Effect of Temperature on Nanoscale Slip Mechanisms in Fault Gouge: Postprint

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Abstract

Fault slip behavior is crucial for understanding earthquake nucleation and rupture mechanisms. In nature, due to friction and wear caused by fault activity, faults predominantly exist in the form of fault gouge, and their frictional properties are controlled by mineral composition and temperature conditions. To investigate the influence of temperature on fault slip mechanisms, this study employs the Steered Molecular Dynamics (SMD) method based on the CLAYFF force field to conduct friction simulations at a constant shear rate (100 m/s). The slip behavior of a quartz-kaolinite-quartz system within the temperature range of 200 K-500 K is analyzed, and the influence mechanism of kaolinite as a weak-phase mineral on fault frictional characteristics is investigated. By analyzing the friction process, shear stress, friction coefficient, and interfacial interactions, the regulatory patterns of temperature on the slip behavior of gouge-bearing faults are revealed, providing further insight into the weakening phenomenon of fault mechanical properties in deep high-temperature environments. The results demonstrate that significant stick-slip effects exist at the friction interface, with higher normal loads leading to stronger stick-slip effects. The presence of clay significantly reduces the frictional strength of quartz. The friction coefficient increases with decreasing temperature, while thermal fluctuations at high temperatures assist the system in overcoming energy barriers, manifesting as a reduction in steady-state frictional stress. The findings provide an atomic-scale interpretation of the pressure-temperature coupling effects in gouge-bearing faults.

Full Text

Thermal Effect on Nano-Scale Sliding Friction of Fault Gouge

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Abstract

Fault slip behavior is key to understanding the mechanisms of earthquake nucleation and rupture. In nature, due to friction and wear caused by fault activity, faults mostly exist in the gouge-bearing form, whose frictional properties are controlled by their mineral composition and temperature conditions. To investigate the influence of temperature on fault slip mechanisms, this study employs the steered molecular dynamics (SMD) method based on the CLAYFF force field, conducting friction simulations under a constant shear rate (100 m/s). The slip behavior of a quartz-kaolinite-quartz system was analyzed within the temperature range of 200 K-500 K, with the influence mechanism of kaolinite as a weak-phase mineral on the frictional properties of gouge-bearing faults being investigated. Through examination of the friction process, shear stress, friction coefficient, and interfacial interactions, the regulatory effects of temperature on the slip behavior of fault gouge were revealed, leading to deeper insights into the weakening phenomenon of fault mechanical properties under high-temperature conditions in deep geological environments. The research results indicate that there is a significant stick-slip effect at the friction interface, with the stick-slip effect becoming stronger as the normal load increases. The presence of clay minerals markedly reduces the frictional strength of quartz. The friction coefficient exhibits an inverse temperature dependence, where thermal fluctuations at elevated temperatures facilitate the system to overcome energy barriers, resulting in decreased steady-state frictional stress. These findings provide atomic-scale insights into the pressure-temperature coupling effects in clay-bearing faults.

Keywords: temperature effect; molecular dynamics; fault gouge; stick-slip

Introduction

Faults are widely distributed structural weak zones in the Earth's crust, and their slip behavior directly controls earthquake nucleation, rupture propagation, and energy release. Under natural conditions, long-term tectonic activity generates frictional wear, leading to the development of fault gouge composed of fine-grained minerals such as clay and quartz. The mechanical properties of these gouge-bearing faults differ significantly from intact rock, with frictional characteristics controlled by mineral composition, temperature-pressure conditions, and fluid environment, among which temperature effects are particularly critical. Experimental studies have demonstrated that temperature exerts significant regulatory effects on the frictional behavior of clay-bearing faults. For instance, natural fault gouge from the Longmenshan fault zone exhibits decreasing steady-state friction coefficients with increasing temperature in the range of 25-150°C; while biotite-bearing fault gouge shows increasing friction coefficients with temperature from 25-600°C. Furthermore, elevated temperatures promote plastic deformation of clay minerals, reducing shear strength of fault gouge and

even triggering dynamic weakening mechanisms. However, conventional experimental methods have limitations under high-temperature and high-pressure conditions, such as difficulty in precisely controlling microstructures, inability to directly observe atomic-scale energy dissipation and interfacial interactions, and unclear temperature-pressure coupling mechanisms in high-velocity friction experiments.

