Thermoelectric Amplification of Phonons in Graphene

K. A. Dompreh\textsuperscript{a,1,*}, N. G. Mensah\textsuperscript{b}, S. Y. Mensah\textsuperscript{a}, S. K. Fosuhene\textsuperscript{1}

\textsuperscript{a}Department of Physics, College of Agriculture and Natural Sciences, U.C.C, Ghana.
\textsuperscript{b}Department of Mathematics, College of Agriculture and Natural Sciences, U.C.C, Ghana
\textsuperscript{c}Ghana Space Science and Technology Institute. Ghana Atomic Energy Commission.

Abstract

Amplification of acoustic phonons due to an external temperature gradient (\(\nabla T\)) in Graphene was studied theoretically. The threshold temperature gradient (\((\nabla T)\_0\)) at which absorption switches over to amplification in Graphene was evaluated at various frequencies (\(\omega_q\)) and temperatures (\(T\)). For \(T = 77K\) and frequency \(\omega_q = 12THz\), \((\nabla T)\_0 = 0.37Km^{-1}\). The calculation was done in the regime at \(ql >> 1\). The dependence of the normalized (\(\Gamma/\Gamma_0\)) on the frequency \(\omega_q\) and the temperature gradient (\(\nabla T/T\)) are evaluated numerically and presented graphically. The calculated (\((\nabla T)\_0\)) for Graphene is lower than that obtained for homogenous semiconductors (\(n - InSb\)) (\((\nabla T)\_0^{hom} \approx 10^3Kcm^{-1}\)), superlattices (\((\nabla T)\_0^{SL} = 384Kcm^{-1}\)), and cylindrical quantum wire (\((\nabla T)\_0^{cqw} \approx 10^2Kcm^{-1}\)). This makes Graphene a much better material for thermoelectric phonon amplifier.

Key Words: Thermoelectric, Graphene, Acoustic phonon, Amplification

*Corresponding author
Email: kwadwo.dompreh@ucc.edu.gh

Preprint submitted to Journal of Templates
Introduction

The amplification (absorption) of acoustic phonons in Graphene \cite{1, 2, 3} and other low dimensional materials such as superlattices \cite{4, 5, 6, 7}, carbon nanotubes (CNT) \cite{8} and cylindrical quantum wires (CQW) \cite{9} has attracted lots of attention recently. For Graphene, Nunes and Fonseca \cite{3} studied amplification of acoustic phonons and determined the drift velocity $V_D$ at which amplification occurs but Dompreh et. al. \cite{11} further showed that even at $V_D = 0$, absorption of acoustic phonons can occur. Acoustoelectric Effect (AE) involves the transfer of momentum from phonons to conducting charge carriers which leads to the generation of d.c. current in the sample. This has been studied both theoretically \cite{10, 11} and experimentally \cite{12} in Graphene. The interaction between electrons and phonons in the presence of an external temperature gradient ($\nabla T$) can lead to thermoelectric effect \cite{13, 14, 15, 16} and thermoelectric amplification of phonons. Thermoelectric amplification of phonons has been studied in bulk \cite{17, 18} and low dimensional materials such as cylindrical quantum wire (CQW) \cite{19} and superlattices \cite{20, 21}. This phenomena was predicted by Gulyeav and Ephstein (1967) \cite{17} but was thoroughly developed by Sharma and Singh (1974) \cite{22} from a hydrodynamic approach $ql << 1$ ($q$ is the acoustic wave number, $l$ is the electron mean free path). Ephstein further explained this effect for sound in the opposite limiting case, $ql >> 1$ and showed that amplification is also possible in an electrically open-circuited sample (i.e., in the absence of an electric current) \cite{23}. In $n - InSb$, Epstein calculated a threshold gradient of $\approx 10^3 K cm^{-1}$ for a chemical potential $\mu = 8 \times 10^5 cm^2 V^{-1} s^{-2}$ at 77$K$. However, in superlattices, Mensah and Kangah (1991) \cite{24} calculated the threshold temperature
gradient necessary for amplification to occur to be \((\nabla T)_{0}^{hom} = 2.6(\nabla T)_{0}^{SL}\)
(where \((\nabla T)_{0}^{SL}\) is the threshold temperature gradient of superlattice) but in the lowest energy miniband \((\Delta = 0.1eV)\) obtained \((\nabla T)_{0}^{SL} = 384Kcm^{-1}\).
In all these materials, the threshold temperature gradient for the amplification was found to depend on the scattering mechanism and sound frequency where the relaxation time is independent of energy [20].

