Cylinder–flat contact mechanics during sliding

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Using molecular dynamics (MD) we study the dependency of the contact mechanics on the sliding speed when an elastic block (cylinder) with a \( \cos(q_0 x) \) surface height profile is sliding in adhesive contact on a rigid flat substrate. The atoms on the block interact with the substrate atoms by Lennard-Jones (LJ) potentials, and we consider both commensurate and (nearly) incommensurate contacts. For the incommensurate system the friction force fluctuates between positive and negative values, with an amplitude proportional to the sliding speed, but with the average close to zero. For the commensurate system the (time-averaged) friction force is much larger and nearly velocity independent. For both type of systems the width of the contact region is velocity independent even when, for the commensurate case, the frictional shear stress increases from zero (before sliding) to \( \approx 0.1 \) MPa during sliding. This frictional shear stress, and the elastic modulus used, are typical for Polydimethylsiloxan (PDMS) rubber sliding on a glass surface, and we conclude that the reduction in the contact area observed in some experiments when increasing the tangential force must be due to effects not included in our model study, such as viscoelasticity or elastic nonlinearity.

INTRODUCTION

The contact between a spherical (or cylindrical) body and a flat surface is perhaps the simplest possible contact mechanics problem, and often used in model studies of adhesion and friction\[1-3]. For stationary contact with \( F_x = 0 \), where \( F_x \) is the applied tangential force, the adhesive interaction is well described by the Johnson-Kendall-Roberts (JKR) theory\[4, 5\] which has been tested in great detail. However, when the tangential force \( F_x \) is non-zero the problem becomes much more complex and not fully understood\[6-11].

Here we consider the contact between an elastic block with cylinder shape with the height profile \( z = h_0 \cos(q_0 x) \), and a rigid solid with a flat surface. We will refer to this system as curved-flat. In Ref. \[10\] and \[11\] we studied the opposite situation of an elastic block with a flat surface in contact with a rigid solid with the height profile \( z = h_0 \cos(q_0 x) \). We will refer to this system as flat-curved. When \( F_x = 0 \) the curved-flat and flat-curved systems are both described by the JKR theory. However, as will be shown here, during sliding the two systems exhibit very different properties.

MODEL

A curved elastic block can be obtained by “gluing” an elastic slab to a rigid upper surface profile. Here we use a slab of thickness \( L_z \approx 86 \) Å attached to a rigid surface with the height profile \( z = h_0 \cos(q_0 x) \), where \( h_0 = 100 \) Å and \( q_0 = 2\pi/L_x \). We use periodic boundary conditions in the \( xy \)-plane with \( L_x = 254 \) Å and \( L_y = 14 \) Å. The number of atoms in the \( x \)-direction is \( N_x = 128 \) for the block, and for the substrate we consider two cases where \( N_x = 128 \) (commensurate interface) and \( N_x = 206 \). In the latter case the ratio between the lattice constant of the block and the substrate is \( a_b/a_s = 206/128 \approx 1.609 \), which is close to the golden mean \((1 + \sqrt{5})/2 \approx 1.618\), i.e. the interface is nearly incommensurate. The block is treated using the smart-block description (with 13 layers with the same spacing as for the first layer plus 4 layers on top of it, where at every step we double the lattice spacing in the \( x \) and \( z \)-directions) discussed in Ref. \[10\], where the bending and elongation spring constants are chosen to give the Young’s modulus and the Poisson ratio \( E = 10 \) MPa and \( \nu = 0.5 \), respectively. The interaction potential between the block and wall atoms at the interface is of the Lennard-Jones (LJ) type:

\[
V(r) = 4V_0 \left[ \left( \frac{r_0}{r} \right)^{12} - 2 \left( \frac{r_0}{r} \right)^{6} \right],
\]

