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The phonon wind as a nonlinear mechanism of dislocation dragging(*)

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THE THEORY of dynamic friction due to the scattering of phonons by the dislocation moving in an anisotropic medium with an arbitrary anharmonicity is presented. The drag of straight dislocations (both edge and scrue) and circular loops is considered. General expressions for the magnitude and the temperature dependence of the dislocation drag coefficient B are derived in integral form. The following calculations explicitly taking into account the anharmonicity are performed for Murnaghan's model. The influence of finite dimensions of the dislocation core on the temperature dependence of drag coefficient B is analysed in a simple scheme.

W pracy przedstawiono teorię hamowania ruchu dyslokacji w ośrodku ciągłym o dowolnej anizotropii pod wpływem wiatru fononów. Zagadnienie przedyskutowano szczegółowo dla dyslokacji prostoliniowej i dla okrągłej pętli dyslokacji. Znaleziono wielkość i zależność od temperatury współczynnika hamowania ruchu dyslokacji (w postaci całkowej) korzystając z metody funkcji Greena. Obliczenia w postaci jawnej zostały przeprowadzone w przybliżeniu Murnaghana. Przeanalizowano poprawki, jakie wnosi do otrzymanych wyników uwzględnienie skończonych rozmiarów jądra dyslokacji.

Развита теория динамического трения в результате рассеяния фононов на дислокации, движущейся в анизотропной среде с произвольным ангармонизмом. Рассмотрено торможение прямолинейных (краевых и винтовых) дислокаций и круговой петли. Получены общие выражения (в квадратурах), описывающие величину и температурную зависимость коэффициента торможения дислокаций $B(T)$. Последующие вычисления с явным учетом ангармонизма выполнены в модели Мурнагана. В упрощенной схеме проанализировано влияние конечных размеров ядра дислокации на температурный ход коэффициента торможения B.

1. Introduction

ONE of the fundamental problems of the contemporary theory of solids is establishing the nature of dissipative processes which determine the kinetics of the plastic deformation of crystals. To solve the problem on the microscopic level it is necessary to study the mechanisms of energy losses caused by moving dislocations.

Stimulated by the requirements of time, the intensive work on dislocation dynamics over the last decade has provided better understanding of many factors which influence dislocation movement. In particular, the role of dynamic dislocation dragging caused by the interaction of moving dislocations with elementary excitations of the crystal (phonons, electrons etc.) has been determined in the general picture of physical processes accompanying plastic deformation.

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Dynamic friction appears, for example, in a clear form in the case of high dynamic loads (of the types of shock loads or deformations by explosions) when fast dislocations, with kinetic energy greater than the potential barriers, interact with the phonon or electron gas with results in viscous dragging.

Of the same nature is viscous damping of vibrating dislocation segments determining the level of amplitude independent internal friction when the ultrasound is traversing a crystal. This phenomenon is the basis of one of the well-known methods of measuring dynamic dislocation dragging.

Finally, the kinetics of the thermofluctuational overcoming of energetic barriers by dislocations depends on the level of viscous dragging experienced by dislocations also in the process of random walk in the potential relief of a crystal. As a consequence, the velocity of thermoactivated movement of a dislocation and the velocity of overbarrier movement of the dislocation appear to be inversely proportional to the mentioned dynamic viscosity.

In most cases the important part in the dynamic dragging of dislocations falls to the dissipative processes in the phonon subsystem. The hierarchy of these processes depending on the temperature and other factors was discussed in detail [1]. One of the most important mechanisms of dragging is the so-called phonon wind(¹), caused by the scattering of phonons on moving dislocations as a result of nonlinear properties (anharmonicity) of the medium. The moving dislocation is "blowed" by the wind of phonons which scatter and impart to the dislocation an entire momentum proportional to its velocity. This was shown for the first time in the paper by LEIBFRIED [2]. The quantum mechanical estimations of the contribution of the phonon wind to the dragging of straight dislocations [3, 4] and dislocation loops [5] were described. The results in papers [3, 4] were obtained in the isotropic approximation and in paper [5] anharmonicity was estimated with the accuracy of the order of magnitude of one phenomenological constant.

The aim of the present paper is to develop a theory of the phonon wind taking into account the full influence of anisotropic harmonicity. In Sect. 2 the quantum mechanical formulation of the problem is given. General expression has been found for the energy dissipation which relates the characteristics of the phonon subsystem with an elastic dislocation field. In Sect. 3 the formulae of Fourier transforms of a distortion field of straight dislocation and dislocation loops for an arbitrary anisotropic medium are derived. In Sect. 4 the magnitude (in the integral form) and the temperature dependence have been determined for the coefficient of the dragging of the straight dislocation. The analogous result for a dislocation loop is found in Sect. 5. In Sect. 6 the above general results have been utilized to determine explicitly the concrete form of the coefficient of dragging taking into account the tensor of elastic constants of the third order in the Murnaghan model. Sect. 7 presents what corrections should be introduced into the previous results to take into consideration the existence of the dislocation core.

(¹) According to [1] at very low temperatures more important can be flutter effect, connected with re-radiation of phonons by the dislocation vibrating in the field of thermal vibrations. At high temperatures the relaxational processes (e.g. relaxation of "slow" phonons) have to be taken into account together with the phonon wind.

2. Formulation of the problem

As it was shown in [1] there exists such a range of not very low temperatures in which the phonon wind plays a more important part than the flutter effect and the relaxation processes and the phonon-phonon interactions may not be taken into account. In this temperature region it is possible to disregard phonon-phonon processes and the heat vibrations of the dislocation line and consider only the long-range component of the elastic field of the moving dislocation that can be expressed by the quasi-static transport of the static field of the rigid dislocation ([2]). Besides, we can also use, for the investigated range of temperatures, the Debye approximation of the phonon spectrum and the continuum theory of dislocations not taking into consideration the existence of the dislocation core.

