Theory of energy dissipation in sliding crystal surfaces

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The average force of kinetic friction that occurs when layered compounds (which are commonly used as solid lubricants) are sheared in steady state is calculated for a model for such substances, assuming that the dissipation is caused by the excitation of lattice vibrations in one surface by the other. Because at slow speeds shearing is believed to be due to dislocation motion, a model for slow-speed shearing due to dislocation motion has been formulated. The force of friction is found to be inversely proportional to the sliding velocity for velocity small compared to the velocity of sound in the material and proportional to the area of the slipping surfaces. The dissipative stress at a sliding speed of 1 cm/s is calculated to be 10^8 dyn/cm^2. The dissipative stress, calculated for slippage of two incommensurate surfaces, is found to be only 10^{-4} dyn/cm^2, however, which opens up the question of whether lubrication is caused by slippage of the lubricant relative to the sliding surfaces rather than by shearing of the solid lubricant crystal.

I. INTRODUCTION

It has recently been shown[1] that when surfaces coated with MoS_2 by sputtering slide relative to each other, the MoS_2 crystallites orient with their basal planes parallel to the sliding surfaces. This supports the generally accepted notion that the fact that layered compounds such as graphite and MoS_2 shear extremely easily in the direction parallel to their basal planes is one of the reasons for the low coefficient of friction of surfaces coated with them. This is also quite likely to be true for some other solid lubricants (such as graphite and graphite fluoride and certain dichalcogenides[2]). Therefore, a study of the resistive force which occurs when such layered compounds shear as a function of a load pushing the layers together and the rate of shearing would be an important step towards understanding lubricating properties of these solid lubricants on a microscopic level. The problem of the shearing of an fcc structure under a shear stress and a load has recently been treated using molecular-dynamics techniques.[3] Molecular dynamics is suitable for treating transient behavior. The present approach treats steady-state shearing (i.e., beyond the elastic limit) of an infinite crystal, which is not easily treated by molecular dynamics. In the problem of sliding friction, it is necessary to study a model with an infinite number of atoms in order to understand the way in which the sliding kinetic energy is dissipated among the macroscopic number of vibrational modes of the crystal because steady-state sliding friction is precisely the process by which sliding motion of a body as a whole is converted into thermal (i.e., vibrational) energy. A conceptually simple model for studying this problem consists of a slab of a layered crystal structure with its lower surface in contact with a rigid periodic potential with the same periodicity as a single layer (meaning that each atom in the lower surface moves in a periodic potential) which is driven at constant speed, with the upper surface held stationary. The interface between the lower surface and the periodic potential represents the slip plane, and the periodic potential itself represents the part of the crystal below the slip plane. This model is a direct application of the work of Ref. 4 to the problem of the shearing of layered solid lubricants. This article will discuss this model, but it should not be much more difficult to generalize this to the more realistic case of two such slabs slipping over each other. At high sliding speeds, the atomic vibrational amplitudes generated by the moving potential are small and hence can be neglected in the argument of the periodic potential. The possible justification of this procedure is studied by examining the amplitudes of the atomic vibrations generated in the crystal by its sliding motion in the potential and seeing if they are small compared to the lattice spacing. In performing these calculations, it will be assumed that the layers which are being slid over the potential contain edge dislocations. If this is not assumed, the force necessary to cause shearing is considerably larger. This is a well-known phenomenon in the mechanics of plastic deformation.[5] Furthermore, the actual crystals certainly contain such defects. The calculated force of friction was found to be inversely proportional to the sliding velocity and proportional to the surface area. The case of very slow-speed sliding is then treated in Sec. VI by assuming that at slow speeds the slippage occurs by dislocation motion. Using the known behavior of dislocations, a model is formulated for the frictional force due to dislocation motion, which is similar to recent work on the damping of solitons in one-dimensional lattices.[6] In Sec. V, the frictional force generated when a crystal slides relative to the surface of an incommensurate crystal is calculated. For the case of a defect-free crystal, it is found to be 13 orders of magnitude smaller than for the case of shearing of commensurate layers considered above, which opens up the question of whether solid lubricants lubricate because of slippage between the surface and the lubricant rather than by shearing of the lubricant

itself. It should be possible to make the model quite realistic by using the known atomic structure of the layers (appropriate for specific compounds), using known force constants between the atoms in a layer and between the layers. Thus, it is quite likely that the present approach will allow one to study properties specific to particular solid lubricants because the method is quite general.

