Adiabatic theory of boundary friction and stick-slip processes

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An adiabatic approach is developed for the problem of boundary friction between two atomically smooth and incommensurate solid surfaces, separated by a monolayer of lubricant atoms. This method permits to consider very slow macroscopic motion of the parts in contact, separately from fast thermic motions of individual atoms. A characteristic "stick-slip" behavior of the tangential force on the contact is obtained within a simple 1D model, relevant for the tip and sample system in friction force microscopy (FFM). This behavior reflects the specific mechanism of stress energy accumulation, through formation of long-living metastable states (defects) within the monoatomic lubricant layer, and their subsequent collapse with energy conversion into heat. This is similar to the dislocation mechanism of irreversible deformation in bulk solids. The peculiar feature predicted by the present theory is the twofold periodicity of "stick-slip" spikes with relative displacement: the shorter period \( a \delta \) (where \( a \) is the tip lattice periodicity and \( \delta \) the relative tip-sample lattice mismatch) relates to defect skips by one elementary cell, and the longer period \( a(1 − \delta) \) relates to defect annihilation or nucleation at the boundaries of contact area.

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INTRODUCTION

Atomic mechanisms underlying the phenomenon of friction attract now a still increasing interest of many investigators. Particularly, this is motivated by the need of better understanding the physical principles that govern the image formation in friction force microscopy (FFM) [1]. Commonly, we call friction the process of energy dissipation during the relative displacement of two solid surfaces in contact [2]. The friction force \( F(x) = -dW(x)/dx \), where \( W(x) \) is the work performed to reach the position \( x \) (Fig. 1), is always directed contrarywise to the displacement. The empirical "Amon-tons' law" relating this force to the normal load \( N \) on contact: \( F = kN \), where the friction coefficient \( k \) depends only on the nature of the contacting materials, is known for about three centuries [3]. The modern tribology much dealt with the linear relation between \( N \) and the effective contact area \( A \), through deformations of microscopical rugosities [4], so that \( F = S_c A \) with a certain load independent constant \( S_c \) (the Bowden-Tabor law).

Nowadays, it is being progressively conceived that essential physics is already contained in the fundamental process of friction between two atomically smooth solid surfaces, not accompanied by any morphologic changes (wearless friction). It is also well recognized that a rather necessary premise for such a regime is the presence of some intermediate (lubricant) layer of relatively inert atoms between the surfaces. Usually, this friction regime is referred to as boundary friction [2]. The most evident source of dissipation at wearless friction is the generation, by microscopic interactions at the contact, of various kinds of quasiparticles. Those should bear away a part of mechanical energy from the external drive and finally transform it into heat.

To the date, a plenty of experimental material on this sort of friction is obtained. Particularly, a lateral force contrast was discovered in FMM scans along an atomically smooth surface containing domains of different materials [5, 6], thus showing the constant \( S_c \) in the Bowden-Tabor law to be material dependent. Furthermore, in FFM experiments with the best resolution, the friction force vs time (or displacement) isn’t constant but reveals a sawtooth-like, or the so-called stick-slip, behavior [1]. This should indicate occurrence of certain mechanical instabilities during the displacement, either within the contact itself or/and within the measurement apparatus (cantilevers, drives, etc.). The theory related to cantilever instabilities [7, 8] has its main disadvantage in that it doesn’t account for the irreversible (microscopic) processes. The models for the contact instabilities, such as the independent oscillator model [9, 10] or the Frenkel-Kontorova model [11, 12], though being able to explain the energy losses, were limited so far to only direct solid-solid interactions (see also [13]), not mediated by the lubricant. For the processes of boundary friction, the most elaborated approach is that considering the sequence of “freezing-melting” transitions within lubricant layers of few atoms thickness as a source of stick-slip discontinuities [14]. However, the FFM conditions can already reach to ultrathin boundary layers, monoatomic or even

![FIG. 1: Friction force \( F \) vs applied load \( N \) at given velocity \( v \) of relative displacement of two bodies.](image-url)
submonoatomic. In this situation, the interlayer viscosity and hence the melting transitions are most probably excluded, nevertheless the indication of still present discontinuous friction forces (atomic contrast in FMM) poses a challenge for atomic friction theory. The treatment in this paper just concerns the contact instabilities between two solids separated by a monoatomic lubricant layer and define microscopic mechanisms for irreversible energy losses with atomic periodicity at slow relative displacement. To fulfill this program, it is of special importance to choose an adequate calculation method.

