Friction in the zero sliding velocity limit

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Using an adiabatic approximation method, which searches for Tomlinson model-like instabilities for a simple but still realistic model for two crystalline surfaces, with mobile molecules present at the interface, sliding relative to each other, we are able to account for the virtually universal occurrence of ''dry friction'' at zero temperature. A modified version of this method allows us to calculate the kinetic friction at nonzero temperature as well. We have also considered the static friction, and have demonstrated that the model is able to account for static friction being larger than kinetic friction.

I. INTRODUCTION

Muser and co-workers have argued that clean surfaces should not exhibit static friction [1] at the point of contact of an asperity from each surface, but the presence of mobile molecules (so called ''third bodies'') at the interface can lead to static friction. This is a surprising result because one usually expects such lubricant molecules to reduce rather than enhance friction. On the other hand, if the mobile molecules are much more strongly attached to one surface than the other, they will act as randomly distributed pinning sites belonging to the surface to which they are strongly attached, and it was argued in Ref. [2] that molecular level random defects on the surface will not lead to static friction. Thus, an important ingredient in these molecules leading to static friction is the relative strength of the interactions of the lubricant molecules with the two surfaces. In the present work, we concentrate mainly on the study of ''dry friction'' (i.e., kinetic friction in the slow sliding speed limit). If a dilute concentration of molecules is initially randomly distributed over the interface, they will in time diffuse to the deepest potential wells. These occur at the locations on the interface at which potential minima from the two surfaces nearly coincide, as the potential at the interface will be minimum there. As the surfaces slide relative to each other the minima from the two surfaces producing the potential minimum occupied by this molecule will no longer coincide, and at some point during the sliding, the minimum often becomes unstable (i.e., ceases to be a minimum), allowing the molecule to drop into a deeper minimum. This is considered as the source of energy dissipation due to kinetic friction in the slow sliding speed limit. It was argued by Caroli and co-workers, based on an earlier suggestion by Brillouin and by Tomlinson [3] that without multistability there is no static or dry friction. The existence of dry friction due to Tomlinson-like potential instabilities has been studied in both one and two dimensions using molecular dynamics [4]. We have presented a way to study dry friction for the model of Ref. [1] (see Ref. [5]). Our method treats the problem in the slow sliding velocity (i.e., the adiabatic) limit quite naturally. It also makes it possible to study the important question of the relationship between static and dynamic friction.

In Ref. [5], we initially studied the case of a dilute concentration of single globular molecules adsorbed at an interface between two triangular lattice surfaces rotated at an arbitrary angle such that the interface is incommensurate. While the triangular lattice surfaces considered in Ref. [5] might be more realistic, the square lattice surface model is much simpler, allowing us to get more insight into this problem without having to deal with the additional complications of the triangular lattice model. Therefore, in this work, we will initially consider surfaces that are square lattices. In reality, the interasperity interface that we are trying to model is more likely to be disordered than periodic or quasiperiodic, and hence, both of these periodic surface models represent only a first step towards a truly realistic treatment of this problem.

The model we have have studied consists of two rigid surfaces with a dilute concentration of particles trapped between them. To zeroth order, we neglect the particle-particle interactions. The surfaces are represented by two identical two-dimensional periodic potentials, which are rotated relative to each other at an arbitrary angle, as this is the usual situation at an interface. We model the potential function acting on a mobile molecule due to each surface by the Steele potential [6]. To a good first approximation, the potential may be represented by the lowest-order term in the Fourier series for it.

In Ref. [5], the problem was studied at zero temperature. In the present paper, the method is discussed in more detail and is extended to nonzero temperature. At zero temperature, frictional dissipation comes about because as the surfaces slide relative to each other, the interface potential well minimum in which each mobile molecule resides eventually becomes unstable, allowing the molecule to drop to a lower energy well. (In this paper, the term interface potential well refers to the potential $v_1 + v_2$, due to the two surfaces.) The kinetic energy so generated is assumed to get quickly dissipated. At nonzero but low temperatures the molecule can drop to a lower well before the well that it presently occupies becomes unstable by hopping over the potential barrier separating it from the deeper well. At very high temperatures, in contrast, it can get just as easily thermally excited back up into the higher well, making the higher interface potential well under consideration no longer contribute because it no

longer represents a metastable state of the molecule under consideration.

II. THE SEARCH FOR INSTABILITIES

We model the potential function acting on a mobile molecule due to each surface by the Steele potential [5]. To a good first approximation, the potential may be represented by the lowest-order term in the Fourier series for it. For one surface (surface 1), it is given by

