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Theory of energy dissipation in sliding crystal surfaces at nonzero temperature

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Previous zero-temperature model studies of friction in a crystal undergoing plastic shear are extended to nonzero temperatures. For the case of a commensurate interface and most incommensurate interfaces without defects, thermal effects on the force of friction are found to be small. For the nearly commensurate case, however, it is argued that the force of friction should increase with increase in temperature. For the case of a commensurate interface with sliding taking place by the motion of dislocations, it is found that at temperature T small compared to the Debye temperature, thermal effects will be small, but as T becomes comparable to the Debye temperature, thermal effects dominate the force of friction.

I. INTRODUCTION

In previous work by the present author,[1] a simple model for kinetic friction was studied. It consists of a crystal lattice being dragged at constant speed in a periodic potential. The model is illustrated in Fig. 1. This can be used as a model for either this crystal sliding on the surface of a second crystal, in which case the potential represents the potential due to the surface of the second crystal, or as a model for the plastic shear of a crystal, in which case the potential represents the potential due to the atoms in the crystal below the shear plane. The problem was studied in lowest-order perturbation theory in the strength of the potential for both the case of a potential which is commensurate and the case in which it is incommensurate with the crystal surface. It was also studied for the case in which the sliding motion occurs by the motion of edge dislocations in the crystal with a slip plane coinciding with the interface between the crystal and the potential. The approximation used in this calculation corresponds to the high speed limit of Al'shitz, Indenbom, and Shtol'berg[2] in which the dislocation has enough kinetic energy to climb over the Peierls barrier. The calculations of Ref. 1 were all done at zero temperature. It is generally accepted, however, that the interaction of a dislocation with thermally excited phonons is an important mechanism for the damping of dislocation motion,[3] and hence, it is important to consider thermal effects, at least for the dislocation model of friction considered in Ref. 1. Therefore, the models of Ref. 1 will be studied at nonzero temperature in the present article. The treatment is in the spirit of the treatment of dislocation damping at nonzero temperature of Flytzanis and Celli.[4]

II. PERTURBATION-THEORETIC TREATMENT OF FRICTION AT $T \neq 0$

In order to extend the perturbation-theory treatment of kinetic friction of Ref. 1 to nonzero temperature, it is only necessary to add to the displacement of the atoms from equilibrium due to the sliding motion a displacement due to the vibrational modes, which are excited at a

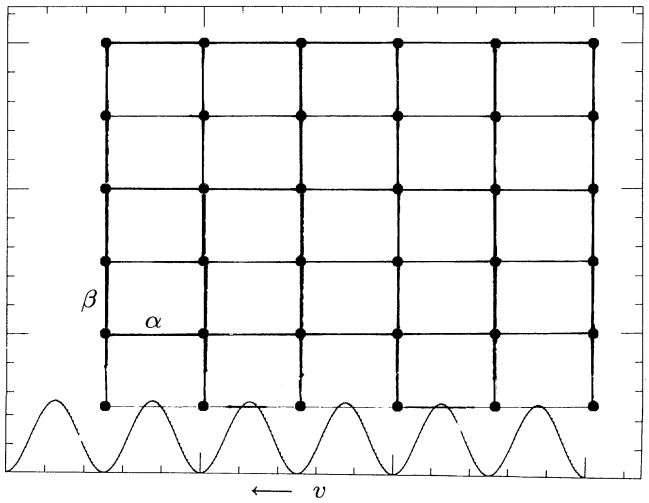

FIG. 1. The model for the sliding friction which was studied in this article is illustrated in this figure. Solid dots are atoms and the lines connecting them represent springs. The vertical and horizontal force constants β and α are labeled. The atoms at the top layer are fixed in place, and the periodic potential at the bottom moves to the left with velocity v, as indicated.

