Effects of Defects on Friction for a Xe Film Sliding on Ag(111)

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The effects of a step defect and a random array of point defects (such as vacancies or substitutional impurities) on the force of friction acting on a xenon monolayer film as it slides on a silver (111) substrate are studied by molecular dynamic simulations and compared with the results of lowest order perturbation theory in the substrate corrugation potential. For the case of a step, the magnitude and velocity dependence of the friction force are strongly dependent on the direction of sliding respect to the step and the corrugation strength. When the applied force $F$ is perpendicular to the step, the film is pinned for $F$ less than a critical force $F_c$. Motion of the film along the step, however, is not pinned. Fluctuations in the sliding velocity in time provide evidence of both stick-slip motion and thermally activated creep. Simulations done with a substrate containing a 5 percent concentration of random point defects for various directions of the applied force show that the film is pinned for the force below a critical value. The critical force, however, is still much lower than the effective inertial force exerted on the film by the oscillations of the substrate in experiments done with a quartz crystal microbalance (QCM). Lowest order perturbation theory in the substrate potential is shown to give results consistent with the simulations, and it is used to give a physical picture of what could be expected for real surfaces which contain many defects.

I. INTRODUCTION

In previous simulations of a xenon film sliding on a silver substrate, using a periodic (i.e., defect-free) substrate, a viscous force of friction (i.e. one proportional to the sliding velocity) was found in agreement with the experimental results of Krim et. al. In contrast, perturbation theory calculations give a velocity independent contribution to the friction (i.e., "dry friction") when there are point defects (i.e., a point defect denotes a defect which is centered around a point in the lattice), such as vacancies or substitutional impurities in the substrate. Since, real surfaces, even very smooth ones, always contain defects, the viscous friction found in these experiments is a surprising result. Perturbation theory results for straight line defects, i.e., defects that extend along a line such as steps or facet boundaries, however, are consistent with viscous friction. In this article, we perform molecular dynamics simulations for a film of Xe atoms sliding on a Ag(111) substrate containing a step and also for a substrate with a random array of point defects. The point defects are found to pin the film for an applied force below a critical value, whereas a step generally does not pin the film. The pinning force due to a 5 percent concentration of point defects comparable in strength to the corrugation potential, however, is still much lower than the effective inertial force per film atom in the experiment done by krim. This force can be expressed as $m\omega^2 A$, where $m$ is the atomic mass and $\omega$ and $A$ are the frequency and amplitude, respectively, of the quartz crystal microbalance used in the experiment. Lowest order perturbation theory in the substrate corrugation potential for the system treated in the simulations is found to be consistent with the simulations. The perturbation theory results are then used to try to give a physical picture of what one would expect for real substrate surfaces, which contain many defects.

II. SIMULATIONS

A. The model used in the simulations

The model Hamiltonian used in Ref. for $N$ film atoms of mass $m$ at positions $\mathbf{r}_k$ ($k = 1, \ldots, N$) is given by

$$H \equiv \sum_{k=1}^{N} \frac{p_k^2}{2m} + U(\mathbf{r}_1, \ldots, \mathbf{r}_N),$$

where $p_k$ is the momentum of the atom $k$, and the total potential $U(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is given by

$$U(\mathbf{r}_1, \ldots, \mathbf{r}_N) \equiv \sum_{k=1}^{N} U_s(\mathbf{r}_k) + \sum_{j<k=1}^{N} V(|\mathbf{r}_j - \mathbf{r}_k|).$$

Here, $U_s(\mathbf{r}_k)$ is a single particle potential describing the interaction between the $k$-th film atom and the substrate, and $V(|\mathbf{r}_j - \mathbf{r}_k|)$ is the pair potential interaction between the $j$-th and $k$-th atoms in the film.

The interaction between two Xe atoms is given by a Lennard-Jones potential

$$V(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right],$$

where $\varepsilon$ is the energy, $\sigma$ is the distance of closest approach, and $r$ is the distance between the atoms.
where \( \varepsilon = 19.83 \text{ meV} \), and \( \sigma = 4.055 \AA \). The interaction between a Xe atom and the substrate can be described by a substrate potential without internal degrees of freedom given by

\[
U_s(\mathbf{r}_\parallel, z) = U_0(z) + U_1(z) \sum_{\{G\}} \cos(\mathbf{G} \cdot \mathbf{r}_||),
\]

where \( \mathbf{r}_\parallel = (x, y) \) are the coordinates of the Xe atom parallel to the substrate, and \( \{G\} \) is the set of the six shortest reciprocal lattice vectors of the substrate. The first term in Eq. (2.4) describes the mean interaction of the atoms with the substrate, and the second term describes the periodic corrugation potential.

Expressions for \( U_0(z) \) and \( U_1(z) \) were derived by Steele assuming that the substrate potential \( U_s(\mathbf{r}) \) is a sum of Lennard-Jones potentials between one film atom and all of the atoms in the substrate. However, a potential like \( U_s(\mathbf{r}) \), which is a sum of Lennard-Jones potentials is not a correct description of the interaction of a metallic surface with a noble gas atom. The corrugation potential is reduced (from the value found by summing Lennard-Jones potentials) due to electronic screening. For this reason we employ a weaker corrugation potential, as did Cieplak et al. in Ref. [1]. The corrugation potential we use is

\[
U_1(z^*) = \alpha e^{-g_1 z^*} \sqrt{\pi / 2g_1 z^*} \left[ \frac{A^* 6}{30} \left( \frac{g_1}{2z^*} \right)^5 - 2 \left( \frac{g_1}{2z^*} \right)^2 \right],
\]

where \( \alpha = 4\pi \varepsilon_{Xe/Ag} A^*/\sqrt{3} \), \( z^* = z/a \), \( a = 2.892 \AA \) is the lattice constant of the substrate, \( A^* = \sigma_{Xe/Ag}/a \), \( g_1 = 4\pi /\sqrt{3} \). We calculate the Lennard-Jones parameters \( \sigma_{Xe/Ag} \) and \( \varepsilon_{Xe/Ag} \) by fitting (i) the position of the minimum of \( U_0(z) \) to the distance between a Xe atom in the first layer and the ion cores of the substrate \( (z_0) \), and (ii) the attractive well depth to the binding energy of one Xe atom to the Ag substrate \( (U_0(z_0) = -211 \text{ meV}) \), from [1]. We find \( \sigma_{Xe/Ag} = 4.463 \AA \) and \( \varepsilon_{Xe/Ag} = 13.88 \text{ meV} \).

