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The influence of twist disclinations on the specific heat and internal friction of disordered semiconductors

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Abstract
The heterogeneous string model for a twist disclination, which is an extended defect of rotational type, is considered. Within the framework of this model, the contribution of twist disclinations to the specific heat and internal friction of disordered semiconductors is calculated.

1. Introduction

Recently, the low-temperature thermal conductivity of some polycrystalline semiconductors was found [1] to reveal a glass-like behaviour typical for amorphous materials. We remark that amorphous semiconductors are of steady current interest. There is reason to believe that extended defects such as dislocations and disclinations can play a significant role in the description of transport properties of amorphous solids [2]. Therefore, it is interesting to find the contribution of the extended defects to other thermal characteristics of disordered semiconductors. In this paper, we calculate the contribution to the specific heat and internal friction due to twist disclinations within the heterogeneous string model.

2. The specific heat

In dislocation theory, the line tension is determined by a conventional line-tension formula of the form $F = T/\rho$, 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, of opposite sign (see, e.g., [3, 4]). The Peach–Koehler force can generally be written (per unit length of the disclination line) as

$$F_r = \varepsilon_{rak}\tau_a u_i^P \sigma_{ik}, \qquad (1)$$

where σ_{ik} is the stress tensor, ε_{rka} is the fully antisymmetric tensor, $\vec{\tau}$ is the unit vector tangent 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

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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. For line tension and effective mass 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 function (see, e.g., [5])

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

where c_{ijkl} is the elastic modulus, G_{jn} is the Green tensor function, δe_{kl}^{pl} is the variation of the plastic part of the strain tensor. Hereafter, the summation over repeated indices is assumed and $G_{jn,i} = \partial G_{jn}/\partial x_i$. Let us apply this scheme to twist disclination. The problem of motion of disclinations and disclination loops was examined in [6–8]. It was shown in [6] that straight wedge disclinations have no slip surfaces and cannot move conservatively. In contrast, the straight twist disclination has a 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 equation (1) the force on a disclination line can be written as

$$F_1 = -\Omega(X_3\sigma_{12} - X_1\sigma_{32}), \qquad F_2 = -\Omega(X_1\sigma_{31} - X_3\sigma_{11}), \qquad F_3 = 0. \tag{3}$$

The condition for conservative motion of a linear defect is generally written as $\mathrm{d}V = 0$ (no vacancies are created or absorbed). It was shown for disclinations in [6] 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 only the component F_1 is of interest for sliding twist disclination. We suggest that the motion of the disclination line is oscillatory and $\vec{\delta x} = (\epsilon, 0, 0)$. Then the displacement fields are written as [9] (see also [8])

$$u_n(\vec{r}) = \mu\Omega \int_{-\infty}^{\infty} (G_{yn,x} + G_{xn,y})\epsilon(z') z'\, \mathrm{d}z'. \tag{4}$$

Performing straightforward calculations one obtains in the linear-in-ϵ approximation (for $ka \ll 1$)

$$T(z) = \frac{\mu\Omega^2 z^2}{2}. \tag{5}$$

The last step is to determine the mass of the twist disclination. The calculations are similar to those for the case of a dislocation (see, e.g., [10, 11]) and the result is

$$m(z) = \frac{\rho\Omega^2 z^2}{2}. \tag{6}$$

Thus, both the linear tension and the mass of the disclination depend on z. This means that a twist disclination can be represented as a string, with the understanding that this is a *heterogeneous* string. The equation of motion (without damping) for heterogeneous string is written as

$$m(z)\frac{\partial^2 \epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T(z)\frac{\partial \epsilon(z,t)}{\partial z}\right). \tag{7}$$

By using of the boundary conditions in the form $\epsilon(-L) = \epsilon(L) = 0$ one finally obtains

$$\epsilon(z,t) = \frac{\epsilon_0 v}{\omega z} \sin\frac{\omega z}{v} \cos\omega t, \tag{8}$$

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

$$\omega_n = v|k_n|, \qquad k_n = \pi n/L, \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{9}$$

Now, we are interested in the contribution to the specific heat. The internal energy is written as

$$U = \sum_n \frac{\hbar\omega_n}{\exp(\hbar\omega_n/k_B T) - 1}, \tag{10}$$

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, one finally obtains the specific heat per mole:

$$C_v = p\frac{\pi^2}{3}\frac{\Lambda a_0^2}{Z} N k_B \frac{T}{\Theta}, \tag{11}$$

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. To make estimates, let us use the values $\Lambda = 10^{14}$ m^{-2}, $a_0 = 10^{-9}$ m. Equation (11) takes then the form $C_v = 3.3 \times 10^{-4}(pNk_B/Z)(T/\Theta)$ J K^{-2} mol^{-1}. Notice the linear variation of the heat capacity with temperature which is typical for amorphous materials.