Molecular dynamics simulations can reveal microscopic temperature regulation mechanisms of fault slip through atomic-scale modeling. For example, Ying et al. verified through simulations that the friction angle of montmorillonite increases with temperature due to water loss at elevated temperatures. Compared with kaolinite and illite, montmorillonite's shear performance is least affected by temperature, as slow water molecule movement in clay minerals at low temperatures partially increases shear resistance. Molecular dynamics simulations can precisely set mineral components and temperature-pressure conditions while directly calculating microscopic processes such as interfacial bonding and dislocation motion, providing new perspectives for understanding thermal weakening of clay-bearing faults.

This study employs steered molecular dynamics based on the CLAYFF force field to simulate shear behavior of quartz-kaolinite-quartz systems across 200-500 K. By analyzing friction evolution, friction coefficients, and interfacial interactions in clay-bearing faults, we explore high-temperature and high-pressure effects on fault friction performance, demonstrating at the molecular scale how kaolinite as a weak-phase mineral weakens fault slip resistance. Through analysis of how thermal fluctuations affect energy barrier crossing, we investigate temperature dependence of clay-bearing faults and mechanical property evolution under deep high-pressure and high-temperature environments. The results will provide atomic-scale foundations for parameterizing earthquake physical models and advance multiscale modeling of fault friction constitutive relationships.

2.1 Model Construction

Quartz is a major rock-forming mineral composed primarily of silicon dioxide. Kaolinite is a common component in natural fault gouge and represents non-expansive clay well. Therefore, we constructed a clay-bearing fault model using a kaolinite supercell to simulate fault gouge, with three silica supercells representing the slider and substrate. The crystal cells were derived from Bish and Antao's data models. Both quartz and kaolinite were cut along the (0 0 1) plane, with oxygen atoms on exposed surfaces saturated by hydrogen atoms and silicon atoms saturated by hydroxyl groups. The quartz slider, kaolinite interlayer, and quartz substrate were assembled sequentially from bottom to top to create the clay-bearing fault model shown in Figure 1: see original paper. A 50 Å vacuum layer was set in the z-direction to avoid boundary atom interactions, yielding final quartz-kaolinite-quartz system dimensions of $54.01 \times 51.03 \times 98.47$ Å^3.

To ensure CLAYFF force field compatibility with the quartz-kaolinite-quartz system, we validated kaolinite and quartz from three aspects: density, radial distribution function before and after relaxation, and tensile strength. Quartz and kaolinite blocks with dimensions of 54.05 × 51.06 × 32.43 $Å^3$ and 56.69 × 53.62 × 32.43 $Å^3$ were constructed, respectively. The simulated densities of 2.649 g/cm^3 and 2.608 g/cm^3 closely match actual values. The models were fully relaxed in NVT and NPT ensembles at 300 K and 1 atm. [Figure 2: see original paper] shows partial radial distribution functions. Pre- and post-relaxation curves follow similar trends, with probability peaks remaining essentially unchanged in position and slightly increased in magnitude, indicating stable relative distances between different atom types and stable crystal parameters and equilibrium configurations for both quartz and kaolinite under CLAYFF.

Uniaxial tension was applied at constant strain rate until total strain reached 0.3. The stress-strain curves are shown in [Figure 3: see original paper], consistent with previous studies using the same force field. Therefore, the CLAYFF force field environment established in this study can effectively simulate mechanical behavior of the quartz-kaolinite-quartz system.

2.2 Force Field

Simulations were performed using the CLAYFF force field through the LAMMPS simulator. CLAYFF is specialized for clay minerals and related materials, effectively characterizing structures, properties, and behaviors of hydroxides, oxyhydroxides, and clay phases, making it widely applicable in multicomponent mineral system simulations. The total system potential energy (Etotal) comprises bond stretching energy (Ebond stretch), angle bending energy (Eangle bend), van der Waals energy (EVDW), and Coulombic electrostatic potential energy (ECoulomb).