The corrugation potential \( U_1(z) \) in Eq. (2.3) falls off exponentially at large \( z \). The above parameters give \( U_1(z_0^*) \sum_{\{G\}} \cos(\mathbf{G} \cdot \mathbf{r}_\parallel) = 2.025 \text{ meV} \) (for the maximum value of this sum) in contrast to the corresponding value of 10.13 \text{ meV} \) for Steele’s potential at \( z_0 \). Our corrugation gives good agreement with the experimental value of the slip time.

Our simulations are carried out at an equilibrium temperature of \( T = 77.4^\circ K \), and the particles move in a three dimensional box of size \( 20 \times 10 \sqrt{3} \times 10 \sigma \). The time scale for vibrations of the adsorbed film atoms is \( t_0 = \sqrt{(m \sigma^2 /2)} = 3.345 \text{ ps} \), with \( m = 2.16 \times 10^{-22} \text{ g} \). Periodic boundary conditions in the \( x \) and \( y \) directions are employed along with a hard wall boundary condition in the \( z \) direction at the top of the box.

We change the coverage by changing the number of Xe atoms \( N \). We use \( 60 \leq N \leq 370 \). All atoms are initially in the gas phase. The atoms condense in \( 250 t_0 \) or less, forming a triangular lattice incommensurate with the substrate fcc(111) surface.

For the simulations done with a step present, the potential in equation (2.4) has the \( z \)-coordinate replaced by \( z - g(x) \). The use of this function guarantees that we have the same corrugation as we used for a substrate free of defects in Ref. [3]. Here \( g(x) = 0.58 \sigma |f(x_1 - x) - f(x - x_2)| \) where \( f(x) \) is the Fermi function, \( 1 / [e^{-x/\omega} + 1] \). (See Fig. 1.) We choose \( \omega \) to be equal to \( 1.1 \sigma \), AS THE width for the step edge, where \( \sigma \) is the distance parameter for the Lennard-Jones potential between a film and substrate atom.

![FIG. 1. A plot of \( g(x) = 0.58 \sigma [f(x_1 - x) - f(x - x_2)] \) where \( f(x) \) is the Fermi function.](image)

We take \( x_1 \) and \( x_2 \), the locations of the beginning and end of the step, equal to \( L_z/3 \) and \( 2L_z/3 \), where \( L_z \) is the length of the box (along \( x \)) in which the simulations are done. We thus assume a straight step in the substrate, (see Fig. 2 (a and b)), which runs along the \( y \)-axis. The height of the step is about 0.8 of an atomic distance. The use of a function \( g(x) \), which varies smoothly with \( x \), is a reasonable choice because the nonzero radius of a surface atom makes the potential that acts on the atom vary smoothly as the atom moves over the surface.

Most of our simulations were done with a coverage corresponding to the uncompressed monolayer (163 particles). Periodic boundary conditions in the \( x \) and \( y \) directions are employed along with a hard wall boundary condition in the \( z \) direction at the top of the box. Because of our use of periodic boundary conditions, we are technically simulating a periodic array of defects. We feel, however, that the cell length used in our simulations of about 13 xenon atom spacings is sufficiently long for the coherence from one cell to the next to be unimportant for most values of the sliding velocity. This is justified using perturbation theory [4,5] for reasonable values of the phonon damping constant in appendix A.
In the present simulations, we use the same method as Cieplak, et. al., in which a constant external force $F$ is applied to each atom in the plane of sliding, and the resulting steady-state velocity is calculated (see Fig. 4). Throughout the simulation a thermostat that rescales the three velocity components is used to maintain constant temperature. The rescaling is done in the center of mass reference frame so as not to change the center of mass velocity and thus introduce an unphysical force of friction due to the thermostat. It renormalizes the atomic velocities every time step, so that the total kinetic energy per atom in the center of mass frame is maintained at $(3/2)k_B T$, where $k_B$ is Boltzmann’s constant and $T$ is the desired absolute temperature of the system ($T = 77.4^o K$ in our case). This method allows us to determine conveniently the velocity dependence of the friction force. The velocity of the film is affected by the inhomogeneities of the medium, in this case the corrugation and the defects. In the absence of defects, the film can move for an arbitrarily weak applied force, but when there is a step present, the film can be pinned for $F$ less than a critical value $F_c$, the force is applied perpendicular to the step. In other words, there are the following two phases, a pinned phase when the external force $F < F_c$, and a moving phase. The depinning transition takes place at a critical threshold force $F_c$. In the vicinity of the depinning transition the average velocity has the form $V \sim (F - F_c)^{\beta}$ where $\beta$ is the velocity exponent.

The potential for a substrate containing point defects is of the form:

$$V_i(\vec{r} - \vec{r}_d) = V_0 e^{-|\vec{r} - \vec{r}_d|^2/\ell^2}$$

where $V_0$ and $\ell$ are the strength and range of the potential respectively and $\vec{r}_d$ is the location of the defect. The defect positions are chosen to be potential minima of the corrugation potential chosen at random with probability $c$, where $c$ is the defect concentration. (The simulations done for point defects were done with $U_1$ having the opposite sign than for the $U_{1}$ used in the step simulations, because this sign of $U_1$ gives the correct corrugation potential minima. For the step simulations it did not really matter what sign we chose, but for the point defect problem it is more important to place the point defects at the correct positions. For example if we want $V_{i}$ to represent the potential due to a vacancy we can choose $V_0$ positive and equal to the depth of the corrugation potential minimum, so that that minimum, presumed to be due to a substrate ion located at that position, is canceled out by $V_0$.) Because of the use of periodic boundary conditions, it was necessary to include the eight nearest neighbor cells to the cell containing the film in which the simulations were done. Each of these neighboring cells contained the defect potentials reflected into these cells. The impurity positions and the reflected impurity positions are shown in Fig. 3. Only interactions between a film atom and a defect (or an image of a defect) which is less than $4 \sigma$ away from the atom are included in the calculation of the force or potential acting on the atom.

