

have

$$\begin{aligned} \delta\eta_{iklm}(\omega, k) = & \frac{T}{6\pi} \left( \frac{\rho}{2\gamma} \right)^{\frac{1}{2}} (i-1) \omega^{\frac{1}{2}} \left\{ \frac{k_i k_h k_l k_m}{k^4} (3F_1 - 15F_2 + 35F_3) \right. \\ & + \frac{1}{k^2} (\delta_{ih} k_i k_m + \delta_{im} k_h k_l) [-F_1 + 3F_2 - 5F_3 + (\varphi - \psi) (-4F_1 + 6F_2)] \\ & + \frac{1}{k^2} (\delta_{ii} k_h k_m + \delta_{im} k_h k_l + \delta_{il} k_i k_m + \delta_{hm} k_i k_l) (-F_1 + 3F_2 - 5F_3) \\ & \quad + (\delta_{ii} \delta_{hm} + \delta_{im} \delta_{il}) \left[ F_1 - F_2 + F_3 + \frac{7}{40} \left( \frac{2\gamma}{\eta} \right)^{\frac{1}{2}} \right] \\ & + \delta_{ih} \delta_{im} \left[ F_1 - F_2 + F_3 + 4(\varphi - \psi) (2F_1 - F_2) + 8(\varphi - \psi)^2 F_1 \right. \\ & \quad \left. \left. + \frac{3}{2} \theta^2 \left( \frac{\gamma c_p}{2\kappa} \right)^{\frac{1}{2}} + 3 \left( \frac{\gamma}{2\eta} \right)^{\frac{1}{2}} \left[ \left( \psi - \frac{2}{3} \right)^2 - \frac{14}{45} \right] \right] \right\}. \end{aligned} \quad (p)$$

The phase velocity of the sound  $c(\omega)$  and its absorption  $\Gamma(\omega)$  are given by the formulae

$$\begin{aligned} c(\omega) = & c \left\{ 1 + \frac{T}{12\pi\rho c^2} \left( \frac{\rho\omega}{\gamma} \right)^{\frac{1}{2}} \Phi \right\}, \\ \Gamma(\omega) = & \frac{\gamma\omega^2}{2\rho c^2} \left\{ 1 - \frac{\rho T}{6\pi\gamma^2} \left( \frac{\rho\omega}{\gamma} \right)^{\frac{1}{2}} \Phi \right\}, \end{aligned} \quad (q)$$

where

$$\begin{aligned} \Phi = & \frac{1024}{14553} + \frac{48}{175} \left( \psi - \frac{2}{9} \right)^2 + \left( \psi - \frac{6}{5} \right) \left( \psi + \frac{11}{35} \right)^2 \\ & + \frac{3}{2} \theta^2 \left( \frac{\gamma c_p}{4\kappa} \right)^{\frac{1}{2}} + 3 \left( \frac{\gamma}{4\eta} \right)^{\frac{1}{2}} \left[ \left( \psi - \frac{2}{3} \right)^2 + \frac{28}{45} \right]. \end{aligned} \quad (r)$$

As  $\Phi$  is positive it follows from this that in any liquid

one should find at sufficiently low frequencies a positive sound dispersion.

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## Interaction of moving dislocation with a soft phonon mode in a displacement-type phase transition

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We consider the anomalies of dynamic slowing down of dislocations as a result of their interaction with the soft phonon mode in a displacement-type phase transition. It is shown that when the phase transition temperature  $T_c$  is approached and the corresponding critical frequency  $\omega_c$  decreases, the dislocation dragging coefficient  $B_c$  increases in proportion to  $\ln(\omega_s/\omega_c)$ , where  $\omega_s$  is of the order of the Debye frequency. The possibilities of observing in experiment the predicted anomalies in the temperature dependence of the viscous component of dislocation friction is discussed.

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It is known<sup>1,2</sup> that in phase transitions of the displacement type there appear in many crystals the so-called phonon modes, which are characterized by a dip in the dispersion law  $\omega_k = \omega(k)$  in the vicinity of a certain wave vector<sup>1)</sup>  $k = k_0$ . It is important that as the phase-transition temperature  $T_c$  is approached the depth of this dip increases, and the corresponding frequency  $\omega_c(T) = \omega(k_0)$  tends to zero as  $T \rightarrow T_c$ . The width of the energy level of the soft mode ( $T$ )—the reciprocal phonon relaxation time—increases and near  $T_c$  it can even exceed the frequency  $\omega_c$ .<sup>2</sup> Recognizing that the lattice-anharmonicity-induced scattering of a phonon by a dislocation from a state with wave vector  $k$  and frequency  $\omega_k$  into a state  $\{k', \omega_{k'}\}$  is characterized by a matrix element