$$v_1(x,y) = V_0 \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

$$= 2V_0\{\cos[(2\pi/a)x] + \cos[(2\pi/a)y]\}, \quad (1)$$

where the vectors $\mathbf{G}$ denote the smallest reciprocal lattice vectors of a square lattice of lattice constant a and V_0 is the strength of the potential. As mentioned in the Introduction, we will initially discuss results for the square lattice, in order to clarify the physics of the problem because the physics of the square lattice model is easier to understand. For all positive loads, V_0 is positive. This is easily seen to be correct because the maxima of the expression in curly brackets in Eq. (1) occur at the positions of the atoms making up surface 1. Clearly, the adsorbed molecules would be expected to lie in the interstitial positions (where the quantity in curly brackets is minimum). This is easily verified by explicit calculation using the Steele potential [5], which is a reasonable approximation for the potential of interaction between an adsorbed molecule and a crystalline surface. We chose for the potential of the second surface (surface 2) the potential given in Eq. (1) rotated by ϕ and translated by $(\Delta x, \Delta y)$. Then this potential is given by $v_2(x,y) = v_1(x',y')$, where $x' = (x+\Delta x)\cos(\phi) + (y+\Delta y)\sin(\phi)$ and $y' = -(x+\Delta x)\sin(\phi) + (y+\Delta y)\cos(\phi)$, where, ϕ is the rotation angle, and the displacement parameters Δx and Δy are given by $\Delta x = s_0\cos(\theta) + b\sin(\theta)$ and $\Delta y = s_0\sin(\theta) - b\cos(\theta)$. Here, $s_0 = vt$, where v is the velocity of sliding of surface 2 relative to surface 1 along a direction making an angle θ with the x axis. The maximum at the origin of surface 2 is moving along a path displaced a distance b, the distance of closest approach, normal to the path passing through the minimum at the origin of surface 1.

Since we are neglecting intermolecular interaction, we study a single molecule placed at random within the Wigner-Seitz unit cell of surface 1 at a time. We assume that each molecule will move to the nearest minimum of $v_1 + v_2$. The resulting potential minimum reaches its lowest value when the two surfaces have slid until a minimum of v_1 and a minimum of v_2 are at their distance of closest approach. Therefore, the resulting potential minimum can only become unstable and disappear after this point, since before it the minimum is getting deeper. Thus we need only begin our search for instabilities for wells that are at their distance of closest approach. Because this potential is a function of time, the existence of these minima is time dependent. As a minimum containing a particle disappears, the particle will drop to another potential minimum of lower energy, resulting in a
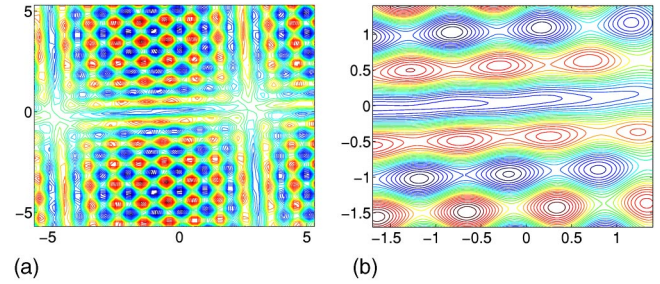

FIG. 1. (Color online) (a) A contour plot of the interface potential for square lattice surfaces for a typical displacement of the surfaces for surfaces of equal strength, for $\phi=7.5°$ and $\theta=22.6°$. The x and y axes are in units of a lattice constant. (b) The contour plot of (a) plotted over a smaller range of x and y. Unstable wells are seen in the row of relatively shallow wells in the middle of the figure.

gain of kinetic energy, which is assumed to get quickly transferred to phonons and electronic excitations of the surfaces. As the surfaces continue to slide relative to each other, the depth of the new minimum occupied by the molecule decreases and the potential eventually becomes unstable so that the process described above repeats itself. This is our mechanism for frictional energy dissipation. We will refer to the fact that each potential well is able to become unstable as the surfaces slide relative to each other as instability renewal. If it does not occur for a particular model for the surface potentials, there will be no dissipation for long time sliding, because the molecules will get sorted into potential wells which never become unstable as the surfaces slide. We have done extensive studies of this problem for the surface potential in Eq. (1) using this method, but it is equally applicable to any two periodic or disordered potentials, representing the two surfaces.

Before discussing the numerical procedure for calculating the frictional energy loss and from it the force of kinetic friction, let us first present some plots of the potential which illustrate how this process occurs and why we feel that it is reasonable to expect it to occur for general surfaces in contact. They are presented in Fig. 1. It is easy to see from Fig. 1(a), as a consequence of the rotation of the surfaces relative to each other, that the interface consists of Moiré patterns with domains in which the interface potential is relatively deep separated by domain wall boundaries, in which the net potential is relatively shallow because on these boundaries the potentials from the two surfaces tend to cancel each other. When instabilities occur, they do so on these domain boundaries. Such an instability is illustrated in Fig. 1(b).

By studying the evolution of the interface potential wells as the surfaces slide relative to each other, we can look at the issue of instability renewal raised earlier in this section. We find that as the surfaces slide relative to each other, potential wells within a domain boundary become unstable, allowing any molecule that might occupy such a well to drop to a deeper well. Eventually, the domain boundary moves away from the the well that the molecule presently occupies, and the well becomes located closer and closer to the center of a domain. As it does so, it becomes deeper (i.e., more stable),

as this is the characteristic of wells in the center of a domain. Eventually, however, another domain wall will move towards the vicinity of this well. As this occurs, the well becomes shallower. When this well is located inside a domain wall, it too becomes unstable, allowing the process to repeat.