where \( V_0 = 0.04 \) meV and \( r_0 = 3.28 \) Å. With this interaction potential we calculate the (adiabatic) work of adhesion \( w \approx 0.0023 \) J/m\(^2\) for the commensurate interface, and \( w \approx 0.0027 \) J/m\(^2\) for the incommensurate interface. We note that in the present system, when the adhesion is removed \((w \rightarrow 0)\) the contact width decreases from 85.3 Å to 25.8 Å when the nominal pressure \( p = 0.1 \) MPa, and from 101.1 Å to 61.5 Å when \( p = 1 \) MPa. Thus,
in spite of the small work of adhesion, the adhesion interaction is very important, which is due to the small size of the system (in the JKR theory the width of the contact region depends on the (dimensionless) parameter $w/(pR)$, where $R$ is a length characterizing the size of the system; $w/(pR)$ is of order unity in the present case).

Fig. 1 shows for the incommensurate interface the system (a) before contact, and (b) after squeezing the block against the substrate with the nominal contact pressure $p = F_z/(L_x L_y) = 0.1$ MPa (blue), and $p = 1$ MPa (red). We also show the contact for the flat-curved case studied in Ref. [10] and [11].

**NUMERICAL RESULTS**

Fig. 2 shows the friction coefficient $\mu = F_x/F_z$ as a function of the distance $vt$ moved by the top of the elastic block (curved-flat system). For the incommensurate (a) and the commensurate (b) interface. The nominal contact pressure $p = 0.1$ MPa and the speed $v = 0.1$ m/s.

Fig. 3 shows the friction coefficient $\mu = F_x/F_z$ as a function of the sliding distance for the commensurate system. The sliding speed $v = 0.1, 0.2, 0.5$ and $1$ m/s, and the contact pressure $p = 0.1$ MPa. For the incommensurate system the average friction coefficient nearly vanish ($\mu < 10^{-2}$) while for the commensurate system it is of order unity ($\mu \approx 0.9$). The oscillations in $F_x/F_z$ for the incommensurate system is due to the abrupt start of sliding where the upper surface of the block abruptly start to move with the speed $v = 0.1$ m/s.
at time $t = 0$ (see movie [12]). This result in an elastic wave propagating (with the transverse sound velocity $c_T = (G/\rho)^{1/2} \approx 56$ m/s) towards the interface so that only after the time $t = d/c_T$ the atoms at the interface will start to move. The periodicity of the fluctuation in the tangential force $F_x$ in Fig. 2(a) is given by the time it takes for an elastic wave to propagate back and forth between the two surfaces, i.e., the distance $2d$ giving the time $\Delta t = 2d/c_T$ or sliding distance $\Delta s = v\Delta t = 2dv/c_T$. Using $v = 0.1$ m/s, $c_T = 56$ m/s and $d = 8.6$ nm this gives $\Delta s = 0.031$ nm. The numerical calculations show that the period (in time) of the oscillations in $F_x$ is independent of the sliding speed $v$, and the contact pressure $p$, while the amplitude of the oscillations is proportional to $v$.

For the commensurate interface the friction is much larger and nearly velocity independent (see Fig. 3). This is the expected result when at the sliding interface rapid slip events occur, involving velocities independent of the driving speed $v$. Observations of movies (see Ref. [13]) shows that the sliding motion involves domain-wall excitation (solitones), which propagate with high speed (of order the Rayleigh sound velocity; see Fig. 4), unrelated to the sliding speed $v$, while energy is radiated into the block giving rise to the observed high friction force.

For both the commensurate and the incommensurate systems the contact width does not change with sliding speed in the studied velocity range ($v < 1$ m/s). For the incommensurate system this is expected because of the nearly vanishing (average) friction force, but for the commensurate system the friction is large but still the contact width is independent of the sliding speed. In particular,
there is no change in the contact width between \( v = 0 \) with \( F_x = 0 \) and sliding at a finite velocity where the frictional shear stress is of order 0.1 MPa (as is typical for PDMS sliding on a glass surface\(^\text{14}\)).

