Transport in Materials with Disclination Dipoles: Applications to Polycrystals and Amorphous Dielectrics

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The problem of both electron and phonon scattering by wedge disclination dipoles (WDD) is studied in the framework of the deformation potential approach. The exact analytical results for the mean free path are obtained within the Born approximation. The WDD-induced contribution to the residual resistivity in nanocrystalline metals is estimated. Using the WDD-based model of a grain boundary, the thermal conductivity, \( \kappa \), of polycrystals and amorphous dielectrics is studied. It is shown that the low-temperature crossover of \( \kappa \) experimentally observed in LiF, NaCl, and sapphire can be explained by the grain-boundary phonon scattering. A combination of two scattering processes, the phonon scattering due to biaxial WDD and the Rayleigh-type scattering, is suggested to be of importance in amorphous dielectrics. Our results are in a good agreement with the experimentally observed \( \kappa \) in a-SiO\(_2\), a-GeO\(_2\), a-Se, and polystyrene over a wide temperature range.

I. INTRODUCTION

There exist many varieties of extended defects in crystals, topological in their origin. The most known examples are dislocations, disclinations, twins, grain boundaries, stacking faults etc. These defects play a significant role in description of various phenomena in real crystals as well as in non-crystalline materials. In particular, there is reason to believe that linear defects like dislocations and disclinations are the principal imperfections of liquid crystals, some amorphous solids, and polymers.

The contribution to the transport characteristics due to dislocations is now well understood (see, e.g., Ref.\([1]\)). Some aspects of the qualitative behavior of the disclination-induced electron scattering have been recently presented\([2]\). In particular, it was found that both dislocations and disclinations can be effective scattering centers for conducting electrons, especially at low temperatures when other scattering mechanisms are suppressed. Thus, along with point impurities, these defects give a contribution to the residual resistivity. In real crystals, however, the isolated disclinations are rather exotic objects. Instead, for topological reasons, the dipole configurations are more favourable. In addition, the creation energy for a single disclination considerably exceeds that for a disclination dipole.

There is another reason to call attention to dipoles of disclinations. As a matter of fact, the wedge disclination dipoles (WDD) simulate finite dislocation walls. In turn, dislocation walls describe the low-angle grain boundaries.\([3]\) Thus, one can expect that the results obtained for disclination dipoles will be useful in description of the grain-boundary scattering problem. This allows us to extend the possible applications to a study of the transport properties of polycrystals where grain boundaries are of importance. In particular, there is experimental evidence that the grain boundaries give contribution to the resistivity in metals (see, e.g., review in Ref.\([4]\)) which in part depends on the size of the grain boundary. Notice that though the problem of the grain-boundary-induced scattering has been formulated many years ago the proper solution is still absent.

A theory of the phonon scattering by grain boundaries has been developed within the Born approximation in Ref.\([5]\). A grain boundary was considered as a wall of edge dislocations with a rather strong assumption that the dislocation wall is infinitely long. Nevertheless, the main properties predicted by this model have been confirmed by experiments\([6,7]\). In particular, the phonon mean free path was found to be a constant over a wide temperature range. As a result, the low-temperature thermal conductivity in polycrystals varies as \( T^3 \) in agreement with the experimental data. However, the model of an infinitely long dislocation wall failed to describe a remarkable increase in thermal conductivity observed below some characteristic temperature \( T' \) (\( T' \sim 0.1K \) for LiF\([8,9]\)).

Recently\([10]\), the grain boundary phonon scattering problem has been investigated within the more realistic model which takes into account the finiteness of the boundary. The basis for this model was the known analogy between disclination dipoles and finite walls of edge dislocations\([3,11]\). It was found that the proper consideration of the finiteness of the boundary results in the low-temperature crossover of the thermal conductivity in agreement with experiments\([12,13]\).

A more intriguing application is an attempt to describe the physics of amorphous dielectrics by considering...
WDD as the basic structural elements. This point of view agrees with the cluster picture proposed earlier for glasses. In accordance with this picture there exist many small crystalline grains (microclusters with average diameters of order 20-30Å) in the amorphous state. On the other hand, the concept of elastic dipoles for orientational glasses was introduced and successfully explored in Refs. 1, 12. The authors considered elastic dipoles as the additional to two-level systems (TLS) structural elements of glasses. This assumption allows them to describe both the specific heat and the thermal conductivity of some glasses in the plateau region and above (up to 100K). The physical nature of these dipoles, however, has not yet been clarified. As is known, a possible way to understand the microstructure as well as the nature of principal imperfections is to study the transport properties of a material. It will be shown below that the concept of the elastic dipole can be successfully realized via dipoles of wedge disclinations without considering TLS. Namely, the WDD-induced phonon scattering is found to provide the correct description of the low-temperature thermal conductivity of amorphous dielectrics. Notice also that in accordance with the geometrical consideration disclinations are expected to always be present in the amorphous state (see also Ref. 11).

The main goal of the paper is twofold. First, we outline the general formalism of the WDD-induced scattering for both electrons and phonons. The most important details needed for a better understanding of calculations are given. Second, we apply the results obtained for description of two important problems. The first one is the experimentally observed deviation of the thermal conductivity from a $T^3$ dependence below 0.1 K in LiF and NaCl. The second problem is the thermal conductivity of amorphous dielectrics. It was shown in Ref. 13 that the experimentally observed behavior of thermal conductivity of a-SiO$_2$ over a wide temperature range can be explained by a combination of two scattering processes. The first one comes from the phonon scattering due to biaxial WDD while the second one is the Rayleigh type scattering. In the present paper we extend our investigation to other glasses and discuss some unsolved questions.