$\Gamma_{kk'} \propto (\omega_k \omega_{k'})^{-1/2}$ , and also the fact that near the transition the density of the critical phonons increases in proportion to  $\omega_c^{-1}$ , it is natural to expect the intensity of the phonon-dislocation interaction to increase in the vicinity of the point  $k = k_0$  of reciprocal space near the transition temperature  $T_c$ . This can manifest itself in integral fashion in the appearance of singularities of the phonon slowing down of the dislocations at  $T \approx T_c$ . We attempt below to investigate the character of these singularities within the framework of a simple model.

Ultrasound damping anomalies of similar origin were investigated earlier in a number of studies (see, e.g., the review by Garland<sup>3</sup>). Unfortunately, these results

cannot be used directly in our analysis inasmuch as shown earlier,<sup>4</sup> ultrasound absorption and dislocation dragging are limited by phonon processes of different kinds.

We consider a straight-line dislocation with a Burgers vector  $\mathbf{b}$  that moves uniformly with velocity  $v$  in a crystal of unit volume. We assume  $v$  to be small compared with the speed of sound  $c$ , but large enough for the kinetic energy of the dislocation to exceed significantly the height of the energy barriers in the crystal; these barriers can be connected with the periodic Peierls potential relief in the discrete lattice, or with other defects.

The interaction of optical oscillations in a crystal with "acoustic" deformations is of striction origin and is described by the Hamiltonian<sup>2</sup>

$$H_{int} = \rho_e^2 \int d^3r \eta_{ijmn} x_i(r) x_j(r) u_{mn}(r). \quad (1)$$

Here  $\rho_e$  is the effective charge density of the critical branch,  $\eta_{ijmn}$  is the electrostriction tensor,  $x(r)$  is the optical-displacement operator, and  $u_{mn}$  is the deformation tensor of the external distortion field. As applied to a moving dislocation<sup>5</sup>

$$u_{mn}(r) = \sum_q \frac{b}{q} \varphi_{mn} \left( \frac{\mathbf{q}}{q} \right) e^{iq(r-vt)}, \quad (2)$$

where  $\varphi_{mn}(q/q)$  is an orientation vector that differs from zero only in a plane perpendicular to the dislocation.

After substituting (2) in (1), together with the usual Fourier expansion of the operator  $\mathbf{x}(r)$  (Ref. 2), the Hamiltonian of the interaction of the soft phonon mode with the moving dislocation can be represented in the form<sup>2</sup>

$$H_{int}(t) = \sum_{\mathbf{k}, \mathbf{k}'} \Gamma_{\mathbf{k}\mathbf{k}'} \xi_{\mathbf{k}} \xi_{\mathbf{k}'}^* \exp(-i\Omega_{\mathbf{k}} t), \quad (3)$$

where  $\xi_{\mathbf{k}} = a_{\mathbf{k}} + a_{-\mathbf{k}}^*$ ;  $a_{\mathbf{k}}$  and  $a_{-\mathbf{k}}$  are the operators of creation and annihilation of a phonon with wave vector  $\mathbf{k}$ ;  $\Omega_{\mathbf{k}} = \mathbf{q} \cdot \mathbf{v}$ ,  $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ ;

$$\Gamma_{\mathbf{k}\mathbf{k}'} = \frac{b\omega_0^2}{8\pi} \frac{\delta_{q_z, 0}}{q} \frac{\Phi(\mathbf{k}/k, \mathbf{k}'/k')}{(\omega_{\mathbf{k}} \omega_{\mathbf{k}'})^{1/2}}, \quad (4)$$

$$\Phi(\mathbf{k}/k, \mathbf{k}'/k') = \eta_{ijmn} l_{\mathbf{k}} l_{\mathbf{k}'} \varphi_{mn}(q/q),$$

$l_{\mathbf{k}}$  is the phonon polarization vector,  $\omega_0$  is the "plasma frequency" of the critical branch,<sup>2</sup>  $\delta_{q_z, 0}$  is the Kronecker symbol, and the  $z$  axis is directed along the dislocation.

