Role of lattice trapping for sliding friction

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On the origin of sliding friction: Role of lattice trapping

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Using molecular dynamics we study the dependence of the friction force on the sliding speed when an elastic slab (block) is sliding on a rigid substrate with a sin(q₀x) surface height profile. The friction force is nearly velocity independent due to phonon emission at the closing and opening crack tips, where rapid atomic snap-in and -out events occur during sliding. The rapid events result from lattice trapping and are closely related to the velocity gap and hysteresis effects observed in model studies of crack propagation in solids. This indicates that the friction force is dominated by processes occurring at the edges of the contact area, which is confirmed by calculations showing that the friction force is independent of the normal force. The friction force increases drastically when the sliding velocity approaches the solid transverse sound velocity, as expected from the theory of cracks.

Introduction—The friction force acting on a block sliding on a substrate is usually nearly velocity independent unless the sliding speed is so low that thermal activation is important, or so high that frictional heating becomes important. A velocity independent friction force results if rapid processes occur at the sliding interface, involving local slip velocities unrelated to the macroscopic drive velocity. One important topic in tribology is to understand the origin and nature of the rapid slip events, which generate the sliding friction force[1].

The friction force is usually proportional to the normal force (Amonton’s law). This result follows quite general from the theory of the contact between elastic solids with random surface roughness[2].1 Thus, the area of real contact is usually proportional to the normal force[3]. This results from the fact that for a large system, when the normal force increases the number of asperity contact region increases proportional to the normal force, but the distribution of asperity contact areas and the (contact) stress distribution are unchanged[11][12]. It follows that the friction force will be proportional to the normal force independent of the nature of the microscopic frictional interaction at the asperity level, e.g., independent of how the friction force acting on an asperity depends on the asperity contact area.

In this paper, we present a molecular dynamics (MD) study of the dependency of the friction force on the sliding velocity when an elastic slab (block) is sliding on a rigid substrate with a sin(q₀x) surface height profile. The atoms on the block interact with the substrate atoms by Lennard-Jones potentials. We show that the friction force is due to lattice pinning: at the opening and (to lesser extent) the closing crack tips atoms snap-out (and -in) of contact in rapid events, with atom velocities unrelated to the block driving speed, followed by “long” time periods where the crack tips are pinned. In the rapid slip events elastic waves (phonons) are emitted from the crack tips (see Fig. 1), resulting (for the opening crack) in a larger crack propagation energy than the adiabatic value.

Model—We consider the contact between an elastic slab and a rigid substrate with the cylinder corrugation (see Fig. 2) z = h₀sin(πLₓ/Lₓ) and 0 < x < Lₓ. We assume periodic boundary conditions in the xy plane with the basic unit having the dimensions Lₓ = 254 Å and Lᵧ = 14 Å. The corrugation amplitude h₀ = 100 Å. In order for the contact mechanics not to depend on the block thickness, one must choose the block thickness larger than the diameter of the block-substrate contact region. In the present study, the block thickness is d ≈ 276 Å.

The substrate is rigid. The springs between the block atoms have elongation and bending stiffness so chosen as to reproduce Young’s modulus E and shear modulus G specified as input for the calculations, and here we use E = 10 MPa and G = 3.33 MPa, corresponding to the Poisson ratio ν ≈ 0.5.

Fig. 2(a) shows the contact between the elastic slab (block) and the substrate at the temperature T = 0 K before start of sliding. We only show the first layer of atoms

![FIG. 1: An elastic block (green) sliding on a substrate (black). At the opening and closing crack tips rapid atomic snap-off and snap-in processes occur which is the origin of the observed sliding friction.](image-url)
of the block and the substrate at the interface. The substrate and the block have \( N_x = 206 \) and 128 atoms along a row in the \( x \)-direction, and \( N_y = 11 \) and 7 atoms in the \( y \)-direction, respectively. The substrate and block-lattice constants \( a_x = L_x / N_x \approx 1.233 \) Å and \( a_y \approx 1.984 \) Å, respectively. The ratio \( a_y/a_x \approx 1.609 \) is close to the golden mean \((1 + \sqrt{5})/2 \approx 1.618\) so the contact is “almost” incommensurate. The block mass density \( \rho = m/a_x^3 \approx 1060 \) kg/m\(^3\).

The atoms at the interface between the block and the substrate interact via the Lennard-Jones (LJ) interaction potential:

\[
V(r) = 4V_0 \left[ \left( \frac{r_0}{r} \right)^{12} - \left( \frac{r_0}{r} \right)^6 \right],
\]

where \( V_0 = 0.04 \) eV and \( r_0 = 3.28 \) Å. This LJ potential gives the adiabatic work of adhesion \( w_0 \approx 0.0027 \) J/m\(^2\). This work of adhesion is very small, and a more typical value is \( w_0 \approx 0.1 \) J/m\(^2\), but this would in the present case result in complete contact at the interface. If the attractive part of the LJ potential is removed (i.e., no adhesion) a “superlubric” sliding state would prevail, with vanishing sliding friction.