The paper is organized as follows. The general formalism of the WDD-induced scattering is presented in Sec.II. We consider all possible types of WDD and calculate the corresponding phonon mean free paths. The principal distinction between the scattering properties of the uniaxial and biaxial dipoles is shown. The developed approach is applied to estimation of the WDD-induced contribution to the residual resistivity of granular metals in subsection A. The phonon scattering due to WDD is studied and the contribution to the thermal conductivity is calculated in subsection B. The obtained results are compared with the experimental data for LiF. In Sec.III we apply the WDD-induced mechanism of phonon scattering to the problem of thermal conductivity in amorphous dielectrics. The results are compared with the experimentally observed $\kappa$ in a-SiO$_2$, a-GeO$_2$ a-Se, and polystyrene (PS). Sec.IV is devoted to the detailed discussion of the results obtained, specifically with relation to the proposed WDD-based model for dielectric glasses.

II. THEORY OF THE WDD-INDUCED SCATTERING

In this section we study the contribution to the effective cross-section which comes from the potential associated with a static deformation of a lattice caused by straight WDD. Two reasonable approximations are in common usage in studies of such problems (see, e.g., Refs. 14, 15). First, we suppose that the scattering processes are elastic and, second, the Born approximation is valid. Besides, we will consider here the simplest case when the only elastic deformations are dilatations.

In this case, an effective perturbation energy due to the strain field caused by a single WDD takes the form

$$U(r) = GSpE_{ij},$$

where $E_{ij}$ is the strain tensor and $G$ is an interaction constant.

Let the disclination lines be oriented along the z-axis, the position of the positive disclination be (0,-L) while of the negative one (0,L) (see Fig.1).

FIG. 1. Schematic picture of a wedge disclination dipole with shifted by distances $l_1$ and $l_2$ axes of rotation. The disclination lines are oriented along the z-axis for both defects.

Notice that in the general case the axes of rotations (with $\Omega_1 = \Omega e_z$ and $\Omega_2 = -\Omega e_z$) are shifted relative to their positions by arbitrary distances $l_1$ and $l_2$, respectively. For $l_1 = l_2 = 0$ one gets the biaxial WDD with nonskew axes of rotation. It was shown that this dipole can be simulated by a finite wall of edge dislocations with parallel Burgers vectors. In particular, the far strain fields caused by biaxial WDD agree with those from a finite dislocation wall.

For $l_1 - l_2 = 2L$ and $l_1 = -l_2$ one gets the uniaxial and the symmetrical uniaxial WDD, respectively. Notice
that uniaxial WDD can be simulated by a finite wall of edge dislocations complemented by two additional edge dislocations at both ends of the wall. The sign of these dislocations is opposite to that of the dislocations in the wall and absolute values of Burgers vectors are equal to $b = 2L \tan(\Omega/2)$ ($b = b_y$ at chosen geometry). As a result, the uniaxial WDD becomes a strongly screened system as opposed to the biaxial WDD (see Fig.2). In the general case, $l_1 \neq l_2 \neq 0$, one gets the biaxial WDD with shifted axes of rotation.

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FIG. 2. Contour plot of the perturbation energy $U(r)$ $U(x, y) = B \left[ \frac{1}{2} \ln \frac{(x + L)^2 + y^2}{(x - L)^2 + y^2} - l_1 \frac{x + L}{(x + L)^2 + y^2} + l_2 \frac{x - L}{(x - L)^2 + y^2} \right]$, (2)

where $B = G \nu (1 - 2\sigma)/(1 - \sigma)$, $\nu = \Omega/2\pi$ is the Frank index, and $\sigma$ is the Poisson constant. Notice that all possible types of WDD are included in Eq.(2).

As is seen from Eqs.(A1) and (A2) in Appendix, all strains caused by WDD are located in the $xy$-plane. In this case, the only components of the wavevector that are normal to the defect lines, $q = q_\perp$, are involved in the scattering process. For the sake of simplicity, let us assume that incident carriers are normal to disclination lines.

The problem reduces to the two-dimensional case with the mean free path given by

$$\Lambda^{-1} = n_i \int_0^{2\pi} (1 - \cos \theta) R(\theta) d\theta.$$ (3)

Here $R(\theta)$ is an effective differential scattering radius, and $n_i$ is the areal density of WDD. Notice that when axes of WDD are oriented randomly, one has to perform an additional averaging over all possible angles of incidents. As was shown for dislocations, however, such averaging leads merely to a modification of the numerical factor in $R(\theta)$.

Within the Born approximation, $R(\theta)$ is determined to be

$$R(\theta) = \frac{q S^2}{2 \pi h^2 v^2} |q | U(r) | q |.$$(4)

where all vectors are two-dimensional, $S$ is a projected area, $v$ is a carrier velocity, the bar denotes an averaging procedure over $\alpha$ which defines an angle between $p = q - q'_\perp$ and the $x$-axis. In other words, it means averaging over randomly oriented dipoles in the $xy$ plane. Evidently, the problem reduces to the estimation of the matrix element in Eq.(4) with the potential from Eq.(2). For this purpose, it is convenient to use the polar coordinates $(r, \phi)$

$$U(p, \alpha) = < q | U(r) | q'_\perp >$$

$$= \frac{1}{S} \int d^2 r \exp[i pr \cos(\phi - \alpha)] U(r, \phi).$$ (5)

For elastic scattering, the matrix element in Eq.(5) depends only on $|q| = |q'|$ and the scattering angle $\theta$. Thus, $p = |p| = |q - q'_\perp| = 2q \sin(\theta/2)$.

