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Atomic-Level Understanding of Contact Potential of Quartz Surface

Lina Ma*

Qinghai Vocational and Technical University, Xining 810000, China.

Corresponding author: Lina Ma, 13299888637@163.com

Abstract: Laboratory and field observations have suggested a correlation between contact dynamics and slow dynamics. The underlying mechanical mechanisms at the contact level require investigation at the nanoscale. This study uses molecular dynamics (MD) simulations to investigate the interactions between two quartz plates separated by a water film, focusing on the relationship between adhesion force and separation distance. The density and orientation angle profiles were calculated from simulation data to investigate the relationship between the interfacial structure of the water film and contact potential. The simulations reveal multiple metastable states of the contact potential, consistent with existing theoretical models. The results show that the contact force is influenced by the structure of the water film, including oscillation forces and stratification. This provided verification and development for existing theoretical models based on metastable contacts

Keywords: Quartz; Molecular simulation; Adhesion; Multiple metastable states; Slow dynamics

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1. Introduction

The softening of near-surface space is caused by strong ground motion generated by large earthquakes. From a physical perspective, near-surface softening and healing are controlled by the dynamic elastic properties of the shallow geomaterials, characterized by strong nonlinear elasticity, stress-strain hysteresis, and slow dynamics, associated with long-term healing processes. The dynamic elastic properties of geomaterials are mainly determined by the contact between grains. For near-surface consolidated geomaterials under low confining pressure, contact mechanics between grains is primarily related to surface energy [1,2]. Therefore, the investigation of surface force and energy on the interface is significant in explaining phenomena during strong earthquakes, such as long-time relaxation and slow dynamics [3,4].

The surface force was first incorporated into the contact deformation analysis between grains by Sharma *et al.* [5]. The existence of a second equilibrium state (metastable state) was theoretically proposed and connected to the hysteresis effect, further confirmed by Smith *et al.* and Averbakh *et al.* [6, 7]. Our group proposed a theoretical contact model between mineral grains in geomaterials containing multiple metastable contacts at slight separations

due to the oscillatory hydration interaction. It was used to explain the two-stage recovery process of the site shear-wave velocity after a strong earthquake [8].

In this study, MD simulation is used to study the thickness of the equilibrium water film between the planes of amorphous quartz particles and obtain the equilibrium thickness and separation force curve. Meanwhile, the density and orientation angle profile are studied to investigate the relationship between the interfacial structure of water film and contact potential.

2. Models, methods, and simulation details

2.1. Construction of the hydroxylated quartz surfaces

A quartz lamella is constructed in the following fashion. Firstly, an α-quartz cubic periodic crystal was built using Materials and Processes Simulations (MAPS) crystal builder. The quartz crystal cell used for simulation was obtained from crystallographic structure databases. After that, the crystal was cleaved to obtain the surface. Considering the widespread existence of water in near-surface geotechnical materials, the quartz surface shall be hydroxylated. The annealing process was applied to turn the crystalline quartz into amorphous quartz. The bulk and surface properties of quartz system are greatly influenced by the annealing procedure. To obtain an amorphous silica slab for simulation with correct structural properties, a fairly high temperature of 4000 K was chosen for annealing. The steps were shown in **Figure 1**.

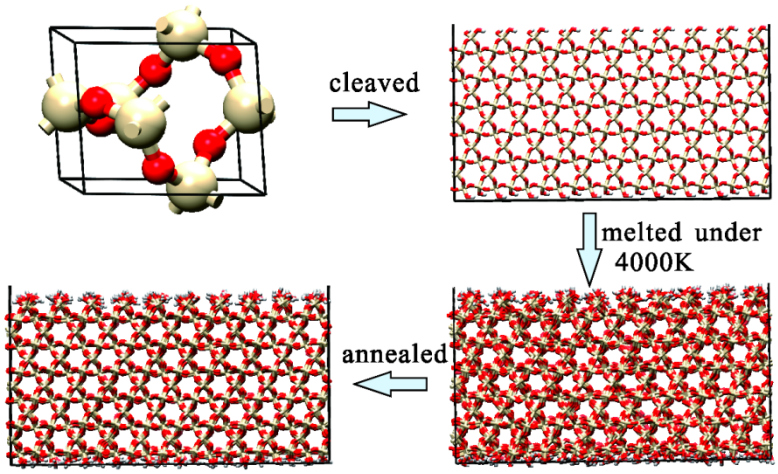


Figure 1. The construction process of quartz slab.