In this work, the unit cell for each surface is chosen to be a Wigner-Seitz unit cell with a potential minimum located at its center. We begin our search with a potential minimum of the top surface at the same location in the x-y plane as a minimum in the bottom surface. We now slide the two surfaces relative to each other by the vector with x and y components Δx and Δy defined below Eq. (1) and determine if any of the minima have become unstable. As noted earlier, such instabilities are responsible for dry friction.

In order to locate minima, and to track their positions and stability as our surfaces slide past one another, we first place a particle at a random position at the interface and use a Monte Carlo routine to move it to the nearest potential minimum. In order to predict where a minimum will move during sliding, we use the fact that the force on a particle at the potential minimum $(x_0(t), y_0(t))$ remains identically zero for all time in the adiabatic approximation to find velocity at which the minimum is moving. Details of this procedure can be found in Ref. [5].

The main part of our procedure is an iterative method, based on the Taylor series expansion of the potential which allows us to search for minima and evaluate whether a particular minimum is unstable. The second-order Taylor series expansion of the potential, assumed to be with respect to the location of the nearest minimum,

$$v(x,y)=v(x_0,y_0)+\frac{\partial v}{\partial x}\bigg|_0 \delta x + \frac{\partial v}{\partial y}\bigg|_0 \delta y$$
$$+(1/2)\frac{\partial^2 v}{\partial x^2}\bigg|_0 \delta x^2 + (1/2)\frac{\partial^2 v}{\partial y^2}\bigg|_0 \delta y^2 + \frac{\partial^2 v}{\partial x\partial y}\bigg|_0 \delta x\,\delta y,$$
$$(2)$$

is now used to determine more accurately the location of the new minimum. The first-order derivatives vanish, since we assume that we are expanding about the true minimum. The second-order derivatives can, to second-order, be replaced by the second-order derivatives at the present position of the particle, provided we are close to the actual minimum. The quantities $\delta x = (x_{pp} - x_0)$ and $\delta y = (y_{pp} - y_0)$ are then the approximate distances, along the x and y directions, between the particle's present position, and where the actual minimum is. In order to use the force components felt by the particle at its present location to find δx and δy, we differentiate the above second-order approximation with respect to both x and y, obtaining an approximation for the force components near the true minimum,

$$\frac{\partial 6v}{\partial x}=\frac{\partial^2 v}{\partial x^2}\bigg|_{pp}\delta x + \frac{\partial^2 v}{\partial x\partial y}\bigg|_{pp}\delta y,\qquad(3a)$$

$$\frac{\partial v}{\partial y}=\frac{\partial^2 v}{\partial y^2}\bigg|_{pp}\delta y + \frac{\partial^2 v}{\partial x\partial y}\bigg|_{pp}\delta x.\qquad(3b)$$

Equations (3a) and (3b) are solved for δx and δy to give

$$\delta x=\frac{1}{D}\left[\frac{\partial^2 v}{\partial y^2}\bigg|_{pp}\frac{\partial v}{\partial x}\bigg|_{pp}-\frac{\partial^2 v}{\partial x\partial y}\bigg|_{pp}\frac{\partial v}{\partial y}\bigg|_{pp}\right],\qquad(4a)$$

$$\delta y=\frac{1}{D}\left[\frac{\partial^2 v}{\partial x^2}\bigg|_{pp}\frac{\partial v}{\partial x}\bigg|_{pp}-\frac{\partial^2 v}{\partial x\partial y}\bigg|_{pp}\frac{\partial v}{\partial x}\bigg|_{pp}\right],\qquad(4b)$$

where D, known as the Gaussian curvature (for extremum points), is evaluated at the point (x_{pp}, y_{pp}). The derivatives in Eq. (4) are found from the potential $v_1 + v_2$ defined in Eq. (1) and in the discussion under it. If the particle is close to the minimum, this procedure converges very quickly to the true minimum. How quickly it converges, however, is dependent on the size of the quantity D.

The second derivatives of the potential form a two-dimensional second-rank tensor, which is diagonal for appropriate orientation of the coordinate axes (i.e., the principal axes); D is equal to the product of these diagonal elements. The xx component defines a parabola along the x direction, and the yy component defines another along the y direction. If both components are positive, one has a minimum; if both are negative, one has a maximum, and if one is positive and one is negative, then one has a saddle point. When one of the eigenvalues, and hence D, becomes zero, we can have an instability if the third-order terms in the Taylor series expansion of the potential around the critical point under consideration are nonzero. If the third-order terms are zero, we can have a fourth-order minimum or maximum if the fourth order terms are nonzero.

