

Frictional characteristics of brucite (001) plane on the real contact area

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Sheet-structure minerals such as clay minerals are abundant in natural faults. As they are thought to be dominant elements of the slip of faults, it is important to investigate their frictional characteristics. While friction coefficients of general rocks are 0.6-1.0 (Byerlee 1978), sheet-structure minerals have smaller frictional coefficients of 0.2-0.4 (Behnsen and Faulkner 2012). Though this weak friction coefficient is considered to be caused by orientation of relatively weakly bonded (001) plane (Moore and Lockner 2004), no experimental evidence was provided. Recent experiments showed that friction coefficient of single crystal specimens of muscovite was about half of that of polycrystalline muscovite (Kawai et al. 2015), implying that the frictional mechanism of (001) planes is important to explain the low friction of clay gouges. The friction coefficients of sheet-structure minerals were thought to be proportional to the interlayer bonding energy (ILBE) of (001) planes (Moore and Lockner 2004), which is associated with mineral specific electrostatic forces between layers estimated by Giese (1978). However, recent experiments and theoretical calculations showed less relationship between ILBE and friction coefficient (Behnsen and Faulkner 2012; Sakuma and Suehara 2015; Kawai et al. 2015). Hence, it is required to understand a physical process that explains the frictional characteristics of sheet-structure minerals instead of ILBE. Here, we investigate frictional characteristics on real contact area of brucite (001) plane to develop the fundamental physics of the friction between (001) planes. Brucite ($\text{Mg}(\text{OH})_2$) is a sheet-structure mineral richly contained in serpentinite often observed in natural faults. The crystal structure is simple and this mineral is suitable for the first principles calculations without high computational cost.

We calculate the potential energy surface under the friction of (001) planes of brucite by using the first principles calculation of electronic structure based on the density functional theory. The normal and friction forces were derived from the potential energy map as the method proposed by Zhong and Tomanek (1989).

Our preliminary results show internal friction coefficient = 0.048 and cohesion stress = 0.371 GPa in the sliding direction of $\langle 010 \rangle$ on (001) plane.

We will estimate frictional characteristics in any sliding direction on (001) plane and discuss dependence of frictional characteristics on sliding directions. In addition, we will compare frictional characteristics of brucite with those of other sheet-structure minerals such as lizardite, talc, pyrophyllite, and muscovite, investigated by Sakuma et al. (2016) and Kawai et al. (2016) and discuss the difference of frictional characteristics on real contact area among sheet-structure minerals.

Keywords: Sheet-structure minerals, (001) plane, Frictional characteristics, Interlayer bonding energy, The first principles calculation of electronic structure