According to [6] the studied anharmonic effect of the scattering of phonons at a moving dislocation can be described by the time-dependent Hamiltonian

$$H_w(t) = \sum_{\alpha,\beta} \Gamma_{\alpha\beta}\,\xi_\alpha \xi_\beta^+ e^{-i\Omega_{\mathbf{q}}t}. \tag{2.1}$$

The subscripts α, β denote the different phonon states given by a pair of the wave vector $\mathbf{k}$ and polarization λ: $\alpha = (\mathbf{k}, \lambda)$, $\beta = (\mathbf{k}', \lambda')$ where $\mathbf{k}' = \mathbf{k}+\mathbf{q}$, $\Omega_{\mathbf{q}} = \mathbf{q}\mathbf{v}$, $\xi_\alpha = a_{\mathbf{k}\lambda}+a^+_{-\mathbf{k}\lambda}$; $a^+_{\mathbf{k}\lambda}$, $a_{\mathbf{k}\lambda}$ — operators of creation and annihilation of phonons respectively, and

$$\Gamma_{\alpha\beta} = \frac{\hbar A^{jtn}_{ism} l_{\alpha i} l^*_{\beta s} k_j k'_t \hat{u}_{mn}(\mathbf{q})}{4\varrho\sqrt{\omega_\alpha \omega_\beta}}, \tag{2.2}$$

$\hbar$ — Planck's constant, $\mathbf{l}_\alpha$ — vector of the phonon polarization in the state α, ϱ — density of an undeformed crystal, $\hat{u}_{mn}(\mathbf{q})$ — Fourier transform of a static distortion dislocation field and A^{jtn}_{ism} the renormalized anharmonic elastic constants [6], ω_α — phonon frequency in the state α.

It can be shown that in the considered range of low temperatures the Hamiltonian of interaction (2.1) is sufficiently small to use the quantum-mechanical perturbation theory. In the first-order perturbation theory the probability of the scattering of the phonon from the state α to the state β per unit time is given by the formula

$$W_{\alpha\beta} = \frac{8\pi}{\hbar^2}|\Gamma_{\alpha\beta}|^2 \delta(\omega_\alpha - \omega_\beta - \Omega_{\mathbf{q}}), \tag{2.3}$$

where $\delta(\omega)$ — Dirac delta-function.

The number of transitions per unit time from the state α to the state β is given by the product of the probability $W_{\alpha\beta}$ times the density number of phonons in the state α:

$$n_\alpha = \left[\exp\left(\frac{\hbar\omega_\alpha}{k_B T}\right) - 1\right]^{-1}, \tag{2.4}$$

([2]) We shall consider a dislocation uniformly moving with the velocity v which is small as compared to the velocity of sound c; this makes applicable the quasi-static description of the elastic field of the moving dislocation.

where k_B — Boltzmann constant. If we take into account the fact that in every event of scattering the energy $\hbar(\omega_\alpha-\omega_\beta) = \hbar\Omega_{\mathbf{q}}$ is transferred then the dissipation of energy per unit time and per unit length of the dislocation line is given by

$$(2.5)\qquad D = -\frac{8\pi}{\hbar L}\sum_{\alpha,\beta}\Omega_{\mathbf{q}}|\Gamma_{\alpha\beta}|^2 n_\alpha\delta(\omega_\alpha-\omega_\beta-\Omega_{\mathbf{q}}) = -\frac{4\pi}{\hbar L}\sum_{\alpha,\beta}\Omega_{\mathbf{q}}|\Gamma_{\alpha\beta}|^2(n_\alpha-n_\beta)\delta(\omega_\alpha-\omega_\beta-\Omega_{\mathbf{q}}).$$

Here L — the length of the dislocation line (in the case of a straight dislocation, L is the diameter of a crystal along the dislocation line).

If we expand the expression (2.5) into a series of v/c, retain the first non-vanishing term and make use of

$$(2.6)\qquad n_\alpha-n_\beta = n(\omega_\alpha)-n(\omega_\alpha-\Omega_{\mathbf{q}}) \simeq n(\omega_\alpha)-n(\omega_\alpha)+\frac{\partial n_\alpha}{\partial\omega_\alpha}\Omega_{\mathbf{q}} = \Omega_{\mathbf{q}}\frac{\partial n_\alpha}{\partial\omega_\alpha},$$

we can neglect $\Omega_{\mathbf{q}}$ in the argument of the δ-function. The corresponding expression for the dissipation D in this approximation has the form

$$(2.7)\qquad D = -\frac{4\pi}{\hbar L}\sum_{\alpha,\beta}\Omega_{\mathbf{q}}^2|\Gamma_{\alpha\beta}|^2\frac{\partial n_\alpha}{\partial\omega_\alpha}\delta(\omega_\alpha-\omega_\beta).$$

Before starting the discussion of Eq. (2.7) we find the explicit form of the function $\hat{u}_{mn}(\mathbf{q})$ (see Eq. (2.2)) for the straight dislocation and for the dislocation loop.

3. Functions $\hat{u}_{mn}(\mathbf{q})$ for straight dislocation and for dislocation loop

According to [7] the elastic distortion field of an arbitrary dislocation with the Burgers vector $\mathbf{b}$ can be expressed with the help of the Green tensor $G_{ik}(\mathbf{r})$ of the theory of elasticity in the following form:

$$(3.1)\qquad u_{ij}(\mathbf{r}) = -c_{klpq}b_p\int_S dS' n_q\nabla_l\nabla_j G_{ik}(\mathbf{r}-\mathbf{r}')-\mathring{u}_{ij}(\mathbf{r}),$$

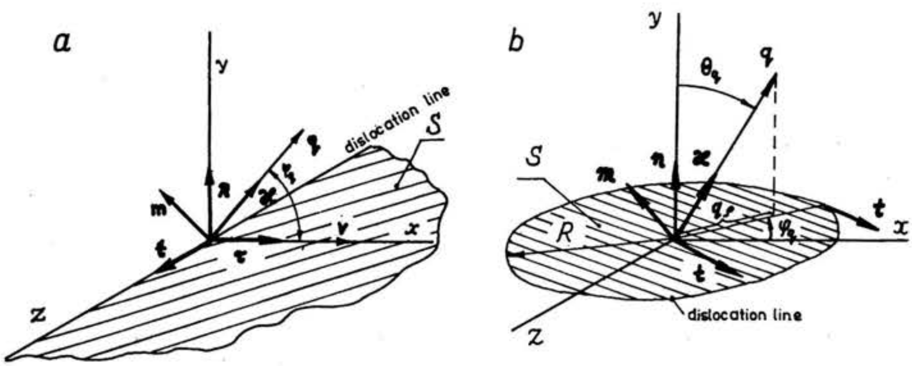

FIG. 1. Coordinate systems: (a) straight dislocation; (b) circular dislocation loop.

where the integration extends over an arbitrary surface S bounded by the line of dislocation and $\mathbf{n}$ is a vector normal to the surface S, c_{klpq} — tensor of elastic constants and $\mathring{u}_{ij}(\mathbf{r})$ — tensor of intrinsic distortions.

