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On the disclination-induced internal friction

D.V. Churochkin [a,*], V.A. Osipov [b]

[a] *Department of Theoretical and Nuclear Physics, Saratov State University, 410 000 Saratov, Russia*
[b] *Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia*

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Abstract

The frequency-dependent loss due to twist disclinations is studied by treating the disclination as a damped oscillating heterogeneous string. The damping parameter is found to vary along the disclination line as z^2 while the decrement has a resonant type behavior similar to that for dislocations. The internal friction is predicted to be proportional to the fourth power of disclination length, which can be tested in experiments with rotationally disordered crystals. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

As is well known, acoustic wave traveling through the matter is partially absorbed. In dislocated crystals, an important source of dissipation is the motion of dislocations (forced by external stress) which is opposed by some damping mechanism. In particular, as it was experimentally found in [1], at low temperatures the vibrating pinned dislocations are the dominant source of scattering. The theory of mechanical damping due to dislocations was developed in [2]. This theory is based on the string model for a dislocation and provides a quantitative interpretation of the dislocation-induced loss. Among other characteristics, the explicit form of the decrement has been found. It should be noted that the vibrating string model proved successful in the description of the contribution of mobile dislocations to the specific heat of crystals [3], in analysis of phonon scattering [4], and in interpretation of the low-temperature thermal conductivity in dislocated crystals [5]. The basic characteristics of the string model are the line tension, the effective mass and the damping parameter. For dislocations they have been calculated in [6], and within a more general approach in [7].

Recently, we have suggested the string model for vibrating pinned twist disclinations [8]. In particular, we have shown that twist disclination can be represented as a heterogeneous string and found a contribution of mobile twist disclinations to the specific heat of crystals. In this Letter we extend the model to take into account the damping. For this purpose we determine the damping constant and formulate the equation of motion. Finally, we calculate the disclination-induced decrement.

2. The general scheme

By analogy with dislocations, we will study the effect of pinned disclinations on the energy lost by the

* Corresponding author.
E-mail address: churochkindv@info.sgu.ru (D.V. Churochkin).

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stress wave traveling through a crystal in the framework of the vibrating string model. The basic characteristic is the logarithmic decrement Q^{-1} which is generally defined by

$$Q^{-1} = \frac{\overline{\Delta W}}{2\bar{W}}, \tag{1}$$

where $\overline{\Delta W}$ is the energy lost per cycle and $\bar{W}$ is the total vibrational energy of a specimen. For a linear defect, $\overline{\Delta W} = \bar{P}T$, where T is a period and

$$\bar{P} = \sum_n \frac{1}{T} \int_0^T \int_{-L}^{L} \mathrm{Re}(F_i)\,\mathrm{Re}(\dot{\epsilon}_i^n)\, dl\, dt \tag{2}$$

determines the mean energy (in a unit time) lost to friction. Here F_i is the Peach–Koehler force acting on unit length of the disclination line due to external stress field, ϵ_i is the displacement of the disclination in the glide plane, and the sum over all normal modes is assumed. The total vibrational energy stored per cycle reads

$$\bar{W} = \frac{\sigma_a^2}{2\mu}, \tag{3}$$

where σ_a is the amplitude of applied stress wave and μ is the shear modulus. To find ϵ_i, one has to study the equation of motion of the disclination. Recently, we have shown that twist disclination can be represented as a string with the understanding that this is a *heterogeneous* string [8]. Let us treat the disclination as a damped oscillating string. The position of the disclination in the glide plane is $\epsilon(z,t)$. In this case, the equation of motion is written as

$$m\frac{\partial^2 \epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T\frac{\partial \epsilon(z,t)}{\partial z}\right) - B\frac{\partial \epsilon(z,t)}{\partial t} + F_i, \tag{4}$$

where m is the mass of twist disclination, T is the line tension, and B is the damping parameter. All these parameters are determined per unit length of the disclination line and can generally be z-dependent.