After integration in Eq.(5) and following averaging of $|U(p, \alpha)|^2$ with respect to $\alpha$ one obtains (see details in Appendix B)
\[ \Re(\theta) = \frac{\pi B^2}{\hbar^2 v^2 \sin(\theta/2)} \left\{ \frac{2}{p^2} \left( 1 - J_0(2pL) \right) - \frac{2A}{p^2} J_1(2pL) + \frac{\Delta^2}{2p} \left( \frac{1}{2} + J_0(2pL) \right) - \frac{J_1(2pL)}{2pL} \right\}, \]  

where \( \Delta = l_1 - l_2 \), \( J_n(t) \) are the Bessel functions. Upon integrating Eq.(3) with respect to \( \theta \) one finally obtains

\[ \Lambda^{-1} = \frac{B^2 L^2 \pi^2 \nu_i}{q\hbar^2 v^2} \left\{ \frac{1}{2} \left( \frac{1}{2} + J_0^2(2qL) \right) - \frac{4}{qL} J_0(2qL) J_1(2qL) \right\}, \]  

where \( z = \Delta t/L \). It should be emphasized that Eq.(7) is the exact result which allows us to describe all types of WDD. Notice, that the behavior of \( \Lambda \) in Eq.(7) is actually governed by the only parameter \( 2L \).

Let us consider two important limiting cases. For biaxial dipoles with \( \Delta = 0 \) \( (z = 0) \) one obtains

\[ \Lambda^{-1}_{bi} = \frac{8B^2 L^2 \nu_i \pi^2}{q\hbar^2 v^2} \left\{ J_0^2(2qL) + J_1^2(2qL) \right\}, \]  

For uniaxial dipoles \( \Delta = 2L \) \( (z = 2) \), and the mean free path \( \Lambda \) is

\[ \Lambda^{-1}_{uni} = \frac{2B^2 L^2 \nu_i \pi^2}{q\hbar^2 v^2} \left\{ 1 + J_0^2(2qL) - J_1^2(2qL) \right\}. \]  

In what follows, we apply the developed formalism to the problem of the WDD-induced electron and phonon scattering.

**A. Electron scattering: WDD-induced residual resistivity in metals**

As is known, the residual resistivity of metals may be caused by electron scattering due to linear defects like dislocations, stacking faults and grain boundaries. It was mentioned in the introduction that the WDD-based model is a good candidate for modelling the grain boundaries. Thus, the previous analysis allows us to study the contribution to the residual resistivity due to grain boundaries.

Let us use the well-known Drude formula for the resistivity in the static regime

\[ \rho = \frac{(m ne^2)}{\pi B^2 \hbar^2} \left( \frac{1}{\tau} \right), \]

where \( \tau \) is the relaxation time, \( m \) and \( e \) are the mass and the charge of the conducting electron, and \( n \) is the electron density. For point impurities and linear defects like dislocations and disclinations, the angle brackets denote the configurational average. In our case, this is averaging over \( \alpha \) in Eq.(4). Thus, one can write the final result

\[ \rho = \frac{(m v_F)}{\pi B^2 \hbar^2} \Lambda^{-1}, \]

with \( \Lambda \) from Eq.(7), where \( q = q_F, \nu = v_F, \) and \( G = G_d \).

Obviously, index \( F \) denotes the Fermi values, and \( G_d \approx (2/3)E_F \) is the deformation potential constant \( \text{[11]} \), where \( E_F \) is the Fermi energy. For simplicity, we restrict our consideration to metals of zinkblende or wurtzite structures. In metals typically \( q_F \approx 0.6 \div 1.2\,\text{Å}^{-1}. \) A dipole separation is chosen to be \( 2L \approx 10^2 \div 10^4\,\text{Å} \) which is of order of the grain size in polycrystals. In this case, \( 2qF L \gg 1 \) and, consequently, the Bessel functions in Eq.(7) can be approximated by their asymptotic values. The results are the following

\[ \rho_{bi} = \frac{16B^2 \pi L \nu_i}{ne^2 mv_F^2}. \]

and

\[ \rho_{uni} = \frac{2B^2 \pi^2 L^2 \nu_i}{ne^2 \hbar v_F^2}, \]

where \( B = B(G = G_d) \).

The main difference in the behavior of \( \rho_{bi} \) and \( \rho_{uni} \) comes from their \( L \)-dependence. As is seen, at fixed \( \nu_i \) \( \rho_{bi} \sim L \) while \( \rho_{uni} \sim L^2 \). As the result, \( \rho_{bi} \) is found to be larger than \( \rho_{uni} \). This agrees with the above-mentioned properties of these dipoles. In the case of biaxial WDD, the main contribution comes from the low-angle scattering processes in view of the long-range character of the perturbation energy in Eq.(2). On the contrary, for uniaxial WDD the large-angle scattering dominates since they are strongly screened systems (see Fig.2). In particular, at \( 2L \approx 10^3 \div 10^4\,\text{Å}, \nu_i \approx 10^9\,\text{cm}^{-2}, \) and \( \nu = 0.01 \) one obtains \( \rho_{bi} \approx 10^{-12} \div 10^{-11} \,\Omega\,\text{cm} \) while \( \rho_{uni} \approx 10^{-9} \div 10^{-7} \,\Omega\,\text{cm} \). Notice that the value of \( \rho_{uni} \) agrees with that in the case of edge dislocations of a similar density.