Our method allows us to track the position of a minimum until it becomes unstable, at which point we can locate the new minimum into which an unseated particle will next fall. This allows us to calculate the drop in potential energy that such a particle would undergo. The total frictional energy loss between our two surfaces is the sum of these energy drops over all of the particles. The quasiperiodic nature of the interface allows us to consider all possible interface potential minima, which are possible positions of molecules on the surface, and all possible sliding distances of the two surfaces relative to each other simply by studying the behavior of the potential minima in a single unit cell of surface 1 as a single minimum from surface 2, which initially coincided with the minimum at the origin of the unit cell of surface 2, which is under consideration, slides in all possible directions. The vector $\Delta \mathbf{r}=(\Delta x, \Delta y)$, the translation of the centers of the two unit cells under consideration relative to each other at which unstable minima occur at some point in the unit cell falls on the curve, which surrounds the point of initial coincidence of the centers of the two cells. We will refer to this as the instability curve, which is shown in Fig. 2(a). The overlap of these minima from surface 1 and surface 2 gives rise to an interface potential minimum for all positions of the minimum from surface 2 under consideration within the interior of the instability curve. Outside of this curve, there can be no interface minimum resulting from these two surface minima (but there can still be one resulting from a different pair of minima). Since the instability curve surrounds the
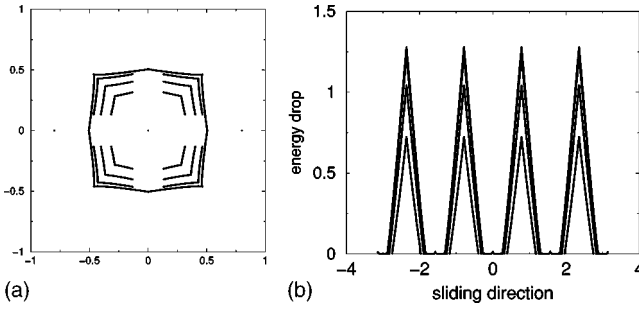
FIG. 2. (a) The instability curve for surfaces of equal strength for $\phi=7.5°$ is the outermost curve; the one inside of it is the effective instability curve for $k_BT/V_0=0.05$; the one inside this curve is for $k_BT/V_0=0.2$; and the innermost curve is for $k_BT/V_0=0.4$ Units of x and y axes are fractions of a primitive lattice vector. The missing parts of the $T\neq0$ instability curves represent values of θ for which the energy drop is so small that the molecule hops back to the higher potential well almost as rapidly as it drops to the lower one. These curves have been rotated by $\phi/2$ in order to make them appear symmetrical. This is equivalent to rotating the top surface by $\phi/2$ and the bottom one by $-\phi/2$, rather than rotating only the top surface by ϕ. (b) The energy drop occurring in an instability in units of $2V_0$ vs the angle (in degrees) θ between $\Delta\mathbf{r}$ and the horizontal axis of a. The tallest curve is for $T=0$; the curve for for $k_BT/V_0=0.05$ falls essentially on top of that for $T=0$; the next tallest is for $k_BT/V_0=0.2$; and the lowest curve is for $k_BT/V_0=0.4$.

origin, there will be friction for almost all directions of sliding (i.e., values of θ). During the sliding, as the minimum from surface 2 slides through successive unit cells, it will not generally coincide with the minimum at the center of the unit cell, but rather it will pass by it at a distance of closest approach, b. Then, in successive unit cells $\Delta\mathbf{r}=\mathbf{b}+\Delta\mathbf{s}$, where $\mathbf{b}$ is a vector of magnitude equal to the distance of closest approach and direction normal to the path followed by the surface 1 minimum and $\Delta\mathbf{s}$ is the displacement along the path followed by the surface 2 minimum under consideration from the point of closest approach to the instability curve.

In order to treat the qualitative effects of nonzero temperature, we use the following arguments. Even before a well becomes unstable, the molecule can hop over the lowest boundary of the well in which it resides and drop into a lower well at nonzero temperature. This will occur if the rate of hopping over the boundary ΔE_b, which is given to a good approximation by $\omega_0 e^{-\Delta E_b/k_BT}$ (where ω_0 is the frequency of the order of the vibrational frequency for the molecule in the higher well), is large compared to v/a, the inverse time for the surfaces to slide a distance of the order of a lattice constant a relative to each other, where v is the sliding velocity. Otherwise the barrier may get higher before the molecule gets a chance to hop over it. In practice, we use a simplified criterion for thermal activation of a molecule over the barrier ΔE_b, namely, that activation will definitely occur whenever k_BT is greater than a certain fraction $\alpha(v)$ of ΔE_b and will definitely not occur if it is less than this energy. How good this crude criterion is for estimating the temperature dependence of the friction will be checked using calcu-

