Kinetics of thin films mechanical oscillations

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Abstract

Thermal conductivity of thin film is analyzed in this paper. It has been shown that at low temperatures, thermal conductivity of film is considerably lower than that of bulk structure. Also, the dependence of activation energy on boundary conditions has been investigated. It has been found that the implantation of light molecules in film boundaries leads to considerably higher activation temperatures. Our theoretical results proved to be in agreement with some of the latest experimental data.
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1. Introduction

Mechanical oscillations are a subsystem, always present when we analyze conductive, semiconductive and dielectric properties of a system. Consequently, the authors are first going to analyze the kinetics of mechanical oscillations in thin films, which can be considered as a ground for investigations of other properties of these structures. In a way this work represents generalization of investigations which were carried out in Refs. [1,2].

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The plane of investigations is as follows. Using the formula

$$\kappa = DC\rho_M \ , \tag{1.1}$$

where κ is the coefficient of the thermal conductivity, D the diffusion coefficient, C the specific heat and ρ_M the density, we shall determine the coefficient of thermal conductivity of thin film. The analysis of this coefficient is of great practical interest, since it determines the heat isolation and a number of other properties of these structures [3].

The diffusion coefficient D (strictly speaking the diffusion tensor D_{ij}) will be found via the use of Kubo formula [4]. The temperature dependence of film density will be determined using the Green's function method. Using this method one can find the internal energy and the average value of the square of molecular displacements.

All calculations will be carried out for ideal boundary conditions in films, and for specific boundary conditions on its surfaces, which can be chosen in a way which leads to some useful effects.

The optimal choice of boundary conditions is the main practical goal of investigations pertaining to deformed structures.

2. The diffusion coefficient

Starting from the Kubo formula [4,5], one obtains the following expression defining the diffusion coefficient:

$$D_{ij} = \lim_{\delta \to \infty} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\delta t} \langle \hat{v}_i(0)\hat{v}_j(t) \rangle \ , \tag{2.1}$$

where $\hat{v}_i$ and $\hat{v}_j$ are the velocity operators in Heisenberg representation, and δ is the perturbation parameter and indexes i, j take values x, y, z.

The averages are taken over great canonical ansamble, i.e.

$$\langle \cdots \rangle = \mathrm{Tr}\{\mathrm{e}^{(\Omega + \mu N - H)/\theta}(\cdots)\} \ , \tag{2.2}$$

where Ω is the thermodynamical potential, μ the chemical potential, and H the Hamiltonian of the system and $\theta = k_B T$.

In order to find the correlation function $\langle \hat{v}_i \hat{v}_j \rangle$ we will find the Green's function [6]

$$\ll p_i(t)| p_j(0) \gg \ ,$$

where $p_i(t)$, $p_j(0)$ are the components of the molecular momentum.

The Hamiltonian of a phonon subsystem is of the form

$$H = \frac{1}{2M} \sum_{\vec{n}} p_{\vec{n}}^2 + \frac{C_H}{2} \sum_{\vec{n}} (u_{\vec{n}}^2 + u_{\vec{n}-\vec{1}}^2 - 2u_{\vec{n}}u_{\vec{n}-\vec{1}}); \quad \vec{n} \in (n_x, n_y, n_z) \ , \tag{2.3}$$

where M is the mass of molecule, C_H are Hook's elasticity constants, u are molecular displacements, and $\vec{1}$ denotes unit elementary cell vector. It should be pointed out that the Hamiltonian of an ideal structure is taken in harmonics approximation and in approximation of the nearest neighbours.

Boundary conditions will be taken into account during the formation of a system of equations defining the Green's function of the system.

We are trying to determine the Green's function

$$G_{n_x n_y f; m_x m_y g} \equiv \ll p_{n_x n_y f}(t) | p_{m_x m_y g}(0) \gg . \tag{2.4}$$