B. Results of the Simulations for the Step

In most of our simulations we have used a corrugation strength (defined as 9 times the value of $f U_1(z)$ evaluated at the value of $z$ at which $U_0(z)$ is minimum) of 2.025 meV ($f=1$), the value that was used in Ref. [3]. In order to examine the effect of using a larger corrugation, we have, in addition, done some runs at a corrugation of 3.56 meV ($f=1.69$).

We apply an external force to all the particles in the monolayer at the following angles with respect to the $x$ axis (which is perpendicular to the step): $0^o$ (force perpendicular to the step), $16^o$, $37^o$, $58^o$, $66^o$ and $90^o$ (force along the step). The case in which the particles move on a substrate which is free of steps (with the force along the $x$-axis) is also studied to make a comparison with the simulations that were done with the step present.

In Fig. 3 the velocity is shown as a function of time for the various values of the applied force for the case of a no step present, and in Fig. 3 for the case of a step present.
The velocity at the top of the plateau is the steady-state velocity, which we will later plot versus the applied force $F$. In order to diminish thermal fluctuations of the velocity vs. time curves, the curves shown in Figs. 4 and 6 are obtained by making averages of several runs. The no-step case was obtained averaging 5 runs and the step cases, by averaging 3 runs each. The steady-state velocity is plotted as a function of $F$ in Fig. 6. We see that the magnitudes of the velocities depend on the orientation of $F$. The velocity is smallest at $0^\circ$ (i.e. when the particles move almost perpendicular to the step). It gets larger when the angle increases, taking on its maximum value for an angle of $90^\circ$ (when particles move along the step).

When the particles move perpendicular to the step (i.e., in the $x$ direction), their motion in $x$ is pinned. For angles of incidence $0 < \theta < 90$ the pinning transition appears to be “softened” or “smeared out.” It is thus of interest to plot the $x$ and $y$ components of velocity vs. the applied force (i.e. $V_{x,y}$ vs. $F$) in order to gain insight into what the atoms do. In Fig. 6, the $x$ and $y$ components of the velocity are shown separately for $58^\circ$ for 2.025 meV corrugation potential strength. We see evidence of pinning in $x$ but not in $y$. (The exponent $\beta$ in this case is $\beta = 1.4$.)

We also made some runs with a corrugation strength of 3.56 meV. The film moves in the same fashion as for 2.025 meV corrugation, but of course with much smaller velocities.

Two cases clearly show linearity between velocity and $F$: no step and $90^\circ$ (along the step). In addition, for angles between $0^\circ$ and $90^\circ$ $v$ shown in Fig. 6 is linear in $F$ to a good approximation for $v$ less than $0.1\sigma/t_0$. This is one possible explanation for why such viscous friction is found in experiment.

### C. Stick Slip and Creep

The results reported in Fig. 6 are obtained by averaging the $V_{cm}$ versus time data for a few different runs for each value of the applied force. These averages are performed in order to suppress the large fluctuations in the data found when a step is present. In order to illustrate this, $V_{cm}$ is plotted as a function of time, without doing any averaging, for one value of the applied force larger than the critical force in Fig. 6. For comparison, a plot of $V_{cm}$ versus time for the case of no step present is also made on the same graph for an applied force chosen so that $V_{cm}$ has about the same value at each time. In this case the driving force is applied at $0^\circ$ with the $x$ axis.

FIG. 4. The velocity is shown as a function of time for the various values of the applied force for the case of no step present. The driving force is applied at $0^\circ$ with the $x$ axis.

FIG. 5. Velocity of the center of mass in the $x$ direction as a function of time, for various values of an applied force, for the case of a step present. In this case the driving force is applied at $0^\circ$ with the $x$ axis.

FIG. 6. Variation of the velocity with $F$ at 77.4$^\circ$ kelvin.

FIG. 7. Variation of $v_x$ and $v_y$ with $F$ for $58^\circ$ for 2.025 meV of corrugation.

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graph the force, for the case in which there is a step, has a value $F = 1.9 \times 10^{-3} \epsilon/\sigma$, slightly above threshold.

It is clear from this figure that the fluctuations in $V_{cm}$ are noticeably larger when there is a step than in the absence of it.

In Fig. 9, a typical plot of $V_{cm}$ is shown for $F$ normal to the step below its threshold value. The $x$ component (normal to the step) and the $y$-component of $V_{cm}$ are shown separately. $V_{cm,x}$ becomes thermally activated for a short period of time and then becomes pinned again. Such behavior is not found in $V_{cm,y}$. The behavior for values of the force slightly above threshold is shown in Fig. 10. In Fig. 11 a similar plot is shown for the applied force at an angle of 37 degrees with the normal to the step. We can again see the thermally activated behavior of $V_{cm,x}$ for a couple of short time intervals. In contrast, $V_{cm,y}$ appears to saturate at a positive value (because the film is not pinned in the $y$-direction). Thermally activated motion of the type that we see here is the type of behavior that would lead to creep of a macroscopic film.

D. Film Rotated Relative to the Step

In the runs discussed so far, the crystallographic axes of the film were lined up with the step. This is not always true for this system. For example, we also did a run for a 173 atom film (a more compressed monolayer film) for the same substrate containing a step. In this case, the film in equilibrium Appeared rotated at an angle with respect to the step, as seen in Fig. 12. In this case, the film attained a steady-state velocity of $0.2\sigma/t_0$ when $F=0.0015\epsilon/\sigma$ was applied normal to the step. As can be seen in Fig. 12, the 163 atom film, which was not rotated with respect to the step, was pinned for $F$ of that magnitude. As we shall see in the next section, this is consistent with the predictions of lowest order perturbation theory.
E. Results of the Simulations done with Point Defects Present

In these simulations $V_0$ in Eq. 2.6 was chosen to be equal to $0.1 \varepsilon$, for which each defect potential has a maximum value approximately equal to the corrugation potential well depth, and the concentration $c$ was chosen to be equal to 0.05. Again, the system was first equilibrated for at least $600,000$ iterations, and then an external force was applied. Simulations were done with the external force making angles of 33, 105 and 203 degrees with respect to the side $L_x$ of the box. The results are shown in Fig. 13. Each point represents the average of the component of the center of mass velocity along the applied force over a time interval equal to at least $10^4 t_0$ (i.e. $2 \times 10^6$ iterations or about $3 \times 10^{-8}$ s.) in order to average out the fluctuations. An average of three runs is also shown for one of the cases. Since it did not look qualitatively different than the single runs, it is clear that single runs are adequate. For all three directions of the applied force the film appeared to become pinned below a critical force of about $2 \times 10^{-4} \varepsilon/\sigma$, even though the detailed shape of the velocity versus force curves might have differed slightly. A run was also done at a temperature of 26 K in order to determine whether the motion of the film might have been partly thermally activated. The results are shown in Fig. 14. It is seen that the critical field is now about $4 \times 10^{-4} \varepsilon/\sigma$, and the curve appears to exhibit a sharp depinning transition, whereas the runs done at $T = 77.4^\circ K$ showed what looked more like a rounded transition. These results imply that some thermal activation of the atoms out of the impurity potential wells is taking place. It is quite unlikely, however, that such thermal activation, which is responsible for creep, will give such a large contribution for a macroscopic film as it does for the small films used in the simulations.

