Correction of the Gas Flow Parameters by Molecular Dynamics

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ABSTRACT

This paper deals with the problem of a mismatch of gas systems parameters modelled by continuum mechanics methods in the conditions of the small sizes of the computational domain. This problem arises in case of simulation of real gas-dynamic processes in technical systems used in nanotechnology. In the provided operation the task of calculating of rarefied gases mixtures microflows in installations of supersonic cold gas dynamic sputtering is considered. The dimensions of individual parts of such units in the cross section can be comparable to the free path length of gases molecules, whereas the overall size of installations reaches several tens of centimeters. For example, in case of implementation of nanoimprinting technology the matrix of micronozzles by few microns diameter each is used. The sizes of the matrix also can vary from hundreds of square microns to tens of square centimeters. Length of the channels which carry gas and entrained nanoparticles can reach tens centimeters or more.

Simulation of such technically complex systems involves various stages. One of them is associated with the calculation of the parameters of the gas jets feeding nanoparticles. Obviously, in this case it is better to use the model of a continuous medium. In this paper it is presented by a system of quasigasdynamic (QGD) equations [1]. This system is very successfully inscribed in the general algorithm of the decision in view of the fact that its natural nondimensionalization parameter is just the mean free path of the molecules. However, for correct calculation this model should be supplemented with real gas equations of state, both on pressure and on heat capacity. Moreover, by interacting a gas mixture with the metal walls of the nozzles and the microchannels and also with nanoparticles phenomena occurs, which are well described only at the molecular level. Therefore, the parameters of QGD system should be consistent with these processes. In this work it is offered pressure, heat capacity and other coefficients of QGD system (viscosity, thermal conductivity, the exchange terms in the case of a mixture of gases, etc.) to calculate (at the initial time) and then to adjust (in the subsequent calculations) by molecular dynamics (MD) method [2]. This will allow to receive far from the walls and nanoparticles a flow which is completely agreed with the molecular dynamic features of the gaseous medium, and near the walls and nanoparticles (i.e., in the boundary layer) to take into account the additional interaction processes on the basis of first principles.

In this paper, by the MD methods the first part of agreement was held, that is, all the coefficient dependences for QGD system were obtained and the transition from the MD to the QGD and back was checked. In the calculations supercomputing technologies were used. The received results confirmed efficiency of the developed approach.

REFERENCES

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