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Contribution of mobile twist disclinations to the specific heat of crystals

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Abstract

Contribution to the specific heat of crystals due to pinned twist disclinations is studied within the vibrating string model. For this purpose, a line tension and an effective mass of a sliding twist disclination is calculated. Both the line tension and the effective mass are found to vary along the disclination line as z^2. On this basis, the model of *heterogeneous* string is formulated for the description of the vibrating pinned twist disclination. A solution to the equation of motion for heterogeneous string is obtained. The specific heat due to twist disclinations is found to be the linear function of the temperature and the defect density.

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1. Introduction

The thermal properties of mobile dislocations have been considered in 1958 by Granato [1]. In particular, he found a contribution of mobile dislocations to the specific heat of crystals by using the Granato–Lücke vibrating string model [2] for a pinned dislocation. The basis for this model is an analogy between the vibration of a pinned dislocation line segment and the forced damped vibration of a string. This simplified model was successful in the description of various aspects of dislocation dynamics. In particular, the vibrating string model offered a clearer view of mechanical damping [2], phonon scattering [3], and low-temperature thermal conductivity in dislocated crystals [4]. It should be noted that the basic characteristics of the string model are the line tension and the effective mass of the defect. For dislocations they have been calculated by Laub and Eshelby [5], and within a more general approach by Ninomia and Ishioka [6].

The dynamics of rotational defects in crystals, disclinations, is poorly understood. One of the most known papers is Ref. [7] where the movement of disclinations and disclination loops has been studied (see also Refs. [8,9]). In particular, a general equation for the force on a disclination loop and its axis as well as the condition for conservative movement were derived. And yet, the question about the real dynamics of disclinations and its influence on physical characteristics of crystals still remains to be answered. Meanwhile, the recent progress in a study of various topologically disordered materials shows clearly an importance of both disclinations and disclination loops

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(see, e.g., [10] and references therein). It is clear that a study of the thermal properties due to mobile disclinations is gaining in importance. In this Letter, we suggest the concept of vibrating string to study the dynamics of pinned twist disclinations and calculate the disclination-induced contribution to the specific heat of a crystal.

2. The general scheme

In dislocation theory, the line tension is determined by a conventional line-tension formula of the form (see, e.g., Refs. [5,11]) $F = T/\varrho$, where T is the static line tension, ϱ is the curvature radius, and F is an appropriate component of the Peach–Koehler force, f_i. The Peach–Koehler force can be generally written as (per unit length of the disclination line)

$$f_r = \varepsilon_{rak}\tau_a u_i^P \sigma_{ik}, \tag{1}$$

where σ_{ik} is the stress tensor, ε_{rak} is the fully antisymmetric tensor, $\vec{\tau}$ is the unit tangent vector to the defect line, and $\vec{u}^P = \vec{u}^+ - \vec{u}^- = \vec{b} + [\vec{\Omega}\vec{R}]$ describes the jump in displacement at point P due to a linear defect. Here $\vec{b}$ is the Burgers vector, $\vec{\Omega}$ is the Frank vector, and $\vec{R} = \vec{r} - \vec{r}_0$ is a vector from any point on the axis of rotation to point P. The stress tensor is determined via the static displacement fields in an elastic body caused by plastic deformation due to defect motion. As is well known, the displacement fields are obtained by using the Green's function (see, e.g., [12])

$$u_n(\vec{r}, t) = -\int c_{ijkl} G_{jn,i} \delta e_{kl}^{\mathrm{pl}}\, dV', \tag{2}$$

where c_{ijkl} are the elastic modulus, G_{jn} is the Green's tensor function, $\delta e_{kl}^{\mathrm{pl}}$ is the variation of plastic part of the strain tensor. Hereafter, the summation over repeated indices is assumed and $G_{jn,i} = \partial G_{jn}/\partial x_i$. Taken together these formulas give us a distinct way to find the static line tension of the linear defect.

