Onset of incommensurate interfacial instability in a minimal model of dry friction

Brad Lee Holian[1] and James E. Hammerberg[2]
[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Applied Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
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We present a minimal model of dry friction between two incommensurate interfaces sliding at high relative velocity. Many of the features of the friction force for the full two-dimensional many-body dynamical system—particularly in the sub-critical velocity regime—are captured by our one-dimensional Einstein model, where the motion of a typical interfacial atom is constrained to be vertical to the sliding plane. Beyond the linear response of force versus sliding velocity, the anharmonic Einstein model predicts a doublet resonance peak, whereupon a catastrophe in the model signals the onset of a plastic deformation mechanism for frictional sliding, namely, the instability of the interface. Higher velocities than this critical value require a much more sophisticated description of the production and coalescence of dislocations into a microstructure.

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Sliding friction between two incommensurate interfaces moving in two dimensions (2D) has been studied by large-scale nonequilibrium molecular-dynamics (NEMD) computer simulations involving up to hundreds of thousands of atoms [1]. In these studies, our focus has been on dry, incommensurate interfaces, under ultrahigh vacuum and completely free of contamination. Under these conditions, no static friction is observed, and dynamic sliding occurs at velocities well above 10 m/s with nonzero friction coefficient [2]. In order to describe the observed behavior in these complex systems, we would like to reduce the number of degrees of freedom to a minimal model that captures as many of the essential features as possible. By minimal, we really mean a single particle, with its motion restricted to 1D, namely, vertical to the sliding plane. As we will show, this simple picture can quantify the tangential force required to obtain a steady sliding velocity above the quasistatic regime, and even to predict the onset of instability at a critical velocity, where many-body plastic deformation mechanisms become dominant [3].

Figure 1 shows the two-dimensional sliding interface. The lower surface is a triangular lattice of close-packed lines parallel to the interface, composed of atoms of type B (solid circles) spaced r_0 apart in the horizontal direction; the close-packed lines are spaced $b=\sqrt{3}r_0/2$ apart in the vertical direction. The upper surface, composed of atoms of type A (rightward-pointing open arrows in the direction of sliding) has close-packed lines perpendicular to the interface, with the x distance between vertical planes equal to b. We also take b to be the y distance between the two surfaces in contact. As the upper surface slides over the lower at relative velocity v, we see that a typical interfacial B atom (depicted as an open circle with a vertical arrow through it) has closest contact with every other A particle, as close as $b\approx 0.87r_0$ and as far as $b+r_0/2\approx 1.37r_0$. Thus, the upper A material has a more open surface structure, which we characterize by the incommensurability ratio of $A{:}B$ atoms; in this case, $2b/r_0{:}1=\sqrt{3}{:}1$.

The response of a typical B atom along the interface is to execute a quasiperiod-two oscillation in the vertical direction, that is, every other atom along the interface is approximately 180° out of phase with its nearest neighbor. This leads inexorably to the minimal Einstein model of a particle driven vertically by the horizontal periodic motion of the upper A atoms.

The Einstein (single-particle) model [4], familiar to the statistical mechanics community, focuses upon a single atom moving in a cage of nearest neighbors (hence, the alternative name, ''cell model''). The Einstein model has been particularly useful in the study of crack propagation [5], where the imposition of a further restriction to one-dimensional motion perpendicular to the crack direction has helped to explain the limiting crack velocity [6]. In the friction literature, Einstein models have been known historically as ''Tomlinson'' models [7], where approximate driving forces are *usually* obtained from a Frenkel-Kontorova (FK) substrate potential, rather than the actual interatomic interactions [8]. When one sees illustrations of the FK potential, it is natural to imagine that the atom moves side to side, *parallel* to the sliding

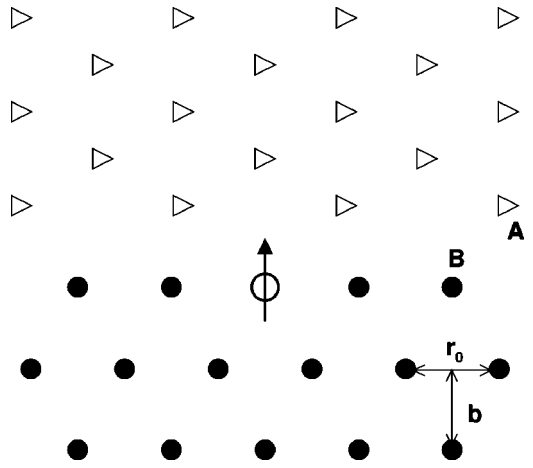

FIG. 1. Incommensurate interface between two triangular lattices in two dimensions. Atoms of type A (open arrow symbol) move to the right at constant relative sliding velocity v; atoms of type B (solid circles) are fixed, except for central Einstein atom (open circle with vertical arrow), which is free to move up and down. Nearest-neighbor spacing is r_0; close-packed rows of atoms are separated by $b=\sqrt{3}r_0/2$, as is A-B interface.