In the expression determining this function, the Green's function of a type $\ll u_{n_x n_y f}(t) | u_{m_x m_y g}(0) \gg$ appears. Using the standard calculation techniques of two time temperature Green's function [6,7], after the transformation:

$$G_{n_x n_y f; m_x m_y g}(t) = \frac{1}{N_x N_y} \sum_{k_x k_y} G_{k_x k_y f; k_x k_y g}(t) e^{ik_x a(n_x - m_x) + ik_y a(n_y - m_y)}, \tag{2.5}$$

one obtains the Fourier component of the function $G_{k_x k_y f; k_x k_y g}(t) \equiv G_f(t)$ (the second index is omitted because it is not essential)

$$G_f(\omega) \equiv \ll p_f | p_f \gg_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} G_f(t) e^{i\omega t} \, dt \tag{2.6}$$

in the form

$$G_{f+1}(\omega) + G_{f-1}(\omega) + \rho G_f(\omega) = \frac{i\hbar}{\pi} M , \tag{2.7}$$

where

$$\rho = \frac{M\omega^2}{C_H} - 4 \left(\sin^2 \frac{ak_x}{2} + \sin^2 \frac{ak_y}{2} \right) - 2 . \tag{2.8}$$

At this stage of calculations we can take into account that the object of our analysis is a thin film and that the boundary conditions have to be included into calculations.

For $f \in (1, \ldots, N_z - 1)$ the equation for the Green's function is of the form

$$G_{f+1}(\omega) + G_{f-1}(\omega) + \rho G_f(\omega) = R; \quad R \equiv \frac{i\hbar}{\pi} M . \tag{2.9}$$

At layer $f = 0$ we have the equation

$$G_1(\omega) + (\rho + \rho_0) G_0(\omega) = R , \tag{2.10}$$

where ρ_0 is the correction of ρ of the boundary $f = 0$, while at the layer $f = N_z$ the corresponding equation is the following:

$$G_{N_z - 1}(\omega) + (\rho + \rho_N) G_{N_z}(\omega) = R , \tag{2.11}$$

where ρ_N is the correction of ρ at the boundary $f = N_z$.

The solution of the system of equations (2.6), (2.8) and (2.10) will be searched for in the form

$$G_f(\omega) = A \sin f k_z a + B \sin(f - 1) k_z a , \tag{2.12}$$

where a is the lattice constant, k_z is the component of wave vector, and A and B are the constants which will be determined in accordance with boundary conditions. After

substitution (2.12) into (2.9), (2.10) and (2.11), we find

$$G_f(\omega) = \frac{i\hbar}{\pi} C_H \frac{1}{\omega^2 - \omega_k^2} \;, \tag{2.13}$$

where

$$\omega_k \equiv \omega_{k_x k_y k_z} = 2\Omega \sqrt{\sin^2 \frac{ak_x}{2} + \sin^2 \frac{ak_y}{2} + \sin^2 \frac{ak_z}{2}} \;. \tag{2.14}$$

The notation used in (2.14) is:

$$\Omega \equiv \sqrt{\frac{C_H}{M}}, \quad k_x = \frac{2\pi v_x}{N_x a}, \quad k_y = \frac{2\pi v_y}{N_y a}, \quad v_{x/y} \in \left[-\frac{N_{x/y}}{2}, +\frac{N_{x/y}}{2} \right], \quad N_{x/y} \sim 10^8 \;,$$

while k_z are the solutions of the transcendental equation

$$\cot(N_z - 1)ak_z$$
$$= \frac{4\cos^3 ak_z - 2(\rho_0 + \rho_N)\cos^2 ak_z + (\rho_0\rho_N - 3)\cos ak_z + \rho_0\rho_N}{-\sin ak_z[4\cos^2 ak_z + 2(\rho_0 + \rho_N)\cos ak_z + (1 - \rho_0\rho_N)]} \;. \tag{2.15}$$

In the "cut-off" case [1,8] (the approximation $\rho_0 = \rho_N = 0$ will be called that) we obtain

$$k_z = \frac{\pi v_z}{N_z + 2} a, \quad v_z = 1, 2, 3, \ldots, N_z + 1 \;. \tag{2.16}$$

It can be seen that the levels k_x and k_y are equidistant, while, due to the structure deformations, levels k_z have lost equidistant properties.