It should be noted that the experiments show an increase of the residual resistivity of nanocrystalline metals with \( L \) decreasing. This can be explained within the above-proposed model due to a direct \( L \)-dependence of \( n_i \). Indeed, it is reasonable to assume that \( n_i \approx L^{-p} \) with \( 1 < p < 2 \) (usually \( p = 2 \)). Thus, in accordance with Eq.(12) \( \rho_{bi} \) increases with \( L \) decreasing. It is interesting to note that in this case \( \rho_{uni} \) decreases with \( L \) (except \( p = 2 \), as is seen from Eq.(13). Let us reiterate that only the biaxial WDD with nonskew axes of rotations (BWDD) simulates the grain boundary.
B. Phonon scattering: low-temperature heat transport in polycrystals

It is clear that phonon scattering due to WDD will also affect the low-temperature thermal conductivity, $\kappa$. We start from the well known kinetic formula

$$\kappa = \frac{1}{3} \int_0^{\omega_D} C(\omega, T) v_s l(\omega, T) d\omega, \quad (14)$$

where $C(\omega, T) d\omega$ is the specific heat contributed by acoustic phonons within the frequency interval $d\omega$, $v_s$ is an average phonon velocity, and $l(\omega, T)$ is the phonon mean free path. It is suggested that $C(\omega, T)$ has standard form with quadratic in $\omega$ density of states and the Debye cutoff $\omega_D$.

The effective perturbation energy caused by the strain field of WDD is determined as\cite{13} $U(q) = \hbar \omega \gamma S p E_{AB}$, where $\omega$ is the phonon energy with wavevector $q$, $\gamma$ is the Grüneisen constant, and $S$ is the sound velocity (for simplicity it is assumed that three acoustic branches are equivalent), and $\gamma$ is the Grüneisen constant. As previously, we suppose that incident phonons are normal to the disclination lines, so that we deal with the two-dimensional scattering problem. The principal difference from the case of electron scattering is the explicit $q$-dependence of the perturbation energy (see details in Ref.14). Namely, the strain tensor due to WDD remains the same while the coefficient $B$ in Eq.(2) should be replaced by $B_{ph} = \hbar q v_s \gamma (1 - 2\sigma)/(1 - \sigma)$. Eqs.(4),(5) preserve their form in this case as well.

For BWDD the phonon mean free path is found to be\cite{23}

$$l_{bi}^{-1} = 2D^2(2\nu L)^2 n_i q \left( J_0^2(2qL) + J_1^2(2qL) \right) - \frac{1}{2qL} J_0(2qL) J_1(2qL), \quad (15)$$

where $D = \pi \gamma (1 - 2\sigma)/(1 - \sigma)$. For uniaxial WDD one obtains

$$l_{uni}^{-1} = \frac{D^2}{2} (2\nu L)^2 n_i q \left( 1 + J_0^2(2qL) - J_1^2(2qL) - \frac{2}{qL} J_0(2qL) J_1(2qL) \right). \quad (16)$$

Fig.3 shows $l(\omega)$ for three types of WDD.

We have used a typical for polycrystals size of the grain boundary $2L = 2700\AA$. As is seen, three curves behave differently. At low frequencies the scattering by uniaxial WDD resembles that by a point impurity. Namely, it strongly depends on $\omega$, $l_{uni} \sim \omega^{-5}$, thus once again confirming a view of uniaxial WDD as a strongly screened system. At high frequencies uniaxial dipoles scatter phonons like dislocations with $l_{uni} \sim \omega^{-1}$. It is interesting that the same $\omega^{-1}$-dependence appears for arbitrary biaxial dipoles both at low and high frequencies. What is more important, there is the only type of biaxial dipoles, BWDD, which shows the unique behavior with $l_{bi} \sim const$ as $\omega$ increases (see Fig.3). It was found that the change in behavior of $l_{bi}$ occurs at $2qL \sim 1$ or, equivalently, at $\omega^* \sim v_s/2L$. It should be emphasized that this intriguing result provides the basis for the following important speculations. Notice that some visible irregularities in Fig.3 came from rapid oscillations of the Bessel functions near the characteristic frequency $\omega^*$.

The BWDD-based model was successfully used for description of the phonon transport in polycrystals.\cite{23} For this purpose, Eq.(14) should be integrated with the phonon mean free path from Eq.(15). The result is shown in Fig.4 together with the experimental data for LiF.\cite{13}

As is seen, the predictions of the theory are in good agreement with the experimental results. It is interesting to note that the behavior of $\kappa(T)$ in our model is governed mainly by $D$, $2\nu L$ and $n_i$ in Eq.(15), that is by parameters which characterize a microstructure of polycrystals. In accordance with the above analysis, the thermal conductivity exhibits a crossover from a $\kappa \sim T^2$ to $\kappa \sim T^3$ at $T' \sim 0.1K$ for a chosen set of model parameters. It should be emphasized that such behavior of $\kappa(T)$ is specific to BWDD (which simulates a finite wall of edge disloc-
tions). For example, for the uniaxial dipoles one obtains that \( \kappa \sim T^{-2} \) at low temperatures and \( \kappa \sim T^{-1} \) for \( T \to \Theta_D \), where \( \Theta_D \) is the Debye temperature.

In accordance with our scenario the mean free path is determined to be

\[
I(\omega) = \left( l_{struc}^{-1} + l_{struc}^{-1} \right)^{-1},
\]

where \( l_{bi} \) comes from Eq.(15), and \( l_{struc} \) should be taken in the most general form describing the Rayleigh scattering over the complete frequency range. The interpolation formula reads (see, e.g., Ref.2)

\[
l_{struc} = Y^{-1} \left( \frac{h\omega}{k_B} \right)^{-4} + l_0,
\]

where \( Y \) is a constant which has been considered as a fitting parameter, and \( l_0 \) appears as the high-frequency limit. Fig.5 shows \( l_{bi} \), \( l_{struc} \), and \( l(\omega; T) \) with the model parameters for a-SiO\(_2\) taken from Table I.