3. The decrement

Making an analogy with dislocations [12], we will study the effect of pinned disclinations on the energy lost by the stress wave travelling 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

$$Q^{-1} = \frac{\overline{\Delta W}}{2\overline{W}}, \tag{12}$$

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

$$\overline{P} = \sum_n \frac{1}{T}\int_0^T \int_{-L}^{L} \mathrm{Re}(F_i)\,\mathrm{Re}(\dot{\epsilon}_i^n)\,\mathrm{d}l\,\mathrm{d}t \tag{13}$$

determines the mean energy (in unit time) lost to friction. Here F_i is the Peach–Koehler force acting on unit length of the disclination line due to the 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 $\overline{W} = \sigma_a^2/2\mu$, where σ_a is the amplitude of the applied stress wave and μ is the shear modulus. To find ϵ_i, one has to study the equation of motion of the disclination. 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

$$m\frac{\partial^2\epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T\frac{\partial\epsilon(z,t)}{\partial z}\right) - B\frac{\partial\epsilon(z,t)}{\partial t} + F_i, \tag{14}$$

where m is the mass of the 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 several damping mechanisms known (see, e.g., [13]). Following Eshelby [14], we suppose here that the damping constant is entirely due to the reradiation damping mechanism. In this case,

$$B = \frac{\overline{D}}{v^2} \tag{15}$$

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 [14], the rate of radiation is

$$\overline{N} = \int f_i \dot{u}_i \, \mathrm{d}V \tag{16}$$

where elastic displacements u_i are caused by fictitious forces f_i. As is known [9], the fictitious forces f_i are determined by

$$f_j = -c_{ijkl}\, \delta e^{\mathrm{pl}}_{kl,i}. \tag{17}$$

The displacement fields can be obtained by using the dynamic Green function

$$u_n(\vec{r}, t) = -\int c_{ijkl} G_{jn,i}\, \delta e^{\mathrm{pl}}_{kl}\, \mathrm{d}V' \tag{18}$$

where G_{ij} is the dynamic Green tensor function. Explicitly (see [14]),

$$G_{jn} = \chi_{,jn} + \delta_{jn}\bar{\omega}, \tag{19}$$

with

$$\bar{\omega} = \frac{\mathrm{e}^{\mathrm{i}\omega(t-R/c_t)}}{4\pi\mu R}, \qquad \chi = \frac{c_t^2}{\omega^2}\frac{\mathrm{e}^{\mathrm{i}\omega(t-R/c_t)}}{4\pi\mu R} - \frac{c_t^2}{\omega^2}\frac{\mathrm{e}^{\mathrm{i}\omega(t-R/c_l)}}{4\pi\mu R}. \tag{20}$$

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. 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. We suggest that the motion and geometry of the twist disclination are the same as above. Then the displacement fields in equation (18) can be written as (see also [8, 9])

$$u_n(\vec{r}, t) = \mu\Omega\epsilon_0 \mathrm{e}^{\mathrm{i}\omega t} \int_{-\infty}^{\infty} (G_{yn,x} + G_{xn,y}) \mathrm{e}^{\mathrm{i}kz'} z'\, \mathrm{d}z'. \tag{21}$$

We will consider the region $k < \omega/c_l$. In this case, for $ka \ll 1$ one finally obtains (see [15] for details)

$$\overline{D} = \frac{\mu\Omega^2 z^2 \epsilon_0^2 c_t^2 \omega^3 \cos^2 kz}{16}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2\omega^2}\right), \qquad \overline{v^2} = \frac{\epsilon_0^2\omega^2\cos^2 kz}{2}. \tag{22}$$

