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Original
The Boltzmann Equation Of Phonon Thermal Transport Solved In the Relaxation Time Approximation – II – Data Analysis / Sparavigna, Amelia Carolina. - In: MECHANICS, MATERIALS SCIENCE & ENGINEERING JOURNAL. - ISSN 2412-5954. - ELETTRONICO. - 2016:3(2016), pp. 1-10. [10.13140/RG.2.1.2026.4724]

Availability:
This version is available at: 11583/2643155 since: 2020-12-19T11:20:53Z

Publisher:
Magnolithe

Published
DOI:10.13140/RG.2.1.2026.4724

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12 October 2024

The Boltzmann Equation Of Phonon Thermal Transport Solved In the Relaxation Time Approximation – II – Data Analysis

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DOI **10.13140/RG.2.1.2026.4724**

Keywords: Thermal Conductivity, Phonons, Boltzmann Equation.

ABSTRACT. As discussed in a previous paper [1], the thermal transport in dielectric solids can be obtained by using the Boltzmann equation of an assembly of phonons subjected to a thermal gradient. Solving this equation in the framework of the relaxation time approximation, from the phonon distribution that we obtain, the thermal conductivity of the solid can be easily given. Here we use such an approach to analyse the data of the thermal conductivities of some dielectric materials.

Introduction. In a dielectric solid subjected to a thermal gradient, the thermal transport is supported by the vibrations of crystal lattice, because other carriers such as electrons freely moving in the solid are absent. Therefore, responsible of the thermal conductivity are the phonons which are coming from the quantization of lattice vibrational modes. In this manner, phonons arise as the quasiparticles occurring because the solid is modelled as an assembly of weakly interacting particles, existing in a free volume coincident to that of the considered solid. In this volume, phonons are giving the thermal transport. The resistive processes producing a finite thermal conductivity are coming from scattering mechanisms due to point- and extended defects of the crystal lattice, from the scattering at the boundaries of the crystal and from the cubic terms of lattice Hamiltonian function, which are giving phonon-phonon scattering processes. They can differ in normal and umklapp processes [1]; in umklapp processes, momentum is transferred to the lattice as a whole, degrading the thermal current.

The thermal transport of phonons in a semiclassical approach can be determined by means of the Boltzmann equation, an equation of statistical mechanics, which is describing system not in the thermodynamics equilibrium [2-4]. For phonons, this happens when an assembly of them is subjected to a thermal gradient. The solution of the Boltzmann equation had been given by means of several approaches; among them, we have proposed a solution based on an iterative method [5-9]. A quite simple solution is that given in [1], where we have discussed the relaxation time approximation. In [1], we have also reported the Callaway's approach to the description of the scattering processes in this approximation [10-12]. In particular, Callaway investigated the role of isotopic defects as source of scattering processes that can strongly reduce the thermal conductivity of solids. Here, we consider the relaxation times to determine the thermal conductivity of some dielectric solids. In particular, we will discuss the thermal conductivity of Germanium, Silicon and Diamond.

The thermal conductivity. In a lattice, phonons move changing position and momentum and are subjected to collisions. They obey to a general equation, which is the Boltzmann equation of the distribution $n_{\mathbf{q}p}(\mathbf{r},t)$, for a phonon state with wave-number **q** and polarization p, about position **r** and time t. Let us suppose a gradient ∇T of temperature $T = T(\mathbf{r})$; the gradient is giving origin to a diffusion process of phonons.

Besides diffusion, phonons are also subjected to scattering mechanisms. Then, in the case of stationary condition, an equation is originated for the phonon distribution:

$$-\mathbf{v}_p(\mathbf{q})\cdot\nabla T\frac{\partial n_{\mathbf{q}p}}{\partial T}+\left.\frac{\partial n_{\mathbf{q}p}}{\partial t}\right|_{\text{scatt}}=0\,. \tag{1}$$

Eq.1 is the general form of Boltzmann equation for phonons subjected to a thermal gradient [2-4]. $\mathbf{v}_p(\mathbf{q})$ is the group velocity of the given phonon mode:

$$\mathbf{v}_{\mathbf{q}p}=\frac{\partial\omega_{\mathbf{q}p}}{\partial\mathbf{q}}\,.$$

For acoustic phonons, this velocity is simply $\mathbf{v}_{\mathbf{q}p}=c_p\,\hat{\mathbf{q}}$, where c_p is the speed of the sound for the given polarization of the wave, and $\hat{\mathbf{q}}$ is the unit vector of $\mathbf{q}$.