II. FORMULATION OF THE PROBLEM

Let us first consider as a simple model of a layered compound a simple tetragonal lattice in which the z axis is taken to be the c axis and the x axis is taken to be the axis along which the sliding takes place. Let us also assume that energy is dissipated by the vibrational motion generated by the sliding along the x axis, which is one of the crystallographic axes. This simple model incorporates the basic physics of the problem. Later, more complicated crystal structures will be considered. Although for graphite and molybdenum disulphide the crystal structure is hexagonal, since dissipation at slow speeds involves the creation of excitations with wavelengths large compared to a lattice constant, the exact details of the crystal structure are not expected to affect the present results significantly. The upper surface of the lattice (i.e., the surface with the lowest z value) will be constrained to be stationary, and the lowest surface is acted on by a sinusoidal potential with period a (the lattice constant of the crystal) which is constrained to move uniformly with a velocity v. This potential results if we include only the first few terms in the Fourier series for the periodic potential due to the crystal below the slip plane. For the lattice considered here, this reduces to a single sinusoidal potential. Thus, the equation of motion for the model is

$$\begin{aligned} m\ddot{x}_{j_1j_2j_3} = &-\alpha(4x_{j_1j_2j_3} - x_{j_1+1j_2j_3} \\ &- x_{j_1-1j_2j_3} - x_{j_1j_2+1j_3} - x_{j_1j_2-1j_3}) \\ &-\beta(2x_{j_1j_2j_3} - x_{j_1j_2j_3+1} - x_{j_1j_2j_3-1}) \\ &- m\gamma\dot{x}_{j_1j_2j_3} , \end{aligned} \tag{1}$$

for j_3 not equal to 1 or N, where the atomic positions are labeled by the lattice vector (j_1a, j_2a, j_3c), m is the atomic mass, γ is the phenomenological damping constant which accounts for the damping of the lattice vibrations, and α and β are the force constants for relative motion of atoms whose x coordinates and whose z coordinates differ, respectively. For $j_3=1$,

$$\begin{aligned} m\ddot{x}_{j_1j_21} = &-\alpha(4x_{j_1j_21} - x_{j_1+1j_21} - x_{j_1-1j_21} \\ &- x_{j_1j_2+1,1} - x_{j_1j_2-1,1}) \\ &-\beta(2x_{j_1j_21} - x_{j_1j_2,2}) - m\gamma\dot{x}_{j_1j_21} . \end{aligned} \tag{2}$$

Here, the atoms with $j_3=0$ are constrained to be stationary. For $j_3=N$,

$$\begin{aligned} m\ddot{x}_{j_1j_2N} = &-\alpha(4x_{j_1j_21} - x_{j_1+1j_21} - x_{j_1-1j_21} \\ &- x_{j_1j_2+1,1} - x_{j_1j_2-1,1}) \\ &-\beta(x_{j_1j_2N} - x_{j_1j_2N-1}) \\ &-\lambda_0\sin(2\pi/a)(x_{j_1j_2N} + vt) - m\gamma\dot{x}_{j_1j_2N} , \end{aligned} \tag{3}$$

where $\lambda_0=(a/2\pi)\beta$ and a is the lattice constant in the x-y plane.