Figure 1 shows a straight dislocation and a circular dislocation loop of the radius R in the Cartesian coordinate system.

If S is chosen as a part of the plane xz, then for the straight dislocation we obtain [8]

$$\mathring{u}^{d}_{ij}(\mathbf{r}) = b_i n_j \delta(y)\eta(x), \tag{3.2}$$

where $\eta(\alpha)$ — Heaviside step-function, and for the dislocation loop we get in a similar way

$$\mathring{u}^{l}_{ij}(\mathbf{r}) = b_i n_j \delta(y)\eta(R^2-z^2)\left[\eta\left(x+\sqrt{R^2-z^2}\right)-\eta\left(x-\sqrt{R^2-z^2}\right)\right]. \tag{3.3}$$

The Green tensor $G_{ik}(\mathbf{r})$ is given as the solution of the equation

$$c_{ijkl}\nabla_k\nabla_l G_{ml}(\mathbf{r})+\delta_{im}\delta(\mathbf{r}) = 0, \tag{3.4}$$

where δ_{ij} is the Kronecker delta.

It is convenient to seek the solution of Eq. (3.4) in the form of the tensor $G_{ml}(\mathbf{r})$ expanded into the Fourier series

$$G_{ml}(\mathbf{r}) = \sum_{\mathbf{q}} \hat{G}_{ml}(\mathbf{q})e^{i\mathbf{q}\mathbf{r}}. \tag{3.5}$$

Inserting Eq. (3.5) into Eq. (3.4) we obtain a simple algebraic equation for $G_{ml}(\mathbf{q})$

$$q^2\Lambda_{im}(\boldsymbol{\varkappa})\hat{G}_{ml}(\mathbf{q}) = \delta_{il}, \tag{3.6}$$

where

$$\boldsymbol{\varkappa} = \mathbf{q}/q, \quad \Lambda_{im}(\boldsymbol{\varkappa}) = \varkappa_j c_{jimn}\varkappa_n. \tag{3.7}$$

Putting the result of Eq. (3.6) into Eq. (3.5) gives

$$G_{ml}(\mathbf{r}) = \sum_{\mathbf{q}} \frac{\Lambda^{-1}_{ml}(\boldsymbol{\varkappa})}{q^2}e^{i\mathbf{q}\mathbf{r}} \tag{3.8}$$

The Fourier transforms of Eqs. (3.1)–(3.3), taking into account Eq. (3.8), are for the straight dislocation

$$\hat{u}^{d}_{ij}(\mathbf{q}) = -\frac{iLS^{*}_{ijkl}(\boldsymbol{\varkappa})b_k m_l}{q}\delta_{q_z,0}, \tag{3.9}$$

for the dislocation loop

$$\hat{u}^{l}_{ij}(\mathbf{q}) = 2\pi RS^{*}_{ijkl}(\boldsymbol{\varkappa})b_k m_l\frac{J_1(q_\varrho R)}{q_\varrho}, \tag{3.10}$$

where

$$S^{*}_{ijkl}(\boldsymbol{\varkappa}) = \delta_{ik}\delta_{jl}-c_{klmn}\varkappa_m\Lambda^{-1}_{ni}(\boldsymbol{\varkappa})\varkappa_j, \tag{3.11}$$

$J_1(x)$ — Bessel function $q_\varrho = \sqrt{q_x^2+q_z^2}$, $\mathbf{m} = \mathbf{t}\times\boldsymbol{\varkappa}$, $\mathbf{t}$ — vector tangent to the dislocation line.

The formula (3.10) can easily be generalized to the case of the ellipse-shaped dislocation loop

$$\frac{x^2}{a^2}+\frac{z^2}{d^2}=1,$$

and the corresponding expression for $\hat{u}^l_{ij}(\mathbf{q})$ has the form

$$\hat{u}^l_{ij}(\mathbf{q}) = 2\pi adS^*_{ijkl}(\varkappa)b_k n_l \frac{f_1(\sqrt{(aq_x)^2+(dq_z)^2})}{\sqrt{(aq_x)^2+(dq_z)^2}}. \tag{3.12}$$

In what follows we investigate the straight dislocation and the circular dislocation loop only.

4. Dragging of the straight dislocation

In this section we present preliminary calculations which allow to discuss the magnitude and temperature dependence of the effect. We restrict ourselves to the contribution of transversal phonons only. The work [1] has shown that these phonons give the main contribution to the dragging of dislocations.

If we put into Eq. (2.7) the formula

$$|\Gamma_{\alpha\beta}|^2 = \left(\frac{\hbar Lb\omega_\alpha}{4q}\right)^2 \delta_{q_z,0}\mathcal{F}_{\alpha\beta}, \tag{4.1}$$

where $\mathcal{F}_{\alpha\beta}$ is dimensionless directional function which, taking into account Eqs. (2.2) and (3.9), is

$$\mathcal{F}_{\alpha\beta} = \left|\frac{A^{jtq}_{isp}l_{\alpha i}l^*_{\beta s}k_j k'_t S^*_{pqkl}(\mathbf{q}/q)b_k m_l}{\varrho b\omega_\alpha\omega_\beta}\right|^2, \tag{4.2}$$

and if summation over $\mathbf{k}$ and $\mathbf{k}'$ is replaced by integration over $\mathbf{k}$ and $\mathbf{q}=\mathbf{k}'-\mathbf{k}$, we obtain

$$D = -\frac{\pi\hbar b^2}{4}\sum_{\lambda,\lambda'}\int\frac{d^3k}{(2\pi)^3}\omega^2_\alpha\frac{\partial n_\alpha}{\partial\omega_\alpha}\int\frac{d^2q}{(2\pi)^2}\frac{(\mathbf{q}\mathbf{v})^2}{q^2}\mathcal{F}_{\alpha\beta}\delta(\omega_\alpha-\omega_\beta). \tag{4.3}$$

