Influence of external temperature gradient on acoustoelectric current in graphene

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Abstract

Recent analyses of thermoelectric amplification of acoustic phonons in Free-Standing Graphene (FSG) $\Gamma_{grap}^q$ have prompted the theoretical study of the influence of external temperature gradient ($\nabla T$) on the acoustoelectric current $j_T^{(grap)}$ in FSG. Here, we calculated thermal field on open circuit ($j_T^{(grap)} = 0$) to be $(\nabla T)^g = 746.8Km^{-1}$. We then calculated acoustoelectric current ($j_T^{(grap)}$) to be $1.1mA\mu m^{-2}$ for $\nabla T = 750.0Km^{-1}$, which is comparable to that obtained in semiconductors ($1.0mA\mu m^{-2}$), the thermal-voltage $(V_T)_{0}^g$ to be $6.6\mu V$ and the Seebeck coefficient $S$ as $8.8\mu V/K$. Graphs of the normalized $j_T^{(grap)}/j_0$ versus $\omega_q$, $T$ and $\nabla T/T$ were sketched. For $j_T^{(grap)}$ on $T$ for varying $\omega_q$, Negative Difference Conductivity (NDC) ($|\frac{\partial j_T}{\partial T}| < 0$) was observed in the material. This indicates graphene is a suitable material for developing thermal amplifiers and logic gates.

Keywords: acoustoelectric, graphene, temperature gradient, Negative Differential Conductivity

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Preprint submitted to Journal of Templates May 4, 2016
Introduction

The ability to acoustically generate d.c current in bulk and low dimensional materials such as Superlattices (SL) [1, 2, 3, 4], Carbon Nanotubes (CNTs) [5, 6, 7, 8] and Quantum wires (QW) [9, 10] have recently become an active field of study. This phenomena is known as Acoustoelectric Effect (AE) and is caused by the attenuation of phonons leading to the appearance of a dc field. In Graphene, this effect has been verified theoretically [11, 12, 13] and experimentally [14, 15, 16, 17]. The high intrinsic carrier mobility (over $2 \times 10^5 cm^2/Vs$) of a 2-D graphene sheet, coupled with its amazingly high value for thermal conductivity at room temperatures ($\approx 3000 - 5000 W/mK$), causes substantial acoustic effect when there is a minimal change in the external temperature gradient ($\nabla T$) [18]. This could lead to activities such as AE [19], amplification of acoustic phonons [20] or Acoustomagnetoelectric effect (AME) in the sample [21, 22]. The influence of non-linear thermal transport in graphene has received little attention as against other non-linear effects such as electric and magnetic fields which are utilised in ideal atomic chains [24, 25, 26, 27], molecular junctions [28] and quantum dots [29]. Daschewski et. al [33], treated the influence of energy density fluctuations (EDFs) on thermo-acoustic sound generation for near-field effects and sound-field attenuation for AirTech 200, UltranGN-55 and thermo-acoustic transducer. Hu et. al. [30] employed classical molecular dynamics to study the non-linear transport in Graphene Nanoribbons (GNRs). The Negative Differential Thermal Conductivity (NTDC) obtained by using the LAMMPS (Large-scale Atomis/ Molecular Massively Parallel Simulator)
package and velocity scaling software vanishes for lengths > 50nm long GNR. Such studies have particular applications in thermal power sources such as thermophones, plasma firings and laser beams [30] but till date there is no theoretical study of the influence of $\nabla T$ on acoustoelectric effect in Graphene.

In FSG, there are two types of phonons: (1) in-plane phonons with linear and longitudinal acoustic branches (LA and TA); and (2) out-of-plane phonons known as flexural phonons (ZA and ZO) [32]. In this paper, we consider a stretched FSG in which flexural phonons are ignored and only in-plane phonons couples linearly to electrons. This study is done in the hypersound regime having $ql >> 1$ (where $q$ is the acoustic phonon wavenumber, $l$ is the electron mean-free path). Here, Negative Differential Conductivity (NDC) in FSG is reported. This is analogous to the electronic NDC [33, 34] which is a useful ingredient for developing graphene based thermal systems such as signal manipulation devices, thermal logic gates and thermal amplifiers [31].