2.3 Simulation Process

The spring towing method via steered molecular dynamics (SMD) was employed to simulate fault slip. In the simulation, constant-velocity SMD was applied to pull the quartz slider horizontally to simulate shear phenomena. Periodic boundary conditions were applied in all three directions. Van der Waals interactions were calculated using Lennard-Jones potential with a cutoff radius of 10 Å. The Verlet algorithm integrated equations of motion, with long-range electrostatic interactions calculated using the Ewald summation method. The simulation timestep was set to 1.0 fs.

To apply SMD simulation, both slider and substrate were divided into three parts: boundary layer, thermostat layer, and Newtonian layer, as shown in Figure 1: see original paper. Upper and lower boundary atoms were set as rigid bodies without ensemble constraints. During simulation, lower boundary atoms remained fixed at initial positions while upper boundary atoms transmitted external loads to the system. The thermostat layer employed a Nose-Hoover ther-

mostat to maintain target temperature. Newtonian layer atoms moved freely, with fault gouge contained within this layer.

First, the conjugate gradient method was used for energy minimization to obtain equilibrium configuration of the quartz-kaolinite-quartz system. The thermostat and Newtonian layers were equilibrated for 200 ps in NVT at temperatures of 200 K, 300 K, 400 K, and 500 K with a damping parameter of 100. Before friction simulation, target normal loads were applied. The thermostat layer ensemble remained unchanged while Newtonian layer atoms and fault gouge switched to microcanonical ensemble (NVE) control for 200 ps. In constant-velocity SMD simulation, mean square displacement of the quartz slider and spring tension were dynamically monitored until slider displacement reached 100 Å. By monitoring system motion throughout the process, we observed that quartz slider and kaolinite interlayer maintained stable uniform motion, allowing virtual spring force to represent friction during shear.

3.1 Friction Process

Figure 4: see original paper-(e) shows the evolution of friction force with sliding distance for clay-bearing faults. Friction force increases from zero, then fluctuates around a stable value, with the mean considered as the fault sliding friction value. Friction force gradually increases with normal stress. During normal stress application, stress transmits through slider boundary atoms to lower structures, causing overall elastic or plastic deformation. As normal stress increases, structural components of the clay-bearing fault become more compact, interlayer spacing gradually decreases, and the number of atoms participating in interfacial interactions increases, enhancing intermolecular forces. Consequently, frictional stress increases with normal load.

Analysis of average friction values under different normal loads reveals a linear relationship between shear stress and normal load stress, as shown in Figure 4: see original paper, following Coulomb's friction law. The friction coefficient is 0.037, close to previous quartz-kaolinite and pure kaolinite system simulation results but significantly smaller than quartz-quartz system friction coefficients. This indicates that overall frictional strength of clay-bearing faults is influenced by weaker kaolinite, with fault gouge presence demonstrating a weakening effect on rock fault friction strength.

Figure 5: see original paper-(d) shows friction curves for the quartz-kaolinite-quartz system at 8 GPa normal stress across different temperatures, where average friction decreases with increasing temperature. Research shows quartz's ultimate strength, Young's modulus, and other mechanical indicators decrease with temperature, suggesting temperature-induced mechanical weakening may be an important factor affecting fault friction. Additionally, at 100 m/s sliding velocity, the quartz-kaolinite-quartz system's average kinetic energies are 5438, 8090, 10670, and 13293 kcal/mol at 200 K, 300 K, 400 K, and 500 K, respectively. Higher temperatures yield higher kinetic energy in the fault system,

facilitating sliding friction.

From an energy perspective, atomic stick-slip effects can be explained as processes of potential energy surface variation and energy dissipation. During the stick phase, potential energy gradually accumulates. When energy becomes sufficient to overcome the barrier, slider atoms jump from current stable positions to next stable positions. During the slip phase, potential energy is suddenly released, causing periodic friction jumps. Thermal fluctuations and applied stress jointly enable atoms to overcome barriers, with thermal energy facilitating atomic sliding over potential barriers. Consequently, higher temperatures promote sliding. As shown in Equation (2), the thermally activated Prandtl-Tomlinson (PT) model predicts relationships between friction, temperature, and velocity:

F = Fc - (βkBT ln(vc/v))

where F is average friction, T is temperature, Fc is critical friction (temperature-independent), β measures potential corrugation curvature, kB is Boltzmann constant, and v and vc are sliding and characteristic velocities, respectively.

