Abstract Submitted
for the DFD15 Meeting of
The American Physical Society

Scattering of water molecules on silicon surface: Molecular beam experiments and molecular dynamics simulations YUSUKE KOTSUBO, IKUYA KINEFUCHI, SHU TAKAGI, The University of Tokyo — The scattering behavior of water molecules on silicon(100) surface was investigated by experimental and numerical approach. Owing to the strong polarity of water molecules, water molecules and surface atoms would interact intricately compared to those of nonpolar gas molecules such as rare gases, nitrogen, and oxygen. In the experiment, we employed the molecular beam method and changed the incident energy of water molecules between 35 and 130 meV, which corresponds to the energy of thermal motion of gas molecules at room temperature. The scattering distribution and the mean translational energy of scattered molecules in each scattering angle were obtained. The experimental results indicated that the scattering distribution was close to that of the cosine scattering due to the roughness of the silicon surface when the incident energy was 130 meV. In contrast, when the incident energy was 35 meV, the scattering distribution had a directivity toward a certain angle close to the specular reflection one. The directivity is usually observed when a surface is flat in an atomic scale and the incident energy is high. To clarify the reason of this anomalous directivity, we are analyzing the interaction between water molecules and the silicon surface using molecular dynamics simulations.

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Date submitted: 31 Jul 2015 Electronic form version 1.4