The most straightforward method, very popular now for modelling various processes on nanoscopic level, is that of molecular dynamics (MD), and it was also applied to boundary friction [15–17]. However, this method has one substantial limitation that was not yet addressed explicitly. The time step for integrating the MD equations is typically of order of femtoseconds, then, in order to meet reasonable computing time requirements (no more than $10^4$–$10^6$ steps), one has to consider the displacement velocities $v$ not slower than $\sim 10^7$ cm/s to model the displacement by only few atomic periods. But in reality, even the faster process of atomic sliding of a free Lennard-Jones adsorbate layer on a single metal surface, subject to a uniform parallel force [18], is characterized by much slower velocities $v \sim 0.1$ cm/s. And the velocities in STM, AFM, FFM, etc. techniques, scale from $10^{-4}$ down to $10^{-7}$ cm/s, thus opening a 10 orders of magnitude abyss beyond the MD capacities. Meanwhile, just such slow adiabatic motions, as will be also seen further, are characteristic for the observable friction phenomena.

The remedy for this problem can be found in focusing the treatment on possible long living metastable states in the boundary layer, similar to those, well-known in physics of solids, as dislocations, domain walls, etc. Then the slow dynamics (SD) of such states can be considered separately from fast thermal motions of MD. Adiabatically, the SD part just follows the scenarios of contact instabilities of Refs. [9–13], while the MD part is accounted for in average, through the temperature dependent factor, triggering the transitions between different (meta)stable states. (This also can be meant as if the adiabatic atomic potentials were defined only within to $\sim \beta^{-1} = T$.)

Each transition is preceded by a certain period when the energy of a metastable state ($m$-state), and so the elastic force on the system, is growing with the macroscopic displacement $x$, while the energy barrier $h$, separating the $m$-state from the nearest stable ($s$-) state, is decreasing (Fig. 2). The adiabaticity condition would require that the $m$-state lifetime, $\tau_m = \tau_a \exp(\beta h)$, does not change too rapidly (see a more precise criterion at the end of Sec. 3). When $\tau_m$ decreases so much that it becomes comparable to the characteristic time $\tau_a = a/v$ of slow displacement by an atomic period $a$ (though still at $\beta h \gg 1$), the barrier can be overcome by a thermal fluctuation. Then, within a very short time $\sim \tau_a$, the system passes from $m$ to another state $s^*$, highly excited by an energy $\epsilon^* \gg \beta^{-1}$ (see Fig. 2) over $s$. Next, within a certain relaxation time $\tau_r \sim 10^8$ s, the energy difference $\epsilon^*$ is released through emission of about $\beta \epsilon^* \gg 1$ quasiparticles.

Since $\tau_r$ is much shorter of the characteristic time ($\sim \tau_m$) of the inverse $s^* \rightarrow m$ transition, the latter possibility can be safely excluded [19]. The considered $m \rightarrow s^* \rightarrow s$ process gives an elementary contribution to irreversible losses and can be compared to an individual spike in the stick-slip picture. The work by displacement $\Delta x$ is written, accordingly to the 1st law of thermodynamics, as

$$\Delta W = \Delta E + \Delta Q \tag{1}$$

Between the transitions, the heat transfer $\Delta Q = 0$ and the force varies continuously (the stick stage). Contrarywise, on a transition, the entire energy change is released into heat: $\Delta E = -\Delta Q$, hence $\Delta W = 0$, and a force discontinuity is generated (a slip). In this first attempt, the model is reduced to the simplified situation of 1D interface between 2D “solids”, however its extension to the realistic 2D (and possibly curved) interface can be also done on the same conceptual basis.
already recognized in literature [20]. For simplicity, we know microscopic models of a lubricant layer over sin-
the bilateral restriction of lubricant layer between two
consists, firstly, in taking into account two atomic period-
vant parameter. The specifics of the above formulation
"solid" arrays: conventionally called "tip" (t) and "sam-
empty circles are lubricant atoms.
lecular arrays: conventionally called "tip" (t) and "sam-
ple" (s), separated by an atomic chain of "lubricants"
(l) at some distance d. We assume the same triangular lattice for both solids, but admit a small mismatch δ be-
tween the lattice parameters. The t-side of the contact
consists of L elementary cells (L + 1 atoms), while the
s-side is unlimited, and the t-chain in contact with t con-
tsists of L atoms. Without loss of generality, we can put
the t-lattice parameter equal a and the s-lattice parameter
a(1 − δ), δ ≪ 1.
These lattice structures are supposed not to vary at
bringing t and s into (l-mediated) contact and during
their posterior mutual displacement by x. Thus we as-
sume the solid-solid links infinitely rigid compared to the
solid-lubricant and lubricant-lubricant links. Hence, the
only variable part in the full system energy is that related
to the l-subsystem:

\[ E(x) = \frac{1}{2} \sum_{n=1}^{L} \left( U(r_n, x) + \frac{1}{2} \sum_{n' \neq n} V(r_{n,n'}) \right), \tag{2} \]

where \( U(r_n, x) \) is the "mean-field" potential on the n-
th lubricant with 2D radius-vector \( r_n \) for given t- s dis-
placement \( x \), and \( V(r_{n,n'}) \) is the l-l interaction \( (r_{n,n'} = r_n - r_{n'}) \). Strictly speaking, the energy, Eq. (2), is also a function of all \( r_n \), but if we only admit them to be-
long to stable (or metastable) l-configurations at a fixed
distance \( d \), the displacement \( x \) remains the single rele-
vant parameter. The specifics of the above formulation
consists, firstly, in taking into account two atomic period-
icities (generally incommensurate) at once and, secondly,
in the bilateral restriction of lubricant layer between two
surfaces. Qualitative difference of this situation from the
known microscopic models of a lubricant layer over sin-
gle solid surface with single periodicity [9–13, 17] was
already recognized in literature [20]. For simplicity, we
will construct all the interactions in Eq. (1) using the
standard Lennard-Jones potential:

\[ f_{\text{LJ}}(y) = y^{-12} - y^{-6}. \tag{3} \]

Particularly, we put

\[ U(r_n, x) = \varepsilon_0 \left[ \sum_{m} f_{\text{LJ}}\left( |r_n - r_m|/r_t \right) \right. \]

\[ + \left. \sum_{m'} f_{\text{LJ}}\left( |r_n - r_{m'} - x|/r_s \right) \right], \]

where \( \varepsilon_0 \) is the adhesion energy, \( r_m \) and \( r_{m'} \) are re-
spectively the coordinates of t- and s-atoms, \( r_t \) and \( r_s \)
the corresponding t-l and s-l equilibrium distances, and
\( x \) the vector of displacement of the t-. Thus, both the
t-l and s-l coupling energies equal \( \varepsilon_0 \), serving as the
energy scale. At least, the l-l interaction is taken
\[ V(r_{n,n'}) = g \varepsilon_0 f_{\text{LJ}}(r_{n,n'}/r_t), \]

where \( g \) is the coupling con-
stant and \( r_t \) the l-l equilibrium distance.

**MEAN-FIELD POTENTIAL AND METASTABLE STATES**

One can reasonably consider the l-l interaction the
weakest one in the above system and, at the first step,
put \( g = 0 \) (this is a good approximation unless the
lubricants approach each other too closely compared with
\( r_t \)). Then the equilibrium states will correspond to vari-
ous distributions of L lubricants over the minima of the
mean-field potential produced by the t- and s-lattices. In
what follows we suppose that the infinite sample moves
with velocity \( v \) in x-direction with respect to the fixed
tip, and the tip-sample distance \( d \) is constant. We de-
define the n-th elementary cell of the boundary layer as the
rectangle limited by the n-th and \( (n + 1) \)-th tip atoms
in x-direction, and \( d \) wide in y-direction, and the entire
contact area corresponds to \( 1 < n < L \) (inset to Fig. 4).
Let the initial tip-sample relative position \( x = 0 \) at the
instant \( t = 0 \) be such that the s-atoms are located symmetri-
cally in the zeroth cell. In what follows, we con-
sider the potential energy \( U_n \) of a lubricant in n-th cell
as a function of \( x_n \) only (as shown in Fig. 4), supposing
\( y_n \) be always adjusted to the relative minimum of this
energy at given \( x_n \) (i.e., supposing the lubricants only
to move along energy "valleys" in 2D cells). Because of
the small mismatch \( \delta \), the static potential relief \( U_n(x_n) \)
(\( 0 \leq x_n \leq a \)) slowly varies (in general, incom-
measurably) from cell to cell along the interface so that the
cells aren’t equivalent. If we neglect the boundary effects (as is the
case in what follows), the potential relief within n-th cell
is fully determined by the "phase parameter" \( p_n = x - n\delta \text{(mod}(1 - \delta))\).

