PHONON THERMAL CONDUCTIVITY OF GRAPHENE

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Abstract: The study of graphene thermal conductivity is of great importance, as its anomalous thermal and electrical conductivities (the largest among the all known materials so far) provide very good perspectives for graphene-based nanoelectronics devices. Thermal conductivity of graphene is phonon-based, since its electronic-based thermal conductivity represents less than 1% of the total thermal conductivity at room temperature. For the consideration of the thermal conductivity of graphene the Boltzmann equation in the approximation of relaxation time is used. The relaxation time is determined, with three mechanisms of phonon scattering accounted simultaneously: at defects, at borders, and on phonons. Temperature dependence of thermal conductivity is determined numerically in the range from 15 K to 400 K. The results obtained are in accordance with some other available results found in literature, obtained either experimentally or by numerical calculations.

Keywords: graphene, thermal conductivity, phonon scattering, relaxation time

PACS Index Numbers: 65.80Ck, 63.22Rc, 61.48Gh

Introduction

In order to fulfill the essential task of phonon engineering [1], to improve the electric and thermal transport properties of the given nanostructure, it is very important to get acquainted with its mechanisms of thermal conductivity. Since the contribution of phonon subsystems to thermodynamic analysis is the first step in research of nano structure properties [2], special attention in this paper is devoted to study of phonon thermal conductivity of graphene.

Graphene is a single layer 2D structure which surface is covered with regular hexagons of 0.142 nm side, with carbon atoms in hexagons' vertices. It can be considered as a structural part of graphite, whose 3D structure is composed of graphene planes located at a distance of 3 nm [3]. Graphene has unique properties such as anomalous high electrical and thermal conductivity, extremely high mobility of charge carriers, dependence of electric properties from the presence of impurities on the surface, the ability to set the size of the band gap, quantum Hall effect and good electromechanical characteristics [4]. All above make graphene a very promising material for nanoelectronics.

Ideal pristine 2D structure cannot be obtained due to thermodynamic instability [5–9]. But, if this structure is strained or has defects, it can exist without contact with the wafer. It is experimentally established that there are free graphene sheets that constitute the complex wavy form [10].

Out of the mentioned properties the most striking is the anomalous high thermal conductivity. The measured thermal conductivity [11] is in the range from 3500 W/mK to 5500 W/mK, the largest among the all known materials so far.

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Based on the measured electrical conductivity and using Wiedemann–Franz law, it is estimated that the share of electronic thermal conductivity in the total thermal conductivity, is less than 1% [11,12]. Therefore, the mechanism of the graphene thermal conductivity is mostly phonon-based. It is the analysis of the grapheme thermal conductivity that can help explaining the paradox of a solid-state physics. This paradox is associated with a monotone growth of the coefficient of phonon thermal conductivity of an ideal crystal (without defects) with the increase of its size, due to enlarged number of phonon modes which can exist in such sample. In real terms, there are several physical mechanisms which limit increase of coefficient of thermal conductivity of a real sample even though increase of its size [3]. By examining the coefficient of thermal conductivity of grapheme it is possible to determine the reasons limiting the thermal conductivity of 2D structures, as well as the changes of the coefficient of thermal conductivity with increasing number of layers. It is assumed that an increase in the number of layers reduces the coefficient of thermal conductivity, because there is another channel for the scattering of phonons, associated with the interaction of layers.

The sheets of ideal graphene of infinite dimensions do not differ among each other. But the real samples differ not only in size but also in the structure of boundaries, which modifies acoustic phonon properties such as phonon group velocity, polarization, density of states, and changes the way acoustic phonons interact with other phonons, defects and electrons [1], cre ating opportunities for engineering phonon spectrum in order to improve thermal properties [2].

