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Structure and physico-chemical properties of interfacial water on a quartz revealed by molecular dynamics simulation

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Structure of water in thin film may have different characteristics compared with that of bulk water. Thin film water can be present at mineral grain boundaries or fractures, and its structure might be influenced by mineral surface. In this study, classical molecular dynamics (MD) simulations were performed to investigate the structure and physico-chemical characteristics of thin film water on a quartz surface.

The model of the quartz surface was characterized by the termination of silanol (Si-OH) group. Water molecules were confined between these surfaces, and we simulated several thicknesses of water in the slab geometry.

Density of water oscillates to be about 1 nm from the quartz surface at 298 K. This structure became less clear with heating, and almost disappeared above 473 K. The self-diffusion coefficients of the confined water were calculated from mean square displacements. These values were lower than that of bulk water indicating that the mobility of confined water is low between quartz surfaces.

These changes in the physical properties of interfacial water on quartz might affect such as slips in the fracture surface of the Earth's crust.

Keywords: interfacial water, quartz, molecular dynamics, self-diffusion coefficient