

## Nature of Mechanical Instabilities and Their Effect on Kinetic Friction

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It has long been recognized that kinetic friction  $F_k$  between two solids must be due to instabilities, sudden “pops” of certain degrees of freedom. Here, such pops are studied with a focus on boundary lubrication. The pops’ characteristics and consequently the friction-velocity relationship depend qualitatively on dimensionality, commensurability, and details of the lubricant wall interaction. It is found that  $F_k$  should be small between commensurate surfaces.  $F_k$  is large for incommensurate surfaces, unless the lubricant’s motion is confined to 1D. The effects of thermal noise are discussed and computer simulations are employed to show the relevance of the predictions to less idealized models.

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When a solid slider is moved laterally with respect to a substrate, the kinetic friction  $F_k$  is usually almost independent of the sliding velocity  $v_0$  [1] with leading corrections in the order of  $\ln v_0$  [2]. This so-called Coulomb friction differs from drag or Stokes friction that states a linear relation  $F_k = \gamma v_0$ . Linear friction can be understood from equilibrium statistical mechanics. The proportionality coefficient  $\gamma$  can be calculated with the fluctuation dissipation theorem [3]. Linear or drag friction arises from the many collisions between the central degree of freedom, for instance a Brownian particle or a phonon, and other degrees of freedom like solvent particles or other phonons.

It has long been recognized that Coulomb friction must be related to instabilities that occur on a microscopic scale [4]. When a slider is moved laterally with respect to the substrate, fast motion (pops) of certain degrees of freedom become unavoidable even if the slider’s center of mass velocity  $v_0$  is extremely small. The microscopic peak velocities in such pops are rather independent of  $v_0$  and consequently the energy dissipated via a Stokes-type mechanism also becomes almost independent of  $v_0$ . The prototypical instability leading to Coulomb friction was suggested by Prandtl and Tomlinson [5]. In their one-dimensional (1D) model, a surface atom in the slider is coupled to its ideal lattice site with a spring of stiffness  $k$  which moves at constant velocity  $v_0$ . Interactions with the rigid substrate are modeled with a potential energy  $V$  periodic in the substrate’s lattice constant plus some drag force linear in the atom’s velocity  $\dot{x}$ . If  $k$  is sufficiently small, pops become unavoidable and if thermal fluctuations are negligible,  $F_k$  remains finite in the limit of zero  $v_0$ . More complex models such as elastic manifolds sliding through ordered and disordered media [6,7] show similar behavior. At small  $v_0$ , the functional dependence for  $F_k(v_0)$  is commonly found to be

$$F_k(v_0) = F_k(0) + c v_0^\beta, \quad (1)$$

where  $\beta$  is a nonuniversal exponent between zero and unity.

While the elastic instabilities considered in those models are important in various contexts, this does not seem to be the case for the atomistic explanation of solid friction: Many detailed calculations reveal that in most cases, interbulk interactions are too weak to lead to instabilities at the atomic scale. If interbulk interactions are very strong, irreversible processes like plastic deformation, material mixing, cold welding, etc. become unavoidable and prevent the instabilities from being elastic [8].

It has been suggested that the presence of adsorbed particles, i.e., a boundary lubricant, confined between two surfaces is a more likely explanation for the commonly observed presence of solid friction [9]: Molecules that are only weakly bound to either surface can accommodate the surface corrugation of both walls simultaneously. This locks the walls together. The argument explains static friction, which is the minimum force to initiate sliding between two solids. However, for kinetic friction, the motion of atoms is relevant. It has become common practice in the context of elastic manifolds [6] to first neglect thermal fluctuations. The resulting athermal motion of the particles, which is intimately linked to the motion of the mechanically stable equilibrium sites, is the key to predict the final dissipation. A similar analysis shall be done here for boundary lubricants, which are first treated in the impurity limit, where interactions between lubricant atoms can be neglected. Such an analysis is not known to the author, although the present model has already been used extensively to predict successfully various tribological phenomena [10,11].