As seen from Fig. 4, besides the general raising or low-
ering of minima with \( p \) (elastic strains), there also exist
some critical values: \( p_{c1}(\approx 0.22 \text{ in that particular case})\)
and $p_{c2} = 1 - \delta - p_{c1}$, when the initial single minimum $U^{(0)}$ splits into two. In the splitted potential, the lower minimum $U^{(1)}$ is separated from the upper one $U^{(2)}$ by a maximum $U^{(3)}$ (a saddle point in the 2D cell). The slow relative $t$-$s$ displacement will result in that the potential relief as if “moves” adiabatically along $x$ with the “phase velocity” $v/\delta$.

If all the lubricants always rest in the lower minima $U^{(1)}$, the distances between them never become too short in this process and we can still neglect the $l$-$l$ interactions. Then no irreversible losses and, hence, no friction occur in the system (the force on external drive $F = -dE(x)/dx$, though non-zero, results fully elastic). However, such an $l$-configuration, even at moderate $L$ (note, however, that a contact area in FMM typically includes $10^9$ or more elementary cells), cannot persist for any macroscopic time by the thermodynamic reasons.

Indeed, with growing displacement, the cell potential splits and then the barriers $h_1 = U^{(3)} - U^{(1)}$ and $h_2 = U^{(3)} - U^{(2)}$ begin to grow and eventually get practically impenetrable. Then there is a finite probability $w > 0$ that at this stage a lubricant atom leaves ”captured” in the upper, metastable minimum $U^{(2)}$. For instance, in the model of linearly growing barriers with time (see Appendix A), this probability is simply given by the Fermi distribution function for the two-level system:

$$w(\Delta E) = \left(e^{\beta \Delta E} + 1\right)^{-1} \quad (4)$$

being $\Delta E$ the energy difference between the two minima. If all $L$ lubricants are initially in $U^{(1)}$ states, the time necessary for at least one of them pass to $U^{(2)}$ is about $1/(Lw)$, which corresponds to the system displacement by only $1/(Lw)$ atomic periods while $Lw$ can easily exceed unity.

Now let the $n$-th lubricant leave ”captured” at $U^{(2)}_n$, the upper minimum of $n$-th cell, while its neighbor in $(n + 1)$-th cell stays at $U^{(1)}_{n+1}$, and follow the system evolution with displacement (Fig. 5). As the distance $r_{n,n+1}$ gets shorter, this particular $l$-$l$ interaction cannot be more neglected. Such a pair of strongly interacting lubricants just realizes a metastable state for the considered system. The Lennard-Jones repulsion will slightly shift the $n,(n+1)$ pair from the mean-field minima $U^{(2)}_n$ and $U^{(1)}_{n+1}$ towards the saddle points $U^{(3)}_n$ and $U^{(3)}_{n+1}$. If the interaction constant $g$ isn’t too small (for the particular case considered in Sec. 4, $g = 1/120$ is already sufficient), such repulsion makes the energy barrier between this $m$-state and the $s$-state to turn from growing

![FIG. 4: Mean-field potential profiles for a lubricant atom in the unit cell of a contact, at different values of the phase variable $p$ (marks at each curve). The mismatch parameter $\delta = 0.05$, the interfacial separation $d = 1.12a$. Inset: the phase variable $p$ is defined as the distance along $x$-coordinate between the midpoints of nearest neighbor $t$- and $l$-atoms within the cell.](image)

![FIG. 5: Relative positions of two interacting lubricant atoms, $n$ and $n + 1$, against the mean-field potential (upper part) and the valley of steepest descent in $xy$-plane (lower part). The mean-field potential is that of Fig. 4 and the interaction constant $g = 1/120$. The phase $p_n$ is close to the transition value $p_t$.](image)
to lowering. The displaced equilibrium positions $U_n^{(2)}$ and $U_{n+1}^{(1)}$ are defined by the compensation between the $l$-$l$ interaction and the crystalline field forces along the valleys:

$$
\Delta_n U_n \cdot (\Delta_n U_n + \Delta_n U_{n+1}) = 0, \quad (5)
$$

$$
\Delta_{n+1} U_{n+1} \cdot (\Delta_{n+1} U_{n+1} + \Delta_{n+1} U_{n+2}) = 0,
$$