Here the integration over $\mathbf{q}$ extends over the plane normal to the dislocation line. This integration will be performed in the polar coordinates, taking the angle $\varphi_\mathbf{q}$ (Fig. 1a) from the direction of the dislocation velocity $\mathbf{v}$ (from the axis Ox). It is convenient to integrate over $\mathbf{k}$ in the spherical coordinate system taking the polar angle $\theta_\mathbf{k}$ from the direction of the vector $\mathbf{q}$, and correspondingly the longitude $\varphi_\mathbf{k}$ in the plane perpendicular to the vector $\mathbf{q}$. The function $\mathcal{F}_{\alpha\beta}$ should be written in these variables:

$$\mathcal{F}_{\alpha\beta} \equiv \mathcal{F}_{\lambda\lambda'}(\varphi_\mathbf{q}, \varphi_\mathbf{k}, \cos\theta_\mathbf{k}). \tag{4.4}$$

Taking into account the above considerations we have

$$D = -\frac{\pi}{4}\frac{\hbar b^2 v^2}{(2\pi c_t)^5}\sum_{\lambda,\lambda'}\int\limits_0^{c_t k_D} d\omega\omega^4\frac{\partial n}{\partial\omega}\int\limits_0^{2c_t k_D} d\omega_\mathbf{q}\omega_\mathbf{q}\int\limits_0^{2\pi} d\varphi_\mathbf{q}\cos^2\varphi_\mathbf{q}\int\limits_0^{2\pi} d\varphi_\mathbf{k} \times\int\limits_0^{\pi} d\theta_\mathbf{k}\sin\theta_\mathbf{k}\mathcal{F}_{\lambda\lambda'}(\varphi_\mathbf{q}, \varphi_\mathbf{k}, \cos\theta_\mathbf{k})\,\delta\big(\omega-\sqrt{\omega^2+\omega^2_\mathbf{q}-2\omega\omega_\mathbf{q}\cos\theta_\mathbf{k}}\big). \tag{4.5}$$

Here k_D — the Debye end point in the phonon spectrum, $\omega_q = q \cdot c_t$, c_t—average velocity of the transversal phonons.

The last integral in Eq. (4.5) can easily be determined:

$$(4.6)\qquad \int_0^{\pi} d\theta_{\mathbf{k}} \sin\theta_{\mathbf{k}} \mathscr{F}_{\lambda\lambda'}(\varphi_{\mathbf{q}}, \varphi_{\mathbf{k}}, \cos\theta_{\mathbf{k}})\delta(\omega - \sqrt{\omega^2+\omega_q^2-2\omega\omega_q\cos\theta_{\mathbf{k}}}) = \frac{\eta(2\omega-\omega_q)}{\omega_q}\mathscr{F}_{\lambda\lambda'}\left(\varphi_{\mathbf{q}}, \varphi_{\mathbf{k}}, \frac{\omega_q}{2\omega}\right).$$

Inserting Eq. (4.6) into Eq. (4.5) we obtain

$$(4.7)\qquad D = -g\frac{\hbar b^2 v^2}{(2\pi c_t)^5}\int_0^{c_t k_D} d\omega\omega^5 \frac{\partial n}{\partial \omega},$$

where g denotes the constant quantity

$$(4.8)\qquad g = \frac{\pi}{2}\int_0^{2\pi} d\varphi_{\mathbf{q}}\cos^2\varphi_{\mathbf{q}}\int_0^{2\pi} d\varphi_{\mathbf{k}}\int_0^1 dt \sum_{\lambda,\lambda'}\mathscr{F}_{\lambda\lambda'}(\varphi_{\mathbf{q}}, \varphi_{\mathbf{k}}, t).$$

Finally, transforming the variable in Eq. (4.7) into dimensionless ones $\hbar\omega/k_B T$, we obtain the following expression for the dragging coefficient $B = D/v^2$:

$$(4.9)\qquad B = g\frac{\hbar}{b^3}\left(\frac{k_D b}{2\pi}\right)^5 f(T/\theta_t),$$

where $\theta_t = c_t k_D/k_B$ — modified Debye temperature, and the function $f(x)$ describing the temperature dependence of the effect is as follows:

$$(4.10)\qquad f(x) = x^5\int_0^{1/x}\frac{e^t t^5 dt}{(e^t-1)^2}.$$

The formula (4.9) involves the parameter $g \sim |A/\mu|$ (A — characteristic value of the anharmonic constant, μ — shear modulus), which is known only with the accuracy of the order of maqnitude. To find the exact value of g, concrete and highly cumbersome calculations are needed. Such calculations for screw and edge dislocations are given below (Sect. 6). But even in the above form, formula (4.9) contains useful information which allows in particular to discuss the temperature dependence (4.10) of the effect.

For low temperatures the phonon wind is quickly "frozen-away": $B \sim T^5$. When the temperature increases the steep behaviour of the function $f(T/\theta_t)$ changes into linear dependence. This occurs already at temperatures considerably below the Debye temperature.

Yet, we notice here that at high temperatures formulae (4.9) and (4.10) overestimate the effect because the existence of the dislocation core is neglected. In Sect. 6 we show that taking into account the core of the dislocation in a simple model leads to a certain renormalization of the integrand (4.10).

5. Dragging of the dislocation loop

The previous calculations were connected with the straight dislocation. The obtained results can be applied to the curved dislocations, for example to loops only in these cases when the mean phonon wavelength is small in comparison with the radius of curvature of the dislocation line, i.e. at not very low temperatures. It is interesting to explain on the example of the phonon wind what corrections have to be made in the temperature dependence of $B(T)$ if the curvature of the dislocation line is taken into account, and to determine the initial temperatures at which this dependence is not considerably different from Eq. (4.10).

The problem has already been investigated by two of the authors in [5] but only in the isotropic case and with representation of the tensor $\hat{u}_{ij}(\mathbf{q})$ in a very inadequate form. For this reason, the discussion was restricted to the estimate of the order of quantity. We return to the problem of the phonon dragging of the circular dislocation loop on the basis of the approach developed here. In particular, the expression (3.10) already obtained for the tensor $\hat{u}^l_{ij}(\mathbf{q})$ will be useful.

