

Abstract Submitted
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Molecular dynamics analysis of reflected gas molecules on self-assembled monolayers¹ HIDEKI TAKEUCHI, National Institute of Technology, Kochi College — In order to investigate the gas flow of high Knudsen number, it is necessary to specify the boundary condition for the reflected gas molecules at a solid surface. In most cases of the analysis, the diffuse reflection is generally assumed, but there are many cases for which this reflection cannot be applied. The characteristics of the reflected gas molecules depend on the state of the solid surface as well as the gas-surface interaction. The present author analyzed the scattering properties of monoatomic and diatomic gases on various solid surfaces based on the molecular dynamics (MD) method and proposed the boundary condition of reflected gas molecule (Phys. Fluids 18, 046103, 2006). Recently, self-assembled monolayers (SAMs) for the functionalization of the solid surface have been used in the development of micro/nano devices such as microarray and nanosensor. Therefore, it is interesting to study the scattering behavior of the reflected gas molecules on the SAM surface and make the scattering model of gases for the boundary condition. In this study, the angular distribution and the trapping probability for gas molecule on the SAM surface are observed by using MD simulation. The scattering probability at different incident energies is also discussed.

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