The equation of motion for a lubricant atom in the impurity regime reads

$$\ddot{x} = -\gamma_b \dot{x} - \gamma_t (\dot{x} - v_0) + \frac{1}{m} \Gamma(t) - \frac{1}{m} \frac{\partial}{\partial x} \{V_b(x) + V_t(x - v_0 t)\}, \quad (2)$$

where  $x$  denotes the atom's position,  $m$  is the atom's mass,  $\gamma_t$  and  $\gamma_b$  parametrize the damping forces from the top and the bottom wall, and  $V_t$  and  $V_b$  denote the interaction of the confined atom with the slider and the substrate.  $\Gamma(t)$  is a Langevin-type stochastic random force defining temperature. For the lubricant wall interactions, various choices will be considered. Centrosymmetric potentials can all be written in the form:

$$V_{t,b} = V_{t,b}^{(0)} \cos(x/b_{t,b}) + V_{t,b}^{(1)} \cos(2x/b_{t,b}) + \dots, \quad (3)$$

where  $2\pi b_t$  and  $2\pi b_b$  are the periods of the top and the bottom wall, respectively. The relevant physical units are defined through the choice  $V_t^{(0)} = 1$ ,  $m = 1$ ,  $b_t = 1$ , and Boltzmann's constant  $k_B = 1$ . Furthermore, we will only consider slightly underdamped dynamics ( $\gamma_b = 1$ ) and restrict ourselves to the symmetric choice of  $V_0 := V_{t,b}^{(0)}$ . The free parameters are thus the degree of lattice mismatch ( $b_t - b_b$ ), the value of the first higher harmonic (for simplicity, we use  $V_1 := V_{t,b}^{(1)}$ ), and temperature  $T$ .

We start the discussion of the athermal, commensurate (com.) system ( $b_t = b_b$ ) without higher harmonics for which the net time-dependent potential is simply given by  $V(t) = 2V_0 \cos(v_0 t/2b) \cos[(x - v_0 t/2)/b]$ . Thus, for times  $\cos(v_0 t/2b) \neq 0$ , the atoms move at velocity  $v_0/2$  as shown in Fig. 1. An infinitely small moment after the equality  $\cos(vt/2b) = 0$  holds, an atom will not be able to find a mechanically stable position in the immediate vicinity of the previous stable position and the atoms should skid towards a new mechanical equilibrium. In order for this to happen, one needs a symmetry breaking element such as thermal fluctuations,  $\gamma_b \neq \gamma_t$ ,  $b_t \neq b_b$ , or round-off errors in numerical calculations, otherwise the atom's velocity simply is  $v_0/2$ . In order to induct the instability, we chose to set  $\gamma_t = 0$ , because thermal fluctuations would result in the trivial  $F_k \propto v_0$  relation at small  $v_0$  and round-off errors would produce meaningless, machine-dependent results. We note that the precise choice of  $\gamma_t$  and  $\gamma_b$  is not relevant for the functional form

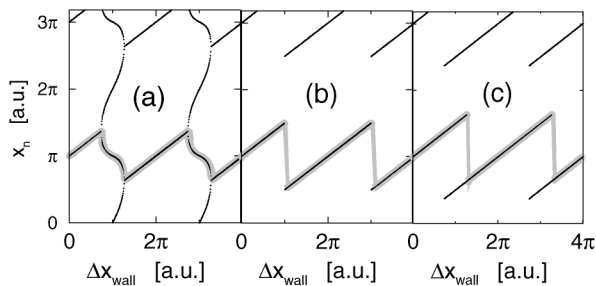


FIG. 1. Mechanical equilibrium positions for adsorbed atoms between two commensurate solid surfaces as a function of the relative displacement  $\Delta x_{\text{wall}}$  between the walls. The grey lines indicate the solutions of Eqs. (2) and (3) if the walls are in slow relative sliding motion. (a) First higher harmonic  $V_1 < 0$ . (b)  $V_1 = 0$ . (c)  $V_1 > 0$ .

of  $F_k(v_0)$  for incommensurate (inc.) surfaces. This is why  $\gamma_t = 0$  is chosen in the following.