The energy dissipation per unit time in a phonon subsystem subjected to the perturbation (3) is described according to Refs. 4 and 5 by an expression of the type

$$D = 4\pi \sum_{\mathbf{k}, \mathbf{k}'} \Omega_{\mathbf{k}}^2 |\Gamma_{\mathbf{k}\mathbf{k}'}|^2 n(\omega_{\mathbf{k}}) \frac{\partial}{\partial \omega_{\mathbf{k}}} \Delta(\omega_{\mathbf{k}} - \omega_{\mathbf{k}'}); \quad (5)$$

here

$$n(\omega_{\mathbf{k}}) = [\exp(\omega_{\mathbf{k}}/T) - 1]^{-1}$$

is the Bose-Einstein distribution function, and

$$\Delta(\omega) = \gamma/\pi(\omega^2 + \gamma^2)$$

is a relaxation factor that goes over into the Dirac delta function  $\delta(\omega)$  as  $\gamma \rightarrow 0$ .

Simulating the soft mode, we assume that the anomaly of  $\omega(\mathbf{k})$  lies in the Brillouin zone in a spherical cavity  $K$  with center at the point  $\mathbf{k}_0$  and with radius  $k_s$ . We assume also that the dispersion law is spherically symmetrical with respect to the center of the cavity and takes the following form<sup>2</sup> at  $\mathbf{k} \in K$

$$\omega^2(\mathbf{k}) = \omega_c^2(T) + \beta(\mathbf{k} - \mathbf{k}_0)^2. \quad (6)$$

The quantity  $\omega_s^2 = \omega_c^2 + \beta k_s^2$  is assumed large enough, so that  $\omega_s \gg \gamma$ .

We confine ourselves next to calculation of only the "critical increment" to the dissipation (5); this increment is due to the phonon transitions within the band  $K$  and makes an increasing contribution to the dislocation slowing down as  $T \rightarrow T_c$ . We neglect the spatial dispersion of the damping  $\gamma$  in region  $K$ .

Changing in (5) in the usual manner from summation to integration over the region  $K$ , we take outside the integral sign a certain mean value of the square of the function of the directions:  $\eta^2 = \langle |\Phi(\mathbf{k}/k, \mathbf{k}'/k')|^2 \rangle$  (the order of magnitude of  $\eta$  is determined by the characteristic values of the components of the tensor  $\eta_{ijmn}$ ). As a result we obtain, after a number of straightforward but cumbersome transformations, which we omit, the following expression for the critical increment  $B_c = D/v^2$  to the dislocation slowing down coefficient:

$$B_c = 2A \int_{\omega_c}^{\omega_s} d\omega n(\omega) \int_{\omega_c}^{\omega_s} \frac{d\omega' \omega'}{(\omega'^2 - \omega_c^2)^{1/2}} \Delta(\omega' - \omega), \quad (7)$$

and

$$A = \left( \frac{\omega_0}{4\pi} \right)^4 \frac{(\eta b)^2}{\beta^{1/2}}. \quad (8)$$

As the temperature  $T$  approaches  $T_c$ , the value of  $\omega_c$  decreases gradually. We consider, for example, a temperature interval in which

$$\gamma \ll \omega_c \ll \Omega. \quad (9)$$

In this case  $\Delta(\omega' - \omega) \approx \delta(\omega' - \omega)$  and expression (7) takes the form

$$B_c = AT \int_0^{\omega_s/T} dt [\exp\{(t^2 + (\omega_c/T)^2)^{1/2}\} - 1]^{-1}. \quad (10)$$

Formula (10) defines a function that diverges logarithmically as  $\omega_c \rightarrow 0$ . For example, at  $\omega_c \ll \Omega = \min\{\omega_s, T\}$  we have in place of (10)

$$B_c \approx AT \ln(\Omega/\omega_c). \quad (11)$$

However, a relation of the type (10), (11) remains qualitatively valid only so long as  $\omega_c \gtrsim \gamma$ . With further decreasing of  $\omega_c$ , the large logarithm  $\ln(\Omega/\omega_c)$  in (11) is replaced in natural fashion by  $\ln(\Omega/\gamma)$ . In fact, in the limiting case  $\omega_c \ll \gamma$  Eq. (7) yields

$$B_c \approx \frac{2A}{\pi} \int_{\omega_c}^{\omega_s} d\omega n(\omega) \arctg \frac{\omega}{\gamma} \approx AT \ln \frac{\Omega}{\gamma}. \quad (12)$$