Graphene differs significantly from the other low-dimensional materials. It has the highest value for thermal conductivity at room temperature \((\approx 3000–5000W/mK)\) [16, 21]. This extremely high thermal conductivity opens up a variety of applications. The most interesting property of Graphene is its linear energy dispersion \(E = \pm \hbar V_F|k|\) (the Fermi velocity \(V_F \approx 10^8 cm/s\)) at the Fermi level with low-energy excitation. At low temperatures, the conductivity in Graphene is restricted by scattering of impurities but in the absence of extrinsic scattering sources, phonons constitute an intrinsic source of scattering of electrons to produce measureable temperature difference \((\nabla T)\).

Acoustic phonon scattering induced by low energy phonons gives quantitatively small contribution of \((\nabla T)\) in Graphene even at room temperature. This is due to the high Fermi temperature of Graphene [25]. To-date, there is no study of thermoelectric amplification of acoustic phonons in Graphene.

In this paper, the effect is theoretically studied in Graphene with degenerate energy dispersion. Here the threshold temperature gradient \((\nabla T)_{0}^{g}\) above which amplification occur is calculated in the regime \(ql >> 1\). Furthermore the frequency at which the graphs converges are calculated. The paper is organised as follows: In the theory section, the equation underlying the thermoelectric amplification of acoustic phonon in Graphene is presented. In the
numerical analysis section, the final equation is analysed and presented in a graphical form. Lastly, the conclusion is presented in section 4.

**Theory**

The kinetic equation for the acoustic phonon population $N_{\vec{q}}(t)$ in the Graphene sheet is given by

$$\frac{\partial N_{\vec{q}}(t)}{\partial t} = \frac{2\pi}{\hbar} g_s g_v \sum_{k,k'} |C_{\vec{q}}|^2 \delta_{k,k'+\vec{q}} \left\{ [N_{\vec{q}}(t) + 1]f_{\vec{k}}(1-f_{\vec{k}'})\delta(\varepsilon_{\vec{k}'} - \varepsilon_{\vec{k}} + \hbar\omega_{\vec{q}}) ight.$$ 

$$- N_{\vec{q}}(t)f_{\vec{k}'}(1-f_{\vec{k}})\delta(\varepsilon_{\vec{k}'} - \varepsilon_{\vec{k}} - \hbar\omega_{\vec{q}}) \right\} \quad (1)$$

where $g_s = g_v = 2$ account the for spin and valley degeneracy respectively, $N_{\vec{q}}(t)$ represent the number of phonons with a wave vector $\vec{q}$ at time $t$. The factor $N_{\vec{q}} + 1$ accounts for the presence of $N_{\vec{q}}$ phonons in the system when the additional phonon is emitted. The $f_{\vec{k}}(1-f_{\vec{k}})$ represent the probability that the initial $\vec{k}$ state is occupied and the final electron state $\vec{k}'$ is empty whilst the factor $N_{\vec{q}}f_{\vec{k}'}(1-f_{\vec{k}})$ is that of the boson and fermions statistics. In Eqn (1), the summation over $k$ and $k'$ can be transformed into integrals by the prescription

$$\sum_{k,k'} \rightarrow \frac{A^2}{(2\pi)^4} \int d^2k d^2k'$$

where $A$ is the area of the sample, and assuming that $N_{\vec{q}}(t) >> 1$ yields

$$\frac{\partial N_{\vec{q}}}{\partial t} = \Gamma_{\vec{q}} N_{\vec{q}} \quad (2)$$

where

$$\Gamma_{\vec{q}} = \frac{A|\Lambda|^2}{(2\pi)^3 \hbar V_F \rho V_s} \int_0^{\infty} dk \int_0^{\infty} k' dk' \int_0^{2\pi} d\phi \int_0^{2\pi} d\theta \left\{ [f(k) - f(k')] \times \delta(k - k' - \frac{1}{\hbar V_F}(\hbar \omega_{\vec{q}})) \right\} \quad (3)$$
with \( k' = k - \frac{1}{\hbar V_F} (\hbar \omega_q) \). \( \Lambda \) is the constant of deformation potential, \( \rho \) is the density of the Graphene sheet. \( f(k) \) is the distribution function, \( V_s \) is the velocity of sound, and \( A \) is the area of the Graphene sheet. Here the acoustic wave will be considered as phonons of frequency \( (\omega_q) \) in the short-wave region \( q l \gg 1 \) (\( q \) is the acoustic wave number, \( l \) is the electron mean free path).