The pinning force of $2.10^{-4} \varepsilon/\sigma$ found at $T = 77.4^\circ K$ is equal to about $1.5 \times 10^{-11}$ dyn per atom.

One might be tempted to think that the fact that point defects do not seem to have much of an influence on QCM friction measurements can be explained by relatively small value that we have found for the pinning force. We do not believe that this is correct, however, because this force is still much larger than the effective inertial force due to the oscillations of the QCM’s substrate which is equal to $m\omega^2 A \approx 10^{-14}$ dyn, where $m$ is a film atom mass ($\approx 10^{-22}$ dyn, $\omega \approx 10^7$ s$^{-1}$ and the amplitude of the substrate oscillations $A \approx 10^2 A^o$.

FIG. 13. The velocity in units of $\sigma/t_0$ versus applied force $f$ in units of $\varepsilon/\sigma$ is shown for a lattice containing a random array of point defects with a 5 percent concentration, the force $f$ applied at 33, 105 and 203 degrees with respect to $L_x$.

An average of three runs is also shown for one case.
FIG. 14. The velocity in units of $\sigma/t_0$ versus applied force $f$ in units of $\epsilon/\sigma$ is shown for a lattice containing a random array of point defects with a 5 percent concentration, with the force making a 33 degree angle with $L_x$. This run was done at a temperature of $T = 26^\circ K$.

III. PERTURBATION THEORETIC TREATMENT

The force of friction acting on a thin film as it slides over a substrate containing defects was recently studied using lowest order perturbation theory in the substrate potential [3]. It was shown there that for most orientations of the film and most directions of sliding over the substrate, the force of friction is viscous (i.e., proportional to the sliding velocity), in agreement with what has to date been observed in QCM friction experiments [3]. The simulations that were discussed in the last section of a xenon film sliding over a silver (111) substrate containing a step show that the film is pinned if we apply a force smaller than a critical value in a direction normal to the step. When a force larger than this critical value is applied, the resulting velocity is a nonlinear function of the applied force. In this case the film’s axes are lined up with the step. For many substrate-adsorbed film systems, the case considered in the simulations, in which the crystallographic axes of the film are lined up with the step, is an important case because one expects that it will be energetically favorable for the film’s axes to line up with the step locally. The reason for expecting this to occur is that adsorbate atoms can lower their energies by lying along a step edge, because in this way each of these adsorbate atoms will be surrounded on two sides by a substrate atom. For the present system, our simulations seem to show, however, that the film does not always line up with the step, and when it is not lined up (for example, for the 173 atom system discussed at the end of the last section), the simulations show that the film is not pinned for forces for which it would be pinned if it were. (For real surfaces, which have many steps, it is expected that because of its stiffness the film in its solid phase will typically not be able to distort in such a way that its crystallographic axes line up locally with each step.) In this section we will try to interpret the results of the simulations reported here using the perturbation theoretic methods of reference [3].

In Ref. [3], it was shown using perturbation theory that for a general nonperiodic substrate force, the mean force of friction acting on a thin film is given by

$$ F_{av} = (mN)^{-1}\sum_{k,\sigma} \frac{\gamma \omega^2 |f(k) \cdot \hat{\epsilon}_{k,\sigma}|^2}{(\omega^2(k)-\omega^2)^2+\gamma^2 \omega^2}. $$

(3.1)

where $\omega = v_x k_x + v_y k_y$, where $v$ is the sliding velocity of the film, $f(k)$ is the Fourier transform of the force due to the substrate, $m$ is the mass of an atom, $N$ is the number of atoms in the film and $\gamma$ is the inverse phonon lifetime.

This expression was obtained by setting the rate at which the substrate force $f(\vec{r} - \vec{v}t)$ does work on the film equal to the rate at which the average force of friction $F_{av}$ does work on the film, i.e., $F_{av}v$. It was also found in that reference that the mean square vibrational displacement of an atom in the film (in the rest frame of the film) is given by

$$ <u^2> = m^{-2}N^{-1}\sum_{k,\sigma} \frac{|f(k) \cdot \hat{\epsilon}_{k,\sigma}|^2}{(\omega^2(k)-\omega^2)^2+\gamma^2 \omega^2}. $$

(3.2)

In Ref. [3], it was found that in two or fewer dimensions for a substrate containing point defects (e.g., vacancies or substitutional impurities), $<u^2>$ diverges as $v$ approaches zero. This signifies that in the zero velocity limit, there will always be significant distortion of the film to conform to the substrate, no matter how small the substrate force, which implies that the film will be pinned in place unless a strong enough external force is applied.

In the $\gamma$ approaches zero limit, Eq. (3.1) becomes

$$ F_{av} = (\pi/m)(a/2\pi)^2 \sum_{\sigma} \int d^d k \omega f(k)^2 \delta(\omega^2(k) - \omega^2). $$

(3.3)

In this limit, a nonzero contribution to $F_{av}$ occurs when the argument of the delta function is zero, which occurs when the plane in the $d+1$ dimensional space defined by $\omega$ and the $d$-components of $k$ whose equation is $\omega = \mathbf{v} \cdot \mathbf{k}$ intersects the phonon dispersion surface [whose equation is $\omega = \omega_{\sigma}(\mathbf{k})$, if $f(\mathbf{r})$ were aperiodic for all directions of $\mathbf{r}$]. This is the case when we have point defects in the substrate. It was shown in Ref. [3] that in this case in lowest order perturbation theory for a two dimensional (i.e., monolayer) film $F_{av}$ is independent of velocity and $<u^2>$ diverges as $1/v$ as $v$ approaches zero, implying pinning of the film at low velocities. In contrast for a three dimensional (i.e., thick) sliding film, $F_{av}$ was found to be proportional to $v$ and $<u^2>$ did not diverge as $v$ became zero, which is consistent with the film not being pinned. In appendix C, these ideas are expanded upon by considering general order in perturbation theory. It is shown that $d=2$ is indeed a critical dimension for this problem.