nonzero temperature. Then, the position of an atom, which would be at the point (j_1a, j_2a, j_3c) in the undistorted lattice (where a and c are the lattice constants perpendicular to and parallel to the crystal axis perpendicular to the sliding direction and the j's are integers) is given by

$$x_{j_1j_2j_3} = x^{00}_{j_1j_2j_3} + x^{0}_{j_1j_2j_3} + u_{j_1j_2j_3} ,$$

where $x^{00}_{j_1j_2j_3}$ is the equilibrium position of an atom at the position (j_1a, j_2a, j_3c) in the corresponding perfect lattice [i.e., $x^{00}_{j_1j_2j_3}$ includes the possible displacement of this atom from the above position when the lattice is distorted because of the presence of dislocations; in the absence of distortions, it is equal to (j_1a, j_2a, j_3c)], $x^{0}_{j_1j_2j_3}$ is the atomic displacement due to thermal lattice vibrations, $u_{j_1j_2j_3}$ is the displacement generated by the moving potential, N is the value of j_3 for the surface of the crystal in contact with the potential and $\langle \cdots \rangle$ represents a thermal average. The equations of motion are then

$$\ddot{x}^{0}_{j_1j_2j_3} + \ddot{u}_{j_1j_2j_3} + \gamma(\dot{x}^{0}_{j_1j_2j_3} + \dot{u}_{j_1j_2j_3}) - \Delta(u_{j_1j_2j_3} + x^{0}_{j_1j_2j_3}) = -\delta_{j_3,N}\lambda_0 \sin[(2\pi/a)(x^{00}_{j_1j_2j_3} + x^{0}_{j_1j_2j_3} + u_{j_1j_2j_3} + vt)] , \tag{1a}$$

where

$$\Delta u_{j_1j_2j_3} = \alpha(4u_{j_1j_2j_3} - u_{j_1+1j_2j_3} - u_{j_1-1j_2j_3} - u_{j_1j_2+1j_3} - u_{j_1j_2-1j_3}) + \beta(2u_{j_1j_2j_3} - u_{j_1j_2j_3+1} - u_{j_1j_2j_3-1}) ,$$

α and β are the force constants normal to and along the c axis respectively, and the term $\gamma(\dot{x}^{0}_{j_1j_2j_3} + \dot{u}_{j_1j_2j_3})$ is a phenomenological damping term which is added for convenience, as was done in Ref. 1. (The limit as γ approaches zero will be taken in the end.) The right-hand side of Eq. (1a) is the force due to the potential which acts on the lowest layer of atoms (see Fig. 1). Since $x^{0}_{j_1j_2j_3}$ represents the atomic displacement due to thermal motion alone (i.e., in the absence of sliding motion), it satisfies the following equation of motion:

$$\ddot{x}^{0}_{j_1j_2j_3} + \gamma\dot{x}^{0}_{j_1j_2j_3} - \Delta x^{0}_{j_1j_2j_3} = -\delta_{j_3,N}\lambda_0 \sin(2\pi/a)(x^{00}_{j_1j_2j_3} + x^{0}_{j_1j_2j_3}) . \tag{1b}$$

At temperatures low compared to the melting temperature, it is reasonable to assume that it is a good approximation to solve Eq. (1b) in the harmonic approximation, and it will be assumed that this has been done in the discussion to follow. Subtracting Eq. (1b) from (1a), we find that $u_{j_1j_2j_3}$ satisfies

$$\ddot{u}_{j_1j_2j_3} + \gamma\dot{u}_{j_1j_2j_3} - \Delta u_{j_1j_2j_3} = -\delta_{j_3,N}\lambda_0\{\sin[(2\pi/a)(x^{00}_{j_1j_2j_3} + x^{0}_{j_1j_2j_3} + u_{j_1j_2j_3} + vt)]\} - \sin[(2\pi/a)(x^{00}_{j_1j_2j_3} + x^{0}_{j_1j_2j_3})] . \tag{1c}$$

Equation (1c) can be formally solved to yield

$$u(t)_{j_1j_2j_3} = -\lambda_0 \sum_{j'_1j'_2} \int dt' G_{j_1j_2j_3,j'_1j'_2N}(t-t') \times (\sin[(2\pi/a)(x^{00}_{j'_1j'_2N} + x^{0}_{j_1j_2N}(t') + u_{j_1j_2N}(t') + vt')] - \sin\{(2\pi/a)[x^{00}_{j_1j_2N} + x^{0}_{j_1j_2N}(t')]\}) . \tag{2}$$