To illustrate this scheme, let us consider the known case of the straight edge dislocation in an isotropic elastic body. For sliding dislocation one has [12]

$$\delta e_{kl}^{\mathrm{pl}} = \frac{1}{2}\big(b_k[\vec{\delta x}\vec{\tau}]_l + b_l[\vec{\delta x}\vec{\tau}]_k\big)\delta(\vec{\xi}), \tag{3}$$

where $\vec{\delta x}$ describes the displacement of the dislocation line and $\delta(\vec{\xi})$ is the two-dimensional delta-function. We consider a dislocation directed along the z-axis and take the xz plane as the slip plane, i.e., the Burgers vector is chosen to be $\vec{b} = (b, 0, 0)$. In this case, $\vec{\delta x} = (\epsilon, 0, 0)$, $\vec{\tau} = (0, 0, 1)$, $[\vec{\delta x}\vec{\tau}] = (0, -\epsilon, 0)$, and $\vec{\xi} = (x', y', 0)$, and Eq. (2) takes the form

$$u_n^d(\vec{r}) = \int c_{ijk2} G_{jn,i}(x, y, z - z') b_k \epsilon(z')\, dz'. \tag{4}$$

For isotropic case,

$$G_{km}(\vec{r}) = \frac{1}{8\pi\mu}\left[\frac{2}{r}\delta_{km} - \frac{1}{2(1-\nu)} r_{,km}\right]$$

and $c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ with λ and μ being the Lamé constants.

We suggest that the displacement of the dislocation line in the x direction is $\epsilon(z) = \epsilon(k)\exp(ikz)$. Performing in Eq. (4) straightforward calculations and substituting the displacement fields in Eq. (1) one obtains

$$\begin{aligned} f_1^d = {} & -2\epsilon(k) e^{ikz} \mu^2 b^2 k^2 \\ & \times \left[2A\left(1 - \frac{8x^2y^2}{a^4}\right) K_2(ka) \right. \\ & \left. - \frac{4Akx^2y^2}{a^3} K_1(ka) + (2A + B) K_0(ka)\right], \end{aligned} \tag{5}$$

where $A = -B/4(1-\nu)$, $B = 1/4\pi\mu$, $a^2 = x^2 + y^2$, and K_ν are the McDonalds functions.

At our choice of $\epsilon(z)$ the curvature radius ϱ can readily be obtained as

$$\varrho^{-1} = -k^2 \epsilon(k) e^{ikz}. \tag{6}$$

Thus, in the first order on ka one finally gets

$$\begin{aligned} T^d(k) = \frac{\mu b^2}{4\pi}\left[-\frac{(1-2\nu)}{(1-\nu)}\left(C + \ln\frac{ka}{2}\right) \right. \\ \left. + \frac{1}{2(1-\nu)}\right], \end{aligned} \tag{7}$$

where C is the Euler's constant. Notice that this result agrees with [5]. In practice, Eq. (7) is usually approximated by introducing the Debye cut-off $k_D \sim 1/a$, so that the value in brackets in Eq. (7) can be roughly estimated as 2π. Thus we arrive at the often-used expression $T = \mu b^2/2$. To complete the string picture one has to determine the effective mass of a dislocation. It can generally be obtained from the kinetic energy of the body containing the dislocation, $E_k = (\rho/2)\int \dot{u}_i^2\, dV$. The calculations are rather simple and can be found, for example, in [6,14]. The well-known approximate result is $m = \rho b^2/2$. Having in hand two main string parameters one can formulate the equation of motion of a pinned dislocation. This program has been performed in [2].

3. String model of twist disclination

The problem of motion of disclinations and disclination loops was examined in [7–9]. It was shown in [7] that straight wedge disclinations have no slip surfaces and cannot move conservatively. On the contrary, the straight twist disclination has its slip plane and can move conservatively. We will study the case 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, i.e., $\vec{\Omega} = (0, \Omega, 0)$, $\vec{\tau} = (0, 0, 1)$. In accordance with Eq. (1) the force on a disclination line can be written as

$$f_1 = \Omega(X_1\sigma_{32} - X_3\sigma_{12}),$$
$$f_2 = \Omega(X_3\sigma_{11} - X_1\sigma_{31}),$$
$$f_3 = 0. \tag{8}$$

The condition for conservative motion of a linear defect is generally written as $dV = 0$ (no vacancies are created or absorbed). It was shown for disclinations in [7] that the motion 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. Therefore the only component f_1 is of our interest for sliding twist disclination. By analogy with the case of edge dislocation we suggest that the motion of disclination line is oscillatory and $\vec{\delta x} = (\epsilon, 0, 0)$. Then the displacement fields are written as [13] (see also [9])

$$u_n(\vec{r}) = \mu\Omega \int_{-\infty}^{\infty} (G_{yn,x} + G_{xn,y})\epsilon(z')z'\, dz'. \tag{9}$$