During sliding lattice vibrations (phonons) are emitted from the contact region, and for a finite system without internal damping, the block will heat up and after long enough sliding distance the thermal fluctuations will influence the contact mechanics and the friction force. For this reason, it is important to choose the thickness of the sliding block relatively large. The thicker this layer is the smaller influence will the thermal fluctuations, resulting from emitted phonons, have on the contact mechanics.

In the present study, we include a Langevin type of damping force (proportional to the atom relative velocity) in the equation of motion for the block atoms during the initial contact formation (no sliding). After we have obtained the initial contact state (at zero temperature) we remove the damping term and consider so short sliding distances that frictional heating is negligible.

In Fig. 2(a) we show pictures of the contact after squeezing the solids into contact (no sliding) for the nominal contact pressure \( p = F_z/(L_x L_y) = 0.1 \) MPa. Fig. 2(b) shows the contact after 3 nm of sliding at 0.1 m/s.

**Results**—Fig. 3 shows the logarithm of the kinetic friction coefficient \( \mu = F_x/F_z \) as a function of the logarithm of the sliding speed. The friction coefficients were obtained after sliding 3 nm at the given sliding speeds. The nominal contact pressure acting on the upper surface of the block is \( p = 0.1 \) MPa. Note that for \( v < 10 \) m/s the friction coefficient is nearly velocity independent and equal to \( \approx 0.6 \).

**FIG. 2:** The contact area between an elastic slab (block) and a rigid substrate at the temperature \( T = 0 \) K. The substrate is corrugated with the height coordinate \( z = h_0 \sin(q_0 x) \) \((h_0 = 100 \) Å and \( q_0 = \pi/L_x \) with \( L_x = 254 \) Å). The nominal contact pressure \( p = F_z/(L_x L_y) = 0.1 \) MPa. (a) before start of sliding and (b) after sliding 3 nm at the velocity \( v = 0.1 \) m/s.

**FIG. 3:** The friction coefficient \( \mu = F_x/F_z \) as a function of the logarithm of the sliding speed and for the nominal contact pressure \( p = 0.1 \) MPa. The vertical dashed line is for \( v = c_T \), where the transverse sound velocity \( c_T = 56 \) m/s.

**FIG. 4:** The friction coefficient as a function of the sliding distance and the nominal contact pressure \( p = F_z/(L_x L_y) \). For the case of adhesion and the sliding speed \( v = 0.1 \) m/s.
friction coefficient $\mu = F_i/F_z$ with the normal force $F_z = L_x L_y p$. Thus

$$\mu = \frac{w_{\text{open}} - w_{\text{close}}}{p L_x}. \quad (1)$$

Using $L_x = 254$ Å, $p = 0.1$ MPa and $\mu \approx 0.6$ this gives $w_{\text{open}} - w_{\text{close}} \approx 0.0015$ J/m$^2$. The crack propagation hysteresis factor $Q = (w_{\text{open}} - w_{\text{close}})/w_0 \approx 0.56$ is very similar to the hysteresis (due to lattice trapping) observed in atomistic MD crack propagation calculations\[16\]–\[20\], e.g., $Q \approx 0.45$ for zero temperature for the 1D-string model studied in Ref.\[18\].

Since $w_{\text{open}}$ and $w_{\text{close}}$ are independent of the applied pressure $p$, (1) predicts that the friction coefficient $\mu \sim 1/p$, i.e., the friction force is independent of the applied normal force. To test this we have performed MD simulations with $p = 0.05, 0.1, 0.2$ and $0.4$ MPa, see Fig.\[4\]. Clearly, within the noise of the calculations, the friction coefficient is proportional to $1/p$ confirming that the friction is entirely due to the emission of phonons from the opening and the closing crack tips.

The calculation above is for $T = 0$ K. As the temperature increases, the hysteresis factor $Q(T)$ decreases\[18\]. Hence the contribution to the sliding friction from the phonon emission from the crack tips decreases with increasing temperature.

From the continuum mechanics theory of cracks, it is known that the crack propagation energy (per unit created surface area) diverges when the crack tip velocity approaches the velocity of elastic wave propagation in the solids (more exactly, the Rayleigh sound speed)\[21\]. This is due to the emission of elastic waves (phonons) from the moving crack tip. In the present case the transverse sound velocity $c_T = (G/\rho)^{1/2} \approx 56$ m/s (the Rayleigh sound speed $c_R \approx 0.95c_T$). Hence we expect the friction to increase drastically as the drive velocity $v$ approaches $c_T$, as it is indeed the case (see Fig.\[3\]).

The emission of sound waves from the opening crack results in a crack propagation energy which is larger than the adiabatic value, while for the closing crack it is smaller than the adiabatic value. This results in an asymmetric contact where $x_{\text{max}} > |x_{\text{min}}|$. This asymmetry is easily observed in pictures of the interfacial separation as a function of the lateral coordinate $x$; see Fig.\[2\]b and Ref.\[22\].