Owing to broken symmetry ( $\gamma_t = 0$ ), the atom can now slide to the next minimum indicated by the gray lines in Fig. 1(b). However, the peak velocities  $\dot{x}_p$  in this process tend to zero as  $v_0$  decreases, because, due to the symmetry of  $V_t$  and  $V_b$ , atoms jump between equivalent positions. Since no lower bound for the dissipated energy can be given, the zero velocity  $F_k$  must be zero. At the same time, the ratio  $\dot{x}_p/v_0$  diverges for  $v_0 \rightarrow 0$ , which can be concluded from Figs. 1(a) and 1(b), so that  $F_k$  must vanish more slowly than with  $v_0$ . As a result  $F_k \propto v_0^\beta$  with  $0 < \beta < 1$  is obtained.

The nature of instabilities changes qualitatively when the first higher harmonic differs from zero. Hence, in the sense of Morse theory [12], which contains Landau's theory of phase transition as a special case, the com. system without higher harmonics can be considered a multicritical point. If  $V_1 < 0$ , the motion of mechanically stable sites  $x_{\text{ms}}(t)$  becomes continuous as shown in Fig. 1, however,  $\dot{x}_{\text{ms}}(t)/v_0$  diverges at some moments of time. If  $V_1 > 0$ ,  $x_{\text{ms}}(t)$  is discontinuous and the pops take place between inequivalent positions as shown in Fig. 1(c). In analogy to phase transitions, pops for which  $V_1 > 0$  shall be called first-order instabilities, those for  $V_1 \leq 0$  continuous instabilities. Only first-order instabilities can lead to finite energy dissipation and thus to finite  $F_k$  when  $v_0$  approaches zero. A numerical analysis shows that in all three cases  $F_k(v_0)$  can be described with Eq. (1) at small  $v_0$ . The results are shown in Fig. 2: The more discontinuous the motion of mechanically stable sites  $x_{\text{ms}}(t)$ , the larger  $F_k$ . Within numerical accuracy, the exponent  $\beta$  (as determined at sufficiently small  $v_0$ ) seems to depend only on the sign of  $V_1$  but not on its precise value provided  $|V_1|$  is not too large.  $\beta$  is difficult to determine

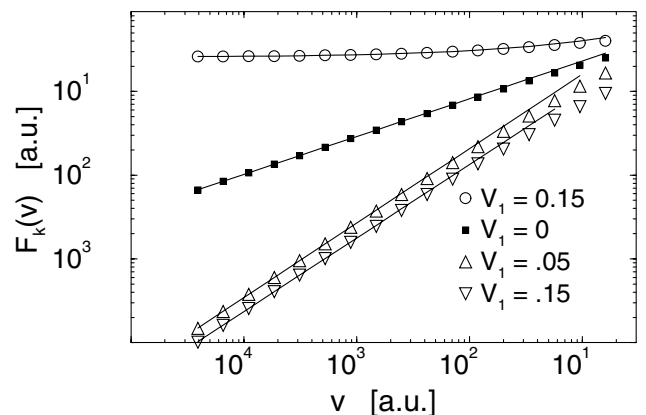


FIG. 2. Kinetic friction force  $F_k$  as a function of sliding velocity  $v_0$  for commensurate walls with different first higher harmonics. Straight lines are fits to low  $v_0$  data according to Eq. (1). The two data sets with  $V_1 < 0$  are fitted with the same exponent  $\beta \approx 0.83$ .

accurately due to nonanalytical corrections of order  $v^{\beta_n}$  with  $\beta_n > \beta$ .

For 1D, inc. surfaces, the basic picture is similar. If  $V_1$  is larger than a (positive) critical value  $V_1^*$ , whose precise value depends on the lattice mismatch, then pops between inequivalent positions are present and  $F_k$  remains finite as  $v_0$  tends to zero. For  $V_1 < V_1^*$ , however, the time derivative of the mechanically stable solution  $x_{ms}(t)$  remains finite at all times. The atoms are dragged with the wall that exerts the maximum lateral force. Hence the microscopic (peak) velocities  $v_p$  scale linearly with  $v_0$ , which implies Stokes-type friction in that regime (1D, inc.). The exponent  $\beta$  depends again only on the sign of  $V_1 - V_1^*$ . It is also independent of the precise choice of the damping coefficient  $\gamma$ .

