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TEMPERATURE DEPENDENCE OF THERMAL CONDUCTIVITY OF TWO-LAYER GRAPHENE

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INTRODUCTION

The heat transport of the two-layer graphene is analyzed, by using different mechanisms of the intra-layer phonon scattering (of both in-plane and out-plane phonons of the graphene mono-layers on defects, boundaries, phonons, and electrons of the corresponding graphene mono-layers) and inter-layer phonon scattering (of out-plane phonons of the one graphene mono-layer on out-plane phonons of the another graphene mono-layer). To consider thermal conductivity of the two-layer graphene, the Boltzmann transport equation in the approximation of relaxation time is used. Temperature dependence of thermal conductivity of the two-layer graphene is presented graphically in the range 0 ÷ 400 K, and compared with the available literature data.

TWO-LAYER GRAPHENE

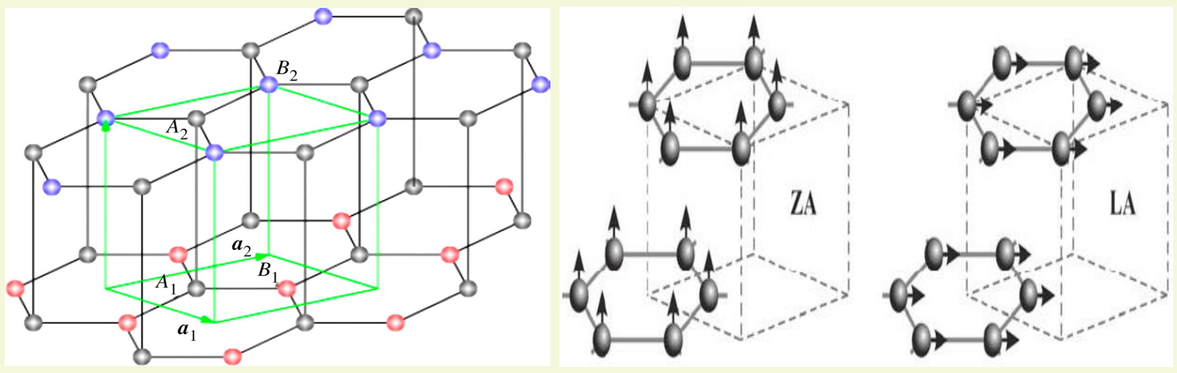


Figure 1. Two-layer graphene with atomic vibrations for ZA and LA branches.

Thermal conductivity of the two-layer graphene is a consequence of phonon scattering on defects, electrons, interlayer phonons, boundaries, and intralayer phonons (U processses). Characteristics of phonon spectrum are determined by 2D structure of graphene. This results in the appearance of six phonon branches in the dispersion spectrum: three acoustic (LA, TA, ZA) and three optical (LO, TO, ZO). The main contribution to thermal conductivity is provided by acoustic branches, while contribution of optical branches is neglected. LA and TA modes correspond to longitudinal and transverse phonon oscillations in a graphene plane, while ZA mode corresponds to oscillations of phonons normal to the direction of LA and TA modes. LA and TA branches have linear dispersion laws: $\omega_1 = v_1 q$, $\omega_2 = v_2 q$, while ZA branch has dispersion law: $\omega_3 = v_3 q^{1.5}$.

THERMAL CONDUCTIVITY OF TWO-LAYER GRAPHENE

The total contribution of all phonon branches in thermal coductivity of the two-layer graphene is analysed. The influence of phonons on thermal conductivity is described by isotropic Debye model. In calculation of the coefficient of thermal conductivity the Boltzmann transport equation in approximation of relaxation time is hereby used:

$$\kappa = \frac{1}{4\pi\hbar k_B T^2} \sum_s \int_{\omega_{\min}}^{\omega_{\max}} (\hbar\omega_s)^2 e^{\frac{\hbar\omega_s}{k_B T}} \left(e^{\frac{\hbar\omega_s}{k_B T}} - 1 \right)^{-2} \tau(\omega_s)\, \omega_s d\omega_s$$

$$\tau = (\tau_1^{-1} + \tau_2^{-1} + \tau_3^{-1} + \tau_4^{-1} + \tau_5^{-1})^{-1}$$

The following reciprocal relaxation times for phonon scattering are applied:

on defects $$\tau_1^{-1} = \frac{A\omega^4 h^3}{k_B^3}$$

on electrons $$\tau_2^{-1} = B\omega \frac{1}{e^{\frac{\Delta-\mu}{k_B T}} + 1}$$

on interlayer phonons $$\tau_3^{-1} = C \tanh\left(\frac{h\omega}{2k_B T} \right)$$

on boundaries $$\tau_4^{-1} = D \frac{v}{L}$$

on intralayer phonons – U processes $$\tau_5^{-1} = E\left(\frac{\hbar\omega T}{k_B} \right)$$

L – length of the sample, d – distance between two graphenee layers, v – phonon velocity, Δ – gap in the dispersion law of quasiparticles,

$$\varepsilon = \sqrt{\Delta^2 + \left(\frac{\hbar^2 k^2}{2m_{ef}} \right)}$$

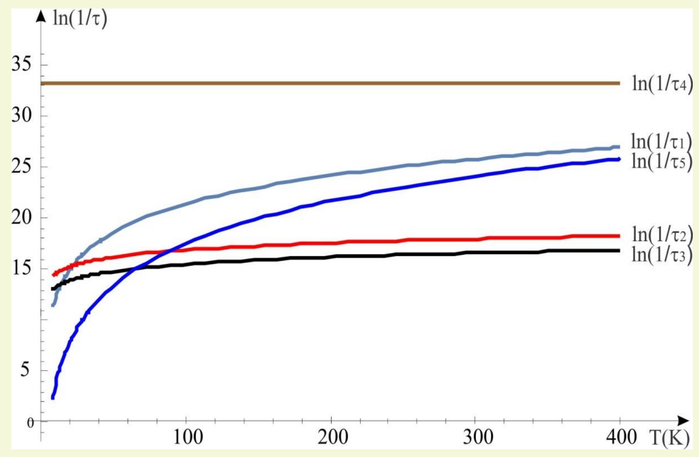
k – wave vector of quasiparticles, m_{ef} – effective mass of quasiparticles in the two-layer graphene.

