Thermoelectric power factor of pure graphene

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Abstract. Thermoelectric power factor (PF) of ultra-pure single layer graphene is investigated over a wide temperature range 6 < T< 300 K. Assuming electrons to be scattered by in-plane longitudinal acoustic phonons, we present numerical results of PF as function of temperature and carrier concentration, \(n_s\). We find PF to increase with increase in temperature. The role and importance of electrical conductivity and the two components of thermopower, namely, diffusion and drag, are discussed. A nonlinear temperature dependent contribution of the diffusion component is noticed at lower temperatures. PF is found to decrease with increase in \(n_s\).

Keywords: Thermopower, power factor, Graphene.

INTRODUCTION

Recent years have witnessed great interest in understanding electronic properties of graphene, characterized by mass-less Dirac fermions as charge carriers and a linear dispersion with a zero band gap. The search for low-dimensional material structures with improved thermoelectric (TE) performance, has led to renewed interest being focused on the TE properties – thermopower, \(S\), electrical conductivity, \(\sigma\), and thermal conductivity, \(\kappa\) – of graphene, which promises potential applications in microelectronics and heat management devices [1].

The effectiveness of a TE material is described in terms of its TE figure of merit, \(Z = P/\kappa\), where \(P = S^2\sigma\) is the TE power factor (PF) of the material. Although efforts are on to reduce \(\kappa\), it is highly desirable to increase the TE power factor \(PF = S^2\sigma\) of the material [3].

In pure graphene, electron transport especially at lower temperatures, is limited by intrinsic scattering mechanisms namely, electron-acoustic phonon scattering. Thermopower, \(S\), is defined by the relation \(E = S\nabla T\) under open circuit conditions, where \(E\) is the effective electric field produced by the temperature gradient \(\nabla T\). In general, there are two contributions to TEP, \(S\), in the presence of \(\nabla T\), carriers diffuse through the specimen to produce the diffusion component, \(S_d\), in addition, the phonons move along \(\nabla T\) to produce the phonon-drag component, \(S_d = S_d + S_v\).

In literature, there exist independent studies of \(S\) and \(\sigma\), in graphene [2,4]. Here, we present a study of the TE PF of pure graphene and estimate the role of acoustic phonons in the PF of graphene.

THEORY

The electron wavefunctions and energy eigenvalues around two points \(K\) and \(K'\) at the corners of graphene Brillouin zone are given by [2]

\[
\psi_{\pm K}(k) = \frac{1}{\sqrt{2}} \left( e^{-i\theta_k/2} \right), \quad \psi_{\pm K'}(k) = \frac{1}{\sqrt{2}} \left( e^{i\theta_k/2} \right) (1)
\]

where \(\pm\) signs correspond to the \(\pi^*\) and \(\pi\) bands, respectively and \(E(k) = \pm h v_F |k|\) where, \(k = (k_x, k_y)\) is the 2D electron wave vector and \(v_F\) is the Fermi velocity.

Transport Coefficients

For the 2D massless Dirac fermions in graphene in presence of electric field \(E\) and temperature gradient \(\nabla T\), the current density, \(J\) and heat current \(U\) are expressed as [2]

\[
J = (4/\pi) \sum_k e v_k f_k
\]

and

\[
U = (4/\pi) \sum_k (E_k - E_F) v_k f_k
\]

Here, \(f_k\), electron distribution function, \(v_k\), the electron velocity and \(E_F\) is Fermi energy.
Figure 1: Temperature dependence of thermoelectric power factor for \( n_s = 1 \times 10^{15} \) and \( n_s = 1 \times 10^{16} \) m\(^{-2}\).

Using linearised Boltzmann transport equation, in relaxation time approximation, the electric and heat currents can be expressed as [3]

\[
\begin{align*}
    j &= e^2 K_{11} E + (e/T) K_{12} (\nabla T) \\
    u &= e K_{21} E + \left(1/T\right) K_{33} (\nabla T)
\end{align*}
\]

(4)

(5)

where the coefficients \( K_{rs} \), are given by

\[
K_{rs} = \frac{1}{\hbar^2} \int_0^\infty E_k \tau^2 (E_k - E_F)^{r-1} \left( - \frac{\partial f}{\partial E_k} \right) dE_k
\]

(6)

In (6), \( \tau(E_k) \) is the relaxation time.

In absence of temperature gradient (\( \nabla T = 0 \)) we obtain electrical conductance as

\[
\sigma = \frac{e^2}{\hbar^2} \int_0^\infty dE_k
\]

(7)

The conductivity can be obtained from conductance using dimensions of sample. Under open circuit conditions (\( j = 0 \)) we obtain expression for diffusion component of thermoelectric power as [3]

\[
S_d = \frac{e}{\hbar^2} K_{11}^{-1} K_{13} \frac{\tau}{T}
\]

(8)

Employing Cantrell and Butcher formalism with \( \nabla T \) in the plane of the sheet and assuming phonons to be scattered at low temperatures by mainly sample boundaries the phonon drag contribution to thermopower can be obtained [5].

RESULTS AND DISCUSSION

Using Eqs. (7) and (8) for \( \sigma \) and \( S_g \) and the equation for \( S_d \) given in [5], we have performed numerical calculations of PF for pure graphene layers for parameters characteristic of graphene [2]: \( v_{ph} = 2 \times 10^4 \) ms\(^{-1}\), \( v_F = 8.15 \times 10^4 \) ms\(^{-1}\), and \( D_{ac} = 4.75 \) eV.

In conclusion, we have investigated thermoelectric power factor in pure graphene. A detailed study of behavior of PF of graphene including other scattering mechanisms is under progress.

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REFERENCES