FIG. 4. Reduced thermal conductivity due to biaxial WDD scattering, \( \kappa \times T^{-3} \) versus temperature \( T \), calculated according to (14) with the same parameter set as in Fig.3. Measured points for the boundary-limited thermal conductivity in LiF (from Ref.2) are indicated by triangles.

III. BWDD IN DIELECTRIC GLASSES: THERMAL CONDUCTIVITY

There are two important consequences of the previous section. First, it was found that the grain-boundary induced contribution to the thermal conductivity behaves like \( T^2 \) at very low temperatures. As is well known, this behavior is peculiar to dielectric glasses, where \( \kappa \sim T^2 \) for \( T < 1K \). Second, the critical temperature \( T' \) depends considerably on a size of the grain. This follows from the condition \( 2qL \sim 1 \) which can be rewritten as \( T \approx \hbar \nu_p/2Lk_B \), where \( k_B \) is the Boltzmann constant (see details in Ref.3). It particular, one obtains \( T \sim 1K \) a \( 2L \sim 20A \). Hence a \( T^2 \) dependence of \( \kappa \) can be extended up to 1K for materials consisting of microclusters with average diameters of order \( 15 \div 30A \). It is intriguing that exactly the same values are expected within the cluster model proposed for dielectric glasses.

This finding have stimulated a detailed study of the problem. It was shown in Ref.4 that the experiment data for the thermal conductivity in vitreous silica (a SiO\(_2\)) can be explained by a combination of two scattering processes. The first one comes from the sound waves scattering due to BWDD while the second one is the known Rayleigh type scattering which appear due to the local variations in structure. In this section, we present the model and extend an analysis to other glasses.

FIG. 5. Phonon mean free paths \( l_{bi} \) (dashed line), \( l_{struc} \) (dotted line) and \( l(\omega) \) (solid line) as functions of frequency. The parameter set for a-SiO\(_2\) is shown in Table I, \( K=2.6 \).

One can see that \( l(\omega) \) has a form typical for glassy materials. At low frequencies, \( \omega < 10^{12} \text{ sec}^{-1} \), \( l(\omega) \sim \omega^{-1} \), and the main contribution is due to the BWDD-induced scattering. In the intermediate region both scattering processes are involved while at high frequencies the Rayleigh scattering becomes dominant. Notice that the region \( 10^{12} \text{ sec}^{-1} < \omega < 10^{13} \text{ sec}^{-1} \) is responsible for the plateau in the thermal conductivity. We have found that the size of this region decreases with \( 2L \) and/or \( l_0 \) increasing.

It is interesting to note that Eq.(17) supports the empirical relation \( l/\lambda \sim 150 \), with \( \lambda \) being the wavelength of a phonon, which holds for many glasses at low temperatures. Indeed, at low frequencies \( l \sim l_{bi} \). Spreading out Eq.(15) at \( qL \ll 1 \) one gets

\[
l_{bi} \frac{1}{\lambda} = \frac{1}{2\pi D^2(2\nu L)^2n_i}.
\]
This is a constant which depends on the model parameters which characterize the structural and elastic properties of a material. It is reasonable to assume that these parameters vary only slightly in different amorphous dielectrics (see also Table I).

This can explain the observed constant-like behavior of $l/\lambda$. In particular, for our choice of parameters for a-SiO$_2$ one gets $l_0/\lambda \sim 135$.

To calculate $\kappa$ with $l(\omega)$ from Eq.(17), it is convenient to use the dimensionless form of Eq.(14)

$$\kappa = \frac{k_B T^3}{2\pi^2 \hbar^3 v_s^2} \int_0^{\Theta D/T} x^4 e^{x^2} (e^x - 1)^{-2} l(x) dx,$$

where $x = \hbar \omega / k_B T$, and the specific heat capacity is chosen in the standard Debye form. The results are shown in Fig.6 and Fig.7.

As is seen, there is a good agreement with the experimental data over a wide temperature range. Notice that we did not use any special fitting programs to get the best fit. Instead, we have fixed the parameters related to BWDD: a dipole separation $2L = 20\AA$, the density of defects $n_i = 2 \times 10^{11}$ cm$^{-2}$ and the Frank index $\nu = 0.1$ (except those for PS, see Table I), and tried to bring the parameters for Rayleigh scattering close to those in Ref. 27. In our opinion, this provides better insight into the essence of the proposed model. Let us stress once again that a characteristic length $20 \AA$ corresponds to the expected average size of clusters suggested in glasses.

FIG. 6. Thermal conductivity vs temperature for a-SiO$_2$ calculated according to Eq.(20) with $l(\omega)$ from Eq.(17) with a set of parameters from Table I. Experimental data from Ref. 27 are indicated by triangles.

IV. DISCUSSION

The results obtained in the previous section call for an additional discussion. First of all, the main question arises of whether the proposed model captures the essence of the glassy state or a good fitting of experiments is purely accidental. At the moment we cannot provide the ultimate answer to this question. It is interesting, however, to consider the peculiarities of our approach in relation to another known ways of tackling the problem.