The correlation function of the Green's function (2.12) is given by a general formula [6]:

$$\langle p_f(t) p_f(0) \rangle = \lim_{\delta \to +0} \int_{-\infty}^{+\infty} d\omega \, e^{-i\omega t} \frac{G_f(\omega + i\delta) - G_f(\omega - i\delta)}{e^{\hbar\omega/\theta} - 1} \;. \tag{2.17}$$

The Green's function (2.12) can be expressed as a sum of elementary fractions. In this way we obtain the correlation function:

$$\langle p_f(t) p_f(0) \rangle = \frac{\hbar C_H}{\omega_k} \left(\frac{e^{-i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} - \frac{e^{i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} \right) \;, \tag{2.18}$$

wherefrom follows

$$\langle v_f(t) v_f(0) \rangle = \frac{\hbar C_H}{M^2 \omega_k} \left(\frac{e^{-i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} - \frac{e^{i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} \right) \;. \tag{2.19}$$

In accordance with the general formula (2.1) the diffusion coefficient is given by

$$D_f \equiv D_{ii}^f(k)$$
$$= \left| \frac{\hbar C_H}{M^2 \omega_k} \int_0^{\infty} \left(e^{-\delta t} \frac{e^{-i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} - e^{-\delta t} \frac{e^{i\omega_k t}}{e^{\hbar\omega_k/\theta} - 1} \right) dt \right| = \frac{\hbar C_H}{M^2 \omega_k^2} \;. \tag{2.20}$$

It can be seen that the phonon diffusion coefficient of the film, as well as of the bulk, does not depend on temperature [9,10].

3. Thermal conductivity

As it has been stated in the Introduction, the determining of the thermal conductivity coefficient, requires (besides the determined diffusion coefficient) the knowledge of specific heat as well as the knowledge of the film density. The specific heat of a thin film has been found in our previous paper [2,11,12]. Taking into account that the energies of the phonons in the film cannot be equal to zero, and applying the long-wave approximation: $4[\sin^2(ak_x/2) + \sin^2(ak_y/2)] \approx a^2 k^2$; $k^2 = k_x^2 + k_y^2$, we obtain from formula (2.14):

$$E(\vec{k}) = \sqrt{a^2 k^2 E_0^2 + \Delta^2} \; , \tag{3.1}$$

where

$$E_0 = \hbar \sqrt{\frac{C_H}{M}}; \quad \Delta = ak_z^{\min} E_0 \; . \tag{3.2}$$

Internal energy of the system will be calculated using the standard formula [9,10]:

$$U_f = 3 \sum_{k_x, k_y, k_z} E(\vec{k}) [e^{E(\vec{k})/\theta} - 1]^{-1} \; . \tag{3.3}$$

Converting the sum in (3.3) to an integral in accordance with the formula: [1]

$$\sum_{k_x, k_y, k_z} \to 3(N_z + 1) \sum_{k_x, k_y} \to \frac{3 N_x N_y (N_z + 1) a^2}{4\pi^2} \int_0^{2\pi} d\varphi \int_0^{k_{\max}} k \, dk$$

and taking $k_{\max} \approx k_D = \sqrt[3]{6\pi^2}$, we obtain the following expression for the internal energy of the film:

$$
\begin{aligned}
U_f = \frac{3 N_f}{2\pi} \left(\frac{\Delta}{E_0}\right)^2 \theta &\left\{ \left[Z_1\left(\frac{\Delta}{\theta}\right) - \varepsilon^2 Z_1\left(\varepsilon\frac{\Delta}{\theta}\right) \right] \right. \\
&\left. + 2\frac{\theta}{\Delta} \left[Z_2\left(\frac{\Delta}{\theta}\right) - \varepsilon Z_2\left(\varepsilon\frac{\Delta}{\theta}\right) \right] + 2\left(\frac{\theta}{\Delta}\right)^2 \left[Z_3\left(\frac{\Delta}{\theta}\right) - Z_3\left(\varepsilon\frac{\Delta}{\theta}\right) \right] \right\} \; ,
\end{aligned}
\tag{3.4}
$$

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[1] The transition $\sum_{\vec{k}} \to \int d\vec{k} = \int d^3 k$ of Decarte's coordinates for film must to be carried out to cylindrical coordinates due to finite thickness.

where

$$E_D = E_0 a k_{max}, \quad E_0 = \hbar\Omega, \quad N_f = N_x N_y (N_z + 1), \quad \varepsilon = \sqrt{1 + (E_D/\Delta)^2} \ ,$$

$$k^2 = k_x^2 + k_y^2, \quad \Delta = a k_z^{min} E_0, \quad Z_r(X) = \sum_{j=1}^{\infty} j^{-r} e^{-jX} \ , \tag{3.5}$$

(The functions Z_r are called Dyson's functions.)