Here, $G_{j_1j_2j_3,j'_1j'_2j'_3}(t-t')$ is the Green's function for the homogeneous equation obtained by setting the left-hand side of Eq. (1c) equal to zero. It is identical to the Green's function used in Ref. 1 and an expression for it is given there. Then, following Ref. 1, the force of kinetic friction is calculated by setting the average rate of doing work by this force equal to the work done on the crystal by the periodic potential. The top atomic layer is held fixed and the sinusoidal potential, which is in contact with the bottom layer, is slid along at a constant speed v. Then, the time-averaged force of friction F_{av} is given by

$$F_{\mathrm{av}}v = t_1^{-1} \int_{-t_1/2}^{t_1/2} dt \sum_{j_1j_2} \langle (\dot{x}^{0}_{j_1j_2N} + \dot{u}^{0}_{j_1j_2N})\lambda_0 \sin[(2\pi/a)(x^{00}_{j_1j_2N} + x^{0}_{j_1j_2N} + u_{j_1j_2N} + vt)] \rangle , \tag{3}$$

where t_1 is a suitable time interval over which we average the rate of doing work. For the commensurate case where the motion is periodic, it is the "washboard frequency." For other cases, for which the motion is not periodic, it is a long time. Lowest-order perturbation theory (i.e., expansion up to second order in λ_0) can be generated by expanding Eq. (3) up to first order and (2) to zeroth order in u and $\dot{u}$ and substituting for u and $\dot{u}$ in Eq. (3) using Eq. (2). The zeroth-order term (in u) in the integrand of Eq. (3) can be written as

$$-\partial/\partial t \langle (a\lambda_0/2\pi)\cos[(2\pi/a)(x^{00}_{j_1j_2N} + x^{0}_{j_1j_2N}(t) + vt)] \rangle - v\lambda_0 \langle \sin[(2\pi/a)(x^{00}_{j_1j_2N} + x^{0}_{j_1j_2N}(t) + vt)] \rangle . \tag{4}$$

Since we are assuming that Eq. (1b) was solved in the harmonic approximation, $x^{0}_{j_1j_2j_3}(t)$, which represents the thermal motion in the absence of sliding, can be written as an expansion in the normal modes of the crystal. Then, it is well known that[5] $\langle e^{\pm i(2\pi/a)x^{0}_{j_1j_2j_3}(t)} \rangle = e^{-W}$, independent of time, where W is the Debye-Waller factor. Using this relationship, Eq. (4) becomes

$$e^{-W}\{(a\lambda_0/2\pi)\partial/\partial t \cos[(2\pi/a)(x^{00}_{j_1j_2j_3} + vt) - \lambda_0 v \sin(2\pi/a)(x^{00}_{j_1j_2j_3} + vt)\} = 0 \tag{5}$$

as expected. In the next two sections, the terms of first order in u will be studied.

III. COMMENSURATE AND INCOMMENSURATE INTERFACES WITHOUT DEFECTS

Expanding the right-hand side of Eq. (3) to first order in u or $\dot{u}$, we obtain

$$t_1^{-1}\int_{-t_1}^{t_1} dt \sum_{j_1 j_2} \lambda_0 \langle \dot{u}(t)_{j_1 j_2 N} \sin Y + \dot{x}^0(t)_{j_1 j_2 N}(2\pi/a) u(t')_{j_1 j_2 N} \cos Y \rangle \ , \tag{6}$$

where $Y=(2\pi/a)[(x^{00}_{j_1 j_2 j_3}+x(t)^0_{j_1 j_2 j_3}+vt]$ and it is understood that we will substitute for u using Eq. (2) with u neglected in the argument of the right-hand side of Eq. (2). For temperatures small compared to the melting temperature of the crystal, since it is expected that the magnitude of x^0 will be small compared to a, we may expand Eq. (6) to second order in x^0. We obtain for this second order in x^0 term