lations based on the Langevin equation in Sec. III. ΔE_b is the lowest potential barrier surrounding the potential well that we are considering. In order to find ΔE_b, we diagonalize the matrix of the second derivatives of the potential evaluated at the potential minimum, as described above. This allows us to determine the principal axes of the potential. The principal axis corresponding to the lowest eigenvalue of this matrix is likely to be close to the direction in which the barrier is lowest. We then do a search for a saddle point of the potential, focusing our search in this direction. The saddle point that we find is the minimum energy barrier ΔE_b, which must be overcome in order for a molecule located in the potential well to get out of the well and then fall into a potential well of lower energy. We found, however, that this does not significantly affect the energy dissipation because even if there were no hopping over the barrier, the well would still at a later time become unstable. As a result, the resulting energy dissipation tends to be comparable to that at zero temperature. As the temperature becomes comparable to $\alpha(v)(\Delta E+\Delta E_b)$, where ΔE is the energy difference between the higher and lower potential well minima, the molecule is quite likely to hop back into the higher potential well shortly after it has dropped to the lower one. This will occur as long as the rate of hopping back to the higher well, which is of the order of $\omega_0 e^{-(\Delta E+\Delta E_b)/k_BT}$ (here ω_0 is the frequency of the order of the vibrational frequency for the molecule in the lower well), is large compared to v/a. This criterion determines $\alpha(v)$. In Fig. 2(a), we plot the instability curve for $T=0$. For $T>0$, we plot an effective instability curve. This is a curve made up of positions of the minimum from surface 2 at which k_BT becomes comparable to the product of $\alpha(v)$ and the lowest barrier, which is our criterion for a molecule occupying this well hopping over the lowest barrier and dropping into a lower minimum. On the basis of Langevin equation calculations as those presented in Sec. III, we find that for $v\approx1$ cm/s, $\alpha\approx0.1$. The missing points on these curves represent places at which k_BT is greater than $\alpha(v)(\Delta E+\Delta E_b)$, and hence the molecule moves back and forth between the higher and lower well. Hence, the picture of the molecule dropping from a metastable to a stable minimum, resulting in energy dissipation, breaks down. The energy drop when a particle drops to a lower stable minimum as a function of the angle that $\Delta\mathbf{r}$ makes with the horizontal axis of Fig. 2(a) is plotted in Fig. 2(b). From this curve, we find the average energy drop, denoted by $\langle\Delta E\rangle$. This average is obtained by considering a series of closely spaced paths for a minimum of surface 2 through a unit cell of surface 1 parallel to the direction of sliding, and hence for each curve the origin passes through this unit cell at a different distance of closest approach b. Because of the incommensurate nature of the interface, this procedure is equivalent to starting with the minimum of surface 2 under consideration coinciding with the minimum in the center of the unit cell of surface 1 which is under consideration. We then follow the path taken by the minimum of surface 2, which is under consideration, through successive unit cells. Unlike the first cell, in successive cells the minima from surface 1 and surface 2 never coincide. Still, when the minimum from surface 2 crosses the instability or effective instability curve, a molecule in the

potential well under consideration will drop to a deeper well. We know that this must be true because it cannot make any difference whether the minimum from surface 2 begins its travel from the origin of the unit cell of surface 1 and then crosses the instability curve or it does not begin from the origin, as actually happens in this case.

In order to calculate $\langle \Delta E \rangle$, and from it the mean force of friction per molecule, we divide the interior of the instability curve into strips of width db along the direction of sliding and a perpendicular distance b from the minimum of surface 1 at the center of its unit cell, where b is the distance of closest approach defined earlier, oriented along the direction of sliding. The place of intersection of this strip with the side of the instability curve in the sliding direction of surface 2 determines ΔE as a function of b, which now must be averaged over b. In reality each point inside the instability curve in the unit cell that we are considering defines an interface minimum residing in one of the unit cells of surface 1 on the interface, but it is convenient to translate them all into one unit cell of surface 1 for the purpose of determining the average energy loss, and from it the mean force of friction. (The minimum will not, however, actually be located at the position of the surface 2 minimum under consideration.) Now let us slide the surface 2 by Δs along the sliding direction that we have chosen. The points in any one of the strips of width Δb that were within a distance Δs of the instability curve before sliding, will pass through it, leading to an energy loss $\Delta E(b)$ for each such point. Each of these strips will have an equal number of points passing through the instability curve. Let us assume that there is a mean concentration of c particles per unit area on the interface. Each such molecule must lie in an interface potential minimum. Since there is a one-to-one correspondence between locations of interface potential minima and locations of a surface 2 minimum within the instability curve, as discussed above, the number per unit area within the instability curve of such points, which correspond to minima containing a molecule, is given by $n = cA/A_i$, where A is the unit cell and A_i is the instability curve area. Then, the total energy loss for sliding by Δs is given by

$$n\Delta s \int_b db \Delta E(b), \qquad (5)$$

integrated over all strips that pass through the side of the instability curve in the direction of sliding. The mean force of friction per molecule is given by the expression in Eq. (4) divided by Δs and by the number of molecules per unit cell, given by cA. Then the mean force of friction per molecule is given by

$$F_{fric} = A_i^{-1} \int_b db \Delta E(b). \qquad (6)$$

For equal values of V_0 for the two surfaces, for $\phi = 7.5°$ and $\theta = 22.5$, using Eq. (5), we obtain $F_{fric} = 1.294 V_0/a$ for $k_B T/V_0 = 0.0$ and 0.05, $F_{fric} = 1.077 V_0/a$ for $k_B T/V_0 = 0.2$, and $F_{fric} = 0.76 V_0/a$ for $k_B T/V_0 = 0.4$. Let us find the frictional force per cm^2 of contact area for a normal load per

