Comment on "First-Principles Theory of Atomic-Scale Friction"

Recent theoretical work[1] has determined the atomic-level kinetic friction observed in atomic-force-microscope (AFM) experiments[2] by equating the force of kinetic friction (f_k) at slow speeds to the mean interfacial force, for a monolayer of palladium on a graphite substrate. In this Comment, it is shown that unlike the monolayer case considered in Ref. 1, for a multilayer solid (a more appropriate model for modeling the AFM experiments[2]) sliding on a similar substrate, one must take into account the strain needed to overcome the force of static friction (f_s), all or part of which is released in the slip of the "stick-slip" motion which occurs at slow-speed sliding. This model accounts naturally for the accepted notion that $f_s > f_k$. Consider the following model: Two macroscopic elastic bodies in contact slide relative to each other, one on top of the other, and the surface of each body at the interface moves in a potential due to the other body. In order for sliding to take place, a critical force f_s must be applied to the upper surface of the upper body (the lower surface of the lower body is assumed to be held in place) sufficiently large to overcome the maximum force due to the potential of interaction at the interface between the bodies. Since the interaction force between the bodies is position dependent, the motion in the slow-speed limit will be stick-slip in nature for an applied force slightly greater than the maximum value of this force. A fraction of the built-up strain in the bodies is released in each slip. If this fraction is very small, the force that must be applied to the upper surface to maintain the motion f_k will remain nearly equal to f_s, but if it is large, as the strain is released, f_k will drop well below f_s between slips, making the average f_k smaller. This correlation between the relative sizes of f_s and f_k and the strain released in each slip should be able to be tested experimentally. In order to calculate the strain released in one slip, consider the following equation of motion, which represents the motion of one of the sliding solids in a periodic potential (assumed to be caused by the second):

$$\ddot{x}_n = -\alpha(2x_n - x_{n-1} - x_{n+1}) - \delta_{n,0}\lambda_0 f(x_0) ,$$

with n running from 0 to $N-1$, where $f(x_0)$ is a force of period a (the lattice constant), x_n is the displacement of the nth layer of atoms (each layer will move rigidly if the periodic force is commensurate with the crystal plane), α is the interlayer force constant, and λ_0 is the strength of the periodic force. The mass has been absorbed into α, and the coordinate x_0 is initially set equal to zero. This is equivalent to the model of Ref. 1. To study the stick-slip motion, the displacement of the top layer, x_N, is set equal to slightly more than the value for which the resulting stress will be just enough to overcome the periodic force with all the other x's at the equilibrium values corresponding to this value of x_N. In the motion that follows, the lowest plane moves one or more periods of the periodic force before getting stuck, as all of the translational motion of the system gets converted into vibrational motion. For $N=1000$ and $f(x_0)=\cos[(2\pi/a)x_0]$ (whose form is close to that of the f of Ref. 1) and $\lambda_0/\alpha=0.158a$ (corresponding to equal intersurface and inter-atomic-layer force constants and comparable to the value of λ_0/α used in Ref. 1), the lower layer was found to slide by about $16a$, implying that all the strain is released in the slip and that $f_k \approx 0.5 f_s$, whereas for $\lambda_0/\alpha=0.0038a$, it slid by only $0.89a$. For the latter value of λ_0/α, and for $N=5000$ and 10000, the lower level slid by about $5a$ and $10a$, respectively, implying that about $\frac{1}{4}$ of the built-up strain is released in each slip. This implies an average f_k which is about 88% of f_s. The slipping distances when there are defects in the crystal planes which are in contact will be smaller than these values because of the excitation of intralayer vibrations (which are not included in this model). Their inclusion would make f_k closer to f_s. These results depend on the form of f. For example, in the exact solution for f due to a "sawtooth" potential, the lowest atomic layer slips either less than one period if λ_0 is less than $2mv_p^2/a$ (m is the atomic mass and v_p is the phonon velocity) or enough to release all the strain if it is stronger.[3]

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