direction—a very natural assumption for the quasistatic (extremely low-velocity) regime—and yet also to assume (subliminally) that the atom moves up and down as well. An earlier two-dimensional Einstein model was proposed for friction which would have included both vertical and horizontal motion, but no analysis of the velocity dependence of the friction force was carried out [9]. When 2D is reduced to 1D, the vertical motion is typically thrown away [10,8] (except for studies of dilatation [11], which are for macroscopic plates, rather than a typical interfacial atom).

In our one-dimensional Einstein model of sliding friction, we use more realistic interatomic forces than the sinusoidal substrate potential. Most importantly, in our model the atom's motion is constrained to be *perpendicular* to the sliding plane, in agreement with what we actually see in movies of large-scale MD simulations. There, the atoms on the denser side of an incommensurate interface bob up and down like loose ties in a dilapidated railroad track as the wheels of a heavy train roll slowly by. As we shall show, our one-dimensional model predicts the onset of a mechanism for dynamical instability of the dry, incommensurate interface at high sliding velocity. With this model, we are able to quantitatively match the full MD simulations for the resonance (critical) velocity, which depends crucially on this out-of-plane motion.

The spatial period of the driving A atom is $2b$, so that the temporal period is $\tau=2b/v$ and the angular frequency of driving is $\omega=2\pi v/(\sqrt{3}r_0)$. The coordinates of the Einstein particle $(x\equiv 0,y)$ are measured from its lattice site at the origin. For simplicity, we imagine that the interaction of this Einstein atom with its four nearest neighbor B atoms is restricted to the pair directly below, and that the effect of its side neighbors is to confine its motion to be in the vertical y direction only. This so-called ''internal'' interaction between the Einstein particle and its two neighbors below at distance $R=[(y+b)^2+(r_0/2)^2]^{1/2}$ is $\Phi(R)=2\varphi(R)$, where we choose $\varphi(R)=\epsilon_0\{\exp[-\alpha(R/r_0-1)]-1\}^2$, the standard Morse potential with bond energy ϵ_0, bond length r_0, and repulsive parameter α (the fundamental bond frequency is ω_0, where $m\omega_0^2r_0^2=mc_0^2=2\alpha^2\epsilon_0$ and $c_0=r_0\omega_0$ is the longitudinal sound velocity); since the atomic mass is m, we can choose the unit of time to be $t_0=r_0(m/\epsilon_0)^{1/2}$. (For a metal such as copper, $r_0\approx 0.3$ nm, $\epsilon_0\approx 0.5$ eV/atom, and $c_0\approx 5$ km/s.)

The Einstein B particle's ''external'' interaction with the upper A atom is described by a purely repulsive short-range Morse potential $\varphi(r)$, cut off at its minimum (i.e., $r_{max}=r_0$), where the x distance between the Einstein B atom and the driving A atom is $x-x_A=-vt$ (the time t is confined to the interval $-\tau/2\leqslant t\leqslant\tau/2$ describing the periodic boundary conditions of the driving A particle), the y distance is $y-b$, and $r=[(-vt)^2+(y-b)^2]^{1/2}$. (In principle, the cross potential between A and B atoms could be different from the A-A and B-B interactions, but we will assume here for simplicity that the two materials across the interface are identical.) In order to achieve the long-time steady state, hundreds of vibrational periods τ are integrated in time to eliminate initial transients, followed by a steady-state average over additional hundreds of τ (the central-difference integration time step is 1/60th of either τ or the fundamental vibrational period, whichever is less).

The Newtonian equation of motion of the Einstein particle includes the effect of dissipation due to the transport of energy away from the interface by sound waves and thermal diffusion, which we represent by the viscous damping coefficient γ:

$$\ddot{y}=\frac{F_y}{m}-\gamma\dot{y}. \tag{1}$$

The total force F_y is the sum of the internal and external (driving) forces:

$$F_y=-\frac{\partial\Phi}{\partial y}-\frac{\partial\varphi}{\partial y}=-\Phi'(R)\frac{y+b}{R}-\varphi'(r)\frac{y-b}{r}. \tag{2}$$

The external force in the x direction required to keep the driving A particle moving at velocity v is

$$F_x=-\varphi'(r)\frac{-vt}{r} \tag{3}$$

which, when averaged over time at the steady state, is the frictional force F_{tang} to be reported as a function of the sliding velocity v.