We now discuss the effect of dimensionality. As one goes from 1D to 2D com. surfaces, the behavior does not change qualitatively, because the interference of  $V_t$  and  $V_b$  remains similar. However, there is a fundamental difference between 1D and 2D inc. surfaces. In 2D inc. interfaces, first-order instabilities will occur even without higher harmonics, because in 2D, atoms can circumnavigate the points of maximum longitudinal force. This induces finite  $F_k$ . This trend remains rather stable beyond the impurity limit and also for more complex lubricant molecules as will be discussed in a separate paper [13]. Our conclusions also provide an explanation of results by He and Robbins. They studied kinetic friction due to boundary lubricants with molecular dynamics and found small  $F_k$  and large  $F_s$  between 2D com. surfaces, while no such gap was seen for inc. systems [14]. Experimentally, signs for the effects of increased *static* friction  $F_s$  between com. surfaces in the presence of a lubricant were also reported [15], however, smooth-sliding kinetic friction should show the opposite trend.

This has potentially measurable implications for the transition from stick-slip motion to smooth sliding. Two-dimensional com. surfaces should show a characteristic drop at this transition, as friction is dominated by  $F_s$  in the stick-slip regime, whereas  $F_k$  is relevant in the smooth-sliding regime. No such drop should happen between 2D inc. surfaces. To support this prediction, we have extended previous simulations [16] that are based on the same model as that used in Ref. [9]. A schematic of the simulation is shown in Fig. 3 together with the average friction, as defined by the energy dissipated per slid distance. The experimental verification of these results requires smooth surfaces, because rough surfaces automatically lead to inhomogeneous energy landscapes [17]. The data shown in Fig. 3 were produced at a normal pressure of 0.4 GPa and a velocity of about 1 m/s using the same conversion of units as in Ref. [9]. Note that the inertia of the slider, which is small compared to experimental values, is responsible for the large velocity at which the transition between the two sliding regimes occurs.

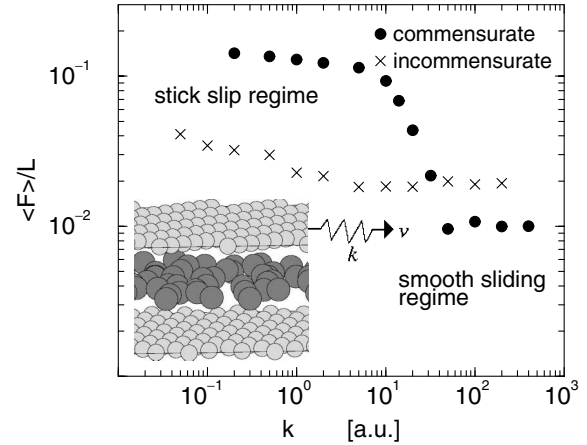


FIG. 3. Kinetic friction force  $F_k$  divided by load  $L$  as a function of spring constant  $k$  for com. and inc. walls lubricated by a quarter layer. A schematic of the simulation is shown as well.

We will now turn to the discussion of thermal fluctuations. He and Robbins found that velocity dependent corrections in a 2D, lubricated, inc. interface satisfy [14]

$$F_k(v_0) = F_k(v_{\text{ref}}) + \mathcal{O}[\ln(v_0/v_{\text{ref}})] \quad (4)$$

over several orders of magnitude in  $v_0$ . This is different from the behavior found in the Prandtl-Tomlinson model, for which rigorous treatments yield corrections of the order  $(T \ln v)^{2/3}$  in agreement with atomic force microscope experiments of nanoscale single-asperity contacts [18]. Hence the Prandtl-Tomlinson model does not explain the usually observed  $\ln v_0$  corrections in a straightforward manner.

