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Electronic thermal conduction in suspended graphene

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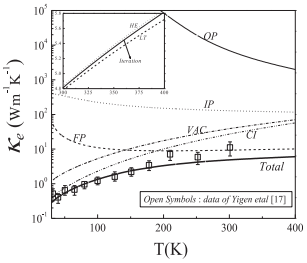
HIGHLIGHTS

- Electronic thermal conductivity, κ_e in suspended graphene is studied theoretically.
- Boltzmann equation directly solved for distribution function by the iteration method.
- Contribution from defects and in-plane, flexural, optical phonons is considered.
- κ_e dominated by flexural phonons (charged impurities) for T greater (less) than 75 K.
- Good fit to recent experimental data on κ_e in suspended graphene samples obtained.

GRAPHICAL ABSTRACT

Electronic thermal conductivity of suspended graphene is studied following Boltzmann formalism by iteration and compared with recent data and low-temperature and high-energy relaxation rate approximations.



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ABSTRACT

The electronic thermal conductivity (ETC), κ_e, of suspended graphene (SG) is studied for $15 < T < 400$ K, following the Boltzmann transport formalism. The electrons are considered to be scattered from defects along with the intrinsic in-plane acoustic phonons, out-of-plane flexural phonons (FPs) and optical phonons. The ETC is evaluated by computing the first-order perturbation distribution function by directly solving the linearized Boltzmann equation by an iterative method. Numerical calculations of the temperature and concentration dependences of κ_e show the dominance of charged impurity scattering at lower temperatures ($T < 75$ K) and of FPs at higher temperatures. The results are compared with the commonly used low-temperature and high-energy relaxation time approximations. Our calculations are in good agreement with recent κ_e data extracted for high-mobility SG samples. The validity of Wiedemann–Franz law is also discussed.

1. Introduction

In recent years, a great deal of interest has been evinced in the study of transport properties of graphene systems which have the potential for use in nano-electronic and thermal management applications. Graphene, a single layer of carbon atoms arranged in a honeycomb lattice is characterized by massless Dirac fermions and linear dispersion and possesses unique properties such as ultrahigh mobility and large thermal conductivity [1–4]. Graphene samples supported on SiO_2 substrates, exhibit a room temperature thermal conductivity of ~600 W m^{-1} K^{-1} [5]. Suspending a graphene layer over a trench is known to improve the electrical and thermal properties of graphene. For instance, the thermal conductivity of suspended graphene (SG) is measured to be ~5000 W m^{-1} K^{-1} [5]. Such an enhancement in thermal conductivity is mainly due to the suppression of the leakage of phonons across the graphene-substrate interface and also due to a large contribution from the scattering of electrons by out-of-plane flexural phonons (FPs) [5]. Being sensitive to the structure and composition of a graphene system the thermal properties are of

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great interest and importance for study in SG.

Thermal conductivity, κ, of a material comprises two contributions, namely the electronic thermal conductivity (ETC), κ_e, and the lattice thermal conductivity, κ_p: $\kappa=\kappa_p+\kappa_e$. In carbon materials, heat conduction is mainly by phonons. In the case of SG, its thermal-transport properties along with the charge-transport properties have been studied extensively [3–18]. There also exist theoretical [5,12–15] and experimental [5,16–18] investigations of thermal conductivity. Seol et al. [5] for their SG samples have reported room temperature thermal conductivity to be 3000–5000 W m^{-1} K^{-1}. Xu et al. [16] have measured temperature dependence of phonon transport in a suspended single layer graphene sheet in the temperature range from 15 K to 380 K using micro-fabricated suspended devices. They find that the thermal conductivity follows a $T^{3/2}$ power law, and that heat in SG is carried mainly by FPs. The theoretical efforts [5,12,13] have focused on κ_p. Using phonon Boltzmann equation, it has been shown that the lattice thermal conductivity of SG is dominated by contribution from the FP modes [5,12,13]. Nika et al. [13] using relaxation time approximation and long-wave approximation showed that the room temperature thermal conductivity of graphene is 4000 W m^{-1} K^{-1}. Lindsay et al. [12] incorporated the inelastic phonon–phonon scattering to describe κ_p of SG and found $\kappa_p \sim 3000$ W m^{-1} K^{-1} for graphene sheet length 10 μm.

The electronic thermal conductivity, κ_e, of graphene, though much smaller than κ_p, is of fundamental interest and can play an important role in determining the performance of nano-scale devices. It describes how the Dirac fermions carry energy. A knowledge of the electronic component of thermal conductivity can complement our understanding of the hot-electron cooling mechanisms involving electron–phonon couplings. It also helps optimizing heat management in highly doped graphene devices, in which κ_e can be dominant [3,17,18]. Foster and Aleiner [14] have computed κ_e within the hydrodynamic regime, and shown that κ_e is independent of the sample length, $L \gg l_Q$, an intrinsic length scale set by the imbalance relaxation rates. Saito et al. [15] have calculated the ballistic thermal conductance and find the temperature dependence of κ_e for gated graphene to change from T^2 to T at low temperatures. Yigen and coworkers [17,18] have extracted κ_e experimentally in high-mobility single-layer, annealed SG samples at moderate temperatures ($T<300$ K) using two-point dc electron transport at low bias voltages. They report κ_e to range from 0.5 to 11 W m^{-1} K^{-1} over a temperature range of 20–300 K and a power law dependence $\kappa_e \alpha T^p$ with $p \sim 1.63$–1.85. They conclude that, their samples are in the diffusive regime at low charge densities and scattering is predominantly due to charged impurities. It would, therefore, be of interest to present a detailed study of the temperature and carrier density dependences of ETC in SG and of relative importance of the scattering mechanisms determining the ETC. However, there do not seem to be reports on a detailed study of ETC in SG.