Eq.1 becomes an integro-differential equation when the scattering term representing the collisions of quasiparticles is explicitly given. In the first part of our discussion [1], we have detailed the scattering terms and discussed them. Here, we just remember that phonons are scattered by others phonons in the three-phonon processes (normal and umklapp), by point- and extended defects of the lattice and by the boundaries of the crystal.

In the case of a small thermal gradient, the equation is solved linearizing it, by considering just small deviations from equilibrium. The deviation is given by $n_{\mathbf{q}p}-n^o_{\mathbf{q}p}$, where $n^o_{\mathbf{q}p}$ is the equilibrium distribution. To have the Boltzmann linearized equation in the general case, let us define $\Psi_{\mathbf{q}p}$ as:

$$n_{\mathbf{q}p}=n^o_{\mathbf{q}p}-\Psi_{\mathbf{q}p}\frac{\partial n^o_{\mathbf{q}p}}{\partial(\hbar\omega_{\mathbf{q}p})}\,. \tag{2}$$

In (2) we have the energy of a phonon, which is $\hbar\omega_{\mathbf{q}p}$. Once function $\Psi_{\mathbf{q}p}$ is evaluated, with the iterative method [4-9] for instance, the density of the thermal current **U** can be determined.

The density current is defined as:

$$\mathbf{U}=\frac{1}{\Omega}\sum_{\mathbf{q}p}\hbar\omega_{\mathbf{q}p}\mathbf{v}_{\mathbf{q}p}n_{\mathbf{q}p}=-\frac{1}{\Omega}\sum_{\mathbf{q}p}\hbar\omega_{\mathbf{q}p}\mathbf{v}_{\mathbf{q}p}\frac{\partial n^o_{\mathbf{q}p}}{\partial(\hbar\omega_{\mathbf{q}p})}\Psi_{\mathbf{q}p}\,. \tag{3}$$

$\Omega = NV$ is the volume of the crystal, N the number of primitive cells of it, having volume V. In a Cartesian frame having unit vectors $\mathbf{u}_i$, current **U** is:

$$U_j=-\sum_i\kappa_{ji}\frac{\partial T}{\partial x_i}\,. \tag{4}$$

Tensor κ_{ij} is the thermal conductivity tensor, that in an isotropic crystal, is having non-null terms $\kappa_{xx} = \kappa_{yy} = \kappa_{zz} = \kappa$.

The main difficulty in evaluating (3) is the determination of the phonon distribution $n_{\mathbf{q}p}$. Let us try to use relaxation times for this task. The relaxation time approximation consists in writing the derivative of the distribution with respect to time as [2]:

$$\frac{\partial n_{\mathbf{q}p}}{\partial t} = \frac{n^o_{\mathbf{q}p} - n_{\mathbf{q}p}}{\tau(\mathbf{q}, p)} . \tag{5}$$

$n^o_{\mathbf{q}p}$ is the equilibrium distribution. In (5) we see the relaxation time for the mode ($\mathbf{q}$, p). Joseph Callaway defined the difference between the distribution existing when there is a temperature gradient and that of equilibrium, which is the Bose-Einstein distribution, as [10-12]:

$$n_{\mathbf{q}p} - n^o_{\mathbf{q}p} = -\tau(\mathbf{q}, p)\ \mathbf{v}_{\mathbf{q}p} \cdot \nabla T \frac{\hbar\omega_{\mathbf{q}p}}{k_B T^2} \frac{e^x}{(e^x - 1)^2} . \tag{6}$$

In (6), we used the dimensionless variable $x = \hbar\omega_{\mathbf{q}p} / k_B T$. The thermal current is given by:

$$\mathbf{U} = -\frac{1}{\Omega} \sum_{\mathbf{q}p} \tau(\mathbf{q}, p) \mathbf{v}_{\mathbf{q}p} \cdot \nabla T \frac{(\hbar\omega_{\mathbf{q}p})^2}{k_B T^2} \frac{e^x}{(e^x - 1)^2} \mathbf{v}_{\mathbf{q}p} . \tag{7}$$

