分子動力学シミュレーションによる石英面間の高温の水の物理化学特性

Physicochemical properties of water confined between quartz surfaces at elevated temperatures by molecular dynamics simulation

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Interfacial water, of which physicochemical properties were different from bulk water, was recognized in the vicinity of solid surface. The physical properties of interfacial water show unique characteristics, for example the self-diffusion coefficient, thermal expansion coefficient and freezing point. The property of interfacial water is essential for understanding geophysical and geochemical phenomena.

Although the phenomena of interfacial water have been studied theoretically and experimentally, the dynamics of the interface at high temperature and pressure remains unclear. In this study, we performed the molecular dynamics (MD) simulations to understand the structure and dynamics of water confined between quartz surfaces at 298-573 K, 10 MPa.

We tested some systems of water confined between quartz surfaces characterized by the termination of silanol (Si-OH) group. At low temperature, the density profiles showed several layered structures near the surface, and the self-diffusion coefficient was reduced in 1.0 nm distance from the surface. At high temperatures, the layered structures were disappeared and the self-diffusion coefficient was reduced in 1.5 nm.

The activation energies of the diffusion process in confined geometries were calculated based on the Arrhenius theory, and these values were close to that of bulk water. This implied that the diffusion mechanism in confined geometries is similar that in bulk and the activation energy may be interpreted by the dissociation energy of hydrogen bond.

Based on these results, the relationship of between geophysical phenomena and interfacial water will be discussed.

キーワード：界面水、石英、分子動力学、自己拡散係数
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