As is well known, the very successful explanation of the very-low-temperature ($T < 1$K) behavior of amorphous dielectrics has been done within the phenomenological TLS model. Namely, at low temperatures the principal scatterers of acoustic phonons in glasses were proposed to be the tunneling states. As is known, however, this view posed some important questions. First, the microscopic basis for the TLS is still unclear. Second, the quantitative universality seen in various glasses at low temperatures (for example, the above-mentioned relation $l/\lambda \sim 150$) has not been explained. Namely, according to TLS model

$$l/\lambda \propto (\bar{P})^{-1} \propto T_g / V_F,$$

where $\bar{P}$ is the density of TLS, $T_g$ is the glass transition temperature, and $V_F$ is the free volume frozen into the glass. However, the experimental data show that the above relation does not depend explicitly on $T_g$ (see, e.g., discussion in Ref. 33).

Third, the universal properties of glasses in the intermediate-temperature range, $1 < T < 10$ K, were not understood even qualitatively within the TLS model. Some of these problems, however, have
been solved later by invoking additional to the TLS concepts. In particular, a reasonable expression for the total phonon mean free path that allows to describe $l$ over a wide temperature range reads (see, e.g., Refs.\textsuperscript{33,34})

$$l(\omega, T) = (l_l^{-1} + l_R^{-1} + l_{add}^{-1})^{-1},$$

where $l_l$ and $l_R$ are due to TLS and the Rayleigh scattering, respectively, $l_{add}$ comes from some additional scattering mechanisms. As a possible candidate there was considered the phonon scattering from some kind of disorder (clusters, fractals, etc.). The modern theories involve the phonon scattering from localized low-frequency vibrations which manifested themselves both experimentally and by computer simulations. All these successful approaches are essentially based on the TLS picture. Unfortunately, the nature of either TLS or the localized vibrations remains still unclear.

Let us discuss these points in the context of our model. Our consideration assumes the new principal scatterer in amorphous dielectrics which has a clear physical origin. Indeed, as indicated above, there is a direct analogy between BWDDs, finite dislocation walls, and grain boundaries. Thus, the BWDD-based model supports the cluster picture of amorphous dielectrics where boundaries between clusters give rise to defects such as BWDD. In this connection the question arises: is there any sound experimental evidence for the existence of either clusters or BWDDs in glasses? At present the answer is no. As a possible reason one can mention a too small average size of clusters as well as their random distribution. In such an event, both clusters and BWDD are difficult to detect. Let us stress that we have considered in our model the randomly oriented dipoles (see averaging in Eq.(4)).

In metals, however, the phase with long-range orientational order and no translational symmetry has been experimentally observed by the x-ray scattering. This finding confirms the proposed point of view that supercooled liquids and metallic glasses can be viewed as defected states, including disclinations, of icosahedral bond orientational order. In particular, in two dimensions liquids are regarded as hexatic fluids interrupted by point disclinations (i.e. local points of 5- and 7-fold symmetry). In accordance with their scenario there is a two-stage pairing process: disclinations first pair to form 5-7 dipoles regarded as dislocations which then pair at lower temperature to form a crystalline solid. It is interesting that grain boundaries are suggested to be linear arrangements of the form \textit{5-7–5-7–5-7–}.  

Regarding Eq.(21), we have shown in the previous section that the WDD-based model predicts a constant for the relation $l/\lambda$ at low temperatures (see Eq.(19)). It is interesting that this constant depends only on the model parameters which characterize the structural properties of amorphous dielectrics. Let us stress also that though Eq.(17) takes into account only two principal scatterers, it allows to describe the thermal conductivity of various dielectric glasses over a wide temperature range.

Another important question is the low-temperature specific heat of glasses, $C_v$. As is known, $C_v$ is characterized by an anomalous linear temperature behavior. An explanation based on the TLS model looks quite correct. While this problem is beyond the scope of our paper, nevertheless, we can discuss briefly an expected contribution to the specific heat due to BWDD. A similar problem has been considered long time ago by Granato. Granato analyzed the pinned-dislocation contribution to the specific heat and found that at low temperatures

$$C_v = \frac{p v_s^2 \rho a^2 N_k b}{3 Z \Theta_D T},$$

where $p = v_s \sqrt{\rho G}$ ($G$ is the shear modulus and $\rho$ the density of a material), $n_d$ is the dislocation density, $a$ the lattice constant, $Z$ the number of atoms per unit cell, and $N$ the number of atoms per mole. This result has been discussed in connection with dielectric glasses in Ref.\textsuperscript{14}. In particular, it was shown that there is a satisfactory agreement with the experimentally observed data for some glasses. As is known, with decreasing of the dipole separation $2L$ the biaxial WDD becomes equivalent to an edge dislocation with the Burgers vector $b = 4L \tan(\Omega / 2)$. Thus, the above result in Eq.(23) for dislocations should be valid for the BWDD-based model where $2L$ is expected to be very small.

Notice also that a possible explanation of the specific heat behavior both at $T \leq 1K$ and $1 \leq T \leq 10K$ has been given within the soft atomic potential model\textsuperscript{15} as well as within the elastic dipole model\textsuperscript{16}. These approaches interpret the specific heat peculiarities in terms of the TLS states and the additional quasilocal harmonic modes. As we have already mentioned, the excess harmonic modes coexisting with sound waves below 1THz actually have been observed in glasses\textsuperscript{17}. It should be recognized that the presence of localized harmonic modes is peculiar to elastic materials with extended defects as well. In particular, the phonon spectrum in the presence of a dislocation was shown to possess localized modes\textsuperscript{18}. Besides, the effect of localized vibration modes due to linear defects on the thermal properties was studied within the framework of the vibrating string model of a dislocation\textsuperscript{19}. It is clear, however, that this consideration should be accompanied by a detailed study within the BWDD model. This problem invites further investigation.