cm^2 of contact area of 1.36×10^{10} dyn/cm^2, which corresponds to the minimum pressure (at lightest loads) in the Greenwood-Williamson model [7] for values of the parameters used in Ref. [2]. This is a standard model for explaining the fact that friction is proportional to the normal force for elastic asperity contact. To determine V_0, we set this pressure equal to the product of the number density of adsorbed molecules per unit area and the component of force on a single molecule normal to the interface, calculated from the Steele potential [6] in order to determine the distance of the molecule from either of the two surfaces (denoted by z in Ref. [6]). This value of z is then used to determine the parameter V_0 used in our calculations. The number density of adsorbed molecules, assuming that 10% of the possible interstitial positions on a surface contain adsorbed molecules is 1.11×10^{14} cm^{-2}. Following this procedure, we obtain $V_0 = 0.0232$ eV. Then, we obtain a force of friction per molecule at the interface of the order for $\theta = 22.5°$ and $\phi = 7.5°$ of 16.0×10^{-7} dyn for $k_B T/V_0 = 0.0$ and 0.05, 13.4 $\times 10^{-7}$ dyn for $k_B T/V_0 = 0.2$, and 9.40×10^{-7} dyn for $k_B T/V_0 = 0.4$. The values of the friction for other values of θ and ϕ that we considered were of similar magnitude. Using the above value for the density of adsorbed molecules, we obtain for the force of friction per unit area of contact 17.8 $\times 10^7$ dyn/cm^2 for $k_B T/V_0 = 0.0$ and 0.05, 14.8 $\times 10^7$ dyn/cm^2 for $k_B T/V_0 = 0.2$, and 10.4×10^7 dyn/cm^2 for $k_B T/V_0 = 0.4$. The ratio of this quantity with the above value of the normal force per unit contact area is the friction coefficient. The value that we obtain is consistent with the value obtained by Muser [8].

Let us now discuss the velocity dependence of the kinetic friction on the basis of this model. Earlier in this section, we argued that if $\omega_0 e^{-(\Delta E + \Delta E_b)/k_B T} \gg v/a$, a molecule that hops over a barrier of height ΔE_b in order to get out of an interface potential well and drop into another well, whose minimum energy lies an energy ΔE below the original well minimum, will just as easily hop back into its original well, implying the higher well will no longer contribute to the kinetic friction. It follows that if $\omega_0 e^{-V_{max}/k_B T} \gg v/a$, where V_{max} is an energy such that if the molecule's energy is above this value, it will be able to get out of all of the interface potential wells and move over the interface through all of the potential wells. This clearly implies that when the above inequality is satisfied, the picture of molecules dropping from metastable equilibria into lower potentials will break down because none of the wells will be metastable. The above condition for the friction being small can also be written as $x = V_{max}/[k_B T \ln(\omega_0 a/v)] \ll 1$, and in the limit $x \gg 1$ the friction will be large. Since we know that in the zero temperature limit we get dry friction, i.e., the friction approaches a constant independent of the velocity, it is reasonable to assume that the force of friction is given by $f = F(x)$, where $F(x)$ is an analytic function which approaches zero as x approaches zero and approaches a constant as x approaches infinity. The above scaling theory implies that as v approaches zero, the friction will be proportional to x^n, where n is an integer. There have been several theoretical studies of the Tomlinson model applied to the problem of an atomic
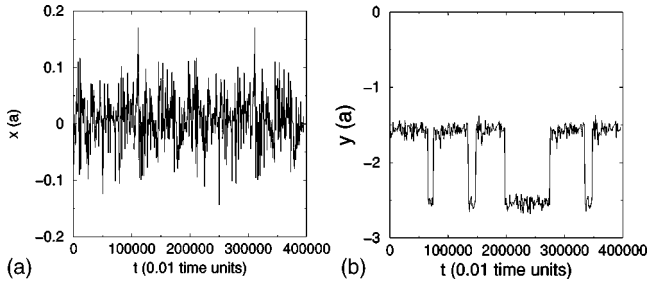
FIG. 3. The x coordinate (a) and the y coordinate (b) of the molecule are plotted as functions of time for $k_B T/V_0 = 0.3$.

FIG. 5. The x coordinate (a) and the y coordinate (b) of the molecule are plotted as functions of time for $k_B T/V_0 = 2$.

force microscope (AFM) tip sliding over a periodic substrate potential at nonzero temperature [9]. These studies give either a $\ln(v)$ or $[\ln(v)]^{2/3}$ dependence of the friction on the sliding velocity v of the AFM tip, which seems to agree with experiment [10]. These models differ from the model that we are studying in the sense that in these studies the instabilities that give rise to the friction are macroscopic level instabilities due to the AFM itself. In contrast, our model ascribes the friction to microscopic level instabilities of the mobile molecules assumed to be at the interface. Therefore, there is no reason to expect that both mechanisms should give the same velocity dependence. Nevertheless, while our velocity dependence is not the $\ln(v)$ dependence found in these studies [9,10], its shape does not look qualitatively different from a $\ln(v)$ velocity dependence.