Here it will be shown that simple logarithmic corrections are obeyed even in the impurity limit. Moreover, the crossover to linear response at extremely small sliding velocities will be included in the discussion. Figure 4 shows the normalized friction force obtained at thermal energy  $T = 0.07$  for the com.  $V_1 > 0$  model. Three regimes can be identified. At very small velocities, friction is linear in  $v_0$  and one may associate this regime with the creep regime. At intermediate  $v_0$ , Eq. (4) is rather well satisfied. At “large” velocities, thermal fluctuations become less relevant and the motion is close to that of the athermal system. The data obtained at different temperatures can be collapsed on a single master curve using time-temperature superposition principles. This requires a dimensionless scaling function  $s(T)$  and in addition at large temperatures a correction function  $r(T)$  close to unity. This latter correction factor, which will be discussed in more detail elsewhere [13], must become necessary at large  $T$  when the thermal equilibrium velocity distribution overlaps with the distribution generated through pops. The collapse is done via  $F_k(v, T) = r(T^*)F_k(v^*, T^*)/r(T)$  with  $s(T) \ln[v^*(T^*)/v_1] = s(T^*) \ln[v(T)/v_1]$  where  $v_1$  is a

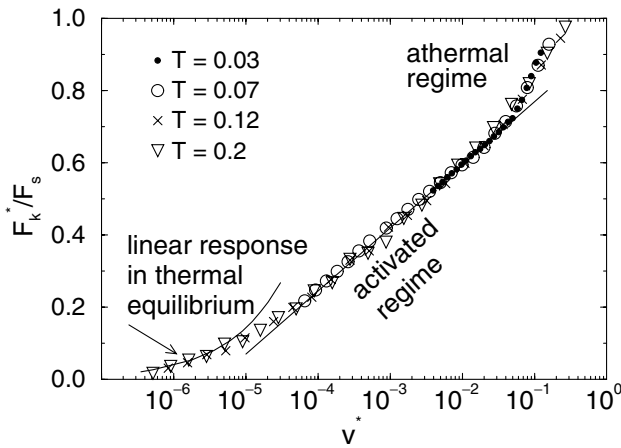


FIG. 4. Scaling plot of kinetic friction  $F_k^*(v)$  normalized by athermal zero-velocity limit  $F_s = F_k(v=0, T=0)$ . The reference temperature in this plot is  $T=0.07$ . In the regime of thermal equilibrium a linear law  $F_k(v) \propto v$  is drawn to guide the eye. The critical  $v^\beta$  contribution is subtracted from all data.

constant. For  $s(T)$  we find  $s(T) \approx k_b T / \Delta E$  so that  $\Delta E$  can be interpreted as an effective (free) energy barrier.  $r(T)$  is set to unity, except at the largest temperature, for which  $r(T) = 1.2$  gave the best fit to our data. Qualitatively similar crossover from the linear response regime to the activated regime occurs in many other systems such as single particles in a static periodic potential [19], driven thermal elastic manifolds [20], and shear-thinning fluids [21].

In conclusion, this Letter provides a classification scheme for instabilities that can occur when two solids are in relative sliding motion. First-order instabilities are defined as pops of atoms (or other degrees of freedom) between inequivalent positions. They lead to kinetic friction that remains finite when the sliding velocity  $v_0$  goes to zero provided the system is athermal. The exponent  $\beta$  of the velocity corrections  $v^\beta$  depends on the details of the model, however,  $\beta$  only changes its value at certain critical points in the parameter space defining interactions and geometry. Continuous instabilities are defined as pops between equivalent positions. They lead to a sub-linear power law  $F_k \propto v^\beta$ . If, however, the positions of mechanically stable sites move at finite velocities at all times, simple Stokes friction follows. Also dimensionality plays a crucial role. It is predicted that kinetic friction would be Stokes like, if it was possible to confine lubricant particles such as Octamethylcyclotetrasiloxane (OMCTS) into trenches of (sub)nanometer depth and width.

While the present study is primarily concerned with dilute boundary lubricants and will presumably break down if several lubricant layers support the load, the concept itself seems to be rather general. For instance  $x_{ms}$  can be a collective order parameter that fluctuates back and forth between two values. Such quasiperiodic

phase transitions have been reported in computer simulations of Ni asperities moving over a Cu substrate [22]. Of course, the situation in those simulations was more complex, because wear was produced as a side effect of the motion. In the other extreme,  $x_{ad}$  may merely denote the position of an electronic orbital.

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