Equations (1)–(3) can be inverted to obtain an expression for $x_{j_1j_2j_3}$,

$$x_{j_1j_2j_3} = -(\lambda_0/m)\sum_{j_1'j_2'}\int dt' G_{j_1j_2j_3,j_1'j_2'N}(t-t')\sin(2\pi/a)(x_{j_1'j_2'N} + vt') , \tag{4}$$

where

$$G_{j_1j_2j_3,j_1'j_2'j_3'}(t-t') = (MLN)^{-1}\sum_{\mathbf{k}}\int d\omega \frac{e^{i\mathbf{k}\cdot(\mathbf{j}-\mathbf{j}')a - i\omega(t-t')}}{-\omega^2+\omega_0^2(\mathbf{k})+i\gamma\omega} , \tag{5}$$

where Ma, La, and Nc are the dimensions of the crystal in the x, y, and z directions, respectively, $\mathbf{j}=(j_1,j_2,j_3)$, and $\omega_0(\mathbf{k})$ is the frequency of the vibrational mode of wave vector $\mathbf{k}$. Equations (1)–(5) represent the system as a set of damped harmonic oscillators (i.e., the lattice vibrations) driven by a periodic driving force, namely the sinusoidal force in the model. The average force of kinetic friction $F_{\rm av}$ will be defined as follows:

$$F_{\rm av}v = (mT)^{-1}\int_0^T dt \sum_{j_1j_2}\lambda_0\sin(2\pi/a)(x_{j_1j_2N} + vt)\dot{x}_{j_1j_2N} , \tag{6}$$

where T is an appropriate averaging time (which will be defined later for each case considered). Thus, $F_{\rm av}$ multiplied by v is the rate at which work is done by the sinusoidal force on lattice vibrations, or in other words, the rate at which energy is absorbed by the lattice vibrations.

III. THE HIGH-SPEED APPROXIMATION

The main approximation of this section is to replace $x_{j_1j_2N}$ in the argument of the sine function in Eq. (2) by $x^0_{j_1j_2N}$, which represents the shifts in the atomic positions in the bottom layer due to dislocations assumed to be present in the crystal before the sliding started. That is, we are neglecting the displacements of the atoms (due to the sliding) introduced by the interaction with the sinusoidal force field in the argument of the sine, which should be a good approxima-

tion if λ_0 is sufficiently small and the sliding velocity is sufficiently large (so that the atoms cannot relax into new configurations sufficiently quickly). The question of just how small λ_0 and how large v must be will be examined in this section. Combining Eqs. (1)–(6), we obtain

$$F_{\rm av}=(\pi\lambda_0^2/LNMa)\sum_{\mathbf{k}}|S(\mathbf{k})|^2\left[\frac{2\pi v\gamma/a}{[\omega_0^2(\mathbf{k})-4\pi^2v^2/a^2]^2+(2\pi v\gamma/a)^2}\right], \tag{7}$$

where

$$S(\mathbf{k})=\sum_{j_1j_2}e^{ik_xj_1a}e^{ik_yj_2a}e^{i(2\pi/a)x^0_{j_1j_2N}}. \tag{8}$$

Let us set $j_1=j_{d\alpha}(j_2)+j'$ in Eq. (8), where $j_{d\alpha}(j_2)$ gives the location of the center of the αth dislocation along the x axis for a given j_2 value and j' is summed over the width of each dislocation. (The distance between the dislocations is assumed to be large compared to their widths.[7]) Then, Eq. (8) becomes

$$S(\mathbf{k})=LM\sum_{\mathbf{G}}\delta_{\mathbf{G},\mathbf{k}}+f(k_x)\sum_{\alpha j_2}e^{ik_xj_{d\alpha}(j_2)a}e^{ik_yj_2a}.$$

It is reasonable to replace $|S(\mathbf{k})|^2$ in Eq. (7) by its average over all dislocation configurations. This average is given by

$$\langle|S(\mathbf{k})|^2\rangle=(LM)^2\sum_{\mathbf{G}}\delta_{\mathbf{G},\mathbf{k}}+|f(k_x)|^2\sum_{\alpha\alpha'j_2j_2'}\langle e^{ik_x[j_{d\alpha}(j_2)-j_{d\alpha'}(j_2')]a}\rangle e^{ik_y(j_2-j_2')a} \tag{9}$$

$$\approx(LM)^2\sum_{\mathbf{G}}\delta_{\mathbf{G},\mathbf{k}}+N_{\rm dis}M|f(k_x)|^2, \tag{10}$$