Calculations of the type in Sect. 3 allow to investigate how, with the decreasing of temperature and corresponding increasing of the mean phonon wevelength λ_{ph}, the character of the coefficient of dragging changes from the dependence (4.10), valid as long as $\lambda_{ph} \ll R$, to the more sharp temperature dependence for $\lambda_{ph} > R$, when phonons "perceive" the loop as a point defect.

On the other hand, in the limit case when the radius R of the loop descreases to the dimension of the lattice parameter, the expression for B gives the estimate of the phonon dragging for crowdions.

The dissipation of energy per unit time, accompanying the movement of the dislocation loop, is described by the expression (2.7) in which $L = 2\pi R$, and the quantity $\Gamma_{\alpha\beta}$ is given by the expressions (2.2) and (3.10). It is convenient to represent $\Gamma_{\alpha\beta}$ in a form analogous to Eq. (4.1)

$$(5.1) \qquad |\Gamma_{\alpha\beta}|^2 = \left(\frac{\pi R b \hbar \omega_\alpha}{2q}\right)^2 J_1^2(q_\varrho R)\mathscr{F}_{\alpha\beta},$$

where $\mathscr{F}_{\alpha\beta}$ as before is given by the expression (4.2) with the only difference that the vector $\mathbf{m} = \mathbf{t}\times\boldsymbol{\varkappa}$ (Fig. 1b) is defined here by a varying vector $\mathbf{t}$ tangent to the dislocation line. The vector $\mathbf{t}$ rotates according to the changes of the azimuth $\varphi_\mathbf{q}$ of the vector $\boldsymbol{\varkappa}$ but is always perpendicular to the projection of the vector $\mathbf{q}$ onto the plane of the loop.

Putting Eq. (5.1) into Eq. (2.7) we obtain

$$(5.2) \qquad D = -\frac{\pi^2\hbar b^2 R}{2}\sum_{\lambda,\lambda'}\int\frac{d^3k}{(2\pi)^3}\omega_\alpha^2\frac{\partial n_\alpha}{\partial\omega_\alpha}\int\frac{d^3q}{(2\pi)^3}\frac{(\mathbf{qv})^2}{q^2}J_1^2(qR)\mathscr{F}_{\alpha\beta}\,\delta(\omega_\alpha-\omega_\beta).$$

The next calculations will be made for the prismatic dislocation loop. This loop moves in the direction of the Burgers vector $\mathbf{b}$, perpendicular to the loop plane. It is convenient to perform integration over $\mathbf{k}$, as before, in the spherical coordinate system taking the polar angle $\theta_\mathbf{k}$ from the direction of the vector $\mathbf{q}$. Integration over $\mathbf{q}$ is performed in the spherical coordinate system, too (Fig. 1b), but with the azimuth $\varphi_\mathbf{q}$ in the loop plane and polar angle $\theta_\mathbf{q}$ measured from the direction of the velocity $\mathbf{v}$. Accordingly the function $\mathscr{F}_{\alpha\beta}$ is expressed in the corresponding coordinates

$$(5.3) \qquad \mathscr{F}_{\alpha\beta} \equiv \mathscr{F}_{\lambda\lambda'}(\varphi_\mathbf{q}, \cos\theta_\mathbf{q}, \varphi_\mathbf{k}, \cos\theta_\mathbf{k}).$$

Calculations quite analogous to those in Sect. 3 lead to the following expression for the dragging coefficient of the dislocation loop

(5.4) $$B = \frac{\hbar}{b^3}\left(\frac{k_D b}{2\pi}\right)^5 \tilde{f}(T/\theta_t),$$

with the temperature dependence given by the function

(5.5) $$\tilde{f}(x) = x^5 \int\limits_0^{1/x} \frac{e\, t^5 dt}{(e-1)^2}\, \psi(\gamma x t),$$

where $\gamma = 2k_D R$ and the function $\psi(y)$ defining the difference between Eqs. (5.5) and (4.10) has the form

(5.6) $$\psi(y) = \frac{\pi y}{2} \int\limits_{-1}^{1} du\, u^2 \int\limits_0^1 dv\, v J_1^2\left(yv\sqrt{1-u^2}\right) \int\limits_0^{2\pi} d\varphi_{\mathbf{k}} \int\limits_0^{2\pi} d\varphi_{\mathbf{q}} \sum_{\lambda,\lambda'} \mathscr{F}_{\lambda\lambda'}(\varphi_{\mathbf{q}}, u, \varphi_{\mathbf{k}}, v).$$

The formulae (5.4)–(5.6) allow to analyze the temperature dependence of dragging of the loop at low and high temperatures.

For $T \ll \theta_t/\gamma$ the main contribution to the integral (5.5) is given by the values $t \sim 1$. Therefore, to calculate the function $\tilde{f}(T/\theta_t)$ in this temperature region it is sufficient to know the behaviour of the function $\psi(y)$ for small values of the argument. Taking into account that for $y \ll 1$

(5.7) $$J_1^2\left(yv\sqrt{1-u^2}\right) \simeq \frac{1}{4} y^2 v^2 (1-u^2),$$

the function $\psi(y)$ in this region has the form

(5.8) $$\psi(y) = \tilde{g} y^3,$$

where

(5.9) $$\tilde{g} = \frac{\pi}{8} \int\limits_{-1}^{1} du\, u^2(1-u^2) \int\limits_0^1 dv\, v^3 \int\limits_0^{2\pi} d\varphi_{\mathbf{k}} \int\limits_0^{2\pi} d\varphi_{\mathbf{q}} \sum_{\lambda,\lambda'} \mathscr{F}_{\lambda\lambda'}(\varphi_{\mathbf{q}}, u, \varphi_{\mathbf{k}}, v) \sim g/30.$$

Taking into account Eq. (5.8), the function $\tilde{f}(T/\theta_t)$ for $T \ll \theta_t/\gamma$ can be represented in the form

(5.10) $$\tilde{f}(T/\theta_t) \approx \frac{(2\pi)^8}{60} \tilde{g}\gamma^3 \left(\frac{T}{\theta_t}\right)^8.$$

Thus, at very low temperatures the dragging of the dislocation loop is "frozen-away" more rapidly than that of straight dislocation.