2.2. Construction of contact model

Considering the existence of water film, the slab-on-slab geometry was adopted instead of the conventional ball-on-slab model to control the number of water molecules confined within the slabs under periodic boundary conditions. **Figure 2(a)** illustrates the simulation system used for studying the relationship between adhesion force and separation distance on the nanoscale contact of quartz surfaces. Detailed heights of each portion are shown in **Figure 2(b)**. Our research chose amorphous quartz due to its wide distribution on rock and soil [9].

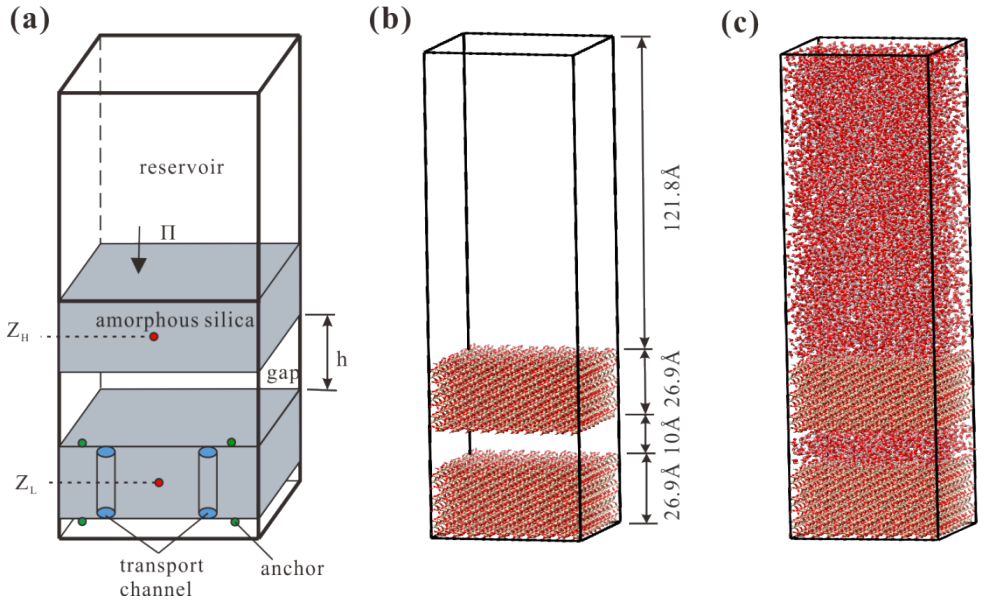


Figure 2. (a) schematic diagram of contact model. The pressure is applied to all atoms in the top quartz slab; due to the squeeze effect, the water molecules will migrate between the interlayer and reservoir through the channels till the applied pressure is balanced by force between the two slabs. (b) contact model without water. (c) contact model filled with water

2.3. Force fields

Simulations were performed with the extended Amber force field, as implemented in the large-scale atomic/ molecular massively parallel simulator (LAMMPS) [10, 11]. Considering that the materials involved in the simulation are mainly quartz and water, the parameter set developed by Emami *et al.* was employed [12].

2.4. Simulation settings

Initially, the upper quartz slab was placed above the substrate at h, beyond the expected equilibrium gap. As simulation starts, the top slab moves toward the substrate until equilibrated. Due to the uneven water film, the following formula was used to calculate the effective thickness.