Our choice for the scaling parameter x is not unique since, for example, we could alternatively have chosen $x = (v/\omega_0 a)e^{V_{max}/k_B T}$. This choice would give f proportional to v^n, but for $k_B T \ll V_{max}$, f will still rise very rapidly to its zero temperature value. This feature of the velocity dependence is independent of how we choose x.

III. LANGEVIN EQUATION CALCULATIONS TO TEST OUR TREATMENT OF TEMPERATURE

In order to test the validity of our approximate method of treating the effects of temperature, we will now give some results of calculations that we have done based on the Langevin equation, which should give an accurate treatment of the effects of temperature. In these calculations, the molecule is
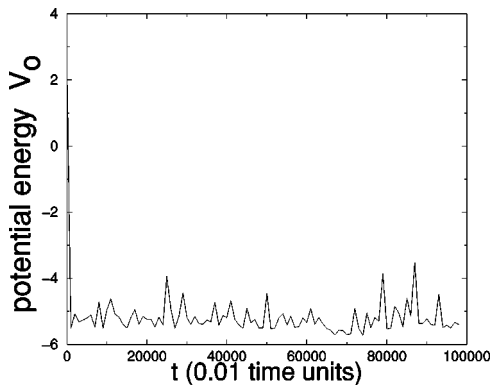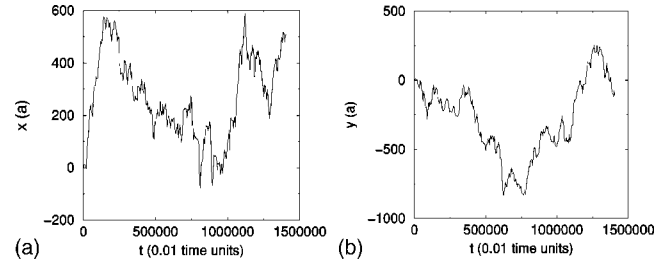
initially placed in a potential well which is close to becoming unstable, meaning that one of its boundaries is relatively low. In these calculations, the surfaces are not sliding. We solve the standard Langevin equation with a damping proportional to the velocity of the molecule. The damping constant is equal to 1.3 of (our time unit)$^{-1}$. This time unit is equal to $(ma^2/V_0)^{1/2}$, where m is the mass of the molecule. We present results for the x and y coordinates in Fig. 3 for $k_B T/V_0 = 0.3$ and in Fig. 4, the potential energy of the molecule as a function of time.

In Fig. 5 we show the x and y coordinates, and in Fig. 6 we show the potential energy of the molecule as a function of time for $k_B T/V_0 = 2.0$.

We observe that for $k_B T/V_0 = 0.3$, the molecule drops out of its original well to a deeper well and then essentially does not move very far from the location of this new well in the time of the simulation, which is the time necessary for a surface sliding at about 1 cm/s to slide about $0.15a$. Similar behavior was found for $k_B T/V_0$ as high as 0.7. For just slightly higher T, the molecule wanders out of its present well into other wells at the interface, which supports the "step function" approximation for the temperature dependence used in Sec. II. For $k_B T/V_0 = 2.0$, we can see that the molecule wanders over many lattice constants throughout the interface, presumably passing through a wide range of potential energies. Here it is clearly reasonable to assume that the molecule can be considered to be in thermodynamic equilibrium at all times. At such a high temperature, molecules will
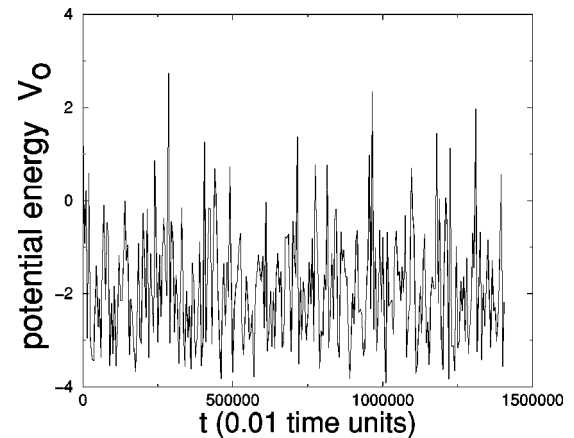

FIG. 4. The potential energy is plotted as a function of time for $k_B T/V_0 = 0.3$.

FIG. 6. The potential energy is plotted as a function of time for $k_B T/V_0 = 2.0$.

never find themselves in metastable equilibrium positions, which are needed for the mechanism for "dry frictional dissipation" discussed in this paper to occur. Hence, for such temperatures there will be no dry friction. Only viscous friction will be possible.

IV. CONCLUSION AND SPECULATIONS ABOUT STATIC FRICTION

We have extended an adiabatic approximation method, which we had previously used to calculate kinetic friction in the low velocity limit at zero temperature for the Muser-Robbins model, to nonzero temperature. We have obtained values of the kinetic friction for reasonable values of the parameters in the model. Our method, which focuses on Tomlinson model-like instabilities that are expected to dominate the frictional dissipation in the slow sliding limit, allows us to gain insight into how this physical mechanism is able to account for kinetic friction.

Let us now make some speculations based on the model studied in this work about a possible physical reason for static friction being larger than kinetic friction in general.

