# 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 $\boldsymbol{E} = S\nabla T$ 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, $S_g$ : $S = S_d + S_g$.

In literature, there exist independent studies of S and σ, 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 eigen values around two points $\boldsymbol{K}$ and $\boldsymbol{K}'$ at the corners of graphene Brillouin zone are given by [2]

$$\psi_{\pm,\boldsymbol{K}}(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\theta_k/2} \\ \pm e^{i\theta_k/2} \end{pmatrix},\ \psi_{\pm,\boldsymbol{K}'}(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\theta_k/2} \\ \pm e^{-i\theta_k/2} \end{pmatrix} \quad (1)$$

where ± signs correspond to the π* and π bands, respectively and $E(\boldsymbol{k}) = \pm\hbar v_F |\boldsymbol{k}|$ where, $\boldsymbol{k} \equiv (k_x, k_y)$ 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 $\boldsymbol{E}$ and temperature gradient $\nabla T$ , the current density, $\boldsymbol{J}$ and heat current $\boldsymbol{U}$ are expressed as [2]

$$J = (4/A)\sum_{\boldsymbol{k}} e\, v_{\boldsymbol{k}}\, f_{\boldsymbol{k}} \quad (2)$$

and

$$U = (4/A)\sum_{\boldsymbol{k}}(E_{\boldsymbol{k}} - E_F)\, v_{\boldsymbol{k}}\, f_{\boldsymbol{k}} \quad (3)$$

Here, $f_k$, electron distribution function, $v_k$, the electron velocity and $E_F$ is Fermi energy.

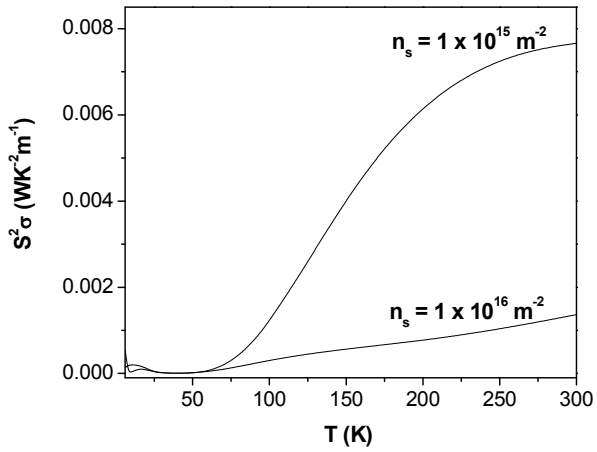


**Figure1:** Temperature dependence of thermoelectric power factor for $n_s$ = 1 x $10^{15}$ and $n_s$ = 1 x $10^{16}$ $m^{-2}$.

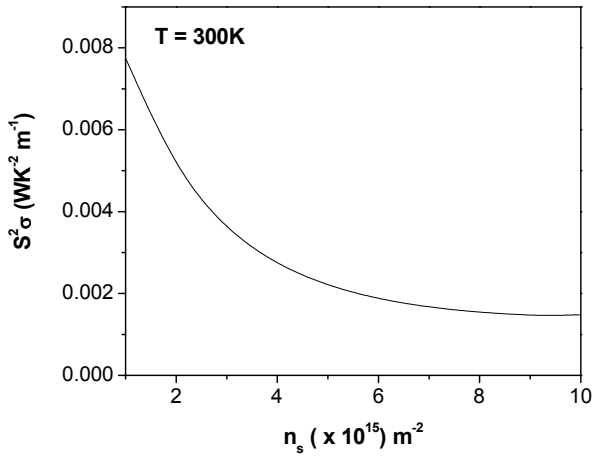


**Figure 2:** Thermoelectric power factor as function of electron concentration for T = 300K.

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

$$J = e^2 K_{11} \boldsymbol{E} + (e/T) K_{12} (-\nabla T) \quad (4)$$

$$U = e K_{21} \boldsymbol{E} + (1/T) K_{3\,1} (-\nabla T) \quad (5)$$

where the coefficients $K_{rs}$, are given by

$$K_{rs} = \frac{1}{\pi\hbar^2} \int_0^\infty E_{\boldsymbol{k}} \tau^s (E_{\boldsymbol{k}}) (E_{\boldsymbol{k}} - E_F)^{r-1} \left( - \frac{\partial f^o}{\partial E_{\boldsymbol{k}}} \right) dE_{\boldsymbol{k}} \quad (6)$$

In (6), $\tau(E_{\boldsymbol{k}})$ is the relaxation time.

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

$$\sigma = e^2 K_{11} \quad (7)$$

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]

$$S_d = \frac{1}{e^2} K_{11}^{-1} K_{12} \frac{e}{T} \quad (8)$$

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 by sample boundaries the phonon drag contribution to thermopower can be obtained [5].

## RESULTS AND DISCUSSION

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

The electrical and thermal transport properties *S* and $\sigma$, and hence the TE efficiency of graphene depends on temperature and on the carrier concentration, $n_s$. Fig.1 shows the results of our numerical calculations of the temperature dependence of PF for two values of electron concentrations. We find PF to increase with increase in temperature.

Fig.2 shows the variation of thermoelectric power factor as function of electron concentration from 1 x $10^{15}$ $m^{-2}$ to 1 x $10^{16}$ $m^{-2}$ for T = 300K. For range of $n_s$ considered, we find power factor decreases with increase in the electron concentration.

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.

## ACKNOWLEDGEMENT

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