where $\mathbf{G}$ is a reciprocal lattice vector in the x-y plane, and

$$f(k_x)=\sum_{j'}e^{ik_xj'a}(e^{i(2\pi/a)x^0_{j_d+j'}}-1),$$

where we have used the fact that for a completely random configuration the average over dislocation configurations vanishes unless $\alpha=\alpha'$. Also, the average must vanish for $|j_2-j_2'|$ large. To a first approximation, we have neglected terms in the summation with j_2 not equal to j_2'. The first term in Eq. (10) should generally dominate. In order to test the internal consistency of the approximation used in this section let us calculate the mean-square atomic displacement of an ion in the $j_3=N$ plane (i.e., the plane in contact with the periodic potential) within that approximation, which is defined by

$$\langle x^2\rangle=(LM)^{-1}\sum_{j_1j_2}x^2_{j_1j_2N}.$$

Using Eqs. (4), (5), (9), and (10), we find to zeroth order in $n_{\rm dis}=N_{\rm dis}/L$,

$$\langle x^2\rangle=(\lambda_0/m)^2\left|N^{-1}\sum_{k_z}[-\omega^2+\omega_0(\mathbf{k})+i\gamma\omega]^{-1}\right|^2, \tag{11}$$

where $\omega=2\pi v/a$, which in the small-γ limit becomes, if we use the Debye model [i.e., $\omega_0^2(\mathbf{k})=v^2_{\text{ph-}z}k_z^2+v^2_{\rm ph}(k_x^2+k_y^2)$],

$$\langle x^2\rangle^{0.5}=0.25(\lambda_0ca)/(2\pi mv_{\text{ph-}z}v),$$

where $v_{\text{ph-}z}$ is the phonon velocity along the z axis. If we take $\lambda_0=0.17\times10^{-5}$ (calculated from the elastic constants of graphite[8] by requiring that the force constant generated by the sinusoidal potential for small displacements gives the observed shear elastic constant c_{44}), $m=10^{-22}$ g, $v_{\text{ph-}z}$, the phonon velocity along the c axis, equal to 10^4 cm/s, $v=10^3$ cm/s, and $a=3\times10^{-8}$ cm, we find $(\langle x^2\rangle)^{0.5}=0.723\times10^{-6}$ cm. Since this is much larger than a lattice constant and only becomes smaller than a lattice constant for v comparable to the sound velocity, the present approximation is probably not suitable for calculating the force of friction for this case. Nevertheless, if we try to calculate the force of friction from Eq. (7) for this case, we find using the Debye model

$$F_{\rm av}/(LM)=(\pi\lambda_0^2/maN)\sum_{k_z}\delta(-\omega^2-\omega_0^2(k_z\hat{z}))$$

$$=0.25(\lambda_0^2a)/(mv_{\text{ph-}z}v)=0.25\times10^{-7} \tag{12}$$

(in dyn) for the above parameters but with v 100 times larger (in order to make $\langle x^2\rangle$ small compared to a lattice constant). If we divide this by the area per surface atom a^2, we obtain a dissipative contribution to the stress of 0.25×10^8 dyn/cm^2.

In the above discussion, we assumed that the film thickness is large compared to the lattice constant c, so that we could treat k_z as continuous. In the opposite limit, we must not replace the sum over discrete values of k_z in Eq. (7) by an integral. In that case, we find that in the small-γ limit if we use only the first term in Eq. (10), we obtain an energy conserving δ function which is not satisfied for most values of v. Thus in the case of films which are only a few atomic layers thick, it is the second

term in Eq. (10) which contributes to the force of friction. Consider the $k_z=0$ term in the summation over k_z (which should dominate because we shall see that it is inversely proportional to v). Then, using the above result, we find that in the γ approaches zero limit (it really only needs to be small compared to the maximum lattice vibrational frequency for the following results to be valid), $\langle x^2\rangle$ becomes for small $n_{\rm dis}$