($\Delta_n$ stands for the 2D gradient along $r_n$). Notably, the numeric results (see Fig. 5 and Sec. 4) show that the energy difference $U_n^{(1)} - U_{n+1}^{(1)}$ for the $(n+1)$-th lubricant increases much faster than $U_n^{(2)} - U_{n+1}^{(2)}$ for $n$-th one. Hence, as the repulsion grows with $x$, the barrier $h_n^{(1)} = U_n^{(3)} - U_n^{(1)}$ decreases, while $h_n^{(2)} = U_n^{(3)} - U_n^{(2)}$ remains increasing, and the $(n+1)$-th atom will be finally pushed out by a thermal fluctuation from the $(n+1)^{(1)}$ position to $U_{n+1}^{(1)}$. Then the distance $r_n, n+1$ will suddenly increase and therefore the $n$-th atom will relax from $U_n^{(2)}$ to $U_n^{(3)}$. The overall energy gain

$$
\Delta \varepsilon = U_{n+1}^{(1)} + U_n^{(2)} - U_n^{(2)} - U_{n+1}^{(2)}
$$

(not to be confused with the energy difference $\Delta E$ in Eq. (4)) is released through emission of quasiparticles. Supposing isometric conditions, this energy is eventually transferred from the external drive to the thermostat.

Further on, the $n$-th lubricant stays always at $U_n^{(2)}$ (until it returns to the unsplit position $U_0^{(0)}$ at $p_n \rightarrow 0$) while the metastable pair is now formed by the $(n+1)$-th and $(n+2)$-th lubricants (that is, skipped by one cell) and so on. For the hierarchy of times specific for our system, the transition time $t_{tr}$ (related to the corresponding phase value $p_{tr}$ through $p_{tr} \sim v t_{tr}$) has a very small statistical dispersion around its mean value $\langle t_{tr} \rangle$ (see Appendix B). The mismatch parameter $\delta$ can be chosen so that either the "capture" and "skipping" processes affect only single metastable pair at a moment, not its nearest neighbors, thus avoiding possible complications due to interacting fluctuations.

Once randomly initiated, each skipping process described above provides a rather regular and stable generator of energy losses within a "phase domain" of length $l_d \approx a(1 - \delta)/\delta$ in the $l$-chain. Along such a domain, the phase $p$ changes from $0$ to $1 - \delta$, and the lubricants are in the $U_n^{(2)}$ position at all the sites with $p_n \sim \langle p_{tr} \rangle = v \langle t_{tr} \rangle$, and in $U_n^{(1)}$ position at $p_n > \langle p_{tr} \rangle$ (for more details see in 6). The spikes in the friction force from subsequent skips have approximate periodicity $\approx a \delta / v$ in time, or $\approx \delta a$ in displacement. Since this is much smaller of atomic periodicity, it may be difficult to resolve such fine structure in actual experiments.

But the atomic periodicity itself can result from another source. The described generators move along the chain with phase velocity $v_p = v/\delta$ and, at sufficient distances from the beginning of chain $(n = 1)$, they exist within each domain, $l_d$ apart. The friction force, averaged over the $\delta$-periods, is $(F)_{\delta} \approx n_g \Delta \varepsilon / (\delta a)$, where $n_g$ is the total number of generators in the chain. When a generator reaches the chain end $(n = L)$, it disappears (like a dislocation when it reaches the sample surface) and $n_g$ decreases by unity. Hence a jump to down occurs in the average force $(F)_{\delta}$. Otherwise, when a new generator appears near the chain beginning, $(F)_{\delta}$ increases. These events have the periodicity $\approx l_d / v_p = a(1 - \delta)/v$ in time, that is just the sample cell periodicity $a(1 - \delta)$ in displacement.

The averaged friction force $(F)$ over many atomic periods results simply $(F) \approx L \Delta \varepsilon$, that is proportional to the "contact area" $L$ with the Bowden-Tabor coefficient $\Delta \varepsilon$, which depends both on the material parameters and the interfacial distance $d$ (related to the pressure).