The total energy of the Einstein particle, $E=\frac{1}{2}m\dot{y}^2+\Phi(R)+\varphi(r)$, is subject to the following rate of change:

$$\dot{E}=m\ddot{y}\dot{y}+\Phi'(R)\dot{R}+\varphi'(r)\dot{r}=(F_y-\gamma m\dot{y})\dot{y}+\Phi'(R)\frac{y+b}{R}\dot{y}$$

$$+\varphi'(r)\frac{v^2t+(y-b)\dot{y}}{r}=-\gamma kT+F_xv, \tag{4}$$

where $kT=m\dot{y}^2$ is the temperature in this one-dimensional externally driven Einstein model. At the steady state, the long-time average of the rate of change in energy is $\overline{\dot{E}}=0$, which implies that the frictional force is [12]

$$F_{tang}=\overline{F_x}=\frac{\gamma}{v}k\overline{T}. \tag{5}$$

While the external force F_x can also be calculated and time averaged at the steady state (so-called direct evaluation), the second equality (temperature evaluation) in Eq. (5) is better behaved, particularly for small values of F_{tang}, simply because the temperature is a positive quantity with smaller fluctuations than the nearly zero force.

The equation of motion [Eq. (1)] for the Einstein particle can also be written in a familiar form, provided that the internal interaction for small displacements $y\approx 0$ can be expressed in the harmonic approximation, with the external driving approximated by a sinusoidal (in time) force:

$$\ddot{y}=-\omega_y^2y-\gamma\dot{y}-g_0(1+\cos\omega t), \tag{6}$$

where the amplitude of the external driving $g_0 = -\omega_y^2 \overline{y^{ss}}$ is determined from the steady-state ($t=0$) displacement $\overline{y^{ss}} = -(2-\sqrt{3})/5 = -0.054$ (where external and internal forces balance in the harmonic approximation). The fundamental frequency ω_y for the internal interaction potential is given by

$$\frac{m\omega_y^2 r_0^2}{\epsilon_0} = 3\alpha^2. \tag{7}$$

For this damped and driven harmonic oscillator, the temperature can be obtained analytically as [13]

$$k\overline{T} = \frac{mg_0^2}{2} \frac{\omega^2}{(\omega_y^2-\omega^2)^2+\gamma^2\omega^2}. \tag{8}$$

The temperature exhibits a resonance peak at $\omega_{critical} = \omega_y$, which implies a critical velocity

$$v_{critical} = \frac{\sqrt{3}}{2\pi} r_0 \omega_y. \tag{9}$$

The peak amplitude is inversely proportional to γ^2, and its width in frequency is proportional to γ. (The underdamped regime, where $\gamma \ll \omega_y$, is the most physically relevant for atomistic systems.) For small velocities, temperature is quadratic in velocity and goes like v^{-2} at large velocities.

As a result, in the low-velocity regime, F_{tang} is linear in v—so-called linear response to the amplitude of the driving—as well as linear in the damping coefficient, and quadratic in the amplitude of the cross potential between the two surfaces (i.e., proportional to g_0^2). (Analogous results are obtained in the linear regime for somewhat more sophisticated models [14].) Then there is a resonance peak near the critical velocity and a tailoff for large velocities that goes as v^{-3}. When the driving is weak, the system responds nearly adiabatically; likewise, when the velocity is very high compared to the resonance condition, the system is unable to respond well. It is only in the resonance peak regime that the driving is well coupled to the system.

Of course, this harmonic analytic behavior is modified by the anharmonicity of the interactions, both internal and external. The most obvious modification due to anharmonicity is that the resonance peak is split into two (a doublet), along with the appearance of overtones of this resonance doublet at multiples of the critical frequency, or velocity. Since this minimal Einstein model has three degrees of freedom (y, $\dot{y}$, and v), anharmonicity guarantees chaotic behavior, which manifests itself as undertones of the resonance doublet at one-half and one-quarter of the critical velocity, i.e., period doubling and quadrupling.

Even more interesting is the possibility of catastrophic behavior, which could herald the breakdown of the Einstein (single-particle) approximation for sufficiently high velocities. The emergence of a correlated (many-particle) mechanism—or mechanisms—for the response of the system could include a dynamic phase transformation, for example.

In Fig. 2, we show the tangential friction force as a function of sliding velocity. The harmonic approximation is shown as a dashed line, with a peak velocity whose value is about 2.85 ($v/c_0 = 0.34$). The anharmonic result is the solid curve, which is rich in complexity. (The comparison of the direct calculation of F_{tang}, shown as a dash-dot curve, essentially overlays the solid curve, which was computed from the steady-state temperature.) The harmonic result agrees with the anharmonic result in the linear response regime.