Graphene of sufficiently large size cannot have an ideal structure, because the grapheme surface contains structural defects depending on the synthesis and external conditions. These defects are: vacancies or adsorption of some functional group on the surface (which represent the most common type of defects), Stone-Wales defect, isotopic defect, dislocations, etc. [3]. The existence of these defects and boundaries significantly affects the coefficient of thermal conductivity and other transport properties of graphene.

Thermal conductivity of graphene

Thermal properties of nanomaterial graphene (specific heat, thermal expansion coefficient, the coefficient of thermal conductivity) significantly depend on phonon characteristics. Characteristics of phonon spectrum are determined by 2D structure of graphene. Graphene has a hexagonal structure with two carbon atoms in each cell. This causes the appearance of the six phonon branches in the dispersion spectrum: three acoustic (LA, TA and ZA) and three optical (LO, TO and ZO). LA and TA modes correspond to longitudinal and transversal phonon oscillations in a graphene plane. Mode ZA corresponds to oscillations of phonons in the direction normal to the direction of oscillation modes LA and TA. LA and TA modes have a linear dispersion law [12,13]: $\omega = \upsilon q$, with the velocities: $\upsilon_{\text{LA}} = 18.4 \, \text{km/s}$ and $\upsilon_{\text{TA}} = 16.5 \, \text{km/s}$. There is no agreement related to the dispersion law for mode ZA. In our calculation we adopted the dispersion law $\omega_3 = \upsilon q^{3/2}$ (instead of usually used $\omega_3 = \upsilon q^2$, as experimentally better fitted [13]) and the velocity $\upsilon(ZA) = 9.2 \, \text{km/s}$ [14,15].

The phonon thermal conductivity is determined from Boltzmann transport equation [14–16]:

$$\frac{\partial n_s(\vec{q})}{\partial t} + v \cdot \frac{\partial n_s(\vec{q})}{\partial x} = \frac{\partial n_s(\vec{q})}{\partial t} \bigg|_{coll}, \tag{1}$$

where $n_s(\vec{q})$ is a distribution function of phonons of polarization s, and $\frac{\partial n_s(\vec{q})}{\partial t}\Big|_{coll}$ is the

collision integral. Unlike the ordinary gas, the total number of phonons and quasi-total phonon momentum are not conserved in the phonon gas. The total quasi-momentum is not conserved

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due to the so-called U process (process of transfer) where the general quasi-momentum can change for the value of the reciprocal lattice vectors:

$$\sum_{i} \vec{q}_i = \sum_{i} \vec{q}_i + \vec{b} \ . \tag{2}$$

In ordinary, so called, normal N-processes, total quasi-momentum is conserved [14–16].

The usual approach for the Boltzmann equation solving lies in the linearization of collision integral around the equilibrium of phonon distribution function. This approach is possible if temperature gradient is not large, when the phonon distribution function is close to equilibrium, and the temperature which determines the distribution function slowly changes along the graphene sheet.

Heat flux is defined as:

$$\vec{W} = -\kappa \nabla T V \; ; \; W_{\alpha} = -\sum_{\beta} \kappa_{\alpha\beta} \frac{\partial T}{\partial x_{\beta}} V \tag{3}$$

where *V* is the volume of graphene sheet.

For the stationary case, $\frac{\partial n_s^0(\vec{q})}{\partial t} = 0$. The left side of the Boltzmann equation (1) becomes:

$$\frac{\partial n_s(\vec{q})}{\partial x} \cdot \upsilon_s(\vec{q}) = \frac{\partial n_s(\vec{q})}{\partial T} \frac{\partial T}{\partial x} \cdot \upsilon_s(\vec{q}) = \frac{\partial n_s(\vec{q})}{\partial T} \nabla_x T \cdot \upsilon_s(\vec{q})$$
(4)

Collision integral is linearized near the equilibrium distribution, i.e.

