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A THEORETICAL AND COMPUTATIONAL STUDY OF SUPERLUBRICITY AND THE ROLE OF THE ROUGHNESS EXPONENT

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ABSTRACT

Superlubricity can only be achieved if the intra-bulk elastic interactions dominate interfacial shear forces at every single length-scale in a contact. Otherwise, there will be some type of plucking motion which will lead to friction-velocity relationships akin of Coulomb's friction law. For nominally flat surfaces, it has been predicted theoretically and demonstrated experimentally that plucking motion and hence kinetic friction can be avoided under certain circumstances. We present theoretical arguments, why these findings may extend to fractal surfaces. The theories are checked by molecular dynamics simulations. It turns out that the roughness exponent and the absolute magnitude of the roughness both play a crucial role in determining whether there can be superlubricity.

INTRODUCTION

It has been shown a long time ago that the source of kinetic friction with weak velocity dependence must be due to what one may best describe as plucking motion. As discussed in detail in a recent review article [1], many different terms were used to describe the underlying dynamics of such processes: stick slip, instabilities, (Hopf) bifurcation, pops, and (molecular) hysteresis, to name a few.

The reason for plucking motion is that an atom, or more generally speaking, a degree of freedom, becomes unstable at its present position due to externally imposed driving. Once unstable, the atom quickly moves into the next available energy minimum. The energy dissipated during this process is the energy difference between the old and the new position. The generic model for such processes is the Prandtl-Tomlinson (PT) model, in which an atom (or a reasonably rigid unit such as an atomic force microscope tip) is pulled over a substrate via a spring of stiffness k. Depending on the ratio of k and the maximum curvature of the substrate potential $\kappa_{\max}$, the kinetic friction $F_{\rm k}$ is zero ($\kappa_{\max}/k \leq 1$) or finite ($\kappa_{\max}/k > 1$). This simple theory was validated experimentally only very recently in an atomic force microscope experiment, in which $\kappa_{\max}/k$ could be modified by varying the normal load [2].

Real solids are, of course, three dimensional, and it is thus necessary to study, whether instabilities occur when two solids slide over one another. Neglecting effects from the boundary of the contact, Hirano and Shinjo's pioneering calculations of copper placed on copper showed that the instabilities do not occur at an atomic scale, if the two (identical) solids are placed sufficiently far out of registry [3]. Here, we will present an analysis of elastic surfaces in relative sliding motion with roughness on many different length scales.

THEORY

If the stiffness of the spring k in the Prandtl-Tomlinson model is greater than the maximum curvature of the potential $\kappa_{\max}$, then there is always a unique equilibrium position for the atom and no plugging motion will occur, which implies a vanishingly small kinetic friction force $F_{\rm k}$ at small sliding velocities v_0. However, if $\kappa_{\max}/k > 1$ and thermal fluctuations are irrelevant, then there will be "pops" and $F_{\rm k}$ will remain finite.

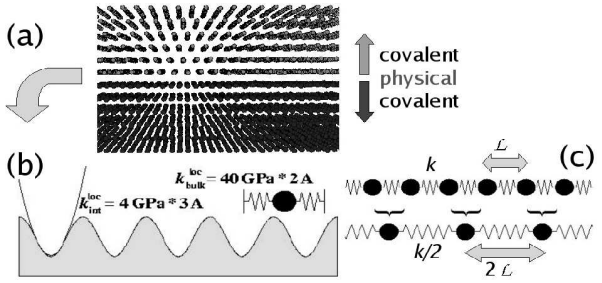

Figure 1. Schematic view of the interaction between two chemically passivated solids.

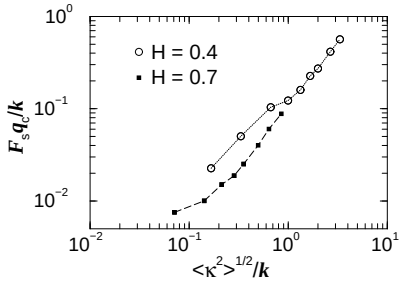

Figure 2. Normalized friction $F_s q_c/k$ as a function of the normalized, average surface or potential energy curvature $\sqrt{\langle\kappa^2\rangle}/k$ for two different Hurst exponents H.

For three-dimensional solids, a similar analysis can be done as in the PT model [4], although now, one has to evaluate the ratio of $\kappa_{\max}/k$ not only at the atomic scale, but at every length scale. The main idea of such an analysis is illustrated in figure 1. Part (a) of that figure shows a snapshot of a friction simulation, whose results have been reported in Ref. [5]. The assumption is that there are no chemical reactions between the solids and that there is no contamination. Part (b) represents the coupling of a surface atom to its neighbors (reflected by the harmonic springs) and to the substrate (reflected by the sinusoidal line). An estimate of a typical value of k is given. The parabola drawn into the substrate potential would indicate the local curvature $\kappa = k^{\rm int}_{\rm loc}$. The estimate for κ is based on the assumption that there are only Lennard Jones type interactions between different solids, as is the case, for example, between hydrogen-terminated diamond surfaces. The last step of the analysis is shown in part (c), which shows how the value of k would change if we were to describe the system on a more coarse-grained scale. It is important to also analyze how κ would scale with the length scale. If $\kappa > k$ holds at any length scale, then superlubricity is lost automatically due to the competition of roughness and elasticity. The results of such studies generally depend on the dimensionality of the systems and the order of the surfaces (commensurate/incommensurate/ disordered/roughness exponent) [4].

SIMULATIONS

In our simulations we generate a rough, fractal surface for which the height, or alternatively, the potential energy $V(x)$ satisfies the following equation:

$$\left\langle \{V(x+\Delta x)-V(x)\}^2 \right\rangle = \tilde{V}_H \Delta x^{2H}. \qquad (1)$$

$\langle ... \rangle$ indicates a statistical average, x is a position on the surface, $\tilde{V}_H$ a proportionality coefficient, and H the Hurst roughness exponent. We also impose a cutoff on the roughness in reciprocal space at a wavelength $2\pi/q_{\rm c}$ similar to atomic dimensions. An elastic chain, in which adjacent atoms are coupled elastically via springs of stiffness k, is placed into this potential and an external, lateral force is exerted on each atom. For small forces, the chain remains typically pinned, until a threshold force, the static friction force, $F_{\rm s}$ is reached. We take $F_{\rm s}$ as an estimate and an upper bound for $F_{\rm k}$.

In figure 2, we show the friction force as a function of the average roughness of the surface. For the one-dimensional model studied here, the friction force never disappears unless the roughness amplitude is exactly zero. This result is in agreement with predictions for one-dimensional, elastic manifolds, which also predict the possibility of superlubricity in higher dimensions [4]. Simulations of systems of higher dimensions have been started as well, but the results are not yet sufficiently satisfactory for publication. We have nevertheless strong indications that self-similar surfaces can remain superlubric even at large length scales. However, the roughness exponent H as well as the atomic scale roughness must stay below a critical value.

ACKNOWLEDGMENT

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