Atomic scale dynamics of frictional processes

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Friction is one of the most fundamental processes in nature, and a key design concept in machines and devices. Friction and wear are the main source of failure in every kind of machinery, macro- and microscopic, as well as biological applications. As the scientific effort pushed towards understanding the nanoscale origin of friction, atomic force microscopy became the tool of choice for creating a controllable nanocontact with a surface, where the friction and wear properties and can be studied with such detail. Combining the conventional NC-AFM technique with the torsional resonance (TR) in the so called bimodal AFM, allows simultaneous mapping of normal and lateral forces gradients via frequency shifts Δf; the energy lost to atomic scale frictional processes is obtained from the TR excitation signal, but its interpretation remains challenging as the underlying non-conservative processes are unknown at the atomic scale. We study the NaCl (001) surface, which is an important benchmark system for theoretical models and easily prepared in the laboratory, using bimodal AFM and computer simulations. Our experiments revealed a weak tip-sample vertical interaction, giving a faint topographic contrast of the surface and no significant dissipation was measured in the flexural channel; the lateral Δf, on the other hand, provided sharper images, showing the typical checkerboard pattern of ionic crystals, although the TR damping image presented double peak features around one surface atomic type. Using a simple mathematical model for the tip-surface interaction, we can deduce that the highest lateral force should be measured not on the atomic sites, but in the gap between them. Under such intense stress, the tip apex is more likely to change shape, causing hysteresis in the oscillation cycle and therefore energy dissipation. We performed classical molecular dynamics (MD) simulations of such oscil lations using a realistic model tip [1] treated to inhibit flexural dissipative processes. The simulated scanline shows how the tip feels the strongest force between two surface atoms, and this indeed triggers reversible tip changes, responsible for the observed hysteresis. The calculated dissipation is in good agreement with the experimental measurements.

[1] S. Kawai, F. Federici Canova, T. Glatzel, A. S. Foster and E. Meyer, *Physical Review B* **84**, 115415 (2011).