Let us now consider a line defect, such as a step or facet boundary. If we choose the $x$ and $y$ axes (i.e., the coordinate axes in the plane of the film) so that the $y$-axis is along the defect (i.e., along a step or facet boundary, which are taken in the present discussion to be straight lines) $f(k)$ will be non-zero only if $k_y$ is a multiple of the $y$-component of one of the reciprocal lattice vectors of the substrate, since the substrate is periodic in that direction if the crystallographic axes of the substrate are lined up with the defect and quasiperiodic otherwise. As a consequence, the plane whose equation is $\omega = v_x k_x + v_y k_y$ gets fragmented into a series of parallel lines at values of $k_y$...
equal to $Q_y$, the y-component of one of the smaller reciprocal lattice vectors of the substrate. For a facet boundary or step, $F$ can be written as $f(r) = g(x)F(x)$, where $F$ is periodic but $g$ is not. (This was illustrated for the model for the potential that was used in the simulations presented in Ref. [3]). A reasonable model potential for other line defects, such as facet boundaries, for example, will have a similar form. This is discussed in appendix B. Since we can write $F$ as $F(r) = \sum_{Q} F_{Q} e^{iQ \cdot r}$, we find that
\[
F(k) = \int d^2r e^{-ik \cdot r} f(r) = \sum_{Q} \delta_{k_x, Q_x} g_{k_x, -Q_x} F_{Q_x}.
\] (3.4)
where $Q$ denotes a reciprocal lattice vector of the substrate. It is only when one of these lines in k-space intersects the phonon dispersion surface that Eq. (3.3) gives a nonzero contribution to $F_{av}$. If this does not occur, we must keep $\gamma$ nonzero in Eq. (3.1). We then find that $F_{av}$ is proportional to $v$.

Let us now consider the case in which the crystallographic axes of the film are not lined up with the direction of the defect but are close to being so. Furthermore, let us keep $\gamma$ nonzero for this discussion, in order to examine what happens if a line passes within a phonon linewidth of the phonon dispersion surface. Then taking the defect to be lined up with the y-axis, if we convert the summation over wavevector in Eq. (3.2) to an integral along a line perpendicular to the step in the usual way, we obtain
\[
< u^2 > /a^2 = \frac{a}{2\pi m^2 a^2} \sum_{\sigma} \int dk_x F(k_x, k_y, G, v) \] (3.5)
where $F(k_x, k_y, G, v)$ is given by
\[
\frac{|f(k_x, k_y) \cdot \hat{\epsilon}_{k,z}|^2}{(v_p^2 k_x^2 + k_y^2) - \omega^2 \gamma^2 / \omega^2}.
\] (3.6)
where $\omega = v_y k_y + G_x v_x$ and $k_y$ is the amount that the line, which would have passed directly through the point in k-space denoted by the film reciprocal lattice vector $G$, if the film’s crystallographic axes were lined up with the defect, misses going through this point in reciprocal space. On doing the integral over $k_x$ by contour integration we find that $< u^2 > /a^2$ is equal to
\[
(ma)^{-2} v_p^{-1} \frac{3\pi}{2} |f \cdot \hat{\epsilon}|^2 \frac{\pi |f \cdot \hat{\epsilon}|^2}{2 \sin(\theta_1/2)(v_p^2 k_y^2 + \gamma^2 G_x^2 v_x^2)^{3/4}},
\] (3.7)
where $|f \cdot \hat{\epsilon}|$ is evaluated at the wavevector corresponding to the pole in the integrand of Eq. (3.3) and where $\theta_1 = \arctan[\gamma v_x G_x/(v_p^2 - k_y^2)]$. (Note that $\sin \theta_1/2$ becomes 1 rather than zero as $v_x$ approaches zero, since $\theta_1$ approaches $\pi$ rather than zero.) From these results, we see that if $k_y \neq 0$, $< u^2 > /a^2$ does not diverge as $v_x$ approaches zero, which implies that the film is not pinned. Furthermore, if $|f \cdot \hat{\epsilon}|$ is of the order of $10^{-7} \text{dyn}$, $m \approx 10^{-22} \text{g}$, $a \approx 10^{-8} \text{cm}$, $G_y \approx 10^6 \text{cm}^{-1}$ and $k_{y_0} \approx 10^7 \text{cm}^{-1}$ (or about 1/10 of the Brillouin zone radius), we estimate that $< u^2 > /a^2$ is of the order of $10^{-3}$. Thus, we conclude that for a reasonable value of the mis-orientation parameter $k_{y_0}$, lowest order perturbation theory should be a correct description of the friction, even as $v$ approaches zero. It is easily seen from Eqs. (3.1) and (3.2) that for this case, in which $< u^2 > /a^2$ does not diverge as the sliding velocity approaches zero, the force of friction will be proportional to the velocity.

### IV. SPECULATIONS ON THE BEHAVIOR OF REAL INTERFACES

We propose the following physical explanation for why a line defect, such as a step, will pin the film if it is oriented along a crystallographic axis of the film but will not pin it if it is not lined up. When the line defect is lined up with a crystal axis, a line of atoms running across the width of the film will pass over the defect at all the same time as the film slides over the defect. Consequently, the force exerted by the defect on the film will be an extensive quantity, in the sense that it will scale with the width of the film. In contrast, when the defect is not lined up with an axis, atoms in the film will pass over the defect one at a time. The defect will act on one atom at a time with a force that does not scale with the width of the film. Thus, if we consider a situation in which the velocity of the film is studied as a function of a force applied to each atom in the film, when the film’s axes and the defect are not lined up, it will clearly be much easier for the applied force to overcome any nonextensive pinning force due to the defect than an extensive one. A real substrate surface will contain a finite density of line defects along a line drawn along the sliding velocity. These defects will most likely not run across the width of the film, and they certainly will not be straight over that distance. Then, although the pinning force due to one of these line defects will not be extensive, the force due to a finite density of them will.