THERMAL CONDUCTIVITY CALCULATIONS FOR TWO-LAYER GRAPHENE

The adopted values of parameters applied for finding thermal conductivity:

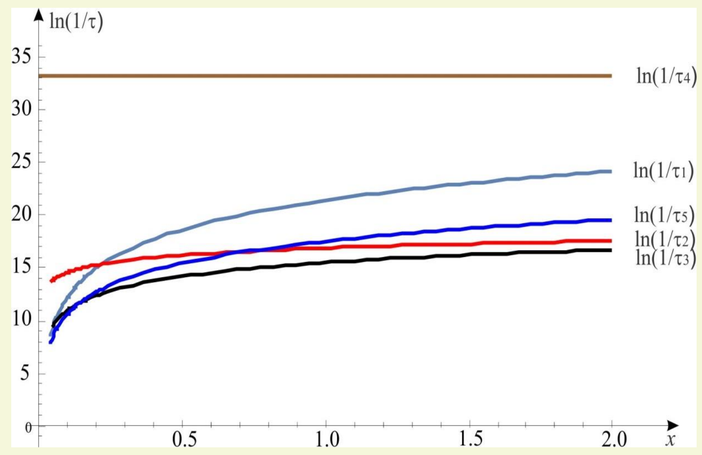
A	B	C	D	E
$1{,}9\times10^{-11} K^{-3}$	$3{,}3\times10^{-6}$	$0{,}9\times10^{-6}$	$5{,}3\times10^{3}$	$4{,}1\times10^{-5} K^{-6} s^{-1}$
L	d	Δ	μ	v
$10\mu m$	$0{,}335 nm$	$0{,}13\times10^{-19} J$	$4{,}168\times10^{-19} J$	$1{,}8\times10^{4} m/s$

Reciprocal relaxation time versus temperature for constant x is given in Fig. 2, while reciprocal relaxation time versus x for constant temperature is given in Fig. 3.



$$x^o \equiv \frac{\hbar\omega}{k_B T} = 1$$

Figure 2. Reciprocal relaxation time versus T for constant x .



$T = 100K$

Figure 3. Reciprocal relaxation time versus x for constant T.

Temperature dependance of total thermal conductivity of the two-layer graphene in the interval 0 ÷ 400 K is given in Fig. 4.

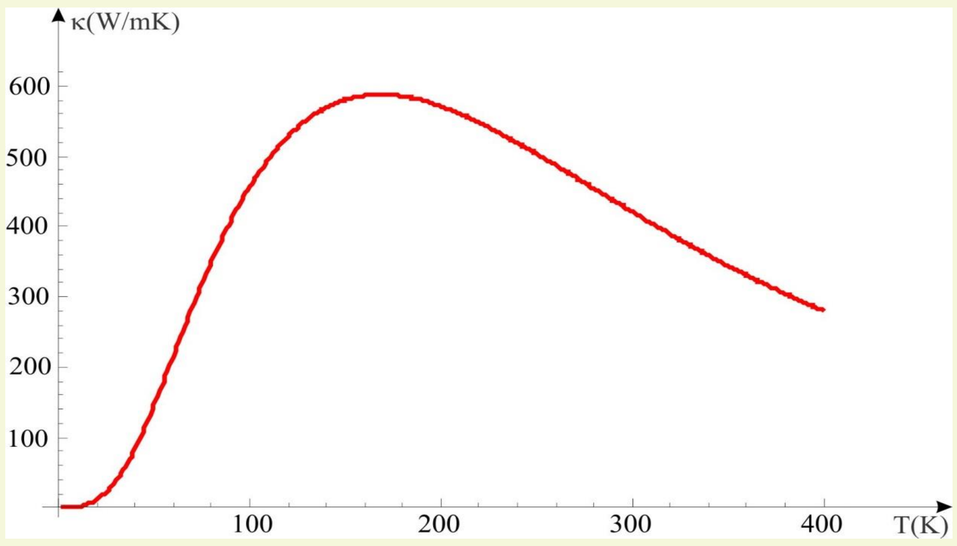


Figure 4. Total thermal conductivity versus temperature of the two-layer graphene

CONCLUSION

For constant phonon frequencies (constant x), from Fig. 2 it can be concluded that reciprocal relaxation time increases in the region of lower temperatures (up to 100 K), afterwards reaching saturation. The highest contribution is due to phonon scattering on boundaries, and lowest contribution is due to phonon scattering of interlayer phonons (of ZA branch) in the two-layer graphene.

For constant temperature, from Fig. 3 it can be concluded that reciprocal relaxation time behaves similarly with increase of phonon frequencies (variable x), but with observation of higher reciprocal relaxation time and lower thermal conductivity, compared to those obtained in Fig. 2.

Temperature dependance of total thermal conductivity has standard behaviour, as observed in Fig. 4. At lower temperatures (up to 150 K) it increases with $T^{1.2}$ behaviour, reaching maximum of 587 W/mK at 218 K, and then decreases with T^{-1} behviour. Maximum of total thermal conductivity is a result of concurent mechanisms of the increase of number of phonons with temperature increase, and decrease of the mean free path of phonons due to intralayer phonons scatternig in the so called U processes. Our results obtained by numerical integration are in accordance with the available experimental data.