$$h = \int_{Z_L}^{Z_H} \frac{\rho_W(z)}{max(\rho_W(z))} dz \qquad (1)$$

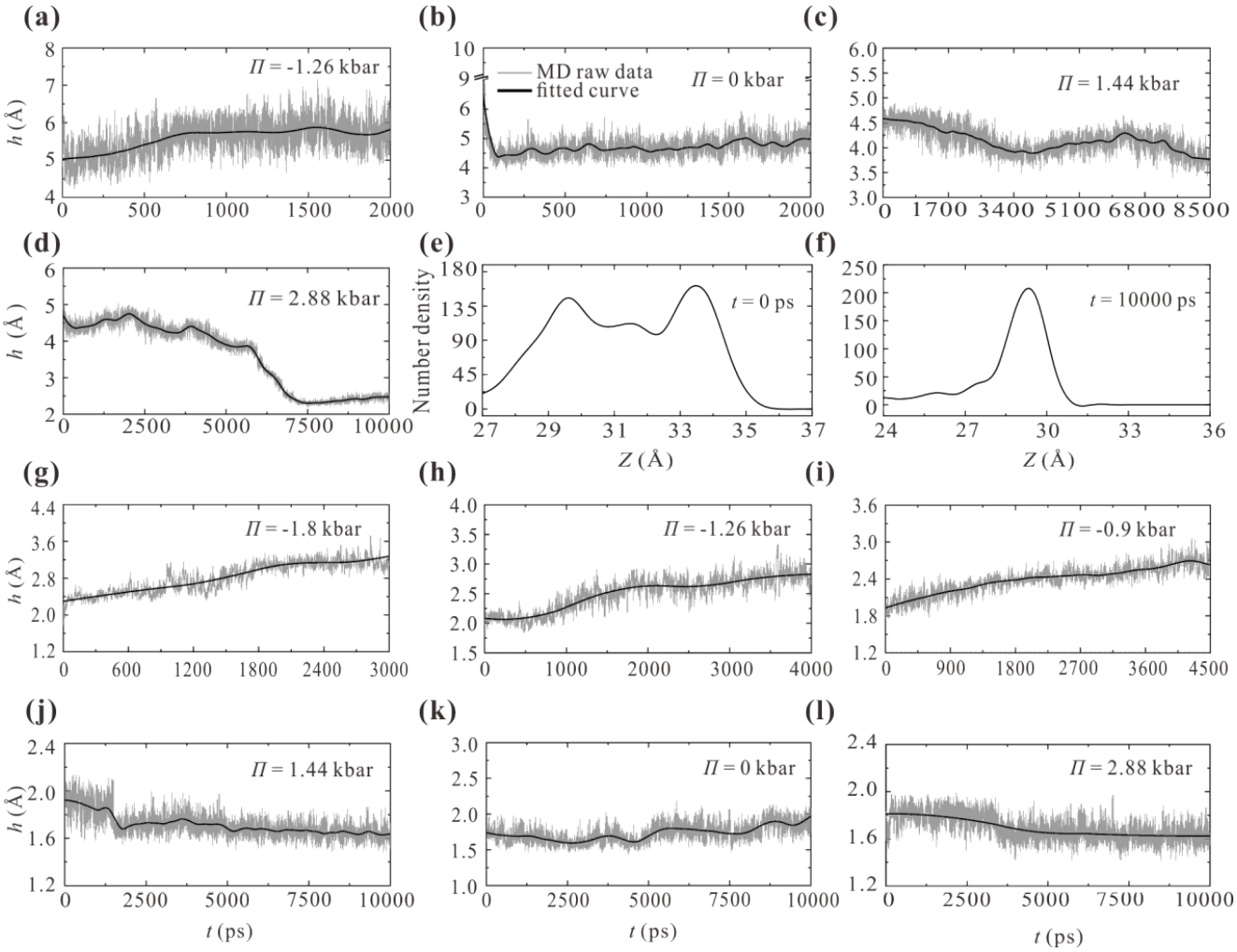
Among them, Z_H, Z_L are the barycentric coordinates of the top and bottom quartz slab respectively. $\rho_W(z)$ is the number density of water molecules in the z-direction.

3. Results and discussion

Although the theoretical model proposed by our group fits well with the two-stage recovery process of the site after a strong earthquake, the relationship between thickness and separation force within 1 nm still lacks verification from atomic level. Therefore, it is necessary to study the contact potential between quartz surfaces with nano water film using MD. In this study, the force-distance curves were shown in **Figures 3** and **4**.

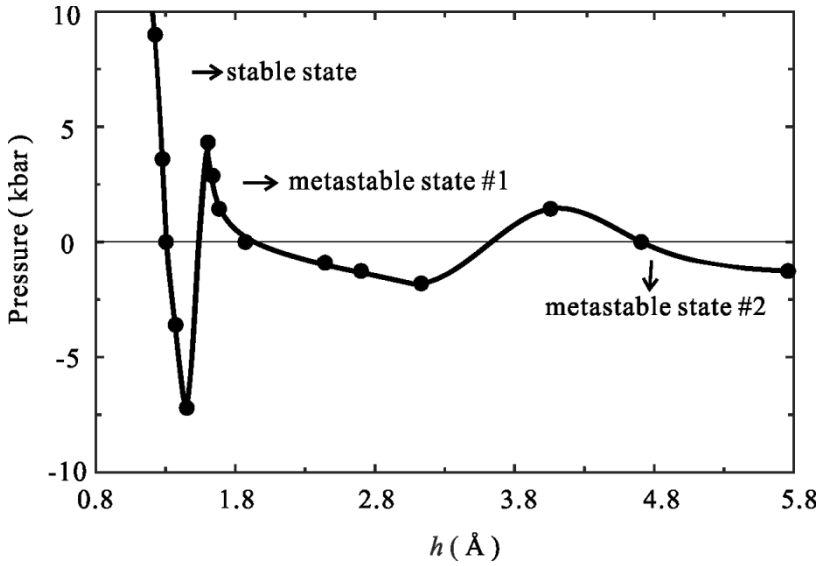
Figure 3 shows the time changes of h under different pressure. In **Figures 3(a)** and **3(b)**, the contact system reached equilibrium without a trend of change. The effective thickness h for applied pressure was calculated by averaging the stable section. As shown in **Figure 3(c)**, the equilibrium under positive pressure took more time than under negative pressure, due to the repulsive interaction between the slabs. Although the h fluctuated after