$$\langle x^2\rangle=(n_{\rm dis}a/2\pi v)(\lambda_0/m)^2(a/2\pi)^2\int dk_x dk_y |f(k_x)|^2\delta(\omega^2-\omega_0^2(k_x,k_y,0))$$
$$=0.5(2\pi)^2(n_{\rm dis}N_\omega^2 a^3\lambda_0^2/\gamma m^2 v v_p^2)\ , \tag{13}$$

where N_ω is the width of the dislocation in units of a. Substituting the values for the above parameters quoted earlier in this section as well as $v=10$ m/s, $N_\omega=10$, and γ equal to 10% of the frequency $2\pi v/a$, and $n_{\rm dis}\approx 10^{-4}$ (found from Ref. 6), we find $(\langle x^2\rangle)^{0.5}\approx 0.3\times 10^{-6}$ cm, which again implies that v must be comparable to the sound velocity for our approximation to be consistent, implying that this method is not valid unless v is 100 times larger. For this "thin film" limit, Eq. (7) becomes

$$F_{\rm av}/(LM)=(n_{\rm dis}\pi^2\lambda_0^2/am)N^{-1}(a/2\pi)^2\int dk_x dk_y |f(k_x)|^2\delta(-(2\pi v/a)^2+\omega_0^2(k_x,k_y,0))$$
$$=\pi n_{\rm dis}\lambda_0^2 a/(Nmv_p^2)\approx 10^{-12} \tag{14}$$

(in dyn) for N of the order of 1, and the other parameters the same as above. This gives a dissipative contribution to the shear stress of order 10^3 dyn/cm^2. Although $F_{\rm av}\propto LM$, the area of the surface in units of the square of a lattice constant, the appropriate area to use for real lubricated surfaces in contact is known to be the actual contact area, which increases with increasing load,[9] so that the force of friction for lubricated surfaces could still be independent of the total surface area and proportional to the load. Since the number of atoms in contact increases in proportion to the load, the supporting force provided by each atom would remain independent of load, and hence, it is reasonable to take λ_0 to be nearly independent of the load.

IV. THE FORCE OF KINETIC FRICTION AT SLOW SPEEDS

Slow-speed shearing is believed to occur by dislocation motion. Layered compounds are known to possess edge dislocations with a slip plane at the interface between two layers.[7] When slippage occurs between two layers at slow speeds, it occurs by the motion of these dislocations. In our model, the region below the slip plane is replaced by a periodic potential. Therefore, the dislocations in question occur in the crystal above this potential. The atomic displacement due to such a dislocation can be represented by[7]

$$x_{j_1 j_2 N}=u(j_1 a-v_d t-x_{d,j_2}) \tag{15}$$

and

$$\sin[(2\pi/a)u(j_1 a-v_d t-x_{dj_2})]=g(j_1 a-v_d t-x_{d,j_2})\ ,$$

where x_{dj_2} is the x coordinate of the center of the dislocation, which is taken to be a function of j_2 to take account of the fact that the dislocation line is in general not straight, and v_d is the dislocation velocity. For a dilute concentration of dislocations, g is replaced by

$$\sum_\alpha g(j_1 a-v_d t-x^\alpha_{dj_2})\ ,$$

where the index α labels the dislocations. Substituting this expression into Eq. (6) and using Eqs. (4) and (5), we obtain

$$vF_{\rm av}/LM=(\lambda_0^2 v_d/mLa)(LNM^2)^{-1}\sum_{k_x k_y k_z}\int d\omega\frac{\gamma\omega^2|\bar g(\omega)|^2}{[-\omega^2+\omega_0^2(\mathbf{k})]^2+\gamma^2\omega^2}$$
$$\times\sum_{G_x}\delta_{k_x,\omega/v+G_x}\sum_{j_2 j_2' \alpha\alpha'}e^{iky(j_2-j_2')a}e^{-i(\omega/v_d)(x^\alpha_{d,j_2}-x^{\alpha'}_{d,j_2'})}\ , \tag{16}$$

where we have taken the averaging time T in Eq. (6) to be La/v_d, the time for a dislocation to traverse the surface and where

