Molecular dynamics study on clay particles in clay-rich crustal fault

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The frictional resistance on a fault controls the earthquake dynamics via solid contact surfaces. Recent studies have revealed that the abundance of clay (smectite) can result in low apparent friction coefficients and facilitate fault slip. A close example is the March 2011 Tohoku-Oki earthquake that produced huge displacement and a disastrous tsunami, while the shallow regions of the plate-boundary thrust were thought to slip aseismically. The drilling survey revealed the fault zone is characterized by 60 to 80 wt% of smectite and a solid fraction of about 0.6. While clay can be simply thought of as a weaker material compared to rocks and minerals, it is distinguished from other fault-zone inclusions in terms of the smaller size and activeness to water. In addition, these properties may largely depend on the clay type. Rheological experiments reveal that the clay-water mixture at low solid fractions behaves as a viscous fluid with thixotropy and can reproduce stick-slip behavior. However, it is still unclear how clay would behave under high pressure and high solid fraction. The underlying mechanism of low shear resistance is also unknown. In this study, we examine the feasibility of nanometer scale simulation of clay particles using molecular dynamics. Individual clay particles are modeled as disc-like ellipsoids with large aspect ratios. Long-range interactions between particles are simplified as Gay-Berne potentials with mid-range attraction and short-range repulsion. The system is compressed and sheared to reach a target configuration of a given pressure or a given solid fraction. Our results show that molecular dynamics can be a promising approach for further study into the rheology and slip behavior of clay-rich faults.