In accordance with equation (15), the damping parameter B takes the form

$$B = \frac{\mu\Omega^2 z^2 c_t^2 \omega}{8}\left(\frac{1}{c_t^4} + \frac{1}{c_l^4} - \frac{2k^2}{c_l^2\omega^2}\right). \tag{23}$$

Thus, the damping parameter becomes z-dependent. Let us consider the equation of motion (14). The Peach–Koehler force is the same as in (1). We consider twist disclination moving in the glide plane xz. In this case, only the component F_1 will be incorporated in equation (14). Thus, the equation of motion takes the form

$$m(z)\frac{\partial^2\epsilon(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left(T(z)\frac{\partial\epsilon(z,t)}{\partial z}\right) - B(z)\frac{\partial\epsilon(z,t)}{\partial t} - \Omega(z\sigma_{12} - x\sigma_{32}). \tag{24}$$

In our case, equation (24) takes the form

$$z^2\frac{\partial^2\epsilon}{\partial z^2} + 2z\frac{\partial\epsilon}{\partial z} - \frac{z^2}{v^2}\frac{\partial^2\epsilon}{\partial t^2} - \frac{z^2\gamma}{v^2}\frac{\partial\epsilon}{\partial t} - \frac{\Omega z\sigma_{12}}{v^2\alpha} = 0. \tag{25}$$

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

$$\sigma_{12} = \sigma_0 \mathrm{e}^{-\mathrm{i}\omega t} = \sum_n \sigma_n \sin(k_n z)\mathrm{e}^{-\mathrm{i}\omega t}, \tag{26}$$

where σ_0 is the shear stress component of σ_a resolved in the glide plane xz and $\sigma_n = 4\sigma_0/\pi n$ is the Fourier coefficient. The exact solution to equation (25) for the nth normal mode is found to be

$$\epsilon_n(z,t) = \frac{C_n}{k_n z}\sin(k_n z)\mathrm{e}^{-\mathrm{i}\omega t}, \qquad C_n = \frac{k_n \Omega \sigma_n}{\alpha}\frac{1}{(\mathrm{i}\gamma\omega + \omega^2 - k_n^2 v^2)}. \tag{27}$$

The last step is to substitute equations (3) and (27) into (13). We obtain

$$\overline{P} = \sum_n \frac{\Omega^2 \gamma \omega^2 \sigma_n^2 L}{2\alpha(\gamma^2\omega^2 + (\omega^2 - k^2 v^2)^2)}. \tag{28}$$

Then, the loss per cycle takes the form

$$\Delta W_L = \sum_n \frac{\pi \Omega^2 \gamma \omega \sigma_n^2 L}{\alpha(\gamma^2\omega^2 + (\omega^2 - k_n^2 v^2)^2)}, \tag{29}$$

and, finally, the internal friction is found to be

$$Q^{-1} = \frac{\Delta W}{2W} = \frac{N\,\Delta W_L}{2W} = \frac{8\Omega^2 q^2 \gamma \omega \mu \Lambda}{\pi \alpha} \sum_n \frac{1}{n^2(\gamma^2\omega^2 + (\omega^2 - k_n^2 v^2)^2)} \tag{30}$$

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., [16]).

The main contribution to the internal friction comes from the first term of series in equation (30). In this case, one has

$$Q^{-1} = \frac{8\Omega^2 q^2 \gamma \omega \mu \Lambda}{\pi \alpha} \frac{1}{(\gamma^2\omega^2 + (\omega^2 - \omega_1^2)^2)}, \tag{31}$$

where $\omega_1^2 = k_1^2 v^2 = \pi^2 v^2/L^2$.

4. Conclusions

In this paper, we have calculated the specific heat and the frequency-dependent loss due to vibrating twist disclinations within the heterogeneous string model. We have found that the decrement in equation (30) has a resonance-type character and is proportional to the fourth power of the disclination length. In turn, the heat capacity varies linearly with temperature and density of defects. An important conclusion can be drawn: that the individual (local) properties of linear defects get lost within the string model. That is, 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 [17] that the experimental study of internal friction phenomena serves as an indirect method for detecting dislocations in crystals. As follows from our consideration, the same method can be used for detecting of disclinations in semiconductors.

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