$$\bar g(\omega)=\int d\omega\, e^{-i\omega t}g(v_d t)\ . \tag{17}$$

The last summation in Eq. (16) may be replaced by its average over all possible dislocation configurations, which are taken to be completely random. Then, its summand will be zero unless $\alpha=\alpha'$. The summand will also be zero if j_2 and j_2' are sufficiently far apart (i.e., more than a few lattice constants). To a first approximation, they will be taken to be equal in this summation. Then, converting the summations over k_x,k_y,k_z to an integral and converting the Kronecker data on k_x to a delta function using

$$\sum_{k_x} \delta_{\omega/v,k_x+G_x} = \int dk_x \delta(\omega/v_d, k_x+G_x) , \tag{18}$$

we obtain in the γ approaches zero limit

$$(LM)^{-1}F_{\rm av}v = v_d n_{\rm dis} c(2\pi m)^{-1}\lambda_0^2 \sum_{G_x} \int d^3k\, |\bar{g}[v_d(k_x+G_x)]|^2 v_d(k_x+G_x)\delta[v^2k_x^2-\omega_0^2(\mathbf{k})] \tag{19}$$

or

$$(LM)^{-1}F_{\rm av}v = 0.5 n_{\rm dis} v_d^2 \lambda_0^2 c(2\pi m)^{-1} \sum_i \int dk_y dk_z |\bar{g}(vk_{xi})|^2 |v_d - v_p|^{-1} , \tag{20}$$

where v_p is the phonon velocity in the x-y plane and k_{xi} is the ith solution to the equation

$$v_d^2 k_x^2 - \omega_0^2(\mathbf{k}) = 0 , \tag{21}$$

where k_y, k_z are restricted to the first Brillouin zone but k_x runs throughout all of k space. If we write

$$\bar{g}(v_d k_x) = \int dt\, e^{-ivk_x t} g(vt) = v_d^{-1}\bar{g}(k_{xi}) , \tag{22}$$

where

$$\bar{g}(k_{xi}) = \int dx\, e^{-ik_{xi}x} g(x) ,$$

then

$$F_{\rm av}/(LM) = 0.5(2\pi)^{-2} n_{\rm dis}\lambda_0^2 c(mv)^{-1} \times \sum_i \int dk_y dk_z |\bar{g}(k_{xi})|^2 |v_d - v_p|^{-1} . \tag{23}$$

The present treatment is quite similar to the treatment of the damping of the motion of solitons in a discrete lattice given in Ref. 10. Since in the limit of continuum dislocation theory $\omega_0(\mathbf{k})$ takes the form $v_p k$, Eq. (21) has no solutions in this limit, implying that the frictional force obtained here comes about from the discreteness of the lattice, as it does in soliton theory.[10] The discrete changes in the soliton damping rate found in Ref. 10 occur because as the soliton velocity decreases, certain phonon modes which were excited by the sliding soliton at higher speeds are no longer excited. It is easy to see from the arguments in Ref. 10 that this results from there being a gap in the phonon spectrum which is about $\frac{1}{4}$ of the phonon bandwidth. In our case, at least for thick films, there is no gap in the phonon spectrum. Even for thin films, since we are considering proportionally smaller values of the ratio of λ_0 to the phonon bandwidth than were considered in Ref. 10, the resulting gap will be smaller compared to the bandwidth. Therefore, such effects should not occur in the present case. Furthermore, we are considering smaller sliding velocities. Using the fact that $v \approx n_{\rm dis} v_d$, we find

$$F_{\rm av}/(LM) \approx (4\pi)^{-1} n_{\rm dis}\lambda_0^2 (amvv_p)^{-1} \sum_i |\bar{g}(k_{xi})|^2 . \tag{24}$$

Using the fact that

$$\bar{g}(k_{xi}) \approx \bar{g}(2\pi/a) = \int dx\, e^{-ik_x x} g(x) \approx 0.01 l , \tag{25}$$

for some reasonable models for $g(x)$ (e.g., the one in Ref. 10), where l is the width of the dislocation and taking $v = 1$ cm/s and $l \approx 10^{-7}$ cm, we obtain (in dyn)

$$F_{\rm av} \approx 0.5 n_{\rm dis}(\lambda_0 l)^2 (mavv_p)^{-1} \approx 10^{-7} , \tag{26}$$

which corresponds to a stress of 10^8 dyn/cm^2, which is comparable to the shear strength of nickel and hence much too large for a lubricant.