In an analogous way for $T \gg \theta_t/\gamma$ the asymptotic behaviour of the function $\psi(y)$ plays the main part for large values of the argument. Putting for $y \gg 1$

(5.11) $$J_1^2\left(yv\sqrt{1-u^2}\right) \simeq \frac{2}{\pi} \frac{\cos^2\left(yv\sqrt{1-u^2}+\pi/4\right)}{yv\sqrt{1-u^2}},$$

into Eq. (5.6) and changing, as usual, the quickly oscillating function $\cos^2(yv\sqrt{1-u^2}+\pi/4)$ into 1/2, we obtain

$$(5.12)\qquad \psi(y) \simeq \frac{1}{2}\int_{-1}^{1}\frac{du\,u^2}{\sqrt{1-u^2}}\int_0^1 dv\int_0^{2\pi} d\varphi_{\mathbf{k}}\int_0^{2\pi} d\varphi_{\mathbf{q}}\sum_{\lambda\lambda'}\mathscr{F}_{\lambda\lambda'}(\varphi_{\mathbf{q}},u,\varphi_{\mathbf{k}},v) \equiv \bar{g} = \text{const}.$$

In other words, at high temperatures $T \gg \theta_t/\gamma$, as it is to be expected, the dragging of the loop has the same temperature dependence as the dragging of the straight dislocation and is described by the formula (4.9) in which the quantity g has to be changed into $\bar{g}$. Such not full coincidence has a simple physical cause associated with the fact that dragging of independent pieces of the loop having different orientations, due to the anisotropy, are different. It is not difficult to state that the parameter $\bar{g}$ is simply a mean value of g taken over all possible orientations, in the plane of the loop, of the straight dislocation line with the Burgers vector $\mathbf{b}$ and the velocity $\mathbf{v}$ perpendicular to that plane

$$(5.13)\qquad \bar{g} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi_t g(t).$$

In the case of the axial symmetry, when the quantity $\mathscr{F}_{\lambda\lambda'}$ does not depend on φ_t, we have $\bar{g} = g$. Disregarding this completely anisotropic effect, connected not with the curvature but with the orientation of the separate elements of the dislocation, we can state that the curvature of the dislocation line influences substantially the dynamic dragging in the region of temperatures $T \leqslant \theta_t/\gamma$ only. This region is considerably large only for crowdions and sufficiently small loops, and for this reason we shall restrict the next calculations to dragging of straight dislocations only.

6. Explicit form of the anharmonicity in the Murnaghan model

The quantity g can be determined in the isotropic approximation when the tensor A^{jtq}_{isp} has, according to [9], the form

$$(6.1)\qquad A^{jtq}_{isp} = 2\left(\frac{5}{3}\mu+\frac{1}{2}K+m-l\right)\delta_{ij}\delta_{si}\delta_{pq}-\left(\frac{\mu}{3}+K+m\right)\delta_{is}\delta_{jt}\delta_{pq}$$
$$-(\mu+m)\delta_{it}\delta_{js}\delta_{pq}-2\left(\frac{4}{3}\mu+K+m\right)(\delta_{ij}\delta_{sp}\delta_{tq}+\delta_{st}\delta_{ip}\delta_{jq})$$
$$-2\mu\delta_{is}\delta_{jp}\delta_{tq}-2\left(\mu+\frac{1}{4}n\right)(\varepsilon_{pis}\varepsilon_{qjt}+\varepsilon_{pit}\varepsilon_{qjs}).$$

Here K — bulk modulus, n, m and l — Murnaghan moduli, ε_{ijk} — fully antisymmetric third order unit tensor. For further determination the isotropic form of the tensor $S^*_{ijkl}(\boldsymbol{\varkappa})$ is also needed

$$(6.2)\qquad S^*_{ijkl}(\boldsymbol{\varkappa}) = \frac{1}{1-\nu}[m_i m_j m_k m_l + t_i t_j t_k t_l + \nu(m_i m_j t_k t_l + t_i t_j m_k m_l)]$$
$$+\frac{1}{2}[m_i t_j t_k m_l + m_i t_j m_k t_l + t_i m_j t_k m_l + t_i m_j m_k t_l] - \frac{\nu}{1-\nu}\delta_{ij}[m_k t_l + t_k m_l].$$

Here ν — Poisson ratio, **m** and **t** — unit vectors being together with $\boldsymbol{\varkappa} = \mathbf{q}/q$ right-handed triplet of vectors. The vector **t** is directed along the dislocation line (Fig. 1a).

Taking into account the explicit form of the tensor $S^*_{ijkl}(\boldsymbol{\varkappa})$ in Eq. (6.2) it is easy to obtain for the screw dislocation with the Burgers vector $\mathbf{b} = b\mathbf{t}$

$$S^*_{pqkl}(\boldsymbol{\varkappa})b_k m_l = \frac{b}{2}[m_p t_q + t_p m_q]. \tag{6.3}$$

For the edge dislocation with the Burgers vector $\mathbf{b} = b\boldsymbol{\tau}$

$$S^*_{pqkl}(\boldsymbol{\varkappa})b_k m_l = \frac{b(\boldsymbol{\varkappa}\mathbf{n})}{1-\nu}[\nu(\delta_{pq} - t_p t_q) - m_p m_q]. \tag{6.4}$$

Putting the expressions (6.1), (6.3) and (6.4) into the formula (4.2) we obtain the explicit form of the quantity $\mathscr{F}_{\alpha\beta}$, directly defining the parameter g in Eq. (4.8). To give an example, for the screw dislocation, neglecting the components corresponding to the contribution of the longitudinal phonons, we have

$$\mathscr{F}_{\alpha\beta} = \Big\{(\mathbf{l}_\alpha \mathbf{l}_\beta)\,[(\boldsymbol{\varkappa}_\alpha \mathbf{m})(\boldsymbol{\varkappa}_\beta \mathbf{t}) + (\boldsymbol{\varkappa}_\alpha \mathbf{t})(\boldsymbol{\varkappa}_\beta \mathbf{m})] + \left(1 + \frac{n}{4\mu}\right)[(\mathbf{l}_\alpha \mathbf{l}_\beta \mathbf{t})(\boldsymbol{\varkappa}_\alpha \boldsymbol{\varkappa}_\beta \mathbf{m}) + (\mathbf{l}_\alpha \mathbf{l}_\beta \mathbf{m})(\boldsymbol{\varkappa}_\alpha \boldsymbol{\varkappa}_\beta \mathbf{t}) + (\mathbf{l}_\alpha \boldsymbol{\varkappa}_\beta \mathbf{t})(\boldsymbol{\varkappa}_\alpha \mathbf{l}_\beta \mathbf{m}) + (\mathbf{l}_\alpha \boldsymbol{\varkappa}_\beta \mathbf{m}) + (\boldsymbol{\varkappa}_\alpha \mathbf{l}_\beta \mathbf{t})]\Big\}^2, \tag{6.5}$$