In the case of anisotropic solids, we have a tensor for the thermal conductivity:

$$\begin{aligned} \kappa_{\alpha\beta} &= \frac{1}{\Omega} \sum_{\boldsymbol{q}p} \tau(\boldsymbol{q}, p) \frac{(\hbar\omega_{\boldsymbol{q}p})^2}{k_B T^2} \frac{e^x}{(e^x - 1)^2} (\boldsymbol{v}_{\boldsymbol{q}p})_\alpha (\boldsymbol{v}_{\boldsymbol{q}p})_\beta \\ &= \frac{1}{\Omega} \sum_{\boldsymbol{q}p} \tau(\boldsymbol{q}, p)\, C_{ph}(\omega) (\boldsymbol{v}_{\boldsymbol{q}p})_\alpha (\boldsymbol{v}_{\boldsymbol{q}p})_\beta . \end{aligned} \tag{8}$$

α and β are corresponding to spatial components x, y, z. We have also used the specific heat $C_{ph}(\omega)$.

Therefore, we have, in the isotropic case:

$$\kappa = \frac{1}{\Omega} \sum_{\mathbf{q}p} \tau(\mathbf{q}, p) C_{ph}(\omega) \mathbf{v}^2_{\mathbf{q}p} \cos^2\theta . \tag{9}$$

In (9), θ is the angle between the group velocity and the thermal gradient. Instead of the summation on the phonon states, we can use an integration:

$$\frac{1}{\Omega}\sum_{\mathbf{q}p} \rightarrow \frac{1}{(2\pi)^2}\sum_p \int d\mathbf{q}\,,$$

Ω is the volume of crystal. Then:

$$\kappa = \frac{1}{(2\pi)^2}\sum_p \int d\mathbf{q}\; \tau(\mathbf{q},p)\, C_{ph}(\omega)\, v_{\mathbf{q}p}^2 \cos^2\theta\,. \tag{10}$$

Callaway's relaxation times and thermal conductivity. First of all, let us note that in [10-12], Callaway used a Debye-like phonon spectrum and a Debye description of the density-of-states. Therefore, the thermal conductivity he derived is suitable for the low temperature region where the model is valid. Moreover, an averaged phonon velocity v_s for longitudinal and transverse branches is used. In [10-12], Callaway proposed the following relaxation times for collisions:

$$\tau_d^{-1} = A\omega^4\ ;\ \tau_b^{-1} = \frac{v_s}{L}\ ;\ \tau_N^{-1} = B_2 T^3\omega^2\ ;\ \tau_U^{-1} = B_1 T^3\omega^2 = b_1 T^3\omega^2 \exp(-\Theta/aT)\,,$$

$A\omega^4$ is the scattering from impurity such as point-like defects and isotope defects. The isotope scattering takes the form proposed by Klemens [13]. The boundary scattering v_s/L contains the average speed of sound and L the characteristic length of the crystal. Callaway model assumes that the scattering at the surface boundary is purely diffusive. The three-phonon normal process is that derived by Herring [14] for longitudinal phonon scattering under momentum conservation conditions at low temperatures. The relaxation time for an umklapp process was suggested by Peierls [15]. Since, in the relaxation time approximation, an addition of the transition probabilities leads to an addition of the reciprocal relaxation times, the total relaxation time for the abovementioned scattering mechanisms is given by:

$$\tau_c^{-1} = \tau_d^{-1} + \tau_N^{-1} + \tau_U^{-1} + \tau_b^{-1} = A\omega^4 + (B_1 + B_2)T^3\omega^2 + \frac{v_s}{L}\,.$$