Recently, experimental techniques have been devised to measure the dissipative force which occurs when a lubricating film is sheared between two oscillating surfaces.[11] Therefore, we will now consider the energy dissipated in a period when a lubricating film is sheared harmonically. To determine this energy, we will use

$$\sin[2\pi a^{-1}u(j_1 a - A\sin\omega_1 t)] ,$$

where ω_1 is the frequency with which it is being sheared and A is the amplitude of the dislocation motion caused by the shearing motion in Eq. (3) for the force which simulates the effect of the part of the crystal below the slip plane. This potential is slid harmonically and the upper plane of the crystal is held fixed, as is assumed in Sec. II. For purposes of obtaining a rough estimate, we assume that the dislocations are shifted rigidly. Substituting this expression into Eq. (6) and multiplying by T, which is taken to be $2\pi/\omega_1$, gives ΔE, the energy dissipated in one period,

$$\Delta E/(LM) = (2\pi/\omega_1)\lambda_0^2 n_{\rm dis} m^{-1}(2\pi)^{-3}a^2 c \int d^3k \int d\omega [\bar{g}(k_x) J_n(k_x A)]^2|_{n=\omega/\omega_1} \delta(\omega_0^2(\mathbf{k})-\omega^2)$$
$$\approx (2\pi/\omega_1)\lambda_0^2 n_{\rm dis} m^{-1}(2\pi)^{-3}a^2 c \int d^3k [\bar{g}(k_x)(k_x A/2n)^n]^2/\omega_0(\mathbf{k})|_{n=\omega_0(\mathbf{k})/\omega_1} , \tag{27}$$

where A is the amplitude of the oscillations and we have taken the large n limit of the Bessel function. Using the fact that for $k_x \ll 2\pi/l$, $\bar{g}(k_x) \approx l$, and replacing $\omega_0(\mathbf{k})$ by $\bar{v}_p k$, where $\bar{v}_p$ is a directional average of the phonon velocity, we obtain

$$\Delta E/(LM) \approx (\lambda_0/\bar{v}_p)^2 n_{\rm dis} ace^{-1}/\ln(2\bar{v}_p/A\omega_1) \approx 10^{-15} \tag{28}$$

in erg, taking $\bar{v}_p \approx 10^5$ cm/s and $A \approx 10^{-5}$ cm, the value

of A used in Ref. 11. From this value of ΔE we find an effective viscosity comparable to that measured in Ref. 11 by the following argument: Dividing this energy by 10^{-15} cm^2, the area of a surface unit cell, we obtain an energy loss per unit surface area of 1 erg/cm^2. Dividing this by the amplitude (10^{-5} cm) of the oscillations gives a mean stress of 10^5 dyn/cm^2. The effective viscosity is obtained by multiplying this by the thickness of the film (which is about 10^{-8} cm) and dividing this by the mean velocity (which is of the order of the amplitude divided by the period, or about 10^{-5} cm/s). We obtain an effective viscosity of the order of 10^2 P, which is comparable to the value found in Ref. 11.

V. SLIPPAGE AT THE INTERFACE BETWEEN TWO INCOMMENSURATE LATTICES

In Ref. 12, films which are incommensurate with an oscillating substrate were found to slip with very low dissipation. In fact theoretical studies have shown that weakly coupled one-dimensional incommensurate structures can slide relative to each other with no dissipation.[13] Therefore, it is of interest to study the frictional stress between two crystals which are incommensurate with each other by the present methods. In the spirit of the preceding sections, we will replace this problem to a first approximation by the sliding of a crystal lattice whose surface interacts with a periodic potential of period incommensurate with the lattice periodicity. This is accomplished by replacing $2\pi/a$ in Eq. (3) by $2\pi/b$, where b/a is an irrational number. In this article the approximation of Sec. III will be used. Also, we will consider only the case of a defect-free crystal, for which $x^0_{j_1 j_2 N}$ is equal to $j_1 a$. Then, from Eq. (4), we obtain