where $\boldsymbol{\varkappa}_\alpha = \mathbf{k}/k$, $\boldsymbol{\varkappa}_\beta = \mathbf{k}'/k'$. The mixed product of vectors is expressed as

$$(\mathbf{ABC}) \equiv \mathbf{A}(\mathbf{B} \times \mathbf{C}). \tag{6.6}$$

The next step consists in expressing the quantity $\mathscr{F}_{\alpha\beta}$ in the corresponding angular coordinates (4.4) and determining the triple integral (4.8). This procedure proves to be rather laborious and we give here the final result only.

The similar determinations were given first in [3] for the screw dislocation. According to [3] in this case

$$g_s \simeq 4 + \left(\frac{n}{\mu} + 6\right)^2. \tag{6.7}$$

For the edge dislocation the quantity g_{ed} is given by means of a more complicated expression presented here for the first time:

$$g_{ed} \simeq \frac{1}{\mu^2}\left(\frac{1-2\nu}{1-\nu}\right)^2 (16.49m^2 + 0.76n^2 - 4.94mn + 13.34K^2 + 55.5\mu^2 + 23.54Km - 3.85Kn + 4.86\mu n + 30.33\mu m + 5.78K\mu) + \frac{1}{\mu^2(1-\nu)^2}(0.63n^2 + 17.41\mu^2 + 5.93\mu n). \tag{6.8}$$

Usually, the main contribution to g_{ed} as well as to g_s is introduced by the Murnaghan modulus n. For example, in copper crystals according to [10],

$$n = -159 \cdot 10^{11}\ \text{dyne/cm}^2, \quad m = -62.10^{11}\ \text{dyne/cm}^2, \quad \mu = 5.46 \cdot 10^{11}\ \text{dyne/cm}^2, \quad \nu = 0.324, \quad K = \frac{2\mu(1+2\nu)}{3(1-2\nu)} = 17.042 \cdot 10^{11}\ \text{dyne/cm}^2. \tag{6.9}$$

Thus we have

$$g_s \simeq 538, \quad g_{ed} \simeq 931, \tag{6.10}$$

and the quantity n gives almost a 80% contribution into g_{ed}.

In such a manner the contribution of the phonon wind into the dynamic dragging of the screw and edge dislocation at low temperatures can be estimated with the the help of Eqs. (4.9), (6.7) and (6.8). In the region of high temperatures the present estimate is not valid because the existence of the dislocation core was disregarded in the determinations. Below we make an attempt to take into consideration the influence of the dislocation core on the basis of a simple model.

7. The phonon wind at high temperatures

As it was mentioned above, there is a need for a more detailed discussion of the behaviour of the elastic field near the dislocation core at not very low temperatures when the phonon wevelength is comparable with the diameter of the dislocation core. In the continuum theory the dislocation is regarded as a linear singularity in terms of an approximation in which the elastic field increases infinitely and proportionally to $1/r$. It is obvious that the continuum theory approach is not applicable to the discrete nature of real crystals, at least near the dislocation core where the relaxation of the elastic field occurs. Virtually, the existence of the dislocation core can be taken into account by using a model in which for small distances from the dislocation line the elastic field is truncated in a smooth manner. For example we can apply the model [11]

$$u_{ij}(\mathbf{r}) = u_{ij}^c(\mathbf{r})\,(1-e^{-r/r_0}). \tag{7.1}$$

Here $u_{ij}^c(\mathbf{r})$ — tensor of elastic deformations introduced by dislocation in continuum theory approximation ($u_{ij}^c \sim b/(2\pi r)$). The model radius of a dislocation core r_0 should be of a few lattice parameters.

It can be shown that to the elastic field in Eq. (7.1) (at least in an isotropic case) there corresponds the Fourier transform

$$\hat{u}_{ij}(\mathbf{q}) = \frac{\hat{u}_{ij}^c(\mathbf{q})}{\sqrt{1+(\mathbf{q}r_0)^2}}, \tag{7.2}$$

where $\hat{u}_{ij}^c(\mathbf{q})$ — Fourier transform of $u_{ij}^c(\mathbf{r})$.

Let us consider, as an example, a straight screw dislocation parallel to the Ox axis, for which

$$u_{ij}^c(\mathbf{r}) = \begin{Bmatrix} u_{zx} \\ u_{zy} \end{Bmatrix} = \frac{b}{2\pi r}\begin{Bmatrix} -\sin\varphi \\ \cos\varphi \end{Bmatrix}, \quad \hat{u}_{ij}^c(\mathbf{q}) = \frac{ib}{2q}\begin{Bmatrix} -\sin\varphi_{\mathbf{q}} \\ \cos\varphi_{\mathbf{q}} \end{Bmatrix}, \tag{7.3}$$

where the angles φ and $\varphi_{\mathbf{q}}$ are measured from the Ox axis. Determining now the Fourier transform of Eq. (7.1), taking into account Eq. (7.3) we have

$$\hat{u}_{ij}(\mathbf{q}) = \frac{b}{2\pi}\int_0^\infty dr(1-de^{r/r_0})\int_0^{2\pi} d\varphi e^{iqz\cos(\varphi-\varphi_{\mathbf{q}})}\begin{Bmatrix} -\sin\varphi \\ \cos\varphi \end{Bmatrix} = \frac{ib}{2q}\begin{Bmatrix} -\sin\varphi_{\mathbf{q}} \\ \cos\varphi_{\mathbf{q}} \end{Bmatrix}\int_0^\infty du(1-e^{-u/(qr_0)})J_1(u) = \frac{\hat{u}_{ij}^c(\mathbf{q})}{\sqrt{1+(qr_0)^2}}. \tag{7.4}$$

