Molecular Study of Rock Friction and Wear Mechanism Using a Pair of α-quartz Asperities

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Frictional instabilities of faults, a significant factor in triggering shallow earthquakes, have widely been recognized as a phenomenon governed by the wear of asperities on fault surfaces. However, there is still a lack of clarity regarding the wear mechanisms of asperities and their dynamical connections to friction. Here, at molecular level, we conducted a series of kinetic simulations with realistic atomic force field to explicitly reproduce multiple 3-D nanoscale wear processes under different normal forces. We extensively explored the friction and wear mechanisms by examining worn surfaces, total wear volume, wear volume rate with distance, and the links of total wear volume to friction work (i.e. integrating friction force over slip).

Our simulation was a sliding friction experiment and focused on the "running-in" period of smoothening asperities (Wang and Scholz, 1984). The surface area of two solid blocks was 23.77 nm×13.73 nm and each block contained an identical semi-sphere α-quartz asperity with radius being 3.40 nm. Initially, the two asperities were not contacted and the distance between semi-spherical centers was a radius. Then we pressed asperities together by applying normal force. The bottom of the lower block was fixed and a constant normal force and velocity were applied to the upper block where it was allowed to move in the fault normal (z-) direction. Additionally, periodic conditions were applied to the x- and y-directions while in the z-direction shrink-wrapping condition was applied. Furthermore, the sliding velocity was set at 10 m/s and the constant normal force was applied ranging from 1nN to 4nN.

Our results showed that the time-averaged friction force had a positive correlation to the normal force at nanoscale and scuffing wear was dominated in the normal force range we applied. This wear type could be due to the high hardness of α-quartz. Moreover, we observed that the total wear volume generally increased with the normal force but it did not show a clear positive correlation. In certain segments of the normal force range, a slight decrease could be observed. A similar phenomenon also occurred at macroscopic rotary shear experiment (Hirose et al., 2012), which could be related to the sliding velocity. On the other hand, we found that the wear volume rate increased nonlinearly with slip distance and it showed a positive dependence on the normal force. Finally, we confirmed that the friction work was proportional to total wear volume, which could be served as a potent indicator for predicting the volume of worn debris. These discoveries will offer a profound understanding of fault friction and wear mechanisms, laying the groundwork for modeling multi-scale friction constitutive laws.