$$n_{s}(\vec{q}) = n_{s}^{0}(\vec{q}) + n_{s}^{1}(\vec{q}),$$
 (5)

where $n_s^0(\vec{q})$ is the equilibrium distribution function of phonons of polarization s while $n_s^1(\vec{q})$ is the corresponding near-equilibrium deviation, and linearization is done in the approximation of relaxation times:

$$\frac{\partial n_s}{\partial t}\bigg|_{coll} = -\frac{[n_s(\vec{q}) - n_s^0(\vec{q})]}{\tau_s(\vec{q})} = -\frac{n_s^1(\vec{q})}{\tau_s(\vec{q})},$$
(6)

where $\tau_s(\vec{q})$ is the relaxation time of phonons of polarization s. Using (4) and (6), Boltzmann equation (1) becomes:

$$-\frac{n_s^1(\vec{q})}{\tau_s(\vec{q})} = \frac{\partial n_s(\vec{q})}{\partial T} \nabla_x T \cdot \nu_s(\vec{q}) \tag{7}$$

Now, heat flux can be expressed as:

$$W_{\alpha} = \sum_{s} \sum_{\beta} n_{s}^{1}(\vec{q}) \hbar \omega_{s\beta}(\vec{q}) \upsilon_{s\beta}(\vec{q}) V. \tag{8}$$

Since the phonon distribution function is close to the equilibrium distribution function, we can use $\frac{\partial n_s(\vec{q})}{\partial T} \approx \frac{\partial n_s^0(\vec{q})}{\partial T}$, and from (7) obtain:

$$n_s^1(\vec{q}) = -\tau_s(\vec{q}) \frac{\partial n_s^0(\vec{q})}{\partial T} \nabla_x T \cdot \upsilon_s(\vec{q}). \tag{9}$$

On the basis of equations (8) and (9), expression for heat flux becomes:

$$W_{\alpha} = -\sum_{s} \sum_{\beta} \tau_{s}(\vec{q}) \frac{\partial n_{s}^{0}(\vec{q})}{\partial T} \nabla_{x} T \cdot \upsilon_{s\alpha}(\vec{q}) \hbar \omega_{s\beta}(\vec{q}) \upsilon_{s\beta}(\vec{q}) V$$
(10)

$$W_{\alpha} = -\sum_{\beta} (\nabla_{x} T)_{\beta} \sum_{s} \tau_{s}(\vec{q}) \frac{\partial n_{s}^{0}(\vec{q})}{\partial T} \cdot \upsilon_{s\alpha}(\vec{q}) \hbar \omega_{s\beta}(\vec{q}) \upsilon_{s\beta}(\vec{q}) V$$
(11)

 $W_{\alpha} = -\kappa_{\alpha\beta} (\nabla T)_{\beta} L_{x} L_{y} L_{z}; \kappa_{\alpha\beta} = \kappa \delta_{\alpha\beta}. \tag{12}$

Wherefrom the diagonal part of tensor of thermal conductivity can be written as:

$$\kappa_{\alpha\alpha} = \kappa = \frac{1}{L_{x}L_{y}L_{z}} \sum_{s} \sum_{\vec{q}} \tau_{s}(\vec{q}) \frac{\partial n_{s}^{0}(\vec{q})}{\partial T} \hbar \omega_{s\alpha}(\vec{q}) \upsilon_{s\alpha}^{2}(\vec{q}) \cos^{2} \varphi =
= \frac{1}{L_{x}L_{y}L_{z}} \sum_{s} \sum_{\vec{q}} \tau_{s}(\vec{q}) \frac{\partial n_{s}^{0}(\vec{q})}{\partial T} \hbar \omega_{s}(\vec{q}) \upsilon_{s}^{2}(\vec{q}) \cos^{2} \varphi.$$
(13)

In the last relation φ is the angle between the graphene direction (x-axis) and the heat propagation direction. Switching from the summation to integration: $\sum_{\vec{q}} \rightarrow \int d^2 \vec{q} \rightarrow \int g_{2D}(\omega) d\omega$ (as in [14]), where the phonon density of states for 2D case, $g_{2D}(\omega)$ is defined from [16]:

$$g_{2D} = \frac{L_x L_y}{2\pi} \frac{\omega_s(\vec{q})}{\upsilon_s(\vec{q})u_s(\vec{q})}.$$
 (14)

 \vec{v} and \vec{u} are group and phase velocity, respectively.