The paper is organised as follows: In the theory section, the equation underlying the acoustoelectric effect in graphene is presented. In the numerical analysis section, the final equation is analysed and presented in a graphical form. Lastly, the discussion and conclusions are presented.

Theory

The acoustoelectric current ($j_T$) generated in a graphene sheet can be expressed as [24] [25]

$$j_T = -\frac{e\tau A|C_q|^2}{(2\pi)^2 V_s} \int_0^\infty kd\phi \int_0^\infty k'd\phi' \int_0^{2\pi} d\theta \int_0^{2\pi} d\theta' \{ [f(k) - f(k')] \times \}
V_i \delta (k - k' - \frac{1}{\hbar V_F}(\hbar \omega_q)) 
$$  (1)
From [26], the matrix element $|C_q|$ in Eqn.(1) is given as

$$|C_q| = \begin{cases} \sqrt{\frac{\Lambda^2 h q^2}{2 \rho \omega_q}} & \text{acoustic phonons} \\ \sqrt{\left[\frac{\omega_0}{q^2}(k_{\infty}^{-1} - k_0^{-1})\right]} & \text{optical phonons} \end{cases}$$

where, $\Lambda$ is the constant of deformation potential, $\rho$ is the density of the graphene sheet, $\tau$ is the relaxation constant, $V_s$ is the velocity of sound, $A$ is the area of the graphene sheet, $\omega_0$ is the frequency of an optical phonon, $k_{\infty}^{-1}$ and $k_0^{-1}$ are the low frequency and optical permeability of the crystal.

The linear energy dispersion at the Fermi level with low-energy excitation is $\varepsilon(k) = \pm \hbar V_F |k|$ (the Fermi velocity $V_F \approx 10^8 ms^{-1}$). From Eqn.(1), the velocity $V_i$ is given as $v(k) = \partial \varepsilon(k)/\hbar \partial k$ (where $V_i = v(k') - v(k)$. yields

$$V_i = \frac{2\hbar \omega_q}{\hbar V_F}$$

From Eqn.(1), the linear approximation of the distribution function $f(k)$ is given as

$$f(k) = f_0(\varepsilon(k)) + f_1(\varepsilon(k))$$

The unperturbed electron distribution function is given by the shifted Fermi-Dirac function,

$$f_0(k) = \{exp(\beta \varepsilon(k) - \beta \varepsilon_F) + 1\}^{-1}$$

where $\beta = 1/k_B T$ ($k_B$ is the Boltzmann’s constant and $T$ is the absolute temperature), and $\varepsilon_F$ is the Fermi energy. At low temperatures, $\varepsilon_F = \xi$ ($\xi$ is the chemical potential) and the Fermi-Dirac equilibrium distribution function become

$$f_0(\varepsilon(k)) = exp(-\beta (\varepsilon(k) - \xi))$$
From Eqn. (3), $f_1(k)$ is derived from the Boltzmann transport equation as

$$f_1(\varepsilon(k)) = \tau[(\varepsilon(k) - \xi)\frac{\nabla T}{T}]\frac{\partial f_0(p)}{\partial \varepsilon}v(k)$$ (6)

