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Prediction of scattering properties for gas molecules on solid surfaces[1] HIROKI KUSUNOSE, HIDEKI TAKEUCHI, National Institute of Technology, Kochi College — In high Knudsen number flows, thermal and flow properties of gas are strongly influenced by the characteristics of reflected gas molecules at solid surfaces. The investigation of scattering properties of gas molecules on solid surfaces therefore is important to analyze the flow fields for micro/nano scale flows or rarefied gas flows. However, the scattering properties of gas molecules depend on many factors such as atomic species, pressure and temperature in a flow field, and solid surface states. It is difficult to completely consider these factors for the investigation of the gas-surface interaction. The purpose of this study is to construct an effective model for predicting the scattering behavior of gas molecules on solid surfaces with adsorbate using machine learning approaches. The molecular velocity distribution functions of the reflected gas molecules were obtained by molecular dynamics simulations for the gas-surface interaction. The parameters of a Gaussian function model which expresses these velocity distribution functions for various adsorbed surfaces were predicted using machine learning. The velocity distribution functions based on the constructed model properly reproduce the results of molecular dynamics analysis.

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