equilibrium, the unchanged position of the top slab confirmed the fact of equilibrium. **Figure 3(d)** showed an irreversible drop of *h* under 2.88 kbar, indicating a state change. Further confirmation in the density profile was shown in **Figures 3(c)** and **3(f)**. **Figure 3(g)-(l)** showed the time changes of *h* in the new state (the first metastable state). The effective thickness *h* decreased with the increase of positive pressure, while it increased with the rise of negative pressure.



Figures 3. The time changes of *h* in different simulation conditions. The gray and black lines represent raw data of MD and its fitted curve. According to their states, (a)–(c) refers to the time changes of *h* for the second metastable state; the shift from the second metastable to the first metastable state was shown in (d)–(f), (g)–(l) refers to the time changes of *h* under different pressure for the first metastable state.

So far, the stable and metastable states were obtained through the process above. The relationship between contact force and effective thickness is shown in **Figure 4**. In addition to the first global minimum, there were another two local minimums in the force-distance curve, indicating the existence of multiple metastable states on the contact of quartz particles in the presence of nanometer water film.



Figures 4. Dependence of the pressure on water layer thickness.

The contact relationship had a double sigmoidal shape. The existence of these states indicated the multiple metastable contacts of quartz with the presence of nano water film. **Figure 5** illustrates the spatial distribution and orientation of water molecules at the interface between two quartz plates.

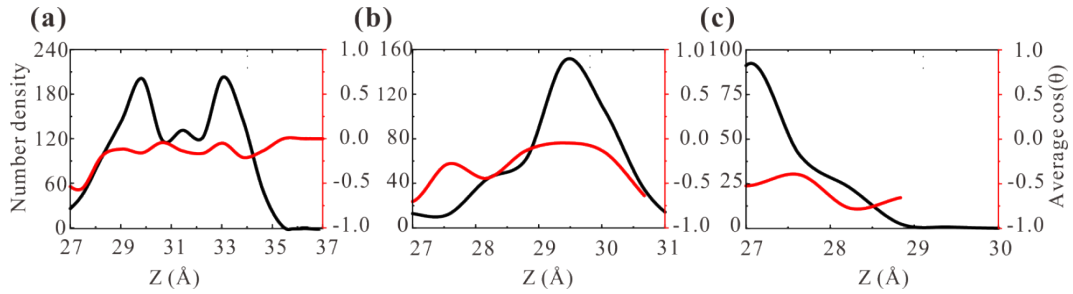


Figure 5. Profiles of density and average cos of orientation angle for the metastable and stable state: (a) For the second metastable state; (b) For the first metastable state; (c) For the stable state

Previous research indicates that water layers between solid surfaces exhibit density oscillations, which may contribute to the multi-stable states of the contact curve. The density profile of the second metastable state shown in **Figure 5(a)** shows two peaks and a middle platform, dividing the water layer into three regions: a lower adsorption layer from 27 Å to 30.65 Å, a stable layer from 30.65 Å to 32.25 Å, and an upper adsorption layer from 32.25 Å to 35.45 Å. The peaks indicate repulsion and attraction between water molecules and the quartz surface. A smaller peak in the stable layer suggests the presence of oscillation forces, consistent with experimental data on mica. The orientation angle profile shows no dominant orientation, indicating minimal polarization force contribution.

In the first metastable state in **Figure 5(b)**, the density profile has a single peak shifted to the right, likely due to transport holes on the lower surface. The distances from the peak to the upper and lower surfaces are 2.42 Å and 1.87 Å, respectively. The orientation angle profile shows a clear orientation angle, with water molecules gradually pointing toward the lower surface. In the stable state shown in **Figure 5(c)**, the density profile decreases monotonically without peaks, indicating that the force between surfaces is primarily Van der Waals. The

correlation between the density profile peaks and the multi-stable states of the contact curve highlights the role of oscillation forces in the interaction between quartz surfaces.