In an earlier publication we have studied sliding friction for the flat-curved situation where an elastic block with a smooth surface is sliding on a rigid surface with the height profile \( z = h_0\cos(q_0x) \). This case differs from the curved-flat configuration studied above since for the flat-curved system there is an important contribution to the friction from phonon emission from the opening and closing crack tips. In fact, for the system sizes we have studied, for the flat-curved case, even for the commensurate interface the contact edge contribution to the friction is larger than the contribution from the internal region of the contact. This is illustrated in Fig. 3 which shows the nominal frictional shear stress \( F_x/(L_xL_y) \) as a function of the sliding distance for the flat-curved case with incommensurate interface (red curve), and for the commensurate interface (blue curve). In the calculations we have assumed the nominal contact pressure \( p = 0.1 \) MPa. The figure also shows the result for a higher contact pressure, \( p = 0.3 \) MPa (green line). Note that the incommensurate interface gives the largest friction. For this system there is negligible contribution to the friction from the internal region of the contact. That is, the friction is entirely due to the phonon emission associated with the rapid atomic snap-out and snap-in at the crack edges (see Ref. \( \text{10} \) and \( \text{11} \)). It is remarkable that the commensurate system gives lower friction than the incommensurate system, in spite of the fact that for this system there is both a contribution from the internal region of the contact and from the crack edges. However, the contribution from the crack edges is smaller than for the incommensurate system due to the higher density of substrate atoms for the incommensurate system (the ratio is \( 206/128 \approx 1.61 \)).

Fig. 6 shows (a) the normal stress \( \sigma_{zz} \) and (b) the shear stress \( \tau_{zx} \) acting on the block as a function of the spatial coordinate \( x \). The red lines are for the curved-flat system, and the green lines for the flat-curved system, in both cases with a commensurate interface (with \( a_y/a_x = 128/128 = 1 \)). The sliding speed \( v = 0.1 \) m/s, and the nominal contact pressure \( p = 0.1 \) MPa. Note that in both cases at the edge of the contact region the normal stress \( \sigma_{zz} \) is tensile and maximal, as expected from the JKR theory, and from the theory of cracks, which predict that the stress has a \( r^{-1/2} \) singularity at \( r = 0 \) (where \( r \) is the distance from the crack tip). Because of the curved contact region in the flat-curved system, at the edge of the contact region the stress \( \tau_{zx} \) will exhibit a similar singular form as the normal stress. However for the curved-flat system the contact region is flat and only the \( \sigma_{zz} \) stress exhibit the singular form.

**DISCUSSION**

We have shown above that within linear elasticity theory the contact area between an elastic cylinder and a rigid flat countersurface does not depend on the applied tangential force, at least not for the systems studied above. This is in contrast to some experimental results for PDMS spheres sliding on smooth glass surfaces. This indicates that the origin of the area reduction in the size of the contact area in Ref. \( \text{15} \) and \( \text{16–18} \) may be due to some effect not taken into account in the model study, such as material viscoelasticity, elastic nonlinearity or contact time-dependent work of adhesion.

In an interesting study Lengiewicz et. al.\(^\text{19}\) have found that the observed contact area reduction for a PDMS rubber sphere in contact with a glass surface can be explained by a theory based on non-linear elasticity without invoking adhesion! They found quantitative agreement with the recent experimental results of Sahli et. al. \( \text{16, 17, 19} \) on sphere-plane elastomer contacts, without adjustable parameters, using the neo-Hookean hyperelastic model. The importance of elastic nonlinearity for the explanation of the contact area reduction have been suggested by us in some earlier papers in particular the Tribology Letters\(^\text{20}\). In another paper\(^\text{10}\) we observed that for a dry clean human finger there is no macroscopic adhesion to a flat glass plate (due to the large surface roughness of the skin) so the fact that for this case too the contact area is reduced upon application of a tangential force must clearly be a non-linear elastic effect. That adhesion itself may not result in a reduction in the contact area upon application of a tangential force was also shown theoretically to be the case in the paper by Menga, Carbone and Dini\(^\text{8}\). Finally, we note that in at least one study the rubber-glass contact area was found to increase upon sliding indicating that other mechanisms may contribute to the dependency of the contact area on the tangential force\(^\text{21}\).