Finally, let us discuss briefly a possible universality of the BWDD-based picture in polycrystals and glasses. In accordance with our results, a principal feature that distinguishes polycrystals from glasses is the size of a cluster. For example, let us consider the alkali halides LiF, NaCl, and KBr:KCN. The first two are polycrystals with the corresponding transport characteristics (see Sec.II) while KBr:KCN is an example of the orientational glass. Within our scenario this markedly different behavior can be explained by the lower average size of a cluster in KBr:KCN. As we have shown above, for this
reason alone the calculated crossover temperature can be moved from very low temperatures to 1K. This means that, e.g., at $2L \sim 1000\text{Å}$ the $T^3$-dependence of $\kappa$ will appear above 0.1K. In addition, one can expect that for such large clusters the Rayleigh scattering will be suppressed while the umklapp processes become of importance at high temperatures. As a result, the behavior of $\kappa$ will be typical for polycrystals. On the other hand, for small clusters the $T^3$ dependence of $\kappa$ goes up to 1K, then the Rayleigh scattering becomes important. As is known, there are no umklapp processes for randomly distributed small clusters. Thus, the proposed within our model scatterers (BWDD and the Rayleigh-type) will be distributed small clusters. Thus, the proposed within our

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**APPENDIX A**

Let us find the exact expression for the perturbation energy in Eq.(1). The WDD-induced strains $E_{ij}$ can be found by using of the Hooke’s law

$$E_{ij} = \frac{1}{2\mu(1+\sigma)} \left[ (1+\sigma)\sigma_{ij}^d - \sigma_{ij} \delta_{ij} \right],$$

(A1)

where $\sigma_{ij}^d$ are the stresses due to the WDD; $\mu$ and $\sigma$ are the shear modulus and the Poisson constant, respectively.

For the chosen in Sec.II geometry (see Fig.1) the WDD-induced stresses $\sigma_{ij}^d$ are

$$\sigma_{xx}^d = \frac{\mu\Omega}{2\pi(1-\sigma)} \left[ \frac{1}{2} \ln \frac{(x+L)^2 + y^2}{(x-L)^2 + y^2} + \frac{y^2}{(x+L)^2 + y^2} \right. \right.$$

$$\left. - \frac{y^2}{(x-L)^2 + y^2} - l_1 \frac{(x+L)(x+L)^2 - y^2)}{(x+L)^2 + y^2} \right]$$

$$+ l_2 \frac{(x-L)(x-L)^2 - y^2)}{(x-L)^2 + y^2} \right],$$

(A2)

$$\sigma_{yy}^d = \frac{\mu\Omega}{2\pi(1-\sigma)} \left[ \frac{1}{2} \ln \frac{(x+L)^2 + y^2}{(x-L)^2 + y^2} + \frac{(x+L)^2}{(x+L)^2 + y^2} \right. \right.$$

$$\left. - \frac{(x-L)^2}{(x-L)^2 + y^2} - l_1 \frac{(x+L)(x+L)^2 + 3y^2)}{(x+L)^2 + y^2} \right]$$

$$+ l_2 \frac{(x-L)(x-L)^2 + 3y^2)}{(x-L)^2 + y^2} \right],$$

(A3)

$$\sigma_{zz}^d = \frac{\mu\Omega}{\pi(1-\sigma)} \left[ \frac{1}{2} \ln \frac{(x+L)^2 + y^2}{(x-L)^2 + y^2} - l_1 \frac{x+L}{(x+L)^2 + y^2} \right. \right.$$

$$\left. + l_2 \frac{x-L}{(x-L)^2 + y^2} \right].$$

(A4)

Notice that Eqs.(A2)-(A4) describe the stresses due to a finite wall of edge dislocations at large distances. Applying Eqs.(A2)-(A4) in Eq.(A1) one gets all the components of the strain tensor $E_{ij}$ and, finally, Eq.(2).

**APPENDIX B**

The perturbation energy given by Eq.(2) takes the following form in polar coordinates

$$U(r, \phi) = B \left[ \frac{1}{2} \ln \frac{r^2 + 2rL \cos \phi + L^2}{r^2 - 2rL \cos \phi + L^2} \right. \right.$$

$$\left. - l_1 \frac{r \cos \phi + L}{r^2 - 2rL \cos \phi + L^2} + l_2 \frac{r \cos \phi - L}{r^2 - 2rL \cos \phi + L^2} \right].$$

(B1)

The matrix element in Eq.(5) with the perturbation energy from Eq.(B1) can be calculated using the following formulas:

$$\sum_{k=1}^{\infty} \frac{z^{2k-1} \cos(2k-1)\phi}{2k-1} = \frac{1}{4} \ln \frac{1 + 2z \cos \phi + z^2}{1 - 2z \cos \phi + z^2}, \quad z^2 \leq 1,$$

(B2)

$$\sum_{k=0}^{\infty} z^k \cos k\phi = \frac{1 - z \cos \phi}{1 - 2z \cos \phi + z^2}, \quad |z| < 1$$

(B3)

Substituting Eqs.(B2) and (B3) into Eq.(B1) and integrating in Eq.(5) one obtains

$$U(p, \alpha) = -i \frac{4\pi BL}{pS} \left[ J_0(pL) \cos \alpha \right.$$

$$\left. + \sum_{k=1}^{\infty} (-1)^k J_{2k}(pL) \frac{\cos(2k+1)\alpha}{2k+1} - \frac{\cos(2k-1)\alpha}{2k-1} \right]$$

$$+ \frac{2\pi B}{pS} \Delta_t \left[ J_0(pL) \cos \alpha + 2 \cos \alpha \sum_{k=1}^{\infty} (-1)^k J_{2k}(pL) \cos 2k\alpha \right],$$

(B4)
where \( \Delta_t = l_1 - l_2 \) and \( J_m(z) \) is the Bessel function. The first term in Eq.(B4) comes from the integration of logarithmic function in Eq.(B1) while the second one comes from two last terms in the r.h.s. of Eq.(B1).