Let us note that the relaxation time for umklapp processes is $\tau_U \propto e^{\Theta/aT}$ [15]. As a consequence, the contribution of such umklapp processes to the thermal resistivity is decreasing when temperature decreases. From Eqs. (16), (19)-(21) of [12], Callaway deduced the following expression for the thermal conductivity:

$$\kappa = \frac{k_B}{2\pi^2 v_s}\left(\frac{k_B T}{\hbar}\right)^3 \left\{ \int_0^{\Theta/T} \frac{\tau_c x^4 e^x}{\left(e^x-1\right)^2} dx + \frac{\left[\int_0^{\Theta/T} \frac{\tau_c}{\tau_N} \frac{x^4 e^x}{\left(e^x-1\right)^2} dx\right]^2}{\int_0^{\Theta/T} \frac{1}{\tau_N}\left(1-\frac{\tau_c}{\tau_N}\right) \frac{x^4 e^x}{\left(e^x-1\right)^2} dx} \right\} \tag{11}$$

In this equation we have k_B Boltzmann constant, v_s speed of the sound, Θ Debye temperature, and x dimensionless variable $x = \hbar\omega / k_B T$. We have the two relaxation times, τ_N and τ_c, as given above.

Thermal conductivity of Germanium. Under standard conditions, Germanium is a material having the same lattice of diamond. Germanium can be produced, for its use in semiconductors, with a very high purity. Since it is an element having five naturally occurring isotopes, of which ^{74}Ge is the most common isotope, in the measurements of thermal conductivity in natural samples and in isotopically enriched samples, we can see the effect of isotope defects. As told in [12], Glen Slack was the researcher that first emphasized the role of isotope effects [16]. Therefore, let us see if expression (11) can give us a good agreement with experimental data of Germanium.

Let us use for Germanium, the following parameters: $v_s = 3.5\times10^5\, cm/s$, $L = 0.18\, cm$, $\Theta = 375\, K$, $a = 1.$, $A = 2.57\times10^{-44} s^3$, $B_2 = 3.\times10^{-23} s/K^3$ and $b_1 = 3.\times10^{-23} s/K^3$. The result of calculation is given in the Figure 1, where some experimental data of Geballe and Hull [17] are also given for comparison. The upper curve represents the isotopically enriched sample, that is a sample were the isotope relaxation time is not considered; the lower curve is giving the thermal conductivity of a natural sample.

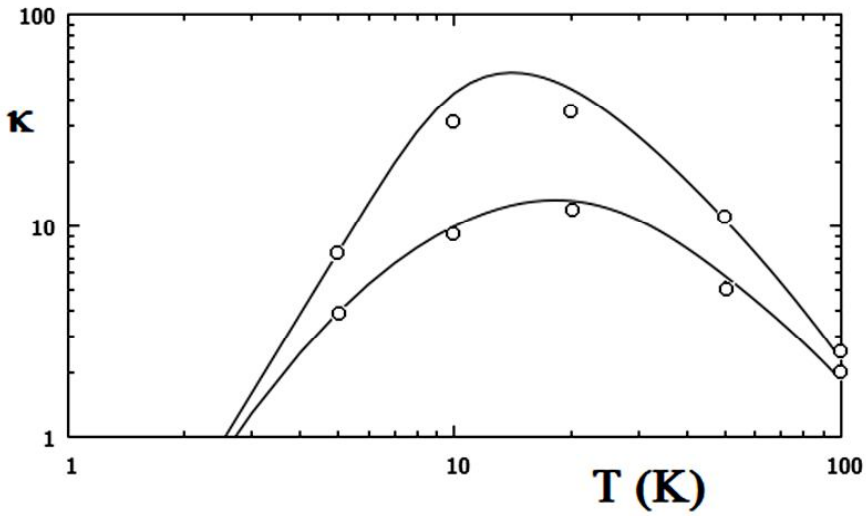

Fig. 1. Thermal conductivity ($W\cdot cm^{-1}\cdot K^{-1}$) of enriched and natural Germanium. The pure sample has the larger thermal conductivity. The dots are representing some of the experimental data of Geballe and Hull [17].

In the Figure 1, the peak of the thermal conductivity in enriched Ge is not perfectly adapted to experimental data; however, this happens also if we use a more precise microscopic model [18]. Probably, this is due to the scattering mechanism from boundaries, which is not properly modelled by the relaxation time.