In dislocation theory, there are known several damping mechanisms (see, e.g., [9]). Following Eshelby [10], we suppose here that the damping constant is entirely due to the re-radiation damping mechanism. In particular, this is true for insulators at low temperatures. In this case,

$$B = \bar{D}\big/\overline{v^2}, \tag{5}$$

where D is the rate of radiation per unit length of the defect line and v is the velocity of a disclination. In accordance with [10], the rate of radiation is

$$\bar{N} = \int f_i \dot{u}_i \, dV, \tag{6}$$

where elastic displacements u_i are caused by fictitious forces f_i. As is known [11], fictitious forces f_i are determined by

$$f_j = -c_{ijkl}\delta e^{\mathrm{pl}}_{kl,i}, \tag{7}$$

where c_{ijkl} are the elastic modulus and $\delta e^{\mathrm{pl}}_{kl,i}$ is the plastic part of the strain tensor. For sliding disclinations, one has

$$\delta e^{\mathrm{pl}}_{kl} = \frac{1}{2}\left(\left[\vec{\Omega}\vec{R}\right]_k\left[\vec{\delta x}\vec{\tau}\right]_l + \left[\vec{\Omega}\vec{R}\right]_l\left[\vec{\delta x}\vec{\tau}\right]_k\right)\delta(\vec{\xi}), \tag{8}$$

where $\vec{\Omega}$ is the Frank vector, $\vec{R} = \vec{r} - \vec{r}_0$ is a vector from any point on the axis of rotation to point P, $\vec{\delta x}$ describes the displacement of the disclination line and $\delta(\vec{\xi})$ is the two-dimensional delta-function. Accordingly, the displacement fields can be obtained by using the dynamic Green's function

$$u_n(\vec{r},t) = -\int c_{ijkl} G_{jn,i} \delta e^{\mathrm{pl}}_{kl}\, dV', \tag{9}$$

where G_{ij} is the Green's tensor function. Explicitly (see [10]),

$$G_{jn} = \chi_{,jn} + \delta_{jn}\varpi \tag{10}$$

with

$$\varpi = \frac{e^{i\omega(t-R/c_t)}}{4\pi\mu R}, \tag{11}$$

$$\chi = \frac{c_t^2}{\omega^2}\frac{e^{i\omega(t-R/c_t)}}{4\pi\mu R} - \frac{c_t^2}{\omega^2}\frac{e^{i\omega(t-R/c_l)}}{4\pi\mu R}. \tag{12}$$

Here c_t and c_l are the velocities of transverse and longitudinal sound waves, respectively, $R = |\vec{r} - \vec{r}'|$, and ω is the frequency. Taken together, these formulas allow us to solve the problem in a self-consistent way.

3. Damping parameter *B*

Let us calculate the damping parameter B. For this purpose, we consider the motion of the rectilinear twist disclination with a fixed axis of rotation. Let the disclination line be oriented along the z-axis and the axis of rotation along the y-axis. In this case, the Frank vector $\vec{\Omega} = (0, \Omega, 0)$ and the unit tangent vector to the defect line $\vec{\tau} = (0, 0, 1)$. The condition for conservative motion of a linear defect is generally written as $dV = 0$ (no vacancies are created or absorbed). It was shown in [12] that the conservative motion of disclinations must be normal to $[[\vec{\Omega}\vec{R}]\vec{\tau}]$. This enables one to define a disclination glide surface as the surface of revolution around the axis $\vec{\Omega}$ containing the disclination line. In our case, this is the xz plane. We suggest that the motion of disclination line in the x direction is oscillatory, $\vec{\delta x} = (\epsilon, 0, 0)$ with $\epsilon(z) = \epsilon_0 \exp(\imath(kz + \omega t))$. Then the displacement fields in Eq. (9) can be written as (see also Refs. [11,13])

$$u_n(\vec{r}, t) = \mu\Omega\epsilon_0 e^{i\omega t} \int_{-\infty}^{\infty} (G_{yn,x} + G_{xn,y}) e^{ikz'} z'\, dz'. \tag{13}$$