By averaging over angle φ , from (11) the expression for the thermal conductivity of graphene is finally obtained:

$$\kappa = \frac{1}{4\pi L_z k_B T^2} \sum_{s} \int_{\omega_{\min}}^{\omega_{\max}} (\hbar \omega_s)^2 \frac{e^{\frac{\hbar \omega_s}{k_B T}}}{\left(e^{\frac{\hbar \omega_s}{k_B T}} - 1\right)^2} \tau(\omega_s) \frac{\upsilon}{u} \omega_s d\omega_s.$$
 (15)

Phonon scattering processes

The main contribution to the thermal conductivity provides acoustic branches, while the contribution of optical branches is negligible. The average time of phonons relaxation, which exists in expression (15), is determined by phonon scattering processes. Average scattering time is defined with Mathisen's rule as:

$$\frac{1}{\tau} = \sum_{i} \frac{1}{\tau_{i}} \tag{16}$$

where i – denotes the number of different scattering processes.

The most common scattering processes are: scattering of phonons at boundaries, scattering of phonons at defects (isotopic impurities, vacancies), and phonon-phonon scattering. Relaxation time for the appropriate type of scattering, considered below, is the estimated time.

At low temperatures in sufficiently pure sample the most important scattering mechanism is scattering at boundaries of the sample. Relaxation time for this case is defined in [14,17] as:

$$\frac{1}{\tau_B} = \frac{1-p}{1+p} \frac{\upsilon}{L_x},\tag{17}$$

where p is a measure of surface roughness, and L_x is the smallest dimension of sheet.

In the case of elastic scattering on isotopes, the relaxation time is defined in [18,19] by expression:

$$\frac{1}{\tau_{pd}} = A_d \frac{2\pi\omega^3}{\omega_D^2},\tag{18}$$

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where is $A_d = c_d \Delta M/M$. Here is c_d concentration of defects and $\Delta M/M$ is a ratio of elementary cell atomic mass change and atomic mass of a cell; ω_D is Debye frequency.

Even for small amounts of defects, the scattering on defects becomes a leading term, so that phonon-phonon scattering becomes negligible.

According to Peierls [5,6] the N-processes do not take part in the heat transmission. But, when it comes to graphene, this statement is questionable because of existence of YA mod with nonlinear dispersion law. Even though this question remains open, the contribution of the phonons which take part in N processes in heat transmission is going to be neglected in this paper. Therefore, for phonon–phonon scattering, so called, U-processes are significant.

For U-processes the relaxation time is defined as [20]:

$$\frac{1}{\tau_u} = 2\gamma_s^2 \frac{k_B T}{M v^2} \frac{\omega^2}{\omega_D} \,, \tag{19}$$

where γ_s is Grüneisen parameter. In case of the three-phonon U-processes only: $\tau_U \to \frac{\text{const.}}{\omega^2}$, $\kappa \to \int \frac{\text{d}\omega}{\omega}$, which leads to the so-called logarithmic divergence of thermal conductivity of 2D systems. Therefore, lower limit of integral is not zero but certain minimum value. Klemens gave a physical interpretation of the choice of this minimum value. He suggested the value ω_{\min} to be determined from the assumption that average free path of phonon is not greater than the characteristic dimension L_x of graphene [20]:

$$l(\omega_s, T) = \frac{1}{2\gamma_s^2} \upsilon \frac{M\upsilon^2}{k_B T} \frac{\omega_D}{\omega_s^2} < L_x.$$
 (20)