In the Figure 2, it is shown the role of the isotope scattering in reducing the thermal conductivity, for different values of parameter *A*. The other parameters are the same as in the Figure 1. In the Figure 3, it is shown the role of the characteristic length *L* of the material in changing the thermal conductivity. Note that at high temperatures, length *L* is irrelevant. In the Figure 3, the isotopic scattering is neglected (*A*=0). The other parameters are the same as in the Figure 1.

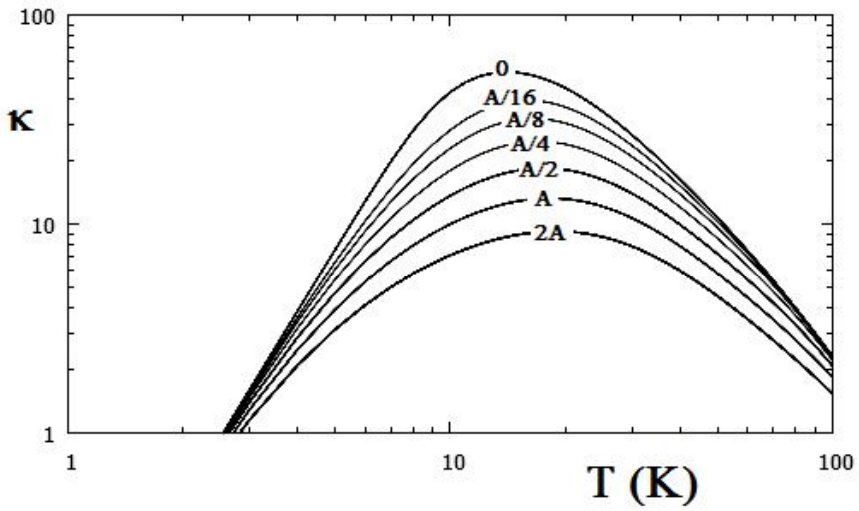

Fig. 2. Role of the isotope scattering in reducing the thermal conductivity ($W \cdot cm^{-1} \cdot K^{-1}$). The curves are giving the thermal conductivity for several values of A. The other parameters are the same as in the Fig.1.

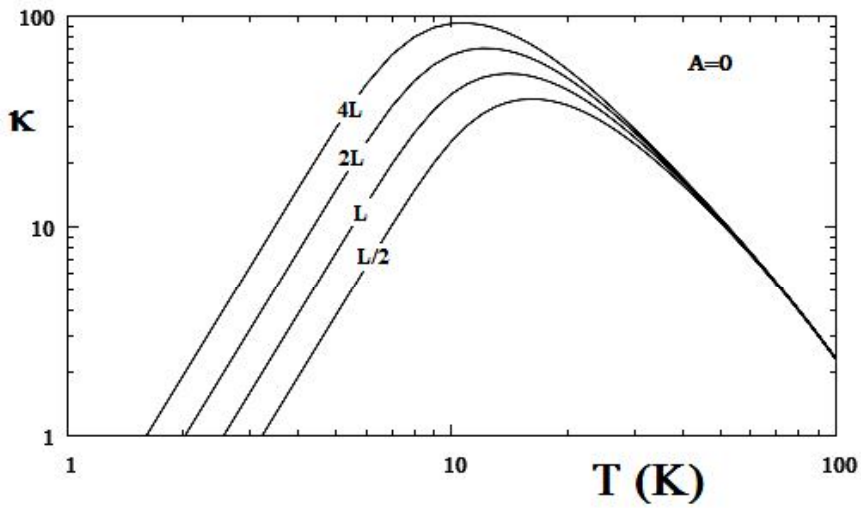

Fig. 3. Role of the characteristic length L of the material in changing the thermal conductivity ($W \cdot cm^{-1} \cdot K^{-1}$). Note that at high temperatures, length L is irrelevant. The isotopic scattering is neglected (A=0). The other parameters are the same as in Figure 1.