We have used the following standard integrals deriving Eq.(B4)

\[
\int_0^{2\pi} \exp(iz \cos \phi) \cos m \phi d\phi = 2\pi i^m J_m(z), \quad (B5)
\]

\[
\int z^k J_{k-1}(z) dz = z^k J_k(z). \quad (B6)
\]

The first sum in Eq.(B4) can be simplified by differentiation with respect to \( \alpha \). The second sum in Eq.(B4) reads

\[
\sum_{k=1}^{\infty} (-1)^k \cos(k \alpha) J_{2k}(z) = \frac{1}{2} \cos[z \cos(\alpha/2)] - \frac{1}{2} J_0(z) \quad \text{(B7)}
\]

After straightforward calculations one obtains

\[
U(p, \alpha) = \frac{B}{S} \left[ -\frac{4\pi i}{p^2} \sin(pL \cos \alpha) + \frac{2\pi i \Delta t}{p} \cos \alpha \cos(pL \cos \alpha) \right].
\]

To find \( \Re(\theta) \) in Eq.(4) one has to make averaging of \( |U(p, \alpha)|^2 \) over \( \alpha \):

\[
|U(p)|^2 = |\langle \mathbf{q}|U(\mathbf{r})|\mathbf{q}' \rangle|^2 = \frac{1}{2\pi} \int_0^{2\pi} |U(p, \alpha)|^2 d\alpha = \frac{2\pi B^2}{S^2} \int_0^{2\pi} \left( \frac{4}{p^2} \sin^2(pL \cos \alpha) - \frac{2\Delta t}{p^2} \cos \alpha \sin(2pL \cos \alpha) \right)
\]

\[+ \frac{\Delta^2}{p^2} \cos^2 \alpha \cos^2(pL \cos \alpha) \right) d\alpha. \quad (B8)
\]

Using

\[
\int_0^{2\pi} \left( \frac{\cos(z \cos \alpha)}{\sin(z \cos \alpha)} \right) \cos(n\alpha) d\alpha = 2\pi \left( \frac{\cos(n\pi/2)}{\sin(n\pi/2)} \right) J_n(z), \quad (B9)
\]

one finally gets

\[
|U(p)|^2 = \frac{4\pi B^2}{S^2} \left\{ \frac{2}{p^2} \left( 1 - J_0(2pL) \right) - \frac{2\Delta t}{p^2} J_1(2pL) \right\}
\]

\[+ \frac{\Delta^2}{2p^2} \left( \frac{1}{2} + J_0(2pL) - \frac{J_1(2pL)}{2pL} \right). \quad (B10)
\]

Substituting Eq.(B10) into Eq.(4) one obtains the effective differential scattering radius in Eq.(6).

The exact expression for the mean free path in Eq.(3) takes the form

\[
\Lambda^{-1} = \frac{n_i B^2}{k^2 v^2} \left\{ \frac{1}{2q^2} I_1(qL) + \frac{\Delta^2}{2q} I_2(qL) - \frac{\Delta t}{q^2} I_3(qL) \right\}, \quad (B11)
\]

where

\[
I_1(qL) = \int_0^{2\pi} \frac{d\theta}{\sin^2(\theta/2)} \left( 1 - J_0(4qL \sin(\theta/2)) \right) = 16q^2 L^2 \pi \left( J_0^2(2qL) + J_1^2(2qL) \right) - 8qL \pi J_0(2qL) J_1(2qL), \quad (B12)
\]

\[
I_2(qL) = \int_0^{2\pi} \left( \frac{1}{2} + J_0(4qL \sin(\theta/2)) \right) \frac{J_1(4qL \sin(\theta/2))}{4qL \sin(\theta/2)} d\theta = 2\pi \left( \frac{1}{2} + J_0^2(2qL) \right) - \pi \left( J_0^2(2qL) + J_1^2(2qL) \right), \quad (B13)
\]

\[
I_3(qL) = \int_0^{2\pi} \frac{d\theta}{\sin^2(\theta/2)} J_1(4qL \sin(\theta/2)) = 4qL \pi \left( J_0^2(2qL) + J_1^2(2qL) \right). \quad (B14)
\]

The final result for the mean free path is given by Eq.(7).

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TABLE I. Parameters used for the numerical fits. Units are the following: $v_s$ ($10^5$ cm/sec), $\Theta_D$ (K), $n_i$ ($10^{11}$ cm$^{-2}$), $2L$ (10$^{-7}$ cm), $\nu$ (cm$^{-1}$ K$^{-4}$), $l_0$ (10$^{-7}$ cm).

| Material | $v_s$ | $\Theta_D$ | $n_i$ | $2L$ | $\nu$ | $l_0$ | $Y$ |
|----------|------|------------|------|------|------|------|-----|
| a-SiO$_2$ | 4.1 | 342 | 2 | 2 | 0.1 | 1.5 | 1 |
| a-GeO$_2$ | 2.6 | 192 | 2 | 2 | 0.1 | 0.6 | 2.9 |
| a-Se | 1.19 | 113 | 2 | 2 | 0.1 | 0.2 | 90 |
| PS | 1.67 | 123 | 5 | 2.4 | 0.1 | 0.5 | 80 |