Thus, the discussed anomalies of the dynamic slowing down of dislocations are not of abrupt character. It is of interest to estimate their scale against the general background of normal phonon slowing down. At the lowest temperatures,  $T \ll \omega_c(T)$  the quantity  $B_c(10)$  is exponentially small and the considered mechanism can-

not compete with the flutter effect,<sup>2</sup> which "freezes out" more slowly than the other phonon mechanism when the temperature is decreased ( $B_{f1} \propto T^3$ ). A more gainful situation from the point of view of observability of the temperature anomalies of  $B_c$  in the vicinity of the phase transition is realized at  $\omega_c(T) \ll T_c \ll \omega_s$ , when the density of the normal phonons is still small while the density of the critical phonons is already large. A comparison of the quantities  $B_c(11)$  and  $B_{f1}$  (Ref. 4) in the indicated temperature region leads to the estimate

$$B_c/B_{f1} \sim (T_c/T)^2 \ln(T/\omega_c); \quad (13)$$

$$T_c \sim 10^{-2} \frac{\eta b \omega_0^2}{(\beta^{1/2}/c^3)^{1/2}} \sim 10^{-1} \eta \frac{\omega_0}{\omega_D} \frac{b \omega_0}{2\pi c} \Theta, \quad (14)$$

$\omega_D$  and  $\Theta$  are the Debye frequency and temperature. Recognizing that usually  $\eta \sim 1$ ,  $\beta^{1/2} \sim c$  and  $\omega_0 \sim \omega_D \sim 2\pi c/b$ , the temperature  $T_c$  should be of the order of  $\Theta/10$ . Thus, in low-temperature ferroelectrics (including virtual ones), for which  $\omega_c < T_c \leq T_0$ , the temperature burst of  $B_c(T)$  in the vicinity of the transition should be perfectly observable.

In the high-temperature region,  $T \geq \omega_s$ , the principal role in the dynamic slowing down of the dislocations is usually played by phonon scattering of anharmonic type (phonon wind).<sup>4,5</sup> In this case both the acoustic and the optical branches make a contribution linear in temperature to the slowing down, and the ratio of the corresponding slowing-down coefficients turns out to be of the order of

$$B_{op}/B_{ac} \sim (\eta \mu/M)^2 (\omega_0/\omega_{op})^4, \quad (15)$$

where  $\mu$  is the shear modulus,  $M$  is the characteristic value of the elastic moduli of third order, and  $\omega_{op}$  is the average frequency of the lowest optical mode at the boundary of the Brillouin zone. Usually  $\eta \sim 1$ ,  $\omega_0 \sim \omega_{op}$ ,  $M \sim 10\mu$  and accordingly  $B_{op} \ll B_{ac}$ . Therefore to assess the relative role of the dissipation mechanism discussed above in the vicinity of the temperature  $T_c \geq \omega_s$ , it is necessary as a rule to compare  $B_c(11)$  with  $B_{ac}$  (Refs. 4, 5); this yields

$$B_c/B_{ac} \sim (\eta \mu/M)^2 (\omega_0/\omega_D)^4 (c/\beta^{1/2})^5 \ln(\omega_s/\omega_c). \quad (16)$$

This ratio, just as  $B_{op}/B_{ac}$ , is apparently usually small, although, taking into account the strong dependence of expressions (15) and (16) on the ratios  $\omega_0/\omega_{op}$ ,  $\omega_0/\omega_D$ ,  $c/\beta^{1/2}$  and some uncertainty in the values of the parameters  $\eta$ ,  $M$ , and  $\omega_{op}$ , one cannot exclude the possible

existence of crystals for which  $B_{ac} \leq B_c$  or  $B_{ac} \leq B_{op}$ . In the latter case the criterion for the observability of the anomalies of  $B_c$  is that the ratio

$$B_c/B_{op} \sim (\omega_{op}/k_B \beta^{1/2})^5 \ln(\omega_s/\omega_c) \quad (17)$$

not be small.

In any case, when choosing objects for an experimental investigation of the discussed effects, preference should be given to crystals characterized by a high level of plasma frequency  $\omega_0$  and electrostriction, and also by a low level of the parameter  $\beta$ , of the damping  $\gamma$ , and of the anharmonicity.

Thus, when the crystal is suitably chosen, the appearance of noticeable temperature anomalies and the dynamic slowing down of dislocations near a displacement type phase transition is perfectly realistic. One can hope to observe them in the dislocation component of high-frequency amplitude-dependent internal friction. They can be investigated also by directly measuring the mobilities of individual dislocations.

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<sup>1)</sup> Most frequently (for a ferroelectric transition of the displacement type)  $k_0 = 0$ . At the same time there are known phase transitions (for example, in anti-ferroelectrics) corresponding to  $k_0 \neq 0$ .

<sup>2)</sup> We shall be interested henceforth only in transitions within the limit of one soft mode, and omit therefore all the phonon polarization indices. The frequency, temperature, and energy will be assumed to have the same dimensionality, i.e., the Planck and Boltzmann constant will be assumed equal to unity.

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