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Atomic-scale interlayer friction of gibbsite is lower than brucite due to interactions of hydroxyls

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Abstract

To investigate the role of atomic-scale structure on the frictional properties of gibbsite, a dioctahedral-type aluminum hydroxide, we calculated the atomic-scale interlayer shear properties using the first-principles method based on density functional theory. We found that the presence of vacant sites within the octahedral sheet of gibbsite enables hydroxyls to move to more stable positions and reduce the repulsive force, leading to a lower atomic-scale shear stress of gibbsite compared with brucite, a trioctahedral-type magnesium hydroxide. We also estimated the macroscopic single-crystal friction coefficient of gibbsite with the assumption that only the atomic-scale interlayer friction controls macroscopic friction. The estimated single-crystal friction coefficient for gibbsite is 0.36(6), which is clearly lower than the experimentally obtained friction coefficient of the powdered gouge of gibbsite (0.74). This difference between the interlayer friction coefficient and gouge friction coefficient suggests the presence of additional mechanisms that affect the frictional strength, such as microstructures within a fault gouge.

Keywords: Layered structure minerals, interlayer friction, gouge friction, gibbsite