$$t_1^{-1}\int_{-t_1}^{t_1} dt\, dt' (\lambda_0^2/m)(2\pi/a)^2 \sum_{j_1 j_2 j_1' j_2'} \langle \dot{x}^0_{j_1 j_2 N} \cos Z G_{j_1 j_2 j_3, j_1' j_2' N}(t-t') x^0_{j_1' j_2' N} + x^0_{j_1 j_2 N} \dot{G}_{j_1 j_2 j_3, j_1' j_2' N}(t-t') x^0_{j_1' j_2' N} \rangle [\cos Z' - \cos X'] \ , \tag{7}$$

where $X=(2\pi/a)(x^{00}_{j_1 j_2 j_3})$, $Z=(2\pi/a)(x^{00}_{j_1 j_2 j_3}+vt)$, and X' and Z' are the same quantities but with primes on the j's. Expressing the x^0's as an expansion in the normal mode coordinates (e.g., as in Ref. 4), we obtain

$$0.5(\lambda_0^2/m)(2\pi/a)^2 (LMN^2)^{-1} \sum_{\mathbf{k}'} \sum_{k_z} \frac{\gamma \omega'^2}{(\omega'^2-\omega^2)^2+\gamma^2\omega'^2} [\hbar/m\omega_0(\mathbf{k}')](e^{\hbar\omega_0(\mathbf{k}')/k_B T}-1)^{-1} \ ,$$

where $\omega=\omega_0(2\pi/a, k_z)$ and $\omega'=\omega_0(\mathbf{k}')+(2\pi/a+k_x')v$. Converting the sums over wave vector to integrals in the standard manner and taking the limit as γ approaches zero, this expression becomes

$$0.5(\lambda_0^2/m)(2\pi/a)^2 (ac/4\pi^2)^2 \int d^3k' dk_z \omega' \delta(\omega'^2-\omega^2)[\hbar/m\omega_0(\mathbf{k}')](e^{\hbar\omega_0(\mathbf{k}')/k_B T}-1)^{-1} \ , \tag{8}$$

which when divided by v gives the second order in x^0 contribution to F_{av}. In the case of a commensurate interface, $2\pi/a$ is also a reciprocal-lattice vector for the crystal, and hence, ω defined above Eq. (8) runs over a range of frequencies whose lower limit is zero as the integral over k_z is performed. Thus, no matter how small v is, the δ function will still be satisfied and hence there will always be a second order in the x^0 contribution to the force of friction. The main way in which this result differs from the zeroth-order term in x^0 is that the vibrational frequency $\omega_0(\mathbf{k}')$ is added to the washboard frequency $v(2\pi/a)$ and the vibrational wave vector $\mathbf{k}'$ is added to $2\pi/a$ in this expression. For low temperatures (compared to the melting temperature), $\mathbf{k}'$ will be small compared to $2\pi/a$. Although $\omega_0(\mathbf{k}')$ can be larger than the washboard frequency, if the temperature is small compared to the Debye temperature, $\omega_0(\mathbf{k}')$ will be small compared to the maximum acoustic mode vibrational frequency and since the washboard frequency is also small compared to the maximum frequency and $[\langle (x^0)^2 \rangle]^{0.5}$ is small compared to all lengths in the system, a large change in the force of friction found in Ref. 1 is not expected. For the incommensurate case, $\omega_0(k_x=2\pi/1, k_y=0, k_z)$ will remain nonzero for all values of k_z. If the interface is far from being nearly commensurate, $\omega_0(k_x=2\pi/a, k_y=0, k_z=0)$ will always be larger than the sum of the washboard frequency and $\omega_0(\mathbf{k}')$ (i.e., ω'), and therefore, the δ function in Eq. (8) will not be satisfied. This means that there will be no friction when the damping constant is set equal to zero, and for the nonzero damping constant, the force of friction will still be very small, as was found at zero temperature in Ref. 1. Thus, we conclude that the force of friction is not affected significantly by temperature. For the nearly commensurate case, however, it is possible for $\omega_0(k_x=2\pi/a, k_y=0, k_z=0)$ to be sufficiently small compared to typical values of $\omega_0(\mathbf{k}')$, which implies that the force of friction will increase as the temperature increases. Since the nearly commensurate case is not expected to be important for most applications, it will not be studied in detail now. One qualitative result that we expect to be true, however, is that the force of friction should increase as the interface passes through a commensurate-incommensurate transition.