From Eqn.(3), the linear approximation of the distribution function \( f(k) \) is given as

\[
f(k) = f_0(\varepsilon(k)) + qf_1(\varepsilon(k))
\]  

(4)

At low temperature \( k_B T << 1 \), the Fermi-Dirac equilibrium distribution function become

\[
f_0(\varepsilon(k)) = \exp(-\beta(\varepsilon(k)))
\]  

(5)

From Eqn. (4), \( f_1(k) \) is derived from the Boltzmann transport equation as

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

(6)

Here \( v(k) = \delta \varepsilon(k)/\hbar \delta k \) is the electron velocity, \( \xi \) is the chemical potential \( \tau \) is the relaxation time and \( \nabla T \) is the temperature difference. Inserting Eqn.(4), Eqn.(5) and Eqn.(6) into Eqn.(3) and expressing further gives

\[
\Gamma = \frac{eA|\Lambda|^2}{(2\pi)V_F \rho V_s} \int_0^\infty \left( k^2 - \frac{\hbar \omega_q}{h V_F} \right) \left\{ \exp(-\beta(\hbar V_F k)) - \beta \hbar V_F q\tau(\hbar V_F k) \times \frac{\nabla T}{\hbar T} \exp(-\beta \hbar V_F k) - \exp(-\beta \hbar V_F (k - \frac{\hbar \omega_q}{h V_F})) - \beta \hbar V_F q\tau(\hbar V_F (k - \frac{\hbar \omega_q}{h V_F})) \times \frac{\nabla T}{\hbar T} \exp(-\beta \hbar V_F (k - \frac{\hbar \omega_q}{h V_F})) \} \right\}
\]  

(7)

Using standard integrals in Eqn(7) and after a cumbersome calculation yields the final equation as

\[
\Gamma = \Gamma_0 \left\{ (2 - \beta \hbar \omega_q)(1 - \exp(-\beta \hbar \omega_q)) - q\tau V_F \left[ 6(1 + \exp(\beta \hbar \omega_q)) - 3\beta \hbar \omega_q(2 + \beta \hbar \omega_q \exp(\beta \hbar \omega_q)) \right] \frac{\nabla T}{T} \right\}
\]  

(8)
where

$$\Gamma_0 = \frac{2A|\Lambda|^2 q}{2\pi \beta^3 h^3 V_F^4 \rho V_s}$$  \hspace{1cm} (9)

The threshold temperature difference \((\nabla T)_0^g\) is calculated. This is achieved by letting \(\Gamma = 0\) as a consequence of the laws of conservation which yields

$$\nabla T_0^g = T \frac{\{(2 - \bar{h}\omega_q)(1 - \exp(-\beta \bar{h}\omega_q))\}}{qT V_F[6(1 + \exp(\beta \bar{h}\omega_q)) - \beta \bar{h}\omega_q(2 + \beta \bar{h}\omega_q \exp(\beta \bar{h}\omega_q))]} \hspace{1cm} (10)$$