Temperature dependence of the coefficient of thermal conductivity

In this paper are analyzed various mechanisms of relaxation. Phonon-phonon scattering (Uscattering) and scattering at boundaries, taken together, provide high thermal conductivity values (as in[12]). If we take into account the scattering at defects, thermal conductivity is significantly reduced even for small concentration of defects. Calculations were carried out on the basis of relation:

$$\kappa = \frac{1}{4\pi L_z k_B T^2} \sum_{s} \int_{\omega_{min}}^{\omega_{max}} (\hbar \omega_s)^2 e^{\frac{\hbar \omega_s}{k_B T}} \left(e^{\frac{\hbar \omega_s}{k_B T}} - 1 \right)^{-2} \frac{\upsilon}{u} (\tau_B^{-1} + \tau_U^{-1} + \tau_{pd}^{-1})^{-1} \omega_s d\omega_s$$
 (21)

by taking into account expressions (17–19). Calculations were performed using the software package *Mathematica 9*. Index s has values $s \in (LA,TA)$, while relevant parameters are given in Table 1.

<i>Table 1: Relevant parameters of thermal conductivity</i>

L_z [μ m]	L_x [μ m]	v_{LA} [km/s]	υ _{TA} [km/s]	υ _{za} [km/s]	$\gamma_{\scriptscriptstyle LA}$	γ_{TA}	γ_{ZA}
0.35	100	18.4	16.5	9.2	1.8	1.6	-1.2
<i>M</i> [kg]	A_d	p	$\omega_{D,LA}$ [Hz]	$\omega_{\scriptscriptstyle D,TA}$ [Hz]	$\omega_{D,ZA}$ [Hz]	$\omega_{\min} = f(\omega, T)$	
2.10-26	$4.5 \cdot 10^{-4}$	0.9	$2.66 \cdot 10^{14}$	$2.38 \cdot 10^{14}$	1.32·10 ¹⁴	_	

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On the basis of our numerical calculations, with scattering at boundaries and phononphonon interaction only, temperature dependence of the graphene thermal conductivity is depicted in Figure 1

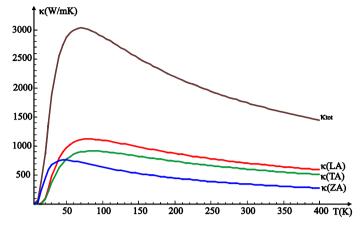


Figure 1: Calculated thermal conductivity of graphene (with no defects and impurities) as a function of temperature for different phonon branches

ZA – blue line, TA – green line, LA – red line, total thermal conductivity – black line

Figure 1 shows that when there is no scattering at defects the coefficient of thermal conductivity for the adopted parameters, reaches the value of $3.1 \text{ kW/(K \cdot m)}$.

The result obtained by taking into account all aspects of the scattering (at the borders, phonon-phonon scattering and scattering at defects) is shown in Figure 2.

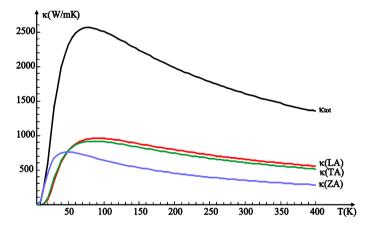


Figure 2:Calculated thermal conductivity of graphene for different phonon branches and all mechanisms of relaxation
ZA –blue line, TA –green line, LA – red line and total thermal conductivity –black line

From the Figures 1 and 2 it can be seen that the total thermal conductivity for the adopted parameters is about 2.6 kW/(K·m), which is consistent with experimental data [21]. Also, in Figure 1 are given temperature dependences of individual phonon branches. The greatest contribution to the thermal conductivity provides LA phonon branch, and branches TA provides only slightly lower contribution. The smallest share of the thermal conductivity provides ZA phonon branch that is about 20% of the total thermal conductivity. This is probably due to the small group velocity of ZA mode and great value of Grüneisen parameter. Interesting is alow-temperature area in which the largest contribution to thermal conductivity provides just ZA phonon branch (Figure 3).