$$\langle x^2\rangle=(\lambda_0/m)^2\left|N^{-1}\sum_{k_z}[-(2\pi v/b)^2+(2\pi v_{\text{ph}}/b)^2+v^2_{\text{ph-}z}k_z^2+i\gamma(2\pi v/b]^{-1}\right|^2, \tag{29}$$

by using the Debye model for $\omega_0(\mathbf{k})$. Making the usual replacement of $N^{-1}\sum_{k_z}\cdots$ by $(c/2\pi)\int dk_z\cdots$, valid for thick films and performing the integration, we find for $v\ll v_{\text{ph-}z}$

$$(\langle x^2\rangle)^{0.5}=\lambda_0 cb/(4mv_{\text{ph-}z}v_{\text{ph}})\approx 0.5\times 10^{-8} \tag{30}$$

(in cm), using the previous values of the parameters in this equation and taking b to be of the order of 10^{-8} cm, implying that the approximation of Sec. III of neglecting atomic displacements in the potential is valid. Equation (6) for the mean force of friction becomes

$$F_{\text{av}}/(LM)=0.25(\lambda_0^2/m)(c/b)\int dk_z\,\text{Im}(-\omega^2+v^2_{\text{ph}}Q^2+v^2_{\text{ph-}z}k_z^2-i\gamma\omega)^{-1}, \tag{31}$$

where $\omega=Qv$ and $Q=2\pi/b$, which gives

$$F_{\text{av}}/(LM)=(16\pi)^{-1}(\lambda_0^2/m)c(v_{\text{ph-}z}v_p)^{-1}(\gamma v/v_p^2Q)$$
$$\approx 10^{-19}$$

(in dyn), which implies a dissipative stress of 10^{-4} dyn/cm^2, if we take $v=1$ cm/s and $\gamma=0.1Qv$ or about 10^7 Hz. Thus the dissipative stress is a factor of 10^{13} smaller for the shearing of an incommensurate interface than that for a commensurate one, which opens up the question of whether solid lubrication occurs by the shearing of the interface between the sliding surface and the lubricant material or by the shearing of the lubricant.

[1] J. R. Lince and P. D. Fleischauer, J. Mater. Res. 2,827 (1987).
[2] M. Gardos, STLE Tribology Transactions.
[3] M. W. Ribarsky and U. Landman, Phys. Rev. **38**, 9522 (1988).
[4] J. E. Sacco, J. B. Sokoloff, and A. Widom, Phys. Rev. B **20**, 5071 (1979).
[5] D. Hull, *Introduction to Dislocations* (Pergamon, London, 1965), pp. 51 and 52.
[6] See D. Hull, *Introduction to Dislocations*, Ref. 5, pp. 28 and 203.
[7] S. Amelinckx, in *Solid State Physics: Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic, New York, 1964), Suppl. 6, p. 267.
[8] A. A. Ahmadieh and H. A. Rafizadeh, Phys. Rev. B **7**, 4527 (1973); H. C. Gupta, J. Malhotra, N. Rani, and B. B. Tripathi, Solid State Commun. **57**, 263 (1986).
[9] J. A. Greenwood, Am. Soc. Mech. Eng. J. Lubrication Technol. **89**, 81 (1967).
[10] M. Peyrard and M. D. Kruskal, Physica **14D**, 88 (1984).
[11] J. Van Alsten and S. Granick, Phys. Rev. Lett. **61**, 2570 (1988).
[12] E. T. Watts, J. Krim, and A. Widom, Phys. Rev. B **41**, 3466 (1990).
[13] S. Aubry and C. Andry, *Proceedings of the Israel Physical Society*, edited by C. G. Kuper (Hilger, Bristol, 1979), Vol. 3, p. 133; S. Aubry (unpublished); J. E. Sacco and J. B. Sokoloff, Phys. Rev. B **18**, 6549 (1978).