**Numerical Analysis**

To understand the complex expression for the absorption, Eqn.(8) was numerically analysed. From Eqn. (10), the threshold temperature gradient \((\nabla T)_0^g\) is dependent on the temperature \((T)\), the frequency \((\omega_q)\) and the relaxation time \((\tau)\) as well as the acoustic wavenumber \((q)\). To evaluate \((\nabla T)_0^g\), the following parameters are used \(\Lambda = 9eV\), \(V_s = 2.1 \times 10^3 m/s\), \(\tau = 10^{-12} s\), \(\omega_q = 10^{12} s^{-1}\) and \(q = 10^8 m^{-1}\). At \(T = 77 K\), \((\nabla T)_0^g\) is calculated to be \(0.37 Km^{-1}\). These values are used in analysing Eqn.(8) numerically and presented graphically (see Figure 1, 2 and 3). In Figure 1a, A normalized graph of \(\Gamma_0/\Gamma_0\) on \(\omega_q\) for varying \(\nabla T\) is plotted. When \(\nabla T = 0\), an absorption graph \((\Gamma_0/\Gamma_0 > 0)\) is obtained. We observed that when \(\nabla T = 0.28 Km^{-1}\), the amplitude of the absorption graph reduces and the absorption switches to amplification at \(\omega_q = 10^{THz}\). Interestingly, when \(\nabla T > (\nabla T)_0^g = 0.37 Km^{-1}\), the graph switches completely to amplification \((\Gamma_0/\Gamma_0 < 0)\) (see Figure 1a for graph of \(\nabla T = 0.38 Km^{-1}\) and \(\nabla T = 0.48 Km^{-1}\)). This agrees with the theory of thermoelectric amplification of phonons. The threshold values above which absorption completely switches to amplification are presented in table 1 for various temperatures and frequencies. In the table 1, \((\nabla T)_0^g\) increases with increase in temperature and frequency. Figure 1b shows the
Figure 1: (a) The normalized graph of $\Gamma/\Gamma_0$ on $\omega_q$ for varying $\nabla T$

Figure 2: The normalized graph of $\Gamma/\Gamma_0$ on $\nabla T/T$ (a) for varying $\omega_q$ (b) for varying $q$
Figure 3: The Dependence of $\Gamma/\Gamma_0$ on $\omega q$ and $\nabla T/T$.

Tab. 1: The frequencies, temperatures and threshold from figure 2a

| Frequency (THz) | 12.0 | 14.0 | 16.0 | 18.0 |
|-----------------|------|------|------|------|
| Temperature(K)  | 77.0 | 90.0 | 109.0| 120.0|
| Threshold (Km^−1) | 0.37 | 0.44 | 0.53 | 0.58 |

graph of various $\Gamma/\Gamma_0$ on $\nabla T/T$ for varying $q$. By increasing $q$, all the graphs switches to amplification at the same point ($\nabla T/T = 0.37$). This shows that, increases in the acoustic wavenumber ($q$) does not alter the threshold temperature gradient($\nabla T)_0^2$ of the material. However, when the graph of $\Gamma/\Gamma_0$ was plotted against $\nabla T/T$ varying the frequency, we notice a shift of the threshold values towards bigger values of $\nabla T/T$ (see Figure 2b). A 3D graph is presented to further elucidate the graphs obtained (see Figure 3). Figure (3a) shows the dependence of $\Gamma/\Gamma_0$ on $\nabla T/T$ and $\omega q$ whilst Figure (3b) is that of $\Gamma/\Gamma_0$ on $\nabla T/T$ and $q$. 

8
Conclusion

Thermoelectric amplification of phonons in Graphenes is studied. We observed that absorption switches over to amplification at values greater than the threshold values. The threshold value calculated at $T = 77K$ and frequency $\omega_q = 10^{12}s^{-1}$ in Graphene is $\langle \nabla T \rangle^0_0 = 0.37Kcm^{-1}$ which is far lower than that calculated in homogenous semiconductor using $n-InSb$ ($s = 2.3 \times 10^5cms^{-1}$, $\mu = 8 \times 10^5cm^2V^{-1}s^{-1}$ at $77K$) and was found to be $\langle \nabla T \rangle^0_{hom} \approx 10^3Kcm^{-1}$, superlattice $\langle \nabla T \rangle^0_{SL} \approx 384Kcm^{-1}$ for miniband width $\Delta = 0.1eV$ at $77K$, and finally for cylindrical quantum wires (CQW) to be $\langle \nabla T \rangle^0_{cwq} \approx 10^2Kcm^{-1}$ at liquid Nitrogen temperature of $77K$. This makes Graphene a much better material for thermoelectric phonon amplification.

Bibliography

[1] Dompreh, Kwadwo A., Natalia G. Mensah, and Samuel Y. Mensah. "Amplification of Hypersound in Graphene with degenerate energy dispersion." arXiv preprint arXiv:1503.07360 (2015).

[2] Dompreh, K. A., S. Y. Mensah, S. S. Abukari, F. Sam, and N. G. Mensah. "Amplification of Acoustic Waves in Graphene Nanoribbon in the Presence of External Electric and Magnetic Field." arXiv preprint arXiv:1410.8064 (2014).