In **Figure 6**, the density profiles have the same double-peak shape under different pressures for the second metastable state. When the positive pressure was applied, the width of the profile decreased from 9.25 Å to 7.56 Å, but the distance between peaks and quartz surfaces did not change. Similarly, the negative pressure increased in the middle stable zone. So, for the second metastable state, the applied pressure mainly led to the change of the stable layer in the middle of the water film and had little effect on the adsorbed layer on the two sides.

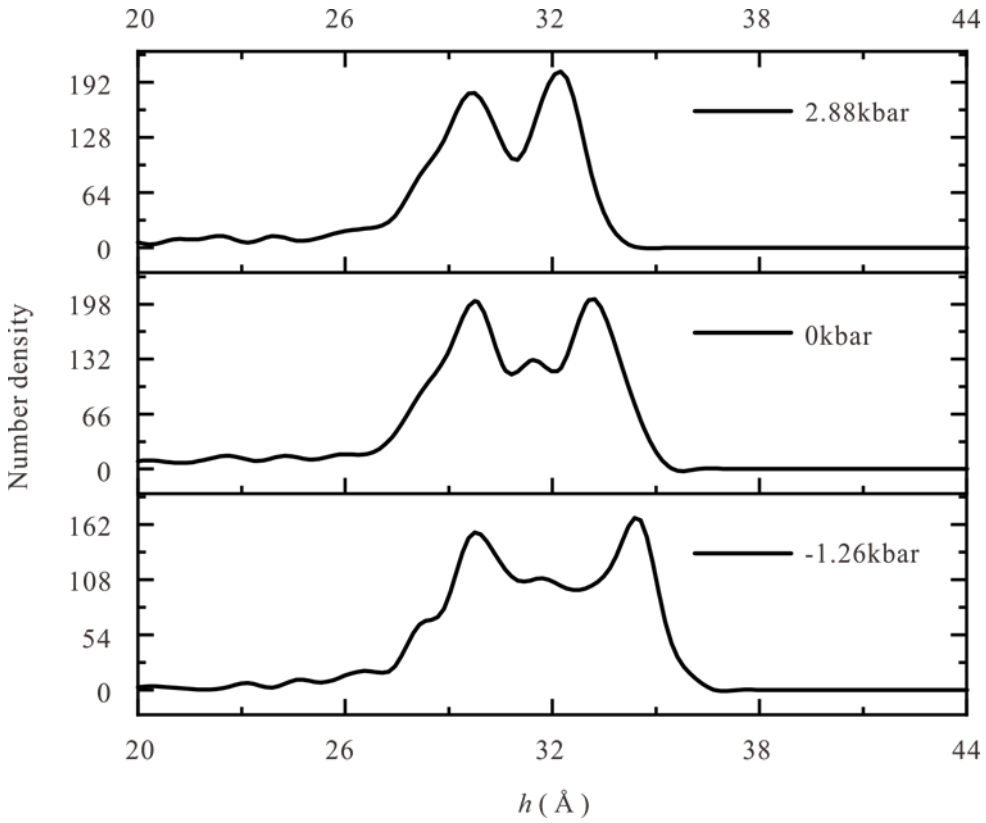


Figure 6. Evolution of density profile under different pressure for the second metastable state.

4. Conclusion

A general model is established to obtain the contact potential between quartz surfaces with nano water film using MD simulations. The contact potential is underpinned by the Lennard-Jones potentials between two quartz and solvation forces related to the structure of the water film. Multiple minima of contact curves are revealed by simulation results, indicating the multiple metastable states of contact potential between quartz. The results agree with the previous atomic microscope tests. Still, the simulation showed that the position of the stable state was closer to the surface, probably due to the difference between the slab and probe. Considering the characteristics of Lennard-Jones potentials, the multiple metastable states are mainly caused by the nano water film between quartz. Density profiles confirm the existence of oscillation force and the stratification of confined water. Due to the consistency of layer number and state, density profiles of different states reveal the relationship between layered water film and metastable states. In addition, the orientation angle profiles show that the polarization force contributes little to the contact force. These provide a preliminary reference for modeling the contact relationship of quartz slabs in the presence of nano water film.

Disclosure statement

The author declares no conflict of interest.

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