Here Eq. (8) is taken into account. By using of Eq. (10) one finally obtains

$$\begin{aligned} u_x(\vec{r}, t) = {} & \frac{\Omega z \epsilon_0 e^{i(kz+\omega t)}}{2\pi} \\ & \times \left[\frac{2y}{a^2} \left(\frac{c_t^2 P_t^2}{\omega^2} K_2(P_t a) - \frac{c_t^2 P_l^2}{\omega^2} K_2(P_l a) \right) \right. \\ & - \frac{2x^2 y}{a^3} \left(\frac{c_t^2 P_t^3}{\omega^2} K_3(P_t a) - \frac{c_t^2 P_l^3}{\omega^2} K_3(P_l a) \right) \\ & \left. - P_t K_1(P_t a) \frac{y}{a} \right] \\ & + \frac{iky\Omega\epsilon_0 e^{i(kz+\omega t)}}{2\pi} \\ & \times \left[\frac{2}{a} \left(\frac{c_t^2 P_t}{\omega^2} K_1(P_t a) - \frac{c_t^2 P_l}{\omega^2} K_1(P_l a) \right) \right. \\ & - \frac{2x^2}{a^2} \left(\frac{c_t^2 P_t^2}{\omega^2} K_2(P_t a) - \frac{c_t^2 P_l^2}{\omega^2} K_2(P_l a) \right) \\ & \left. - K_0(P_t a) \right], \end{aligned} \tag{14}$$

$$\begin{aligned} u_y(\vec{r}, t) = {} & \frac{\Omega z \epsilon_0 e^{i(kz+\omega t)}}{2\pi} \\ & \times \left[\frac{2x}{a^2} \left(\frac{c_t^2 P_t^2}{\omega^2} K_2(P_t a) - \frac{c_t^2 P_l^2}{\omega^2} K_2(P_l a) \right) \right. \\ & - \frac{2y^2 x}{a^3} \left(\frac{c_t^2 P_t^3}{\omega^2} K_3(P_t a) - \frac{c_t^2 P_l^3}{\omega^2} K_3(P_l a) \right) \\ & \left. - P_t K_1(P_t a) \frac{x}{a} \right] \\ & + \frac{ikx\Omega\epsilon_0 e^{i(kz+\omega t)}}{2\pi} \\ & \times \left[\frac{2}{a} \left(\frac{c_t^2 P_t}{\omega^2} K_1(P_t a) - \frac{c_t^2 P_l}{\omega^2} K_1(P_l a) \right) \right. \\ & - \frac{2y^2}{a^2} \left(\frac{c_t^2 P_t^2}{\omega^2} K_2(P_t a) - \frac{c_t^2 P_l^2}{\omega^2} K_2(P_l a) \right) \\ & \left. - K_0(P_t a) \right], \end{aligned} \tag{15}$$

$$\begin{aligned} u_z(\vec{r}, t) = {} & \frac{\Omega \epsilon_0 e^{i(kz+\omega t)}}{2\pi} \\ & \times \left[\frac{2xy}{a^2} (1 + ikz) \right. \\ & \left. \times \left(\frac{c_t^2 P_t^2}{\omega^2} K_2(P_t a) - \frac{c_t^2 P_l^2}{\omega^2} K_2(P_l a) \right) \right] \\ & - \frac{k^2 \Omega \epsilon_0 e^{i(kz+\omega t)}}{\pi} \frac{xy}{a} \\ & \times \left(\frac{c_t^2 P_t}{\omega^2} K_1(P_t a) - \frac{c_t^2 P_l}{\omega^2} K_1(P_l a) \right), \end{aligned} \tag{16}$$

where $K_n(x)$ are the McDonalds functions, $a^2 = x^2 + y^2$, $P_t^2 = k^2 - \omega^2/c_t^2$, $P_l^2 = k^2 - \omega^2/c_l^2$. We will consider the region $k < \omega/c_l$. In this case, the following known relation must be used: $i^n K_n(ix) = (-i\pi/2) H_n^2(x)$, where $H_n^2(x)$ is the Hankel function. For $ka \ll 1$ one obtains

$$\begin{aligned} u_x(\vec{r}, t) = {} & -\frac{\Omega z \epsilon_0 c_t^2 \omega^2 \cos kz \sin \omega t}{16} \\ & \times \left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2 \omega^2} \right) y, \end{aligned} \tag{17}$$

$$\begin{aligned} u_y(\vec{r}, t) = {} & -\frac{\Omega z \epsilon_0 c_t^2 \omega^2 \cos kz \sin \omega t}{16} \\ & \times \left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2 \omega^2} \right) x. \end{aligned} \tag{18}$$