1000 K(W/mK)

800 T*

K(ZA)

600

400

200

10 20 30 40 50 60 70 T(K)

Figure 3: Low temperature dependence of thermal conductivity for different phonon branches; ZA –blue, TA – green, LA –red

It also can be noted from the Figure 3 that the thermal conductivity for ZA branch fastest drops to zero, i.e. it has the steepest decline. At a temperature T^* , slightly lower than 50 K, all three phonon branches give equal contribution to thermal conductivity of graphene. Up to this temperature, the contribution to the thermal conductivity of TA phonon branch is larger than that of the LA branch, and for the values greater than T^* the contribution of these branches is invers.

Defects influence to the probability of scattering of phonons and the coefficient of thermal conductivity of real samples depends on the concentration of defects. The reduction of thermal conductivity coefficient of graphene with increasing concentration of defects is experimentally measured [11,22].

In the case of graphene samples without defects (Figure 1) the contribution of phonon branches of LA and TA is greater than in the case of samples with defects, which affects the growth of the total thermal conductivity, which now amounts to about $3.1 \text{ kW/(K \cdot m)}$. The contribution of phonon branch ZA is approximately the same as in the case of the sample with defects.

When analyzing the effect of different concentrations of defects on the total thermal conductivity of graphene, it can be seen that the thermal conductivity decreases with increasing concentration of defects (Figure 4). In the case of up to 0.5% increase of impurities concentration, for the values adopted in our example, the maximal thermal conductivity is reduced by about 12%, and the total thermal conductivity is reduced by 8.5%. For 1% increase of impurities concentration, the maximal thermal conductivity is reduced by about 24% and the total thermal conductivity is reduced by 15%. In doing so, the maximum values of thermal conductivity move into region of higher temperatures.

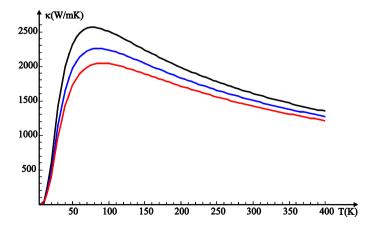


Figure 4: The dependence of coefficient of thermal conductivity for different concentrations of impurities; $A_d = 4.5 \cdot 10^{-4}$ -black line, $A_d = 9 \cdot 10^{-4}$ - blue line, $A_d = 13.5 \cdot 10^{-4}$ - red line

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The certain influence to the phonon properties of graphene at finite temperatures has anharmonic character of oscillations of the crystal lattice. One of the most important characteristic of anharmonic oscillations of graphene is phonon frequency dependence on the dimensions of elementary graphene cell, so called Grüneisen parameter:

$$\gamma_s = \frac{a_0}{2\omega_s^0(\vec{q})} \frac{\mathrm{d}\omega_s(\vec{q})}{\mathrm{d}a} \bigg|_{0}$$

Here are: a- dimension of elementary cell, \vec{q} - the wave vector of Brillouin zone, s- index of phonon mode, and the index 0 indicates the sizes corresponding to the equilibrium structure of the lattice. As a rule Grüneisen parameter is a positive value, because with oscillation amplitude increase, the mean value of the grid dimensions increases and frequency of oscillation decreases. However, under certain conditions, with layered structures type graphene, Grüneisen parameter can be negative [23]. In the paper [24] were calculated values of Grüneisen parameters in graphene and for some mode it is negative. The largest negative values correspond to ZA mode. The frequency of that mode increases with the lattice parameter increase, since during the stretching of graphene layer the movement of atoms is confined in the perpendicular direction to the layer thus increasing the frequency of oscillations of atoms–effect of membrane [25].

In this paper is analyzed the impact of the value of Grüneisen parameters on the total thermal conduction of graphene. In Figure 5 are presented the temperature dependences of the total thermal conductivity for different values of Grüneisen parameters. From Figure 5 is noticeable that the total thermal conductivity decreases for lower values of Grüneisen parameters.