Here $\tau$ is the relaxation time, and $\nabla T$ is the temperature gradient. With $k' = k - \frac{1}{\hbar V_F}(\hbar \omega_q)$, and inserting Eqn.(2), (3),(5) and (6) into Eqn.(1) and expressing further gives

$$j_T = \frac{-eA|\Lambda|^2 \hbar q \tau}{(2\pi)V_F \rho V_s} \int_0^\infty (k^2 - \frac{k\omega_q}{V_F})\{exp(-\beta(\hbar V_F k)) - \beta V_F \tau(\hbar V_F k) \times$$

$$\frac{\nabla T}{T}exp(-\beta \hbar V_F k) - exp(-\beta \hbar V_F(k - \frac{\omega_q}{V_F})) - \beta \hbar V_F \tau(\hbar V_F(k - \frac{\omega_q}{V_F})) \times$$

$$\frac{\nabla T}{T}exp(-\beta \hbar V_F(k - \frac{\omega_q}{V_F}))\}dk$$ (7)

Using standard integrals and after some cumbersome calculations, Eqn(7) yields the current ($j_T$) as

$$j_T = j_0\{(2 - \beta \hbar \omega_q)(1 - exp(-\beta \hbar \omega_q))$$

$$- \tau V_F[6(1 + exp(\beta \hbar \omega_q)) - \beta \hbar \omega_q(2 + \beta \hbar \omega_q exp(\beta \hbar \omega_q))]\frac{\nabla T}{T}\}$$ (8)

where

$$j_0 = \frac{-2eA|\Lambda|^2 q}{2\pi \beta^3 \hbar^2 V_F^4 \rho V_s}$$ (9)

From Eqn.(8), for an open circuit ($j_T = 0$), the thermal field $(\nabla T)^g$ is calculated as

$$(\nabla T)^g = T\frac{\{(2 - \beta \hbar \omega_q)(1 - exp(-\beta \hbar \omega_q))\}}{\tau V_F[6(1 + exp(\beta \hbar \omega_q)) - \beta \hbar \omega_q(2 + \beta \hbar \omega_q exp(\beta \hbar \omega_q))]}$$ (10)

the thermal field $(\nabla T)^g$ is found to depend on the temperature ($T$), the frequency ($\omega_q$) and the relaxation time ($\tau$) as well as the acoustic wavenumber.
The threshold temperature gradient \( \nabla T \) relate the thermal voltage \( V_T = k_B T/e \) as

\[
(\nabla V)_T = -S(\nabla T)^g
\]

where the Seebeck coefficient \( S \) is given as

\[
S = \frac{k_B \{ \tau V_F [6(1 + \exp(\beta \hbar \omega_q)) - \beta \hbar \omega_q (2 + \beta \hbar \omega_q \exp(\beta \hbar \omega_q))] \}}{e(2 - \beta \hbar \omega_q)(1 - \exp(-\beta \hbar \omega_q))}
\]

\[\text{(12)}\]

**Numerical Analysis**

To analyse, Eqn. (8), (9) and (12), we used the following parameters:

\[\Lambda = 9eV, \quad V_s = 2.1 \times 10^3 ms^{-1}, \quad \tau = 5 \times 10^{-10}s, \quad \omega_q = 10^{12} s^{-1}\]

At \( T = 77K \), the thermal field generated on open circuit \( \nabla T \) is calculated to be \( 746.8 Km^{-1} \). To clarify the results obtained, the dependence of the normalized acoustoelectric current \( j_T/j_0 \) on \( \omega_q, T, q \) and \( \nabla T/T \) are analysed graphically. In Figure 1a, the dependence of \( j_T^{(\text{grap})}/j_0 \) on \( \omega_q \) for varying \( \nabla T \) are presented. We observed that at \( \nabla T = 850 Km^{-1} \), the graph rises to a maximum at \( j_T^{(\text{grap})}/j_0 = 2.8 \) then decreased. By decreasing \( \nabla T \) to \( 500 Km^{-1} \), the graph decreases to a minimum at \( j_T^{(\text{grap})}/j_0 = -0.8 \) and then increases.