To conclude this section, we obtain a quantitative criterion for adiabaticity in our system. The limitation on the displacement velocity $v$ can be extracted from the evident condition that the lifetime $\tau_m$ of the metastable state (especially when it becomes comparable to $\tau_v$) doesn’t changes appreciably within the microscopic time $\sim \Omega^{-1}$ (atomic oscillation period): $d\tau_m / dt \ll \Omega \tau_m$, or $\beta h_{max}/dt \ll \Omega$. Since $dh/dt = v dw / dx$ and the barrier height changes from its maximum value $h_{max}$ to zero within a fraction $q \ll 1$ of atomic period, the adiabaticity criterion is given by:

$$
v < v_{cr} = \frac{a \Omega}{\beta h_{max}/q}
$$

(6)

The numerator in the last equation is of the order of sound velocity while the denominator $\beta h_{max}/q$ can be as high as $\sim 10^2$. Thus, the adiabaticity must be definitely violated (with all possible complications, as appearance of shock waves, thermal instabilities, etc.) at $v$ above some $m/s$, as is the case for the most of MD simulations. However, it is well assured at actual FFM velocities, men-
At least, the interfacial distance is chosen so that

\[ d \approx 17 \text{nm} \]

This value is slightly below the equilibrium separation \( d_e \) and corresponds to the normal force on tip \( N \), the mismatch parameter \( \delta \) corresponds to the disappearings of domain boundaries at reaching the sample end.

### FIG. 7: Microscopic tangential force on the contact vs sample displacement

Each fine structure spike corresponds to a skip of the boundary between "spin-up" and "spin-down" areas of Fig. 6 by one cell period, while the "envelope sawtooth" with the periodicity of sample lattice (0.95a) corresponds to the disappearings of domain boundaries at reaching the sample end.

### NUMERICAL RESULTS

We choose the equilibrium distances for Lennard-Jones interactions \( r_1 = 0.8a, r_2 = 0.78a, r_3 = 0.9a \), and the mismatch parameter \( \delta = 0.05 \). The energy parameter \( \varepsilon_0 \) is chosen 10 meV and the cell parameter \( a = 0.3 \text{ nm} \). At least, the interfacial distance is chosen \( d = 1.12a \). This value is slightly below the equilibrium separation \( d_e = 1.24a \) for a cell at the displacement phase \( p = 0 \) and corresponds to the normal force on tip \( N = 17.2 \text{ nN} \). The calculated profiles of mean-field potential for different values of the phase parameter \( p \) are shown in Fig. 4. Next, the equilibrium equations, Eq. (5), are resolved to give the values of barriers \( h^{(1)} \) and \( h^{(2)} \) as functions of \( p \).

The total length of the system was taken \( L = 20 \) and its initial state corresponds to one lubricant at \( U^{(1)} \) (or \( U^{(0)} \)) state in each cell. The displacement velocity \( v = 30 \text{ nm/s} \) corresponds to the characteristic time of displacement by cell period \( t_c = 10^{-2} \text{ s} \), and the elementary time step is \( \Delta t = 10^{-5} \text{ s} \), that is 10 orders of magnitude slower of the respective MD times. The evolution of total energy \( E(x) \) is modelled, using the mean-field and l-l interaction energies (at displaced positions for metastable pairs) at phase values \( p_n \) which vary with \( x = vt \), and the account for capturing and skipping events with probabilities is described in Appendices A,B. The temperature is set \( T = 1 \text{ meV} \approx 11 \text{ K} \).

The resulting plot of the friction force \( F(x) \) is presented in Fig. 7. After some initial period, when the force is almost elastic, the stick-slip behavior with two types of periodicity establishes and the mean level of friction force corresponds to a rather high "friction coefficient" \( k \approx 0.6 \). A more detailed study of the present model, for different values of pressure, temperature and velocity parameters, will be given elsewhere. It is also of interest, that using the above parameter values and \( \Omega = 10^{12} \text{ s}^{-1} \) in the adiabaticity criterion, Eq. (6), we get the critical velocity \( v_{cr} \approx 0.3 \text{ m/s} \), in good accordance with our previous reasoning.