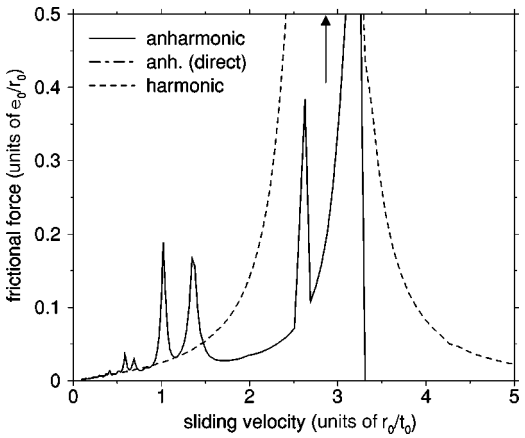

FIG. 2. Frictional force vs sliding velocity for minimal model of sliding friction (anharmonicity parameter $\alpha = 6$ and damping coefficient $\gamma = 1$, i.e., underdamped). Arrow points to harmonic-approximation resonance peak. Direct anharmonic calculation of force overlays temperature evaluation [Eq. (5)].

The anharmonic model of incommensurate sliding friction shows a dramatic catastrophe for velocities above about 3.2. There, the friction coefficient drops to zero, and stays that way to about 6.4. The resonance becomes so strong in this range of sliding velocities that the Einstein particle manages to escape upward beyond the periodic driving A atom. Because of viscous damping, it reaches an asymptotic y position, with zero y velocity; hence, the temperature goes to zero.

Weiss and Elmer simulated a one-dimensional chain of harmonically bonded atoms moving parallel to the sliding direction over a sinusoidal substrate at constant velocity [8]. They find a curve that qualitatively resembles our Fig. 2, but with significant differences: First, their resonance occurs at a higher velocity, because the motion is constrained to the horizontal, rather than vertical direction. Second, no catastrophe occurs near their smooth resonance peak, because no escape from the cage is possible in side-to-side motion.

The real two-dimensional many-body NEMD simulation [1,3] undergoes a dramatic transformation at a velocity very nearly one-quarter of $v_{critical}$, where the first noticeable split peak due to chaotic period quadrupling occurs in our model system (at $v_{instability} \sim 0.6$). The main resonance peak in our model exhibits this $B \rightarrow A$ catastrophe at roughly four times higher velocity than the real many-body simulation, but that is really no surprise, since the period-doubling and -quadrupling subresonances are obvious candidates for the onset of interfacial instability, provided that the resonance exceeds some critical threshold. In fact, the subresonance doublets are amplified in intensity by the push-pull of the actual repulsive-attractive forces between the A driving atoms and the B Einstein atom, as opposed to the purely re-

pulsive interaction we have assumed in our simplified model. It would seem that at the first palpable opportunity (in sliding velocity), the many-body system becomes susceptible to instability, such that each *B* atom joins the upper, more open *A* surface by popping up into an available *A* hole as it moves by. The NEMD force versus velocity curve shows no sign of subresonances at velocities lower than this first peak, indicating that the Einstein model period quadrupling is sufficient to instigate the interfacial instability.

This instability of the incommensurate interface is like an orientational phase transformation; that is, the orientation of the upper *A* atoms becomes more favorable than that of the lower *B* atoms, and the phase front moves downward at a discernible rate, rather than diffusively. A movie of the full many-body dynamical action [3] verifies that our simple Einstein model captures an essential feature of the interfacial instability, namely, that *B* atoms pop up into open *A* positions at a regular rate, such that the $\sqrt{3}$:1 interface appears to move downward at a geometrically predictable velocity: $v_{front} \approx v_{instability}/\sqrt{3} \approx 0.57 v_{instability}$. NEMD simulations [3] reveal that $v_{front} \approx 0.53 v_{instability}$, which is very close indeed to this estimate.

Beyond the point of catastrophic interfacial instability, which occurs at the first period-quadrupling subresonance peak, the Einstein model becomes inappropriate. In any event, this phase-front instability soon gives way to the production of dislocations, and ultimately, to the formation of a microstructure that facilitates the sliding process at higher velocities [1,3]. In reality, the friction force in this plastic regime does not drop to zero, but reaches a peak, and then declines with sliding velocity by a power law $v^{-\beta}$, where $\beta \approx 3/4$. We have recently constructed a plasticity model applicable to this regime [15]. At even higher sliding velocities, the interfacial region commences to melt, so that the harmonic large-velocity limit is never achieved.

In spite of the severe minimalism of our one-dimensional Einstein model, it is nevertheless able to discern the onset of catastrophic structural events at the incommensurate interface sliding at high velocities. The up-and-down, out-of-plane bobbing of atoms at the interface is crucial to the understanding of this instability, which presages the regime of plastic self-lubrication of clean metal interfaces.

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