IV. THE COMMENSURATE CASE WITH SLIDING DUE TO DISLOCATIONS

The sliding motion of a commensurate interface resulting from dislocation motion is expected to be the usual way for commensurate interfaces to slide, as discussed in Ref. 1. The presence of thermally excited lattice vibrations has long been believed to be an important source of damping of dislocation motion. Therefore, we expect temperature effects to be important for this case. In order to treat moving dislocations at the interface, we use the treatment given in Ref. 1 for the "slow speed case," in that we replace the force due to the sinusoidal potential by a potential due to the presence of a dislocation of the form $g(j_1 a - x^{\alpha}_{dj_2} + v_d t)$, where u_d is the dislocation velocity and $x^{\alpha}_{dj_2}$ is the location of the dislocation core at the y coordinate $j_2 a$ for the αth dislocation [$g(x)$ is a function whose magnitude falls off with increasing values of $|x|$]. If the dislocations are on the average far apart, the total contribution to the force due to the dislocations can be written as a sum of such terms. When thermal vibrations are included, this becomes

$$\sum_{\alpha} g(j_1 a - x^{\alpha}_{dj_2} - x^0_{j_1 j_2 N} + v_d t) \ , \tag{9}$$

where the notation follows that of Ref. 1 except that the vibrational displacement $x^0_{j_1 j_2 N}$ has been included in the argument. It represents the vibrational displacement of the atoms near the center of a dislocation. This method of treatment is similar to that used by Flytzanis and Celli[4] in their treatment of dislocation damping. Substituting Eq. (9) for the sinusoidal potential in Eqs. (2) and (3), using Eq. (2) to substitute for $\dot{u}$ in Eq. (3), and replacing the function g by its Fourier transform, we obtain

$$F_{\rm av}v = t_1^{-1}\int_{-t_1/2}^{t_1/2}dt\int_{-\infty}^{\infty}dt'(\lambda_0^2/m)\sum_{\alpha\alpha'}\sum_{j_1j_2j_1'j_2'}\sum_{k_xk_x'} g(k_x)g(k_x')^* \times\langle e^{ik_x[j_1a-x^{\alpha}_{dj_2}-x^0_{j_1j_2N}(t)+v_dt]}e^{-ik_x'[j_1'a-x^{\alpha'}_{dj_2'}-x^0_{j_1'j_2'N}(t')+v_dt']}\rangle \times\dot{G}_{j_1j_2N,j_1'j_2'N}(t-t') ,$$

where the average sliding velocity v is given in terms of the dislocation velocity v_d by $v=v_dN_d/L$, where L is the length of the crystal along the direction of sliding in units of the lattice constant and N_d is the number of edge dislocations at the interface. Following Ref. 1, we first average over dislocation configurations (i.e., over the $x^{\alpha}_{dj_2}$'s) to give to a good approximation

$$F_{\rm av}v = t_1^{-1}N_d\int_{-t_1/2}^{t_1/2}dt\int_{-\infty}^{\infty}dt'(\lambda_0^2/m)\sum_{j_1j_2j_1'}\sum_{k_xk_x'} g(k_x)g(k_x')^*\langle e^{ik_x[j_1a-x^0_{j_1j_2N}(t)+v_dt]}e^{-ik_x'[j_1'a-x^0_{j_1'j_2N}(t')+v_dt']}\rangle \times\dot{G}_{j_1j_2N,j_1'j_2N}(t-t') . \tag{10}$$