One way to understand the case of many finite length line defects, which are not perfectly straight, as occur on real surfaces using the calculation presented above for a single straight line defect is that if the defect is not a straight line over an infinitely long distance, the Fourier transform of the substrate force in Eq. (3.4) will no longer contain a $\delta_{k_y, Q_y}$ factor (since a kroniker delta only occurs if $f$ is periodic over an infinite distance). Rather the Kroniker delta will be replaced by a function of $k_y$ of finite width of the order of $2\pi/\ell$, where $\ell$ is the length of a straight section of the defect, peaked around the values of $Q_y$. Consequently, we can now think of the lines in k-space, defined by $k_y = Q_y$, which must intersect the phonon dispersion surface in order for the delta function in Eq. (3.3) to be satisfied, as being broadened. For real
surfaces, which contain many finite length straight sections of line defects separated by defect-free regions, \( f ( k ) \) will consist of the following contributions: defect-free regions which will give a peak in \( f \) at each reciprocal lattice vector of the film, point defects, which will give a contribution which is not peaked in k-space and straight sections of line defects, which will each give a contribution that is peaked at values of the component of \( k \) along the defect equal to components of a reciprocal lattice vector of the substrate if we move in k-space in a direction parallel to the defect. How sharply it is peaked will depend on the length of the straight section of the defect. In the direction perpendicular to the defect, the contribution to \( f ( k ) \) will not be peaked. The magnitude of each of these contributions to \( f ( k ) \) will be proportional to the number of lattice sites in each of the above elements. Thus, when we take the square of \( f ( k ) \), which enters Eqs. (3.1) and (3.2), we will thus obtain the following contributions: 1. a Bragg peak at each substrate reciprocal lattice vector, 2. a contribution which is not peaked in k (from the point defects), and 3. a series of "mountain ridges" in k-space directed in various directions. These are the lines in k-space that we found for a single line defect except that each one now has a width of the order of 2 \( \pi / L \). 

The point defects will always contribute "dry friction." We assume that the major fact that the observed force of friction generally seems to be viscous in these experiments seems to imply that either the defects are much weaker or have a concentration much lower than the 5 percent concentration used in the present simulations.

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### APPENDIX A: EFFECTS OF PERIODIC BOUNDARY CONDITIONS

We will now use perturbation theory to estimate the effect of using periodic boundary conditions in simulations of films sliding over substrates containing steps and substrates containing point defects (e.g., vacancies, substitutional impurities or add-atoms). What we will do is to calculate the force of friction for a system with periodic boundary conditions and compare our results to the results of the calculation of the force of friction for an infinite system. For the case that we consider, motion takes place perpendicular to the step. Since the finite system with periodic boundary conditions is periodic with the length of the box, the driving force due to the substrate (in which we are doing perturbation theory) is periodic. As a result, the sum over wave-vector in the expression for the force of friction, i.e., Eq. (5) in Ref. 7, becomes Eq. (12) in that reference, which gives the force of friction when the substrate is perfectly periodic with reciprocal lattice vectors with components \( G_x = 2 \pi n_1 / L \) and \( G_y = 2 \pi n_2 / L \), where \( L \) is the length of the box (the reciprocal lattice vectors for a substrate which is periodic only because of the use of periodic boundary conditions). Then the important parameters are \( R \), the ratio of \( 2 \pi / L \) to the reciprocal lattice vector of the substrate, the phonon mode width \( \gamma \), and the sliding velocity \( v \).

To be explicit, we do the sum over wavevector in Eq. (5) of Ref. 7. When periodic boundary conditions are used with a finite size box, this is a sum over discrete values of \( k \) (i.e., \( k_x = n_1 2 \pi / L \) and \( k_y = n_2 2 \pi / L \), where \( L \) is the box length). We make the following assumptions, valid for small sliding velocity: We take the sliding velocity to be along the x-axis. We assume that the major

### V. CONCLUSIONS

Simulations and perturbation theory calculations done for a monolayer film sliding on a substrate containing a step defect gave approximately viscous friction for all sliding directions other than perpendicular to the step. The point defects in the simulations were found to pin the film below a critical applied force For defects of strength comparable to the strength of the corrugation potential (which were used in the present simulations), however, the pinning force was only about \( 10^{-11} \) dyn. This force is still greater than the inertial effective force resulting from the oscillations of the microbalance (\( m \omega^2 A \), where \( m \approx 10^{-22} g \) is the adsorbate atom mass and \( \omega \approx 10^7 s^{-1} \) and \( A \approx 10^{-6} cm \) are the microbalance frequency and amplitude, respectively), which is about \( 10^{-14} \) dyn. The
The summation is evaluated for $R=1/13$, $\Gamma = 0$.

In the infinite $L$ limit, the summation from $0$ to $0.2$, which are parameters appropriate to point defects, Eq. (5) of Ref. [7] can be approximated by

$$F_{av} \propto \sum_k \frac{\gamma G_x^2 v|f \cdot \epsilon|^2}{(v_p^2 k^2 - v^2 G_x^2 + \gamma^2 \omega^2)}, \quad (A1)$$

where $G_x$ is the $x$-component of one of the smallest reciprocal lattice vectors of the film. The k-dependence of $\mathbf{f}(\mathbf{k}) \cdot \epsilon_{k,\sigma}$ is neglected and the origin of k-space has been moved to the point $\mathbf{G}$, one of the smallest reciprocal lattice vectors of the film. Then, we must evaluate the summation

$$\sum_{n_1,n_2} \frac{\Gamma \nu'}{(n_1^2 + n_2^2) R^2 - v'^2 + (\Gamma \nu')^2}, \quad (A2)$$

where $R = 2\pi/(LG_x)$, $\nu' = v/\nu_p$ and $\Gamma = \gamma/\nu_p G_x$. This summation is evaluated for $R=1/13$, $\Gamma = 0.1$ and $\nu'$ ranging from 0 to 0.2, which are parameters appropriate to the simulations. In the infinite $L$ limit, the summation over $n_1$ and $n_2$ can be approximated by the integral

$$R^{-2} \int dq_x dq_y \frac{\Gamma \nu'}{(q^2 - v'^2 + (\Gamma \nu')^2), \quad (A3)}$$

where $q_x = n_1 R$ and $q_y = n_2 R$. The result of doing this integral is

$$(R^{-1})[\pi/2 + \arctan(\nu'/\Gamma)]. \quad (A4)$$

Plots of Eqs. (A2) and (A4) are shown in Fig. 14. As can be seen, the integral (which describes an infinite system) and the summation (which describes a finite system with periodic boundary conditions) agree with each other for $\nu'$ greater than 0.02. Thus, for velocities greater than this value, we are justified in assuming that the simulations will be a good description of a film on an infinite nonperiodic substrate.