Let us now study the stresses acting normal and tangential to the (rigid) substrate profile. These stresses, which we denote as $\sigma^*$ and $\tau^*$, respectively, can be easily obtained from the linear combination of $\sigma = \sigma_{zz}$ and $\tau = \sigma_{xx}$: $\sigma^* = \sigma \cos \theta - \tau \sin \theta$ and $\tau^* = \sigma \sin \theta + \tau \cos \theta$, where $\tan \theta = \frac{\tau^*}{\sigma^*}$ is the slope of the substrate profile. In Fig.\[3\] we show $\sigma^*$ and $\tau^*$ as a function of the spatial coordinate $x$. The nominal contact pressure $p = 0.1$ MPa and the sliding speed $v = 0.1$ m/s. We show results (a) after squeezing the solids into contact (zero sliding distance), and (b) after sliding 3 nm. Note the

![FIG. 5: The normal stress $\sigma^*$ (red line) and the shear stress $\tau^*$ (blue) acting on the block as a function of the spatial coordinate $x$. (a) Only squeezing and (b) after sliding 3 nm at the sliding speed $v = 0.1$ m/s. The nominal contact pressure $p = 0.1$ MPa.](image-url)
large adhesive stress at the edges (crack tips) of the contact region. If \( r \) denotes the distance from a crack tip, from the continuum model of adhesion (the JKR theory for stationary contact), one expects the stress to diverge as \( r^{-1/2} \) as one approaches a crack tip \([21]\).

Note that the friction force is the integral over the surface area, from \( x = 0 \) to \( x = L \), of the stress \( \sigma_{xz} = \tau^* \cos \theta - \sigma^* \sin \theta \). The shear stress \( \tau^* \) in the contact area takes both positive and negative values and the integral of \( \tau^* \cos \theta \) over \( x \) nearly vanish. Hence, the biggest contribution to the friction force comes from the stress \( \sigma^* \) normal to the substrate profile. For the sliding state (Fig. 3(b)) the integral of \( \sigma^* \sin \theta \) over \( x \) is nonzero and relatively large because the adhesive stress \( \sigma^* \) at the opening crack tip is considerably larger than the corresponding stress at the closing crack tip (see Fig. 3(b)).

**Discussion**—We have shown that the friction force is nearly velocity independent for \( v \ll c_T \), where \( c_T \) is the velocity of transverse sound waves in the block. The friction force is mainly due to energy dissipation at the opening crack tip, where rapid atomic snap-off events occur during sliding. This “edge-dominated friction” is very different from the frictional processes found when a macroscopic silicone rubber sphere is sliding on a substrate. In the latter case, one observes an “area-dominated friction” where the shear stress is nearly uniform within the contact area. In this case, the friction force arises from the stick-slip type of motion of nanometer-sized regions everywhere within the contact region (see Fig. 6). For viscoelastic solids like rubber, there is a viscoelastic contribution to the crack-opening energy, which may involve regions in the solid far away from the crack tip, which for high enough crack tip speed may enhance the crack propagation energy with a very large factor, given by the ratio between Young’s modulus in the glassy and the rubbery region (enhancement factor typically of order 100-1000) \([28–31]\). Thus, for high enough sliding speeds the crack tip region may give a very important contribution to the sliding friction force for viscoelastic solids. We note, however, that the higher the sliding speed the further away from the crack tip the dominating viscoelastic energy dissipation will occur, which will result in a finite-size effect: if the asperity contact region is small the viscoelastic contribution to the crack propagation energy may be strongly reduced \([31]\).

Most real surfaces have layers of weakly adsorbed molecules, e.g., hydrocarbons. In this case too, one expects an important contribution to the friction force from the internal area of the contact region. Thus, when weakly bound “contamination” molecules are located between two solids they will adjust to the corrugated potential of both walls and pin the surfaces together. This will result in a non-zero breakloose (or static) friction force. During sliding instabilities occur where the molecules rapidly slip at velocities unrelated to the (macroscopic) block driving speed. After each slip event, the local vibrational motion may occur, which is damped by phonon emission \([14, 15]\), very similar to the processes occurring at the opening crack tip in the model studied above. At low temperature this usually results in a kinetic friction force which is nearly independent of the sliding speed, except at very low sliding speeds where thermal activation becomes important, where the friction force depends logarithmic or linearly on the sliding speed \([1, 32, 33]\).

Finally, we note that elastically hard materials like diamond usually exhibit very low sliding friction. This may result from the large elastic modulus, and the relative small surface energy of diamond (the dangling bonds in the normal atmosphere are passivized by hydrogen or oxygen atoms). Thus, MD calculations for the model studied above, but with increased Young’s modulus \( E > \)
1 GPa, gives so small friction that it cannot be detected within the noise level of the simulations. The Young’s modulus of diamond $E \approx 1000$ GPa makes the ratio $\frac{w_0}{E}$ much smaller than we used above even if $w_0 \approx 1$ J/m$^2$. The large modulus of diamond also results in incommensurate arrangements of the atoms at the sliding interface (unless two single crystals with aligned crystal orientations are used) so for clean smooth surfaces one expects negligible contribution from the internal regions of the contact area. The (small) friction observed in practical applications must be due to contamination molecules (see above).

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Movie 2 (Sliding): https://youtu.be/Hxd7AaS3Mq0