A short note on the values of parameters used for calculating the reciprocal of relaxation times could be interesting. Let us consider a temperature near the value of the peak of thermal conductivity. For instance, we can assume $T = 20K$. Parameters A and B_2 are that appearing in the reciprocal relaxation times $\tau_d^{-1} = A\omega^4$ and $\tau_N^{-1} = B_2 T^3 \omega^2$. We can estimate the phonon frequency that we have in reciprocal of relaxation times as $\omega = k_B T/\hbar$. Therefore, considering $A = 2.57\times10^{-44} s^3$ and $B_2 = 3.\times10^{-23} s/K^3$:

$$\tau_d^{-1} = A\omega^4 = A\left(\frac{k_B T}{\hbar}\right)^4 = 1.2\times10^6 s^{-1},$$

$$\tau_N^{-1} = B_2 T^3 \omega^2 = B_2 T^3 \left(\frac{k_B T}{\hbar}\right)^2 = 1.6\times10^6 s^{-1}.$$

Around the temperature of the peak, these reciprocals of relaxation times are about $10^6 s^{-1}$. The reciprocal of relaxation time of the boundary scattering is $\tau_B^{-1} = v_s / L = 2\times10^6 s^{-1}$. It has a value, which is not depending on temperature; for this reason, at temperatures above that of the peak, the boundary scattering becomes less relevant and negligible, as depicted in the Figure 3. In fact, if we consider a higher temperature, for instance $T = 100K$, and estimate the reciprocal relaxation times as did previously, we obtain:

$$\tau_d^{-1} = A\omega^4 = A\left(\frac{k_B T}{\hbar}\right)^4 = 7.5\times10^8 s^{-1},$$

$$\tau_N^{-1} = B_2 T^3 \omega^2 = B_2 T^3 \left(\frac{k_B T}{\hbar}\right)^2 = 5.1\times10^9 s^{-1}.$$

These reciprocals are quite larger than the term coming from the boundary scattering. Let us also note that the effect of three-phonon scattering is larger than that of the scattering from isotope defects. This is in agreement with an increasing role of phonon-phonon scattering at higher temperatures.

Silicon thermal conductivity. Silicon is a solid at room temperature, with relatively high melting point of 1414 °C. It has a relatively high thermal conductivity. In its crystalline form, its lattice is, like that of Germanium, a diamond cubic crystal structure. Silicon is a semiconductor where the number of free charge carriers increases with temperature.

Let us use for Silicon the following parameters: $v_s = 6.7\times10^5 cm/s$, $L = 1.cm$, $\Theta = 645K$, $a = 1.$, $A = 1.2\times10^{-44} s^3$, $B_2 = 2.\times10^{-24} s/K^3$ and $b_1 = 2.\times10^{-24} s/K^3$. The result of calculation from Eq.11 is given in the Figure 4. The upper curve represents the isotopically pure sample, the lower curve the thermal conductivity of the natural sample.

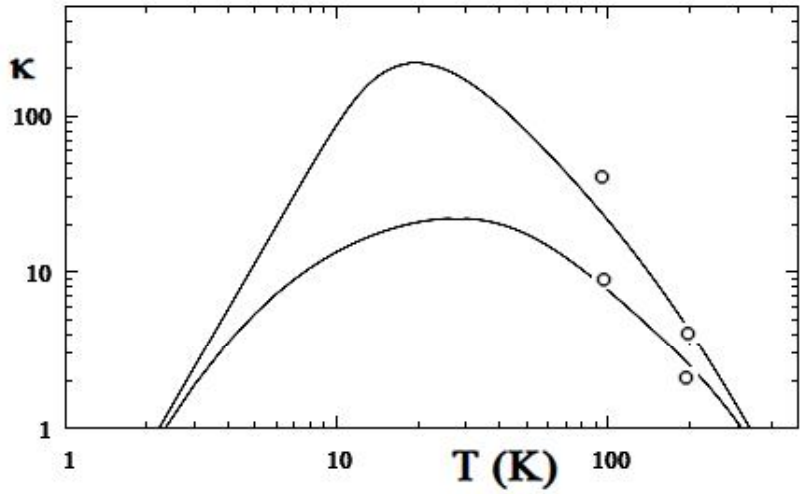

Fig. 4. Thermal conductivity ($W \cdot cm^{-1} \cdot K^{-1}$) of isotopically pure and natural Silicon. The pure sample has the larger thermal conductivity. The dots are representing some of the experimental data of Capinski, Maris and Tamura [19].