For the case of a straight step, the film is periodic or quasiperiodic along the step with a repeat distance or almost repeat distance comparable to a lattice constant. Thus, if we take the step to be along the $y$-axis and consider the sliding velocity to be in the $x$-direction, the expression for $F_{av}$ involves an integral only over the $x$-component of the wavevector for an infinite system. For a finite system with periodic boundary conditions, the summation and integral corresponding to these quantities are respectively

$$\sum_n \frac{\Gamma \nu'}{(n^2R^2 - v'^2 + (\Gamma \nu')^2)} \quad (A5)$$

and

$$R^{-1} \int dq (q^2 - v'^2 + (\Gamma \nu')^2), \quad (A6)$$

where $q=nR$. This integral can easily be performed by contour integration to give $(\pi/(2\gamma))^{1/2}(\nu')^{-1/2}$. This result together with the summation over $n$ are shown in Fig. 10. We again see that the finite system with periodic boundary conditions is an accurate representation of the infinite system for $\nu'$ greater than 0.02.

FIG. 16. A comparison of Eq. (A5) (the curve that is higher near $\nu'=0$) and (A6), which are proportional to the force of friction for a finite and an infinite system, respectively, with periodic boundary conditions.

APPENDIX B: THE SUBSTRATE FORCE WITH A LINE DEFECT PRESENT

A good model for the corrugation potential when there is a step present in the crystal which is parallel to the $y$-axis is

$$v_1(z - g(x)) \sum_{Q_1} e^{iQ_1 \cdot (r-d(x))}, \quad (B1)$$

where $g(x)$ is a Fermi function $z_1/[e^{\beta(x-\delta)} + 1]$ times $z_1$ (where $z_1$ is the height of the step and $\beta$ is the reciprocal width of the step edge, which is of the order of the reciprocal of an atomic spacing). $Q_1$ denotes the 6 smallest reciprocal lattice vectors of the substrate and $d(x)$ is the product of a vector giving projection of the difference between the equilibrium positions of the film atoms in the
first and second Fermi atomic layers parallel to the x-y plane and the above Fermi potential. Then the x and y components of the force \( f_{x/y} \) due to the corrugation potential are given by

\[
\begin{align*}
    f_x &= -\frac{dV_1(z_0)}{dz} \sum_{Q_1} \frac{d}{dx} \left[ g(x) e^{-iQ_1 \cdot d(x)} \right] e^{iQ_1 \cdot \mathbf{r}} + \\
    &+ \sum_{Q_1} Q_{1z} e^{iQ_1 \cdot (r-d(x))} \\
    f_y &= V_1(z_0) \sum_{Q_1} iQ_{1y} e^{iQ_1 \cdot (r-d(x))},
\end{align*}
\]

(Eq. B2)

where \( z_0 \) is the value of \( z \) at which the attractive potential \( V_0(z) \) is minimum. Then it is easily found that each term in \( f_x \) and \( f_y \) will have the form of Eq. (3.4).

Now, let us consider another type of line defect, a facet boundary. In going from one facet to its neighbor, the crystal surface rotates in the x-z plane for a facet boundary along the y-axis. Then a simple phenomenological model for a facet boundary, along the lines of the crystal lattice in an applied electric field [10], can be used to examine the behavior of the \( n^{th} \) order term in perturbation theory in the substrate potential as the sliding velocity approaches zero. (The charge density wave problem differs from the present problem, however, in that in the charge density wave problem, the motion is overdamped, whereas in the present problem it is not.) To accomplish this, let us consider the average rate at which the substrate force does work on the film by generating phonons, as the film slides over it (which can be set equal to \( F_{av \cdot v} \) where \( F_{av} \) is the mean force of friction and \( v \) is the sliding velocity). From previous work on this problem this is given by (Eq. 3.4)

\[
F_{av \cdot v} = (T^{-1}) \int dt \sum_j f(R_j + \mathbf{u}_j - \mathbf{v}t) \cdot \mathbf{u}_j(t),
\]

(Eq. C1)

where

\[
\mathbf{u}_j(t) = \sum_{j'} dt' G(R_j - R_{j'}, t - t') \cdot f(R_{j'} + \mathbf{u}_{j'}' - \mathbf{vt'}),
\]

(Eq. C2)

where the Green’s function is given by

\[
G(R_j - R_{j'}, t - t') = \sum_{k, \sigma} \int dk e^{i(k \cdot \mathbf{R}_j - \mathbf{R}_{j'})} e^{\omega(t-t')/\omega_k^2(k) - \omega^2 + i\gamma\omega}.
\]

(Eq. C3)

The perturbation series in the substrate potential corrugation strength \( f \) can be generated by expanding \( f(R_{j'} + \mathbf{u}_{j'} - \mathbf{vt'}) \) on the right hand side of Eq. (C2) in a Taylor series in \( u_{j'}(t') \). Each factor of \( u_{j'} \) in each term in the Taylor expansion is given by Eq. (C2). We then make a Taylor series expansion of the \( f(R_{j'} + \mathbf{u}_{j'}(t') - \mathbf{vt'}) \) which occurs in each of these expressions. At any given point in this procedure, we can stop it by replacing \( f(R_{j'} + \mathbf{u}_{j'}(t') - \mathbf{vt'}) \) by its zeroth order term in the Taylor series expansion, namely \( f(R_{j'} - \mathbf{vt'}) \). Then the resulting perturbation expansion of Eq. (C2) can be represented schematically by the diagram in Fig. 17.