If the reduction in the contact area upon application of a tangential force can be interpreted as an effective stiffening of the rubber elastic properties by the tangential deformations, then we expect also that the penetration is decreasing by increasing tangential force. This could explain the experimental observation in Ref. \( \text{20} \) that a sharp tip indented in a rubber surface with a given normal force moves upwards when a parallel force is applied in addition to the normal force. Within (small deformation) linear elasticity theory this result is unexpected as there is no coupling between the parallel and the perpendicular deformations when the Poisson ratio is equal to 0.5 (incompressible solid), as is the case in the rubbery region for rubber-like materials.

In this paper, and in Ref. \( \text{10} \) and \( \text{11} \), we have assumed simple crystalline solids. Rubber-like materials are more complex materials with cross-linked long-chain molecules, and may have nanometer-thick surface layers with liquid-like mobility of the polymer segments, which can rearrange in the substrate surface potential and form small regions which are pinned by the substrate. In this case during lateral motion of the rubber block the chain stretches, detaches, relaxes, and reattaches to the surface to repeat the cycle. Here “detaches” stands for rearrangement of molecule segments (in small domains) parallel to
the surface from pinned (commensurate-like) to depinned (incommensurate-like) domains. This result in an “area-dominated friction” where the shear stress is uniform within the contact area as observed experimentally. In this case the friction force arises from stick-slip type of motion of nanometer-sized regions everywhere within the contact region. Theoretical model studies of this process was presented in Ref. [22, 23].

That systems with (nearly) incommensurate interface exhibit smaller friction than systems with commensurate interface, as found above, is a well known, but in practice there are several “complications”. Thus, even if the interface is incommensurate mobile adsorbed contamination molecules will always exist in the normal atmosphere, which will adjust their positions and pin the surfaces together, which may result in a large and nearly velocity independent friction force [24, 25]. Nevertheless, even if there are no strictly incommensurate systems, one expect smaller friction force the closer an interface becomes to a perfect incommensurate system. As an example, if two polymers, say A and B, with very different nature of the bead units, slide on top of each other, a relative small friction coefficient may prevail, while for A sliding on A, or B on B, the friction may be much higher due to the more commensurate-like contact [26, 27]. In the latter cases the friction coefficient is also expected to be nearly velocity independent, assuming the sliding speed is not so high that frictional heating becomes important, or so low that thermal activation becomes important. As an example, in Fig. [7] we show the velocity dependency for PolyOxyMethylene (POM) polymer block sliding on a POM substrate.

**SUMMARY AND CONCLUSIONS**

We have presented molecular dynamics simulations for an elastic cylinder sliding on a rigid flat countsurface (curve-flat). For this system, within linear elasticity theory, the contact area does not depend on the applied tangential force.

The sliding friction of commensurate and incommensurate interface contacts was investigated. For the commensurate interface the friction is large and nearly velocity independent due to rapid slip events involving domain-wall excitation (solitones), which propagate at the interface with a speed of order the sound velocity, radiating energy to the block giving rise to the observed high friction force.

The geometry of contact, whether curved-(rigid) flat contact or flat-(rigid) curved contact decide the energy dissipation mechanism during sliding resulting in observed difference in frictional force. For the curved-flat case the friction force is mainly due to processes occurring inside the contact area, while for the flat-curved case, for the system we studied, the friction force is mainly due to phonon emissions at the crack edges associated with the rapid atom snap-out (at the opening crack) and snap-in (at the closing crack) events.

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