First-principles study on frictional characteristics of gibbsite

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Sheet-structure minerals, which have layered crystal structures, are known to be observed in natural faults (e.g. Chester et al., 2013). The fault slip behaviors are considered to be controlled by the frictional characteristics of sheet-structure minerals because they have lower and diverse friction coefficients than general minerals (Byerlee, 1978; Moore & Lockner, 2004). Recent studies suggested that the low and diverse frictional characteristics of sheet-structure minerals can be estimated by the variation of the potential energy between layers while being sheared (Sakuma et al., 2018; Okuda et al., submitted).

In this study, we focus on the frictional characteristics of two sheet-structure minerals, brucite (magnesium hydroxides) and gibbsite (aluminum hydroxides). Brucite has the friction coefficient of 0.42 and shows stick-slip behavior, whereas gibbsite has the friction coefficient of 0.75 and shows stable sliding (Moore & Lockner, 2004). These two minerals were composed by MgO_6 and AlO_6 octahedral sheets, respectively (Fig. 1). The difference between them was brucite has no vacant site within the octahedral sheet, whereas gibbsite has 1/3 vacancy with in the sheet (Fig. 2). These two octahedral sheets were the main component of phyllosilicates and their influence of crystal structures on frictional characteristics is important for understanding the frictional characteristics of sheet-structure minerals. We theoretically examined the frictional characteristics of brucite in our previous study (Okuda et al., submitted). Here we calculate atomic-scale frictional characteristics of gibbsite using first-principles calculations based on the density functional theory and compare the results of gibbsite with those of brucite.

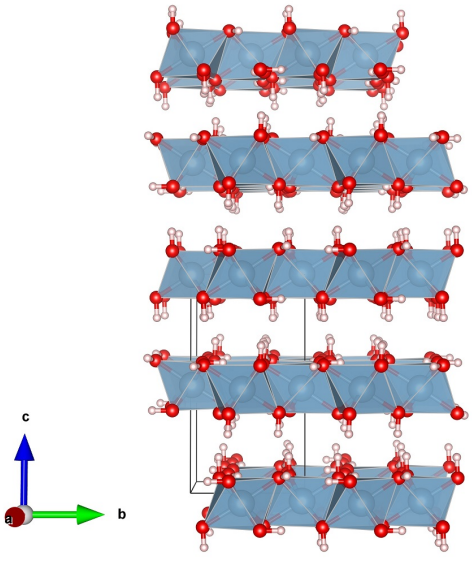
Preliminary results showed that gibbsite has lower atomic-scale shear stress than brucite. This is because the hydroxyls of gibbsite can be easily moved due to the vacancy within the octahedral sheet of gibbsite and that makes the potential energy low and increases the structural stability while being sheared. On the other hand, the yield strength of gibbsite is 1~2 GPa estimated by Mohs hardness (Mehrotra et al., 2015; Broz et al., 2006). This yield strength is lower then that of brucite (4.0 GPa (Okuda et al., submitted)) and this low yield strength increases the macroscopic friction coefficient when considering the adhesion theory of friction. We will quantitatively discuss the atomic-scale shear stress and yield strength of gibbsite and investigate what controls the difference of frictional characteristics between brucite and gibbsite.

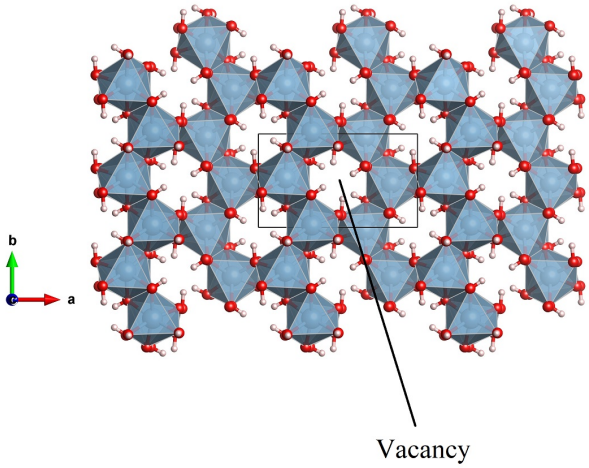
Keywords: Sheet-structure minerals, Crystal structure, Frictional characteristics, Gibbsite, First-principles calculation

Figure 1

Figure 2

Gibbsite ($Al(OH)_3$)





Brucite ($Mg(OH)_2$)