FIG. 17. Diagramatic representation of the perturbation expansion for \( u_j \) in powers of \( f \). The lines and vertices are defined in the text.
Each vertex is labeled by a position and time \((R_{j_n}, t_n)\), where \(n\) is equal to 1 at the vertex that is furthest to the left. It increases as one moves to the right. With the exception of the vertex at the beginning of the “tree” (i.e., the far left hand side of the diagram) each of these variables is summed and integrated over. A line connecting two vertices labeled by \((R_{j_1}, t_1)\) and \((R_{j_2}, t_2)\), for example, represents the Green’s function \(G(R_{j_1} - R_{j_2}, t_1 - t_2)\), and each vertex denotes \((q - 2)\)th order derivative of \(f\) multiplied by a factor of \(1/(q - 2)!\), where \(q\) is the number of lines intersecting at the vertex. It is not difficult to show that the last element in a chain of vertices (i.e., a line of vertices, each one of which has only two neighbors), which ends at the vertex \((R_{j_1}, t_1)\) is a function of \(R_{j_1}\) and \(t_1\) only in the combination \((R_{j_1} - vt_1)\). For example, in \(d\)-dimensions this element is proportional to

\[
\int d^d k \frac{e^{ik \cdot (R - vt)}}{\omega^2(k) - (\mathbf{v} \cdot \mathbf{k})^2 + i\gamma \mathbf{v} \cdot \mathbf{k}} \tag{C4}
\]

In two and three dimensions the above integral can be done by contour integration. In the small \(v\) limit \(\omega(k)\) can be approximated by \(v_p k'\), where \(v_p\) is the sound velocity and \(k = G + k'\), where \(G\) is the nearest reciprocal lattice vector to the region in which \(\omega(k)\) and \(\mathbf{v} \cdot \mathbf{k}\) intersect. Then the above integral becomes

\[
\int d^d k' \frac{e^{ik \cdot (R - vt)}}{v_p^2 k'^2 - (\mathbf{v} \cdot \mathbf{G})^2 + i\gamma \mathbf{v} \cdot \mathbf{G}} \tag{C5}
\]

In one dimension this integral is proportional to

\[
\cos(vG(x_1 - vt_1)) e^{\gamma|x_1 - vt_1|} \tag{C6}
\]

In three dimensions, it is proportional to

\[
\int d^d x e^{i \mathbf{v} \cdot \mathbf{x}} \frac{e^{i \gamma \mathbf{v} \cdot \mathbf{x}} |R_1 - vt_1|}{|R_1 - vt_1|}. \tag{C7}
\]

By building a chain out of these elements and integrating over each of the vertices except the furthest to the left, we find that if \((R_{j_1}, t_1)\) are the labels of the end of the chain farthest to the left, the chain will be a function of these variable in the combination \((R_{j_1} - vt_1)\). On doing the integrals and sums on each of the vertices in the chain except the last one, the Fourier transform of the \(n\)th Green’s function in the resulting contribution to the perturbation theory is

\[
[\omega^2(k_n) - (\mathbf{v} \cdot \mathbf{k}_n)^2 + i\gamma(\mathbf{v} \cdot \mathbf{k}_n)]^{-1} \tag{C8}
\]

where \(k_n\) is one of the wavevectors which are summed over. Each vertex represents the dot product of one of the phonon polarization vectors \(\hat{\epsilon}_n\) and the spatial Fourier transform of one of the functions \(f\), evaluated at the difference between the wavevectors of the Green’s functions on either side of the vertex, multiplied by the dot product of a polarization vector and the argument of the Fourier transforms of \(f\) appearing in the chain. Using the fact that a chain ending at the vertex labeled by \((R_{j_1}, t_1)\) is a function of the variable \((R_{j_1} - \mathbf{v} t_1)\), it is easy to show that a vertex at which \(q\) chains intersect will also have this dependence on the space and time variables with which it is labeled, and it will also contain a factor

\[
\Pi_{m=1}^n [\omega^2(k_m) - (\mathbf{v} \cdot \mathbf{k}_m)^2 + i\gamma \mathbf{v} \cdot \mathbf{k}_m]^{-1}, \tag{C9}
\]

where \(n\) is the order in perturbation theory. Each variable \(k_m\) is summed over. When we take the thermodynamic limit for the film, each of these summations becomes a \(d\)-dimensional integral over the wavevector. If these integrals diverge at small \(v\), the most divergent part will come from the integral over the vicinity of the intersection of the plane \(\omega = \mathbf{v} \cdot \mathbf{k}_m\) with the phonon dispersion surface \(\omega(k_m)\). Therefore, let us consider the integral over just this region of \(k\)-space. Then in the small \(v\) limit, \(\omega(k_m)\) can be expanded in a Taylor series about the film reciprocal lattice vector \(\mathbf{G}\) of the dip in \(\omega(k_m)\) which is intersected by the plane \(\omega = \mathbf{v} \cdot \mathbf{k}_m\). Then, if we write \(k_m = G + k'_m\), \(\mathbf{v} \cdot \mathbf{k}_m\) and \(\omega^2(k_m)\) are, to lowest order in \(k'_m\), \(\mathbf{v} \cdot \mathbf{G}\) and \((v_p k'_m)^2\), respectively. Then the divergent part of one of these integrals is proportional to

\[
\int \frac{d^d k'}{v_p^2 k'^2 - (\mathbf{v} \cdot \mathbf{G})^2 + i\gamma \mathbf{v} \cdot \mathbf{G}}. \tag{C10}
\]

Let us consider this integral in the limit as \(\gamma\) approaches zero since it is expected that the phonon damping will always be small compared to the frequency of the phonon being excited (which is equal to \(\mathbf{v} \cdot \mathbf{G}\)). If we make a change of integration variable to a variable \(x\) equal to \(v_p k/(vG)\) the integral becomes

\[
(vG/v_p)^d (v_p/vG)^2 \int \frac{d^d x e^{i \mathbf{v} \cdot \mathbf{x}}}{x^2 + 1 + i\epsilon}, \tag{C11}
\]

where \(\epsilon = \gamma/vG\), which we are assuming to be \(\ll 1\), since the damping of an acoustic phonon mode is always small compared to its frequency. The smallest value of \(x\) in the range of integration is 0 and the largest value is large compared to 1, but still finite. As long as \(\epsilon\) is small compared to 1 but nonzero, the integral over \(x\) gives a finite number. Then the \(n\)th order term in the perturbation theory diverges as \(v^{d-2}\) if \(d < 2\). Two dimensions is a marginal dimensionality, which could still have logarithmic divergences in \(v\) at small \(v\).