Calculation of nitrogen flow in nickel micronozzle based on numerical approaches of gas and molecular dynamics

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ABSTRACT

Modeling of gas flows in micronozzles is one of the topical problems of modern nanotechnology [1]. The complexity of studying such processes is connected both with the small sizes of technical system that makes it difficult to carry out the natural experiments and with the violation of hypothesis of continuity of the considered gas medium. An additional factor of complexity is the lack of information on the real processes taking place at the gas-metal boundary.

In this paper, an attempt to consider the features of gas flow in a micronozzle of a small cross-section in order to compare two approaches supplementing each other is made. The first approach is based on direct modeling of the flow by the molecular dynamics method taking into account the real surface structure of the micronozzle [2]. The second approach is multiscale two-level approach based on the method of splitting into physical processes [3]. This multiscale approach uses the alternation of computations by the macroscopic quasigasdynamic model [4] and the microscopic model of molecular dynamics [5].

The flow of nitrogen in the nickel micronozzle is considered as an example. Previously for this calculation the parameters of interacting the nitrogen molecules and atoms of the nickel surface were calculated. In this paper they are used to form the material coefficients in the quasigasdynamic equations. The performed preliminary modeling has shown that at low flow velocities in calculations for both techniques it is possible to obtain a flow with a profile of longitudinal velocity close to the Poiseuille flow profile. It means the adequacy of the developed numerical techniques.

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