We obtain

$$u_x(\vec{r}) = 2\mu\Omega\epsilon(k)e^{ikz}yk \times \left[\frac{2Ax^2k}{a^2}\big(zK_2(ka) + iaK_1(ka)\big) - \frac{(B+2A)}{a}\big(zK_1(ka) + iaK_0(ka)\big)\right], \tag{10}$$

$$u_y(\vec{r}) = 2\mu\Omega\epsilon(k)e^{ikz}xk \times \left[\frac{2Ay^2k}{a^2}\big(zK_2(ka) + iaK_1(ka)\big) - \frac{(B+2A)}{a}\big(zK_1(ka) + iaK_0(ka)\big)\right], \tag{11}$$

$$u_z(\vec{r}) = 4A\mu\Omega\epsilon(k)e^{ikz}xyk \times \left[kK_2(ka) - i\frac{zk}{a}K_1(ka) - \frac{3}{a}K_1(ka)\right]. \tag{12}$$

Notice that the first term in f_1 is of the second order in ϵ and can be omitted. Thus, in the linear in ϵ approximation one gets

$$f_1 = -2\mu^2\Omega^2\epsilon(k)e^{ikz}z \times \left[2Azk^2\left(1 - \frac{8x^2y^2}{a^4}\right)K_2(ka) + \left(i(B+4A)k^2a - \frac{4Ax^2y^2k^2}{a^3}(zk + 2i)\right)K_1(ka) - \left(k(B+2A)(2i - kz) + i\frac{4Ax^2y^2k^3}{a^2}\right)K_0(ka)\right]. \tag{13}$$

For $ka \ll 1$ the line tension takes the form

$$T(k,z) = \frac{\mu\Omega^2z^2}{4\pi}\left[-\frac{(1-2\nu)}{(1-\nu)}\left(C + \ln\frac{ka}{2}\right) + \frac{1}{2(1-\nu)}\right]. \tag{14}$$

It is interesting to note that Eq. (14) agrees with Eq. (7) except for the factor Ωz instead of b. An appearance of such space-dependent factor is well-known in disclination theory. In particular, a twist disclination has specific property of a linear divergence of strain fields along its line. This leads to the corresponding quadratic divergence in the energy of twist disclinations that can be directly seen from Eq. (14). By making use of the approximation made in the previous section we finally obtain

$$T(z) = \frac{\mu \Omega^2 z^2}{2}. \quad (15)$$

The last step is to determine the mass of twist disclination. The calculations are similar to those for the case of a dislocation (see, e.g., Refs. [6,14]) and the result is

$$m(z) = \frac{\rho \Omega^2 z^2}{16\pi(1-\nu)^2}\left[2(1-2\nu)^2 + (3-4\nu)\right]\ln\frac{R}{a_0}, \quad (16)$$

where $m(z)$ is the mass per unit length of the disclination, R and a_0 are the cut-off parameters. It should be noted that analogously to Eq. (14) this result agrees with that for a dislocation (cf., e.g., [14]) with the exception of the factor Ωz instead of b. As for a dislocation one can approximate Eq. (16) as

$$m(z) = \frac{\rho \Omega^2 z^2}{2}. \quad (17)$$

Thus, both the linear tension and the mass of the disclination depend on z. This means that twist disclination can be represented as a string with the understanding that this is a *heterogeneous* string. Therein lies the essential difference from the case of a dislocation where the string is considered to be homogeneous.

4. Equation of motion

The equation of motion for heterogeneous string is written as

$$m(z)\frac{\partial^2 \epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T(z)\frac{\partial \epsilon(z,t)}{\partial z}\right). \quad (18)$$

When m and T are constants, which is the case of a dislocation, one obtains the familiar equation for harmonic vibrations. Notice that the linear tension and the effective mass of a dislocation are found to be related by $T = mv^2$ with $v = \sqrt{\mu/\rho}$. In accordance with Eqs. (15) and (17), a similar relation becomes also valid for twist disclination where, however, it holds locally, $T(z) = m(z)v^2$.

