease of density of the vapor. The process of cluster growth is "freezing" at the distance of several radius of the jet's source orifice. Parameters (translational velocity, translational and internal temperatures) of the most abundant clusters were examined. It was shown that in the rarefied flows with approximately same translational velocities and temperatures of monomers and clusters, the internal temperatures of clusters is greater than the temperature of the vapor. The comparisons with available experimental data on condensation were performed for water and copper vapors. The comparisons with analytical solutions and experimentally derived similarity laws were performed as well.

I would like to highlight the solution of a steady problem of metal clusters formation in jets of mixture metal vapor +inert gas presented in the manuscript. This problem has an important practical interest for investigations of the nanostructure films growth dynamics in the vacuum technologies of jet-edge deposition.

It should also be noted the model and numerical algorithm of solution for the joint (thermal and gas-dynamic) problem of condensation processes for the laser ablation products, expanding into vacuum. These model and algorithm are of great practical interest for technologies of cluster beams formation e.g. the laser ablation. Since for the unsteady gas-dynamic problem which takes into account the processes of cluster formation, the solution of the thermal problem (which determines the flux of particles from the surface) provides the input parameters. N.Yu.Bykov has solved this problem in application to the laser ablation of niobium vapor in vacuum, induced by pulses of laser radiation of moderate intensity in nanosecond range. The manuscript presents a number of important conclusions on the influence of the condensation process on the parameters of the flow.

Summarizing my conclusions on the manuscript, I have to state the following. The thesis presents new models and corresponding numerical algorithms for the DSMC of cluster formation in a rarefied vapor. The thesis presents results of researches for a wide class of problems of cluster formation in steady and pulse rarefied jets of atomic and molecular vapors. The studies were conducted on the world class level (which is confirmed by the publications). The research, conducted by N.Yu.Bykov, has made significant contribution in the dynamics of rarefied gas, investigations of flows with physicochemical processes and computational fluid dynamics. Therefore, N.Yu.Bykov deserves to be awarded the degree of a Doctor of Physical and Mathematical Sciences.

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