### CONCLUDING REMARKS

The above analysis gives only a simple illustration for possible irreversible processes within the adiabatic picture of boundary friction. Other types of the system behavior can be obtained at varying the material and external parameters. In particular, with growing separation \( d \) between surfaces (lower or even negative pressure) the potential profiles get lower and the stick-slip behavior is expected to disappear. Contrarywise, at closer separation, the stage of inverse barrier evolution ceases to appear for lubricant pairs, and irreversible transitions (much sharper) can occur already in close clusters of three or more lubricants, however this would greatly complicate the treatment. A special regime can be obtained for the case of two fully commensurate solids (\( \delta = 0 \)). In this case, there is no preference between the two splitted mean-field states in a cell, and the "phase domain" becomes infinitely long. All the skips would occur simultaneously over the whole contact area, at the moment when the transition phase value \( \rho = \rho_{tr} \) is reached at all the cells. This will generate very high and short spikes of friction force with single periodicity of the lattice. Note in conclusion that passing from the above considered 1D to the realistic 2D situation will comply the model, not only by the extension of arrays for computation, but also due to introduction of several types of different metastable states.

### APPENDIX A

To model the initial evolution stage of potential in our system, let us consider a particle in the double-well system (Fig. 8) where the potential barriers for each well \( h_{1,2} \) vary adiabatically with time at \( t \geq 0 \).

Then the probability \( w(t) \) to find the particle in the upper well at the moment \( t \) obey the linear differential equation with the coefficients slowly depending on time (through \( h_{1,2} (t) \)):

\[
\Omega^{-1} \frac{dw}{dt} = - (e^{-\beta h_1} + e^{-\beta h_2}) w + e^{-\beta h_1}.
\]  

(A1)
The solution to Eq. (A1), satisfying the initial condition \( w(0) = 0 \) (that is, at \( t = 0 \) the particle is with certainty in the lower well), is given by the evident expressions:

\[
w(t) = \Omega e^{-\varphi(t)} \int_0^t e^{-\varphi(t')} - \beta h_1(t') dt' \tag{7}
\]

where

\[
\varphi(t) = \Omega \int_0^t \left[ e^{-\beta h_1(t')} + e^{-\beta h_2(t')} \right] dt'. \tag{A2}
\]

Now let us adopt, for simplicity, the model linear law for the growth of the barriers:

\[
h_1(t) = \Delta E + h_2(t), \quad h_2(t) = ut. \tag{A3}
\]

As seen from Fig. 4, Eq. (A.3) is a rather plausible approximation. Then the explicit integration in Eq. (A.2) gives the sought probability:

\[
w(t) = \frac{1 - \exp \left[ -\Omega \left( 1 - e^{-\beta ut} \right) / \beta u \right]}{e^{-\beta \Delta E} + 1}. \tag{A4}
\]

Since the rate of barrier growth is \( u = v h_{\text{max}} / (\Delta \mu) \), we conclude from comparison with Eq. (6) that the dimensionless parameter \( \Omega / \beta u \) is just the adiabaticity ratio \( v_{\text{cr}} / v \) and, for typical FFM conditions, its value is enormous: \( \sim 10^8 \). Thus the exponential in the numerator of Eq. (A.4) rapidly vanishes and we arrive at the result of Eq. (4).

**APPENDIX B**

Let us turn to the stage of reversed evolution (see the paragraph before Eq. (5)), and let the potential barrier (the lower one in Fig. 8) adiabatically decrease in time as \( h(t) = -ut, -\infty < t < 0 \). If at the moment \( t \) the particle is in the well, the probability that it escapes within an infinitesimal time interval \( dt \) is \( dw(t) = \Omega e^{\beta ut} dt \). Then the probability distribution \( \rho(t) \) for the transition to occur at the moment \( t \) is the product of \( dw(t) / dt \) times the probability to survive within the well during the period from \( -\infty \) to \( t \):

\[
\rho(t) = \frac{dw}{dt} \exp \left[ -\int_{-\infty}^t dw(t') \right] = \exp \left[ -\frac{\Omega}{\beta u} e^{\beta ut} - \beta ut \right].
\]

The function \( \rho(t) \), shown in Fig. 9 for different values of \( u \), sharply peaks at \( t^* = \ln(3\mu / \Omega) / \beta u \). Since the parameter \( \Omega / \beta u = v_{\text{cr}} / v \) is huge [21], then: i) the distribution \( \rho(t) \) is very narrow and ii) its form and the critical barrier value \( h^* = h(t^*) = \beta^{-1} \ln(v_{\text{cr}} / v) \) depend on the displacement velocity \( v \) only very weakly.

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