

Effects of adsorbed water on frictional strength of fault gouge minerals

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Introduction

From the studies of various natural fault zones, it is known that phyllosilicates (i.e. clays and micas) are ubiquitous in natural fault zones. Experiments on layer-structure mineral-bearing gouges have shown that the presence of their minerals leads to significantly weaker faults compared to clay-free materials. The lowest strength is observed in gouges containing swelling clays like montmorillonite. The low friction of this clay is probably due to adsorbed water and interlayer water, which are lost at elevated pressures and temperatures. The behavior of adsorbed water has been investigated from the density oscillations of water on the several mineral surfaces by recent remarkable progress of high-resolution x-ray reflectivity measurements and from the molecular ordering of adsorbed water between muscovite mica surfaces by the surface force experiment. They showed that in general the water density profiles oscillate with distance below a few molecular diameters. This indicates that the adsorbed water is limited in a few molecular layers, and for the understanding the behavior of the adsorbed water, the microscopic investigation in molecular level is needed. However microscopic mechanisms of water adsorption on gouge minerals and the water behavior on the mineral surfaces are still unclear. We have examined the adsorption mechanism and dynamic properties of adsorbed water confined between four different mineral surfaces by theoretical study using molecular dynamics (MD) computer simulation method.

Methods

Molecular dynamics simulations were performed by MXDORTO and MXDTRICL.

Results and discussion

Regardless of the thickness of water thin film, orderings of water molecules, which are reflected by density profiles, are noticeable at the brucite and halite surfaces having the large adsorption energy, and the density profile between talc surfaces is flat. The self-diffusion coefficients parallel to the surfaces are 1.4~2.5 times as large as bulk water in the vicinity of the brucite and talc surfaces, while it is 0.6 times as large as bulk water in the vicinity of the halite surface. The reorientation times are 0.7~0.9 times as large as bulk water in the vicinity of the brucite and talc surfaces, while it is 1.0~1.4 times as large as bulk water in the vicinity of halite surfaces. These results indicate that the water molecules in the vicinity of brucite and talc surfaces can move easily, while ones in the vicinity of the halite surface cannot move easily.

The mobility of adsorbed water molecules is not significantly different from the bulk water at ambient conditions even if strongly adsorbed on brucite and halite surfaces. In other words, the adsorbed water molecules have large fluidity. These results imply that adsorbed water layer on a mineral surface significantly lowers the frictional strength of minerals.