The expression for the specific heat per elementary cell is the following [9,10]:

$$C_f = \frac{1}{N_f} \frac{\partial U_f}{\partial T} = \frac{k_B}{N_f} \frac{\partial U_f}{\partial \theta} \ . \tag{3.6}$$

Combining this formula with formula (3.4) one obtains

$$C_f = \frac{3k_B}{2\pi} \left(\frac{\Delta}{E_0}\right)^2 \left\{ \frac{\Delta}{\theta} \left[(e^{\Delta/\theta} - 1)^{-1} - \varepsilon^3 (e^{\varepsilon\Delta/\theta} - 1)^{-1} \right] \right.$$

$$+ 3 \left[Z_1 \left(\frac{\Delta}{\theta}\right) - \varepsilon^2 Z_1 \left(\varepsilon\frac{\Delta}{\theta}\right) \right] + 6\frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta}\right) - \varepsilon Z_2 \left(\varepsilon\frac{\Delta}{\theta}\right) \right]$$

$$\left. + 6 \left(\frac{\theta}{\Delta}\right)^2 \left[Z_3 \left(\frac{\Delta}{\theta}\right) - Z_3 \left(\varepsilon\frac{\Delta}{\theta}\right) \right] \right\} \ . \tag{3.7}$$

To determine the density, we first calculate the density correction caused by molecular vibrations. Starting with the standard expression [13]:

$$\vec{u}_{\vec{n}} = \sum_{j,\vec{k}} \sqrt{\frac{\hbar}{2MN\omega_{\vec{k}}^j}} \left[b_j^+(\vec{k}) e^{-i(\vec{k}\vec{n} - \omega_j(\vec{k})t)} + h.c. \right] \vec{e}_j(\vec{k}), \quad j \in (x, y, z) \tag{3.8}$$

for molecular displacements, we can find the averages of squares of displacements:

$$\sum_{\vec{n}} \langle u_{\vec{n}}^2 \rangle \equiv N_f \langle u^2 \rangle = \sum_{j,\vec{k}} \frac{\hbar}{2M\omega_{\vec{k}}^j} (1 + 2\langle \hat{n}_k \rangle), \quad \langle \hat{n}_k \rangle = \frac{1}{e^{E(\vec{k})/\theta} - 1} \ . \tag{3.9}$$

Introduction of the notation $\langle u_0^2 \rangle = (1/N) \sum_{\vec{k}} \hbar/2M\omega_k$ one can find in (3.9):

$$\langle u^2 \rangle - \langle u_0^2 \rangle = \frac{3}{2\pi} \frac{\hbar}{M\omega_D} \frac{\Delta}{E_0^2} \theta \left\{ Z_1 \left(\frac{\Delta}{\theta}\right) \right.$$

$$\left. - \varepsilon Z_1 \left(\varepsilon\frac{\Delta}{\theta}\right) + \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta}\right) - \varepsilon Z_2 \left(\varepsilon\frac{\Delta}{\theta}\right) \right] \right\} \ . \tag{3.10}$$

The density of the film is given by the formula

$$\rho_M = \frac{M}{\langle a + u \rangle^3} = \frac{M}{\langle a_0 \rangle^3} \frac{1}{1 + 3\langle u \rangle^2/\langle a_0 \rangle^2} \rho_M \approx \rho_0^M \left(1 - \frac{3\langle u \rangle^2}{\langle a_0 \rangle^2}\right) \ . \tag{3.11}$$

Using Debye's approximation [14], we shall substitute $\langle u^2 \rangle$ in (3.11) with $\langle u^2 \rangle - \langle u_0^2 \rangle$ from formula (3.10). Thus, we obtain

$$\rho_M = \rho_0^M \left(1 - \frac{9}{2\pi} \frac{\hbar^2 \Delta\theta}{M\langle a_0 \rangle^2 E_D E_0^2} \left\{ Z_1 \left(\frac{\Delta}{\theta} \right) \right. \right.$$

$$\left. \left. - \varepsilon Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) + \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\} \right) . \tag{3.12}$$