Figure 1b shows the temperature dependence on the normalized acoustoelectric current \( j_T^{(\text{grap})}/j_0 \) for various \( \omega_q \). We observed that for increasing temperatures, the graph raises to a peak value and then decreases. The region of the decrease (negative slope) indicates Negative Differential Conductivity (NDC) \( (|\frac{\partial j}{\partial T}| < 0) \) in the materials. The peak values increases with increases in \( \omega_q \). In Figure 2, the behaviour of \( j_T^{(\text{grap})}/j_0 \) versus \( \nabla T/T \) for varying \( \omega_q \) and \( q \) are presented. For Figure 2, it was noted that the graphs initially attained minimum points then increase for increasing \( \nabla T/T \) to a maximum point then falls off. It is observed that the ratio of the absolute value of the
Figure 1: (a) Dependence of $j_{T}^{(grap)}/j_{0}$ on $\omega_{q}$, (b) a graph of $j_{T}^{(grap)}/j_{0}$ on $T(K)$

Figure 2: the dependence of $j_{T}^{(grap)}/j_{0}$ versus $\nabla T/T$ for varying $\omega_{q}$. 

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maximum peak $|j_T^{(grap)}/j_0|_{max}$ to the minimum $|j_T^{(grap)}/j_0|_{min}$ peak is quite big. In the case where $\omega_q = 1.4THz$, the ratio $|j_T^{(grap)}/j_0|_{max}/|j_T^{(grap)}/j_0|_{min} \approx 3$. A similar observation was made in superlattice for the case of electric field $[4]$. A 3D plot of the dependence of the normalized acoustoelectric current $j_T^{(grap)}/j_0$ on $\omega_q$ and $q$ are presented in Figure 3a and b. The current density $(j_T^{(grap)})$ generated per unit area in the sample at $\omega_q = 0.1THz$ and $\nabla T = 750.0Km^{-1}$ is calculated to be $j_T^{(grap)} = 1.1mA(\mu m)^{-2}$ as compared to that calculated in semiconductors ($\approx 1.0mA(\mu m)^{-2}$). Eqn.(12) is the Seebeck coefficient $S$ which deals with the main thermoelectric properties of the FSG and how efficient it is. Fig. 4a shows the dependence of $S$ on $\omega_q$ for various $\nabla T/T$. The asymmetric distribution is due to electrons moving at the Fermi level in the material with an energy related to the Fermi energy. The value of $S$ ranges from $152\mu V/K$ to $-22.7\mu V/K$ at $\nabla T/T = 0.16m^{-1}$, $215.5\mu V/K$
to $-322.7 \mu V/K$ at $\nabla T/T = 0.22 m^{-1}$, and $278.8 \mu V/K$ to $-417.6 \mu V/K$ at $\nabla T/T = 0.29 m^{-1}$. At $\omega_q > 2.16 \times 10^{13} s^{-1}$, the graph switched from positive to negative values of $S$ indicating that at such frequencies, the n-type FSG changes to p-type FSG. In Fig. 4b, the $S$ is plotted against $T$. Here, the diffusion depends on temperature gradient present in the material which creates the opposite field. From the graph, the $S$ decreases with increasing $T$. At $\omega_q = 1.2 \times 10^{12} s^{-1}$, and $T = 77 K$, the $S = 8.8 \mu V/K$. By increasing the frequencies also increases the value of the Seebeck coefficient.

Figure 4: (left) the graph of $S$ versus $\omega_q$ for various $\nabla T/T$ (right) the dependence of $S$ versus $T$ for varying $\omega_q$

Conclusion

The influence of external temperature gradient $\nabla T$ on AE in FSG is studied. The thermal field $(\nabla T)^g$ is calculated to be $746.8 Km^{-1}$. Negative
differential conductivity \( (|\frac{\partial j}{\partial T}| < 0) \) is observed to manifest in FSG. The current density was calculated to be \( j_T = 1.1 mA \mu m^{-2} \) at \( \omega_q = 0.1 THz \) and the Seebeck coefficient evaluated to be \( S = 8.8 \mu V/K \). FSG is therefore a suitable material for the development of thermal amplifiers and logic gates.

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