It is not necessary to present u_z since it does not enter $\bar{N}$. Indeed, this fact follows directly from Eq. (16)

and the explicit form of the force in Eq. (7) which is written out as

$$f_j = c_{ij12}\big[\Omega z\epsilon(z,t)\delta(\vec{\xi})\big]_{,i} - c_{ij32}\big[\Omega x\epsilon(z,t)\delta(\vec{\xi})\big]_{,i}. \tag{19}$$

Substituting Eqs. (17)–(19) into Eq. (6) one finally obtains

$$\bar{D} = \int (f_x\dot{u}_x + f_y\dot{u}_y)\,dx\,dy = \frac{\mu\Omega^2 z^2\epsilon_0^2 c_t^2\omega^3\cos^2 kz}{16}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2\omega^2}\right), \tag{20}$$

$$\overline{v^2} = \frac{\epsilon_0^2\omega^2\cos^2 kz}{2}. \tag{21}$$

In accordance with Eq. (5) the damping parameter B takes the form

$$B = \frac{\mu\Omega^2 z^2 c_t^2\omega}{8}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2\omega^2}\right). \tag{22}$$

Notice that this result is similar to that for an edge dislocation [10] with the exception of the factor Ωz instead of the Burgers vector b. At first glance, this is the well-known in disclination theory replacement. It leads, however, to the principally new physical situation when the damping parameter becomes z-dependent. This is important in analysis of the equation of motion.

4. Equation of motion and decrement

Let us consider the equation of motion (4). The Peach–Koehler force is written as [11,14]

$$F_r = \varepsilon_{rak}\tau_a u_i^P\sigma_{ik}, \tag{23}$$

where σ_{ik} is the strain tensor, ε_{rak} is the fully antisymmetric tensor, $\vec{\tau}$ is the unit tangent vector to the defect line, and $u_i^P = \vec{u}^+ - \vec{u}^- = [\vec{\Omega}\vec{R}]$ describes the jump in displacement at point P due to a disclination. Thus, we obtain

$$F_1 = -\Omega(z\sigma_{12} - x\sigma_{32}),$$
$$F_2 = -\Omega(x\sigma_{31} - z\sigma_{11}),$$
$$F_3 = 0. \tag{24}$$

We consider twist disclination moving in the glide plane xz. In this case, only the component F_1 will be incorporated in Eq. (4). Thus, the equation of motion takes the form

$$m(z)\frac{\partial^2\epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T(z)\frac{\partial\epsilon(z,t)}{\partial z}\right) - B(z)\frac{\partial\epsilon(z,t)}{\partial t} - \Omega(z\sigma_{12} - x\sigma_{32}). \tag{25}$$

For free motion the last two terms in Eq. (25) are discarded. This problem was studied in [8]. In particular, there were estimated the linear tension and the mass of twist disclination in the form $m(z) = \alpha z^2$, $T(z) = m(z)v^2$, where $\alpha = \rho\Omega^2/2$. Let us rewrite Eq. (22) as $B = \beta z^2$ with

$$\beta = \frac{\mu\Omega^2 c_t^2\omega}{8}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2K^2}{c_l^2\omega^2}\right),$$

and introduce the parameter

$$\gamma = \frac{\beta}{\alpha} = \frac{c_t^4\omega}{4}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2K^2}{c_l^2\omega^2}\right).$$

In this case, Eq. (25) takes the form

$$z^2\frac{\partial^2\epsilon}{\partial z^2} + 2z\frac{\partial\epsilon}{\partial z} - \frac{z^2}{v^2}\frac{\partial^2\epsilon}{\partial t^2} - \frac{z^2\gamma}{v^2}\frac{\partial\epsilon}{\partial t} - \frac{\Omega z\sigma_{12}}{v^2\alpha} = 0. \tag{26}$$

