

## 超薄膜水による鉱物の摩擦係数低下とその安定性の検証

## Water thin film: The effect on the frictional coefficient of minerals and the stability

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**Introduction:** Fluid/mineral interfaces have an effect on fault slips in the Earth's crust. Deformation of rocks in the Earth's crust is often localized within fault zones, and the slip behavior strongly depends on the frictional strength of these fault zones. Phyllosilicates (e.g., clay minerals and mica) are ubiquitous in natural fault zones and these layered-structure minerals can decrease the frictional strength of the fault zones. One of the reasons to explain the low frictional strength is the lubrication due to adsorbed and interlayer water molecules on these phyllosilicate minerals [1]. To know the lubrication properties and the stability of water on mineral surfaces is important to develop the fundamental physics of fault mechanics. Here we investigated the structure, dynamics and stability of water on the muscovite surfaces using classical molecular dynamics (MD) simulations, density functional theory (DFT) calculations, and x-ray crystal truncation rods (CTR) scattering measurements.

**Methods:** (1) Classical MD simulations: The interatomic potential models for muscovite, water, and ions were originally developed. These models succeeded to be applied to water/mineral interfaces [2]. (2) DFT calculations: The calculations were performed by the code Quantum-Espresso to know the stability of water confined between muscovite surfaces. (3) Surface x-ray scattering measurements: The measurements were carried out at Photon Factory, KEK, Japan (BL-4C) by using monochromatic x-rays of 11.0 keV.

**Structure of aqueous NaCl/Muscovite interface [3]:** The sub-Å-scale atomic distribution of muscovite surface in aqueous NaCl solution was measured as a function of the distance normal to the interface. The four distinguished peaks were observed at  $z = 1.4, 2.8, 5.3,$  and  $9 \text{ \AA}$  in the NaCl solution. The electron-density oscillation decayed and disappeared at  $z \approx 12 \text{ \AA}$ . The oscillation of the electron density can be explained by the adsorbed hydrated  $\text{Na}^+$  ions as the inner sphere complexes (IS).

**Implications for the mechanism of lubrication:** The radius of the first hydration shell of  $\text{Na}^+$  ions adsorbed on the muscovite surface was extended over  $4 \text{ \AA}$  from the outermost oxygen layer of the mica surface. In the previous shear measurements of NaCl solution confined between muscovite surfaces [4], the increased viscosity and high lubricity were observed at a surface separation of  $6 \pm 3 \text{ \AA}$ , which corresponds to the distance of contact of the first hydration shell of  $\text{Na}^+$  ions adsorbed on opposite muscovite surfaces. To realize water lubrication, the water molecules must be confined between the muscovite surfaces during the shear. In this context, the hydrated  $\text{Na}^+$  ions adsorbed on the muscovite surface as IS could retain the water molecules around them due to the attractive coulomb forces and be a candidate for an effective lubricant between muscovite surfaces.

**The stability of hydration shell:** The stability of water around  $\text{Na}^+$  ions at high temperature and pressure conditions was discussed by the combined methods of DFT calculations, the thermodynamics, and the shear measurements. The compressive differential stress larger than  $1.7 \text{ GPa}$  was necessary to squeeze out the water film.

**References:** [1] Morrow, C. A. et al (2000) GRL 27 815-818. [2] Sakuma, H. and Kawamura, K. (2011) GCA 75 63-81. [3] Sakuma, H. et al (2011) JPCC 115 15959. [4] Sakuma, H. et al (2006) PRL 96 046104.

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