Again following Ref. 1, we have assumed that this average is small unless $\alpha=\alpha'$ and $j_2=j_2'$ to obtain Eq. (10). Since at temperatures low compared to the melting temperature it is reasonable to assume that x^0 is small compared to all other lengths in the problem, we will now expand each exponential to lowest order in x^0. The thermal average of $x^0_{j_1j_2N}(t)$ is zero and $\langle x^0_{j_1j_2N}(t)x^0_{j_1'j_2'N}(t')\rangle$ is given by

$$\langle x^0_{j_1j_2N}(t)x^0_{j_1'j_2'N}(t')\rangle = (LMN)^{-1}\sum_{\mathbf{k}}[\hbar/m\omega_0(\mathbf{k})](e^{\hbar\omega_0(\mathbf{k})/k_BT}-1)^{-1}e^{i\mathbf{k}\cdot\mathbf{R}}\cos[\omega_0(\mathbf{k})(t-t')] , \tag{11}$$

where $\mathbf{R}=[j_1-j_2')a,(j_2-j_2')a,0]$. The zeroth-order term in the expansion of Eq. (10) in powers of x^0 gives the result of the second of Refs. 1, which is that $F_{\rm av}v$ is proportional to $v_d^2(2\pi/a)^2$. The second-order term is approximately equal to this same result except that $v_d^2(2\pi/a)^2$ in the expression for $F_{\rm av}v_d$ is replaced by the following expression having the same units:

$$(LMN)^{-1}\sum_{\mathbf{k}'}[\hbar(2\pi/a)^2/(m\omega_0(\mathbf{k}')]\{[\omega_0(\mathbf{k}')+v_d(2\pi/a)]^2 +[\omega_0(\mathbf{k}')-v_d(2\pi/a)]^2\theta[\omega_0(\mathbf{k}')-v_d(2\pi/a)]\}(e^{\hbar\omega_0(\mathbf{k}')/k_BT}-1)^{-1} , \tag{12}$$

where $\theta(x)=0$ if $x<0$ and 1 if $x>0$. Replacing the sum over k' by an integral and doing the integral in the Debye model, Eq. (12) becomes, in the limit as v_d approaches zero,

$$[(k_BT)^3\Omega]/(\hbar v_p)^3(k_BT/\hbar)(\hbar/m)(2/a)^2\int_0^{x_D}x^3dx[(e^x-1)^{-1}+0.5] , \tag{13}$$

for v_d in the high dislocation speed limit of Ref. 2, where Ω is the unit-cell volume, v_p is the phonon velocity (for simplicity we neglect the anisotropy of v_p), and $x_D=\Theta_D/T$, where Θ_D is the Debye temperature. For $T\ll\Theta_D$ this expression is of the order of $(10^{25}\ \text{rad}^2/\text{sec}^2)(T/\Theta_D)^2$ for the values of the parameters used in Ref. 1, as compared to a value of $10^{24}\ \text{rad}^2/\text{sec}^2$ for $v_d^2(2\pi/a)^2$. Thus, we conclude that, whereas for $T\ll\Theta_D$ the zero-temperature result for $F_{\rm av}$ is valid, when T becomes comparable to Θ_D, the second-order terms in x^0 calculated above, which represent the contribution to the damping force due to thermal phonons, will dominate. Furthermore, in the case of T comparable to θ_D, $F_{\rm av}v$ will no longer be proportional to v, as it is at $T=0$, which implies a force of friction inversely proportional to v at nonzero temperature.

V. CONCLUSIONS

For the case of a commensurate interface and most incommensurate interfaces without defects, thermal effects on the force of friction were found to be small. For the nearly commensurate case, however, it was argued that the friction should increase with an increase in temperature. For the case of a commensurate interface with sliding taking place by the motion of dislocations, it was found that at T small compared to the Debye temperature, thermal effects will be small, but as T becomes comparable to the Debye temperature, thermal effects dominate the force of friction.

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[1] J. B. Sokoloff, Phys. Rev. B **42**, 760 (1990); **42**, 6745 (1990).
[2] V. I. Al'shitz, V. L. Indenbom, and A. A. Shtol'berg, Zh. Eksp. Teor. Fiz. **60**, 2308 (1971) [Sov. Phys. JETP **33**, 1240 (1971)].
[3] V. I. Al'shitz and V. L. Indenbom, in *Dislocations in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1986), Vol. 7, p. 34.
[4] N. Flytzanis and V. Celli, J. Appl. Phys. **43**, 3301 (1972).
[5] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), p. 449.