The purpose of the present work is to, first, make a systematic study of the electronic component of thermal conductivity taking into account the various contributions arising due to electron scattering in SG and, second, to compare our calculations with recent experimental data. For this, we employ the Boltzmann transport formalism. Section 2 describes the theory employed. The linearized Boltzmann equation is solved directly for the first order perturbation distribution, $\phi(E)$ by an iterative technique. Our numerical results on κ_e are discussed in Section 3.

2. Theory

2.1. Electronic thermal conductivity

The electronic thermal conductivity of a material, is defined under open circuit conditions, as

$$\boldsymbol{U} = \kappa_e\,(-\nabla T) \tag{1}$$

where $\boldsymbol{U}$ is the electron heat current density produced under the temperature gradient $\nabla \boldsymbol{T}$ and κ_e, in general, is a tensor.

We consider a SG sheet of length L and width W. The electron wave functions and energy eigenvalues around the Dirac points $\boldsymbol{K}$ and $\boldsymbol{K'}$, at the corners of the Brillouin zone are given by [1]

$$\psi^{\boldsymbol{K}}_{s,\boldsymbol{k}}(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}.\boldsymbol{r}}}{\sqrt{2A}}\begin{pmatrix} s e^{i\theta_k} \\ 1 \end{pmatrix},\ \psi^{\boldsymbol{K'}}_{s,\boldsymbol{k}}(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}.\boldsymbol{r}}}{\sqrt{2A}}\begin{pmatrix} s e^{-i\theta_k} \\ 1 \end{pmatrix}, \tag{2}$$

and

$$E(\boldsymbol{k}) = \hbar v_F\,|\boldsymbol{k}|, \tag{3}$$

where $\boldsymbol{k} \equiv (k_x, k_y)$ is the 2D electron wave vector, v_F is the Fermi velocity, $\theta_k = \tan^{-1}(q_x/q_y)$, $A=LW$ is the area of SG sheet and $s=+1,\ -1$ corresponds to conduction and valence band, respectively.

Let the occupation probability of the state $\boldsymbol{k}$ by an electron be given by the distribution function, $f(\boldsymbol{k})$. For low electric fields, $\boldsymbol{F}$ and temperature gradients, $\nabla \boldsymbol{T}$, applied along the SG layer the electron distribution function $f(\boldsymbol{k})$ experiences a perturbation, $f^1(E)$ which, neglecting the higher order terms, can be written as [19,20]

$$\begin{aligned} \mathrm{f}(\boldsymbol{k}) &\equiv \mathrm{f}(E) \\ &= f^0(E) + f^1(E) \\ &= f^0(E) + \varphi(E)\boldsymbol{v_k}.\left[\mathrm{e}\boldsymbol{F} + \left(\frac{E-\mathrm{E_F}}{T}\right)(-\nabla T)\right]\left(-\frac{\partial f^0}{\partial E}\right). \end{aligned} \tag{4}$$

here $f^0(E)$ is the Fermi–Dirac distribution function, $\phi(E)$ is the first order perturbation distribution function having the units of time, $\boldsymbol{v_k}$ is the electron velocity and E_F the Fermi energy. The current density, $\boldsymbol{J}$ and heat current density, $\boldsymbol{U}$ due to the 2D fermions in graphene are given by [9]

$$\boldsymbol{J} = (4/A)\sum_{\boldsymbol{k}} \mathrm{e}\boldsymbol{v_k} f(\boldsymbol{k}) \tag{5}$$

and

$$\boldsymbol{U} = (4/A)\sum_{\boldsymbol{k}} (E-\mathrm{E_F})\boldsymbol{v_k} f(\boldsymbol{k}) \tag{6}$$

Using Eqs. (3)–(6) and the transformation

$$\sum_{\boldsymbol{k}} \rightarrow \int d^2\boldsymbol{k} = \int d\theta \mathrm{dk}\ \mathrm{k} = \frac{1}{(\hbar v_F)^2}\int_{-\pi}^{+\pi} d\theta \int_0^{\infty} dE\ \mathrm{E} \tag{7}$$

the expressions for the electric and heat currents can be written as

$$\boldsymbol{J} = e^2 K_{11}\boldsymbol{F} + (e/T)K_{21}(\nabla T) \tag{8}$$

$$\boldsymbol{U} = eK_{21}\boldsymbol{F} + (1/T)K_{31}(-\nabla T) \tag{9}$$

where the coefficients K_{rs} are, in general, tensors and given by

$$K_{rs} = \frac{1}{\pi\hbar^2}\int_0^{\infty} dE\, E(E-E_F)^{r-1}[\varphi(E)]^s\left(-\frac{\partial f^0}{\partial E}\right) \tag{10}$$

Under open circuit conditions ($\boldsymbol{J}=0$), Eqs. (1), (8) and (9) obtain an expression for the ETC as [5]:

$$\kappa_e = \frac{L}{Wt}G_{th} \tag{11}$$