Temperature and friction data under various normal loads were fitted using Equation (2). Results are shown in [Figure 7: see original paper]. Due to small friction values at 1 GPa, fitting error is relatively large (R^2 = 0.782). Under other normal stresses, fitted R^2 values exceed 0.969, confirming that the quartz-kaolinite-quartz model demonstrates temperature dependence at microscale and follows the thermally activated PT model.

3.3 Main Sliding Surface Transition

In tribology, both Arrhenius theory and PT model explain temperature effects on friction. While PT model is universally applicable at microscale, Arrhenius theory is more commonly applied to macroscale fault slip. Analysis of quartz-kaolinite-quartz system friction coefficients at different temperatures reveals a linear relationship between ln( ) and 1/T, consistent with Arrhenius theory and further validating intrinsic consistency of temperature effects on clay-bearing fault slip across micro- and macroscales.

The quartz-kaolinite-quartz system exhibits two sliding surfaces with different displacements during slip. With increasing normal stress, the main slip surface gradually transitions from kaolinite's Si-O plane to Al-OH plane. To investigate factors affecting slip displacement, we fixed slider and substrate under different normal loads, used virtual springs to move the kaolinite layer at constant velocity while maintaining identical layer spacing and normal load conditions as slider-pulling cases. Measuring friction at both interfaces revealed that at low normal stress, Al-OH interface friction always exceeds Si-O plane friction, making Si-O plane more prone to sliding. As normal stress increases, Si-O plane friction increases beyond Al-OH plane friction, causing main friction surface transition. Velocity measurements during slider-pulling simulations show the

slider moves at constant 100 m/s under spring traction, exerting driving force on kaolinite in the positive x-direction, while the fixed substrate layer exerts resistance in the negative x-direction. Under these forces, kaolinite adjusts velocity to balance forces and achieve uniform motion. Therefore, differences in relative velocity between kaolinite and slider/substrate are the direct cause of different slip displacements at the two friction surfaces, while interatomic interaction forces are the fundamental controlling factors.

As shown in [Figure 9: see original paper], under the same normal stress, higher temperatures result in lower kaolinite sliding velocities. Measuring kaolinite velocities under different normal stresses reveals that at 200 K, main slip surface transition occurs between 9 GPa and 10 GPa normal stress. At temperatures between 200 K and 600 K, transition occurs between 8 GPa and 9 GPa. At temperatures $ $600 K, main slip surface transitions from Si-O plane to Al-OH interface at stresses below 8 GPa. With increasing temperature, the critical normal stress for main slip surface transition gradually decreases, indicating that high-temperature and high-pressure environments both favor slip along kaolinite's Al-OH interface in clay-bearing faults.

Conclusions

Through simulations of quartz-kaolinite-quartz system slip behavior at 200 K, 300 K, 400 K, and 500 K, we analyzed temperature effects on clay-bearing fault friction mechanisms, obtaining the following conclusions:

(1) Kaolinite as a weak-phase mineral weakens rock fault friction, significantly reducing fault strength.

(2) Due to temperature-induced mechanical property degradation and sliding promotion, average friction during clay-bearing fault slip decreases with increasing temperature under the same normal stress.

(3) At constant slip velocity, higher temperatures yield smaller friction coefficients in the quartz-kaolinite-quartz system, with ln( ) showing linear relationship with 1/T.

(4) Friction in the quartz-kaolinite-quartz system exhibits temperature dependence, with high temperatures facilitating atomic sliding over potential barriers.

(5) The quartz-kaolinite-quartz system exhibits two friction interfaces (Si-O plane and Al-OH plane) during sliding. Larger normal stress and higher temperature both favor slip along kaolinite's Al-OH interface.

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Note: Figure translations are in progress. See original paper for figures.