Substituting (2.20), (3.7) and (3.12) in (1.1) we finally obtain the expression for the thermal conductivity coefficient of thin film structures:

$$\kappa_f = \frac{3k_B}{2\pi} \frac{\hbar \Omega^2}{M\omega_k^2} \left(\frac{\Delta}{E_0} \right)^2 \left\{ \frac{\Delta}{\theta} [(e^{\Delta/\theta} - 1)^{-1} - \varepsilon^3 (e^{\varepsilon\Delta/\theta} - 1)^{-1}] \right.$$

$$+ 3 \left[Z_1 \left(\frac{\Delta}{\theta} \right) - \varepsilon^2 Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 6 \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right]$$

$$+ 6 \left(\frac{\theta}{\Delta} \right)^2 \left[Z_3 \left(\frac{\Delta}{\theta} \right) - Z_3 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\} \rho_0^M \left(1 - \frac{9}{2\pi} \frac{\hbar^2}{M\langle a_0 \rangle^2 E_D} \left(\frac{\Delta}{E_0} \right)^2 \right.$$

$$\left. \times \frac{\theta}{\Delta} \left\{ Z_1 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) + \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\} \right) . \tag{3.13}$$

Formula (3.13) was analysed numerically as a function of the scaled temperature $x = \theta/\Delta$. The notation

$$\lambda_{b/f}(x) \equiv \frac{\kappa_{b/f}(x)}{\kappa_0} , \tag{3.14}$$

where

$$\kappa_0 = \frac{8}{9} (6\pi^2)^{-2/3} \frac{\hbar}{a^3} \left(\frac{\Delta}{E_0} \right)^3$$

represents scaled thermal conductivity, is introduced into formula (3.13). The dependence of scaled thermal conductivity on the scaled temperature is given in Figs. 1 and 2.

It can be seen from figures quoted that, at extremely low temperatures $T \leqslant 4$ K and at temperatures $T \geqslant 180$ K, the thermal conductivity of a film is lower than that of a bulk. In the temperature range $4 < T < 180$ K the thermal conductivity of a bulk is lower than that of a film.

At the end of this section we would like to point out an important fact: since Eq. (2.15) does not have the solution $k_z = 0$, all phonon energies in film have a gap. Consequently, to excite the phonons in films some activation energy is necessary [6,7,10–12].
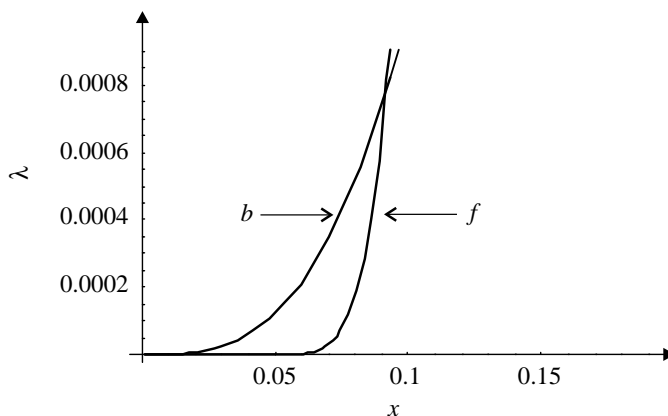
Fig. 1. Thermal conductivity versus temperature at extremely low temperatures (up to 5 K).
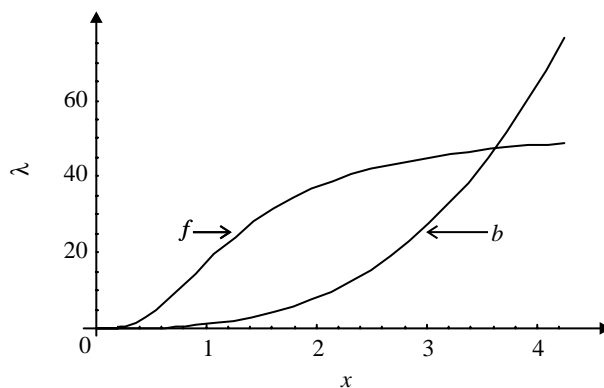

Fig. 2. Thermal conductivity versus temperature at higher temperatures (in the range $T > 4$ K).

4. The influence of boundary conditions

The influence of boundary conditions to the minimum of the activation energy will be discussed here.

It will be assumed that the physical conditions at both boundaries $n_z = 0$ and N_z are the same. It will also be assumed that the lattice constants at boundary layers are the same as in the volume of film. It means that Hook's constants C_H, as well as the trigonometric part of parameter ρ (formula (2.8)) which is independent on molecular mass M, do not change at the boundaries. We shall assume that only molecular masses change at the boundaries. Their boundary values are $M - M'$, where M is the mass of volume molecules.