Notice that we omit here the term with σ_{32} which is responsible for the force along the disclination line. We consider a periodic stress wave in the form

$$\sigma_{12} = \sigma_0 e^{-i\omega t} = \sum_n \sigma_n \sin(k_n z)e^{-i\omega t}, \tag{27}$$

where σ_0 is the shear stress component of σ_a resolved in the xz glide plane and $\sigma_n = 4\sigma_0/\pi n$ is the Fourier coefficient. The exact solution to Eq. (26) for the nth normal mode is found to be

$$\epsilon_n(z,t) = \frac{C_n}{k_n z}\sin(k_n z)e^{-i\omega t} \tag{28}$$

with

$$C_n = \frac{k_n\Omega\sigma_n}{\alpha}\frac{1}{(i\gamma\omega + \omega^2 - k_n^2 v^2)}.$$

The last step is to substitute Eqs. (24) and (28) into Eq. (2). We obtain

$$\bar{P} = \sum_n \frac{\Omega^2\gamma\omega^2\sigma_n^2 L}{2\alpha(\gamma^2\omega^2 + (\omega^2 - k^2v^2)^2)}. \tag{29}$$

Then, the loss per cycle takes the form

$$\Delta W_L = \sum_n \frac{\pi \Omega^2 \gamma \omega \sigma_n^2 L}{\alpha(\gamma^2\omega^2 + (\omega^2 - k_n^2 v^2)^2)}, \tag{30}$$

and, finally, the internal friction is found to be

$$Q^{-1} = \frac{\Delta W}{2W} = \frac{N \Delta W_L}{2W} = \frac{8\Omega^2 q^2 \gamma \omega \mu \Lambda}{\pi \alpha} \times \sum_n \frac{1}{n^2(\gamma^2\omega^2 + (\omega^2 - k_n^2 v^2)^2)}, \tag{31}$$

where $\Lambda = 2NL/V$ is the density of disclinations and $q = \sigma_0/\sigma_a$ is the resolved shear stress orientation factor (cf., e.g., [5]).

The main contribution to the internal friction comes from the first term of series in Eq. (31). In this case, one has

$$Q^{-1} = \frac{8\Omega^2 q^2 \gamma \omega \mu \Lambda}{\pi \alpha} \frac{1}{(\gamma^2\omega^2 + (\omega^2 - \omega_1^2)^2)}, \tag{32}$$

where $\omega_1^2 = k_1^2 v^2 = \pi^2 v^2/L^2$. As is seen from Eq. (32) there is a close agreement between dislocation and disclination-induced contribution to the internal friction (cf. Ref. [2]). Indeed, in both cases the decrement has a resonance-like behavior. For small damping ($\omega_1 \gg \gamma$), the decrement is linear for frequencies below the resonant frequency, passes through a maximum, and then decreases like ω^{-3}. For large damping ($\omega_1 \ll \gamma$), the linear in ω behavior goes to a maximum value which occurs at an earlier frequency than the resonant frequency. It then decreases like ω^{-1} through the resonant frequency range and finally decreases like ω^{-3}. It is interesting to note that both the decrement and the resonant frequency are independent from Ω. This is directly seen from Eq. (31) since $\alpha \sim \Omega^2$. For dislocations the decrement does not depend on the Burgers vector as well. The maximum loss occurs at $\omega = \omega_1$ for small damping and at $\omega = \omega_1^2/\gamma$ for large damping. Finally, near the resonant frequency the loss is inversely proportional to the damping.

5. Conclusion

In this Letter we have calculated the frequency-dependent loss due to vibrating twist disclinations within the heterogeneous string model. We have found that the decrement is similar to that for dislocations. In particular, the decrement in Eq. (31) has a resonance type character and is proportional to the fourth power of the disclination length. An important conclusion can be made that the individual (local) properties of linear defects get lost within the string model (see also our previous Letter [8]). Namely, the main physical characteristics (heat capacity, internal friction) are found to be determined only by some general parameters of linear defects (the length of the defect line, the density of defects) and elastic body (the density of the solid, sound velocities, the shear modulus). It is known [15] that the experimental study of internal friction phenomena serves as an indirect method to detect dislocations in crystals. As it follows from our consideration, the same method can be used for detecting of disclinations in rotationally disordered materials.

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