

## Interlayer energy of pyrophyllite: Implications for macroscopic friction

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### ABSTRACT

Deformation of phyllosilicate can control the dynamics of the Earth's crust. The phenomenological relationship between stress and deformation is known for some typical phyllosilicates; however, the underlying physics originating from the crystal structures is poorly understood. In this study, the deformation mechanism of pyrophyllite along basal planes was revealed through density functional theory calculations and atomic-scale theory of friction. The stable and metastable interlayer structures formed by interlayer slide were consistent with the experimental results reported previously by high-resolution transmission electron microscopy. The difference in potential energies between stable and metastable interlayer structures can be interpreted as the difference in the stacking of dioctahedral sheets between the adjacent layers. The estimated friction coefficient of the pyrophyllite between adjacent layers was consistent with the results of atomic force microscopy, suggesting that atomic-scale friction can be adequately estimated by this method. The calculated shear stress in our simulations has a linear relationship with the normal stress and has no significant crystallographic dependence on sliding direction along the basal planes. The crystallographic isotropy of interlayer friction is explained by the absence of interlayer cations in pyrophyllite, while muscovite showed crystallographic anisotropy as observed in previous studies. The macroscopic friction of a single crystal of pyrophyllite was estimated from atomic-scale friction by using the area of contact. The macroscopic friction coefficient of ideal interlayer sliding was estimated to be 0.134, which was smaller than a reported value (0.276) in shear experiments conducted for wet polycrystalline gouge layers. This difference can be primarily explained by the degree of orientation of pyrophyllite particles in the gouge layers. The friction coefficient estimated by a simple model of randomly oriented pyrophyllite gouge layer was  $0.203 \pm 0.001$ , which was similar to the reported value of 0.276 and clearly smaller than the values (0.6–0.85) of common minerals estimated by the empirical Byerlee's law. These results indicate that weak interlayer friction of phyllosilicates has a large effect on the low frictional strength of gouge layers in natural faults. Our methodology and results are useful for understanding the physics behind the phenomenological friction laws of phyllosilicate gouge.

**Keywords:** Pyrophyllite, friction coefficient, interlayer friction, gouge layers, density functional theory