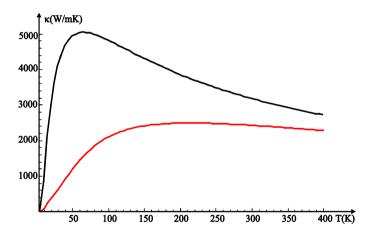


Figure 5: The dependence of the coefficient of thermal conductivity on Grüneisen parameters; $\gamma^{LA} = 1.8$; $\gamma^{TA} = 0.75$; $\gamma^{ZA} = -2 - black$ line, $\gamma^{LA} = 1.5$; $\gamma^{TA} = 0.56$; $\gamma^{ZA} = -1.8 - red$ line

It is interesting how the total thermal conductivity of graphene depends on the graphene sample size given in Figure 6. It is also evident that the thermal conductivity of graphene decreases with the sample size decrease, which is in accordance with the experimentally obtained results [26]. For the selected values and given temperature range in our case, the maximum value of thermal conductivity decreases for 52.23% if the dimensions of sample are cut twice, and the total thermal conductivity falls for 37%. When the dimensions of the sample are cut four times, then the maximum value of thermal conductivity is reduced by 62.13%, and the total thermal conductivity by 52%. In doing so, the maximum values of thermal conductivity are moving in the region of higher temperatures with sample size decrease. It is obvious that reduction of the dimensions of graphene sheet diminish the role of three-phonon U-process, causing a decrease of the coefficient of thermal conductivity.

4000 K(W/mK)

2000

1000

50 100 150 200 250 300 350 400 T(K)

Figure 6: Temperature-dependence of the coefficient of thermal conductivity on the length of the sample; $L_x = 100 \mu m - black$ line, $L_x = 50 \mu m - red$ line, $L_x = 25 \mu m - blue$ line

Conclusion

The study of graphene provides answers to fundamental issues related to the characteristics of two-dimensional crystal structure. The very fact of the existence of graphene is contrary to the principle formulated seventy years ago on the thermodynamic instability of similar structures.

The study of graphene is justified because of its exceptional characteristics and potential significant applications. The high thermal, mechanical and chemical stability associated with exceptional transport characteristics offer great opportunities for practical application of graphene. High value of coefficient of thermal conductivity is one of the important characteristics of graphene and has record levels of all known materials.

Thermal conductivity of grapheme is essentially phonon-based. The analyzed grapheme samples' dimensions exceeded average free path of phonons (800 nm [3]). Otherwise, a so-called ballistic transport would appear, with phonons spreading through the sample without scattering.

The obtained results have been achieved with a simplistic assumption that Grüneisen parameters, group and phase velocity of phonons are constant sizes. These parameters generally depend on the phonons frequency.

Different measurements of the coefficient of thermal conductivity of graphene, as well as different theoretical investigations give different results. It is evident that at low temperatures, the coefficient of thermal conduction is proportional to T^2 , and at high temperatures to T^1 what is in line with the general theory of the coefficient of thermal conductivity for 2D structures [16,17,27,28]. Also, the absolute value of coefficient of thermal conductivity increases with graphene sheet dimensions increase, which is associated with an increase in the number of phonon modes that occur in the sample. However, it is obvious that there are several physical mechanisms that limit the increase of the coefficient of thermal conductivity with increasing dimensions. One such mechanism is the scattering of phonons on defects. Further research should provide the answer about other mechanisms. Also, one direction of research is changing the phonon spectra, density of states and group velocity of phonons [29,30] which contribute to graphene thermal conductivity changes. Since experimental research of such miniature objects is difficult, numerical modeling should greatly provide information on important factors such as, for example, a form of potential interatomic interaction in graphene.

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Acknowledgment

This work was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Projects OI-171039 and TR 34019).

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