We seek the solution to Eq. (18) in the form

$$\epsilon(z,t) = \epsilon(z)\cos\omega t. \quad (19)$$

In this case, Eq. (18) reads

$$z^2\frac{\partial^2 \epsilon(z)}{\partial z^2} + 2z\frac{\partial \epsilon(z)}{\partial z} + \frac{z^2\omega^2}{v^2}\epsilon(z) = 0, \quad (20)$$

with Eqs. (15) and (17) taken into account. The solution is found to be

$$\epsilon(z) = \frac{v}{\omega z}\left(C_1 \sin\frac{\omega z}{v} + C_2\cos\frac{\omega z}{v}\right), \quad (21)$$

where C_1 and C_2 are arbitrary constants. By using of the boundary conditions in the form $\epsilon(-L) = \epsilon(L) = 0$ one finally obtains

$$\epsilon(z,t) = \frac{\epsilon_0 v}{\omega z}\sin\frac{\omega z}{v}\cos\omega t, \quad (22)$$

with ϵ_0 being the maximal amplitude (at $z = 0$) and the spectrum

$$\omega_n = v|k_n|, \quad k_n = \pi n/L, \quad n = 0, \pm 1, \pm 2, \ldots. \quad (23)$$

Thus the vibrations have a rather complex form which is characterized by a decreasing with z amplitude. At the same time nodes are distributed regularly. This makes a study of the contribution to the thermal characteristics due to vibrating twist disclinations similar to that for dislocations.

5. Contribution to the specific heat

We are interested in the contribution to the specific heat. The following calculations are similar to those in the case of dislocations [1]. Namely, the internal energy is written as

$$U = \sum_n \frac{\hbar\omega_n}{\exp(\hbar\omega_n/k_B T) - 1}, \quad (24)$$

where the sum is over all the normal modes of the vibrating disclination, and k_B is the Boltzmann constant. Approximating the sum by an integral in the usual way one finally obtains

$$U = \frac{2L}{\pi v}\int_0^\infty \frac{\hbar\omega}{\exp(\hbar\omega/k_B T) - 1}\,d\omega = \frac{\pi L k_B^2 T^2}{3v\hbar}. \quad (25)$$

Therefore the contribution to the specific heat is

$$c_v = \frac{2\pi L k_B^2 T}{3v\hbar}, \tag{26}$$

and the specific heat per mole is finally written as

$$C_v = p\frac{\pi^2}{3}\frac{\Lambda a_0^2}{Z} N k_B \frac{T}{\Theta}, \tag{27}$$

where a_0 is the lattice constant, Λ is the disclination density, N is the number of atoms per mole, Z is the number of atoms per unit cell, Θ is the Debye temperature, and $p = v_0/v$ with v_0 being the sound velocity in the perfect lattice. Notice that a similar result has been obtained in [1] for dislocations. The most interesting feature of Eq. (27) is the linear variation with temperature. As is known, this behavior is familiar to glassy materials. This fact has stimulated a study of the dislocation contribution to the specific heat of glassy $Pd_{78}Si_{16}Cu_6$ in [15] where a good quantitative agreement with the experimentally measured value of the specific heat was found.

It has recently been shown in [16] that the experimental data for the thermal conductivity in vitreous silica (a-SiO_2) can be explained within the disclination-based model. It is interesting therefore to estimate the contribution to the specific heat due to vibrating disclinations. We will use the parameter set from [16]. Namely, $\Lambda = 2 \times 10^{15}$ m^{-2}, $a_0 = 2.88 \times 10^{-10}$ m, $\Theta = 342$ K, $\rho = 2200$ kg/m^3, $\mu = 3.2 \times 10^{10}$ N/m^2. Additionally, we use in Eq. (27) $p = 1.075$ and $Z = 3$. In this case one obtains $C_v/T = 4.7 \times 10^{-6}$ J/K^2 mol. It is interesting to note that this value is in a reasonable agreement with the experimental data [17]. Actually, this good agreement is scarcely surprising. Indeed, as has been observed by Zeller and Pohl in [17], the linear specific heat anomaly could suggest linear chains. Moreover, they have indicated that about 10^{15} chains per square meter are needed in order to explain the magnitude of the observed anomaly. This is exactly the density of linear defects that we have used in [16] and, accordingly, in this Letter.

6. Summary

In this Letter we have introduced the concept of vibrating string to study the dynamics of pinned twist disclinations. We have considered the case of the conservatively moving twist disclination. The most important conclusion is that the concept of vibrating string becomes valid for twist disclination, however, an important distinction from the case of the dislocation is established. Namely, we have found that the basic characteristics of a string are z-dependent. This finding allowed us to formulate the model of *heterogeneous* string for twist disclination. Although the vibration dynamics is affected in comparison with the case of a dislocation, the spectrum of the vibrating disclination is proved to be precisely the same. The contribution to the specific heat is found to depend linearly on the temperature and the disclination density. The numerical estimation of the specific heat for vitreous silica shows a good agreement with the experiment.

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