Taking all this into account, we obtain the boundary corrections of the parameter ρ:

$$\rho' = \rho_0 = \rho_N = \frac{\omega^2}{\Omega^2} \frac{M'}{M} \ . \tag{4.1}$$

On the other hand, the numerical solution of (2.15) has shown that for $\rho' = 1$ the minimal value of ak_z is $ak_{\min}^z = 1.22$. Substituting this value in (4.1) we obtain

$$\omega_{\min} = 2\Omega \sin \tfrac{1.22}{2} \ , \tag{4.2}$$

wherefrom follows:

$$\frac{\omega_{\min}}{\Omega} = 1.146 \ . \tag{4.3}$$

By combining (4.2) and (4.3) we find $M'/M = 0.76$. This means that the masses of boundary molecules $M - M'$ are about four times smaller than the masses M of volume molecules. More precisely

$$M - M' = 0.24 \ . \tag{4.4}$$

If we assume the Debye's frequency to be $\omega_D \equiv E_D/\hbar = 2\sqrt{3}\Omega = 150 k_B/\hbar$, on the basis of (4.2), it can be concluded that minimal temperature necessary to excite the phonons is around

$$T_{ac} \approx 50 \text{ K} \ . \tag{4.5}$$

The result obtained has shown that the choice of boundary conditions is one of most important elements in the synthesis of high-temperature superconductors.

At the end of the section we quote the general formula for correction of the parameter ρ at the boundaries. If the changes of the boundary lattice constants are $a \to a \mp a', a' \ll a$ then $C_H \to C_H \pm C'_H, C'_H \ll C_H$. If we assume that the mass changes are $M \to M \mp M'$, the correction of the parameter ρ is

$$\rho' = \frac{\omega^2}{\Omega^2} \left(\mp \frac{M'}{M} \pm \frac{C'_H}{C_H} \right) \mp 2a'k_x \sin ak_x \mp 2a' \sin ak_y \ . \tag{4.6}$$

This general formula enables the choice of optimal boundary conditions in films.

5. Conclusion

The results obtained show that the thermal conductivity coefficient of a film is considerably lower than that of a bulk at low temperature, where the thermal conductivity of bulk decreases as T^3. This result is practically applicable: sandwich of several films would be a better thermoisolator than the bulk structure of the same thickness.

In the analysis in Section 4 it has been shown that, by convenient choice of boundary conditions (implantation of light molecules at boundaries), a relatively high activation temperature (about 50 K) can be reached.

It should be noticed that, in the "cut-off" case (boundary corrections of the parameter ρ are equal to zero), the activation temperature is around 20 K for the film of the same thickness.

Higher activation temperatures cause lower thermal conductivity. Consequently, if we implant light molecules in the film boundaries, we shall get several times better thermal isolation.

In accordance with the Viedeman–Frantz rule, the electrical conductivity is proportional to thermal conductivity. This leads to the conclusion that films are worse electrical conductors than bulk structures of the same material.

It could be interesting to estimate the superconductive properties, since worse conductors are, in principle, better superconductors.

The results obtained here are compared to the theoretical results as well as to the experimental data from Refs. [15–18].

The theoretical results are in qualitative agreement with the experimental measurements from Ref. [15]: in the range of temperatures higher 50 K thermal conductivity of thin structure is represented by convex curves. In bulk structure the corresponding curves are concave. In connection with this one can see Figs. 2a and b from Ref. [15] and Fig. 2 on our paper.

We found satisfactory agreement our results with corresponding theoretical results in Refs. [16,17]. The curve for thermal conductivity from Ref. [16] has the same trend as our curve in Fig. 2. In Ref. [17] was shown that phonons in thin structure have gap in dispersion law. The same is obtained in our theory.

In the paper [18] the experimental curve is given for more wide temperature interval. Analysis of the curves given in Fig. 4 from Ref. [18] shows that thermal conductivity of thin structure is higher than that of bulk in the temperature range 1–10 K. For $T > 10$ K thermal conductivity of bulk is higher than in corresponding thin structure. For extremely low temperature, thermal conductivity of thin structure has to be lower than that of bulk due to the presence of gap in phonon spectra. This range of temperatures was not experimentally caught in Ref. [18].

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