Molecular dynamics simulation to reveal slip and lubrication behaviors of interfacial water on quartz at high temperature conditions

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Water-rock interaction has many important roles in Earth’ s events such as earthquake. The relationship between fault friction and geofluid has been studied as represented by Sibson *et al.* (1988). The frictional strength of fault under the presence of fluid is controlled by phenomena occurring at the interfaces of mineral surface and fluids. Such interfaces can be understood from micro- and nano-scale approaches. The physicochemical properties of interfacial water on a solid surface have been studied by both theoretical and experimental methods. In our previous molecular dynamics study (Ishikawa *et al.*, 2016), interfacial water on quartz at 298-573 K showed layered structure and lower self-diffusion coefficient than that of bulk water. This indicates that, even at high temperature condition like underground environment, physicochemical properties of interfacial water on mineral could be different from bulk water. This interfacial water may alter the frictional strength of faults. In this study, we performed molecular dynamics simulations to understand the effects of interfacial water on the friction between quartz surfaces at 298-573K.
We prepared the system of confined water between two quartz surfaces characterized by the termination of silanol (Si-OH). The thickness of confined water layer ranges from 0.3 to 3 nm. In the simulation, surface force balance (SFB) system was used (Leng and Cummings, 2006). One quartz surface was fixed and the other surface was moving with constant velocity. The shear force of moving surface was calculated to obtain the friction coefficient.
In our presentation, we will show the lubrication behavior of interfacial water at 298-573 K and the discussion of frictional behavior on fault with pressurization.

Sibson *et al.* (1988) *Geology*
Ishikawa *et al.* (2016) *J. Mineral. Petrol. Sci.*
Leng and Cummings (2006) *J. Chem. Phys.*

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