In a very similar way the expression (7.2) can be proved also for an edge dislocation, the elastic field of which has the structure very close to Eq. (7.3) if the tensor $u_{ij}^{e}(\mathbf{r})$ is written in polar coordinates

$$u_{ij}^{e}(\mathbf{r}) = \begin{Bmatrix} u_{rr} \\ u_{\varphi\varphi} \\ u_{r\varphi} \end{Bmatrix} = -\frac{b}{4\pi r}\frac{1-2\nu}{1-\nu}\begin{Bmatrix} \sin\varphi \\ \sin\varphi \\ -\dfrac{\cos\varphi}{1-2\nu} \end{Bmatrix}. \tag{7.5}$$

The simple character of the renormalization in Eq. (7.2) of the tensor $\hat{u}_{ij}^{e}(\mathbf{q})$ and the results of the previous section allow to obtain a modified estimate of the phonon wind without cumbersome determination of the parameter g. It can be easily seen that putting Eq. (7.2) into Eq. (2.7) provides the expression (4.5), the integrand of which is multiplied by $[1+(r_0\omega_{\mathbf{q}}/c_t)^2]^{-1}$. The final estimate of the dragging coefficient is given by the formula having a form similar to Eq. (4.9)

$$B = g\frac{\hbar}{b^3}\left(\frac{k_D b}{2\pi}\right)^5 f_\chi(T/\theta_t), \tag{7.6}$$

where the coefficient g is given by Eq. (4.8). The estimates (6.7) and (6.8) of g, for screw and edge dislocations respectively, are valid. The only difference between Eqs. (7.6) and (4.9) is the form of the function $f_\chi(T/\theta_t)$ describing the temperature dependence on the effect.

$$f_\chi(x) = x^5\int_1^{1/x}\frac{e^t t^5 dt}{(e^t-1)^2}\frac{\operatorname{arctg}\chi x t}{\chi x t}, \tag{7.7}$$

where $\chi = 2k_D r_0$. The similar modification of the temperature dependence of the phonon wind was shown for the first time in the papers [1, 12].

The additional term (in comparison with Eq. (4.10)) in Eq. (7.7) arctg $\chi xt/(\chi xt)$ describes the smooth cut of the elastic field in the core of the dislocation. At $r_0 = 0$ this factor is equal to unity and the function $f_\chi(x)$ is the same as that obtained before. As it should be expected at low temperatures $T \ll \theta_t/\chi$, the renormalization considered is not substantial because in this situation the contribution into the integral is connected with values $t \sim 1$, for which $\chi xt \ll 1$ and $\operatorname{arctg}\chi xt \simeq \chi xt$. This reflects the physical fact that the long wave phonons prevailing at low temperatures are weakly detectable for sensitive measuring gauges of the perturbating field along distances which are small as compared to the wavelength.

When the temperature increases, the function $f_\chi(x)$ quite quickly goes over from the dependence $f_\chi(x) \sim x^5$ to the linear one with the slope depending on the parameter χ:

$$f_\chi(x) \simeq \frac{x}{3\chi}\left[\operatorname{arctg}\chi - \frac{\chi^2-\ln(\chi^2+1)}{2\chi^3}\right] \simeq \begin{cases} x/4, & \chi \ll 1, \\ x/(2\chi), & \chi \gg 1. \end{cases} \tag{7.8}$$

For usual estimates of k_D and $r_0 \sim (1\div 3)b$, the quantity χ is about $(10\div 30)$. As it follows from the expression (7.8), taking into consideration the finiteness of dimensions of the dislocation core at high temperatures $T > \theta_t$ leads to the decrease of estimate of the influence of the phonon wind on the dissipation by $\chi/2 = k_D r_0$, i.e. by near by one order.

In Fig. 2 the plot of the function $f_\chi(x)$ is shown for different χ. It is important that the proportion $f_\chi(x)/f_\chi(1)$ (Fig. 3) very weakly depends on the parameter χ up to very low temperatures. This fact considerably facilitates the procedure of theoretical analysis of the experimental data (see e.g. [1, 12 ÷ 14]). We notice in connection with the above considerations that the estimates on the basis of Eq. (7.6) at room temperature give the

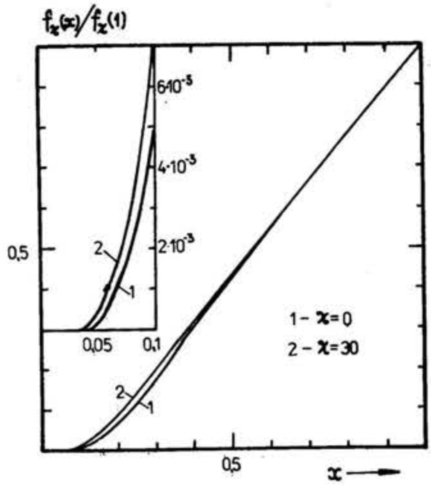

FIG. 2. The plot of the function $f_\chi(x)$ for different χ.

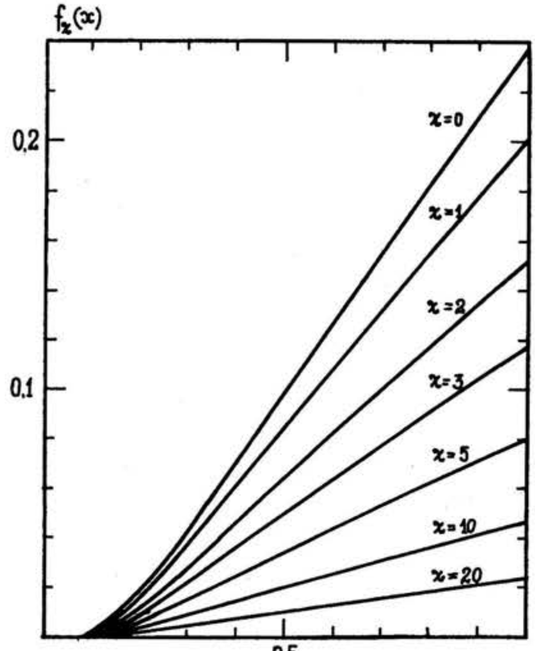

FIG. 3. The plot of the function $f_\chi(x)/f_\chi(1)_1$.

values of the dragging coefficient B comparable with the measured values. Nevertheless we do not use such a comparison, because at high temperatures one has to take into account the so-called relaxation of "slow" phonons [1, 12, 13] in the line with the phonon wind and this is beyond the scope of the present study.

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