The largest possible value of the force of static friction for this model will occur if the molecules have enough time to diffuse to the deepest possible potential minima that can occur at the interface. These will occur whenever a potential minima from each surface exactly coincide. Because of the quasiperiodic nature of the interface, which occurs when the surfaces are rotated at arbitrary angles with respect to each other, there can be at most one point on the interface at which two minima can exactly coincide, but there will be many locations at which minima from the two surfaces can come arbitrarily close to coinciding.

Let us now attempt to slide the surfaces relative to each other. Since the two wells will no longer coincide, the location of the interface potential minimum will no longer be at the location of the minimum of each of the two potential wells. Thus the two wells will exert equal and opposite forces on the molecule. This force for each molecule will be along the line joining the minima of the two wells, which is not necessarily along the sliding direction. The component of the force of static friction along the sliding direction is just $-\partial V/\partial s_0$, where s_0 is the sliding distance. The component perpendicular to the sliding direction was found to be at most

11% of the component along the sliding. Since real crystal surfaces have grains oriented with random axis directions, we expect it to average out. Hence we will not consider it. We have calculated the force on the molecule due to one of the surfaces for the molecule located at an interface potential minimum (which is due to the potentials due to both of the surfaces) as a function of sliding distance, beginning with the situation in which the two wells exactly coincide. This force clearly reaches its maximum possible value just before the interface well minimum occupied by the molecule disappears, i.e. when the well becomes unstable, since that is when the wells from the two surfaces are farthest from coinciding. The force that must be exerted in order to slide the surfaces relative to each other is the vector sum of the force exerted by each molecule on one of the surfaces. The maximum value is the maximum force of static friction, i.e., the force that must be applied in order to make the two surfaces slide relative to each other. The maximum force of static friction per adsorbed molecule is found to be about $14V_0/a$, which is much larger than the largest value of the average force of kinetic friction found in the preceding section (i.e., $1.29V_0/a$). In practice, for k_BT much less than the height of the highest barrier, molecules will not be able to thermally activate over the barriers bounding the deeper wells. Under such circumstances, the static friction will be much closer to the kinetic friction.

The idea that the static friction gets larger as the two surfaces are stationary and in contact is in qualitative agreement with what is observed for macroscopic surfaces [3], although we are certainly not claiming that the present simplified model is able to account for all the complications of general macroscopic interfaces. It may, however, be suggestive of possible mechanisms for such phenomena.

It is clear that when the temperature is nonzero, the molecule is able to get out of its well sooner, before the force that it exerts on one of the surfaces reaches its maximum value. This implies that the maximum force of static friction should decrease as the temperature increases. This point was also made by Aichele and Muser [8].

[1] G. He, M.H. Muser, and M.O. Robbins, Science **284**, 1650 (1999); M.H. Muser and M.O. Robbins, Phys. Rev. B **61**, 2335 (2000); M.H. Muser, L. Wenning, and M.O. Robbins, Phys. Rev. Lett. **86**, 1295 (2001).

[2] J.B. Sokoloff, Phys. Rev. Lett. **2001**, 86 3312 (2001); J.B. Sokoloff, Phys. Rev. B **65**, 115415 (2002).

[3] C. Caroli and Ph. Nozieres, Eur. Phys. J. B **4**, 233 (1998); *Physics of Sliding Friction*, Vol. 311 *NATO Advanced Studies Institute, Series E: Applied Sciences*, edited by B. N. J. Persson and E. Tosatti (Kluwer Academic, Dordrecht, 1996); M. Brillouin, *Notice sur les Travaux Scientifiques* (Gautier-Villars,

Paris 1909); G.A. Tomlinson, Philos. Mag. **7**, 905 (1929).

[4] G. He and M. Robbins, Tribol. Lett. **10**, 7 (2001); M. Muser, Phys. Rev. Lett. **89**, 224301 (2002).

[5] C. Daly, J. Zhang, and J.B. Sokoloff, Phys. Rev. Lett. **90**, 246101 (2003).

[6] W. Steele, Surf. Sci. **36**, 317 (1973).

[7] J.A. Greenwood and J.B.P. Williamson, Proc. R. Soc. London, Ser. A **295**, 3000 (1966).

[8] M. Muser, in *Dynamics in Small Confining System V*, edited by J.M.Drake, MRS Symposia Proceedings No. 651 (Materials Research Society, Pittsburgh, 2001), p. T4.8; M. Aichele and

M. Muser, Phys. Rev. E **68**, 016125 (2003).

[9] E. Gnecco, R. Bennewitz, T. Gyalog, Ch. Loppacher, E. Meyer, and H.-J. Guntherodt, Phys. Rev. Lett. **84**, 1172 (2000); O.K. Dudko, A.E. Filippov, J. Klafter, and M. Urbakh, Chem.

Phys. Lett. **352**, 499 (2002); Yi Sang, M. Dube, and M. Grant, Phys. Rev. Lett. **87**, 174301 (2001).

[10] E. Riedo, E. Gnecco, R. Bennewitz, E. Meyer, and M. Brune, Phys. Rev. Lett. **91**, 084502 (2003).