Diamond. It is a metastable allotrope of carbon, where atoms are arranged in a face-centered cubic crystal structure, which is the diamond lattice. In it, each carbon atom is surrounded by four neighboring carbon atoms, which are forming a tetrahedral shaped unit. Diamond is a material having exceptional physical characteristics. Most notable are its extreme hardness and thermal conductivity (900–2320 $W \cdot m^{-1} \cdot K^{-1}$) [20]. Above 1973 K, and in vacuum or oxygen-free atmosphere, diamond converts to graphite, whereas, in air, transformation starts at ~700 °C [21].

To apply (11), let us use for diamond the following parameters: $v_s = 18. \times 10^5\, cm/s$, $L = 0.7\, cm$, $\Theta = 2230\, K$, $a = 5.$, $A = 0.05 \times 10^{-45} s^3$, $B_2 = 3. \times 10^{-26} s/K^3$ and $b_1 = 12. \times 10^{-26} s/K^3$. The thermal conductivity is given in the Figure 5.

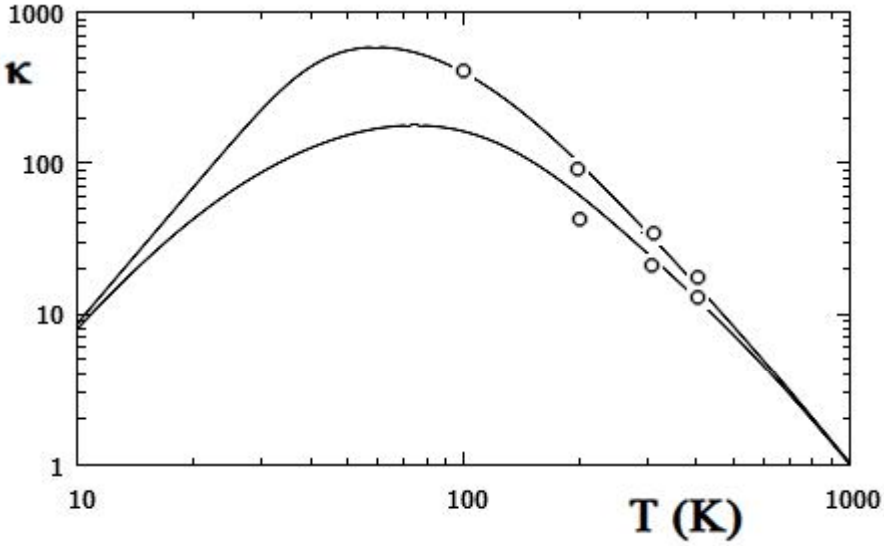

Fig. 5. Thermal conductivity ($W \cdot cm^{-1} \cdot K^{-1}$) of isotopically enriched and natural Diamond. The enriched sample has the larger thermal conductivity. Dots are representing some of the experimental data from Ref.20.

Another approach based on relaxation times. The Callaway model is not considering any distinction between longitudinal and transverse phonon. M.G. Holland in [22], proposed an analysis of lattice thermal conductivity, where longitudinal and transverse phonons have their specific relaxation times. In Holland's model, the relaxation time of the isotope scattering is the same of Callaway's model. In the boundary scattering, Holland introduced a factor to simulate a non-fully diffusive event. However, the main change in his model was in the relaxation times for normal and umklapp phonon-phonon scattering mechanisms, which were arranged to capture the high-temperature behavior of thermal conductivity. The Holland's relaxation time expressions are different for normal and umklapp processes, and are also involving distinct parameters for longitudinal and transverse acoustic phonons. In this manner, the Holland's model can describe the thermal conductivity at higher temperatures, better than the Callaway's model. Of course, in a relaxation time approximation, besides changing the expression of relaxation times it is also possible to add the contribution of other scattering mechanisms, such as the four-phonon scatterings (an expression for them was given by Klemens [23]), to improve the fitting of theoretical model to experimental data.

Let us conclude remembering that, as discussed in [1], several other approaches to the analysis of thermal conductivity in dielectric solids are possible, from variational techniques to first-principle calculations [4, 24-28].

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