[3] Nunes, O. A. C., and A. L. A. Fonseca. "Amplification of hipersound in graphene under external direct current electric field." Journal of Applied Physics 112, no. 4 (2012): 043707.
[4] Shmelev, G. M., S. Y. Mensah, and G. I. Tsurkan. "Hypersound amplification by a superlattice in a nonquantised electric field." Journal of Physics C: Solid State Physics 21, no. 33 (1988): L1073.

[5] Mensah, S. Y., and G. K. Kangah. "Amplification of acoustic waves due to an external temperature gradient in superlattices." Journal of Physics: Condensed Matter 3, no. 22 (1991): 4105.

[6] Mensah, S. Y., F. K. A. Allotey, N. G. Mensah, and V. W. Elloh. "Amplification of acoustic phonons in a degenerate semiconductor superlattice." Physica E: Low-dimensional Systems and Nanostructures 19, no. 3 (2003): 257-262.

[7] Dompreh, Kwadwo A., Samuel Y. Mensah, Natalia G. Mensah, Sulley S. Abukari, Frank KA Allotey, and George K. Nkrumah-Buandoh. "Amplification of acoustic phonons in superlattice." arXiv preprint arXiv:1101.1854 (2011).

[8] Dompreh, K. A., N. G. Mensah, S. Y. Mensah, S. S. Abukari, F. Sam, and R. Edziah. "Hypersound Absorption of Acoustic Phonons in a degenerate Carbon Nanotube." arXiv preprint arXiv:1502.07636 (2015).

[9] Hung, Nguyen Quoc, Nguyen Vu Nhan, and Nguyen Quang Bau. "On the amplification of sound (acoustic phonons) by absorption of laser radiation in cylindrical quantum wires." arXiv preprint cond-mat/0204563 (2002).

[10] Zhao, C. X., W. Xu, and F. M. Peeters. "Cerenkov emission of terahertz
acoustic-phonons from graphene.” Applied Physics Letters 102, no. 22 (2013): 222101.

[11] Dompreh, K. A., N. G. Mensah, and S. Y. Mensah. ”Acoustoelectric Effect in Graphene with degenerate Energy dispersion.” arXiv preprint arXiv:1505.05031 (2015).

[12] Bandhu, L., L. M. Lawton, and G. R. Nash. ”Macroscopic acoustoelectric charge transport in graphene.” Applied Physics Letters 103, no. 13 (2013): 133101.

[13] Mensah, S. Y., F. K. A. Allotey, N. G. Mensah, and G. Nkrumah. ”Differential thermopower of a CNT chiral carbon nanotube.” Journal of Physics: Condensed Matter 13, no. 24 (2001): 5653.

[14] Mensah, S. Y., F. K. A. Allotey, N. G. Mensah, and G. Nkrumah. ”Giant electrical power factor in single-walled chiral carbon nanotube.” superlattices and microstructures 33, no. 3 (2003): 173-180.

[15] Mensah, S. Y., A. Twum, N. G. Mensah, K. A. Dompreh, S. S. Abukari, and G. Nkrumah-Buandoh. ”Effect of laser on thermopower of chiral carbon nanotube.” arXiv preprint arXiv:1104.1913 (2011).

[16] Mensah, N. G., G. Nkrumah, S. Y. Mensah, and F. K. A. Allotey. ”Temperature dependence of the thermal conductivity in chiral carbon nanotubes.” Physics Letters A 329, no. 4 (2004): 369-378.

[17] Gulayev, Yu V. ”Acousto-electric effect and amplification of sound waves in semiconductors at large sound intensities.” Physics Letters A 30.4 (1969): 260-261.
[18] Tenan, M. A., A. Marotta, and L. C. M. Miranda. ”On the thermoelectric amplification of sound in semiconductors.” Applied Physics Letters 35, no. 4 (1979): 321-323.

[19] Nunes, O. A. C., D. A. Agrello, and A. L. A. Fonseca. ”Thermoelectric amplification of phonons in cylindrical quantum well wires.” Journal of applied physics 83 (1998): 87-89.

[20] Mensah, S. Y., and G. K. Kangah. ”The thermoelectric effect in a semiconductor superlattice in a non-quantized electric field.” Journal of Physics: Condensed Matter 4, no. 3 (1992): 919.

[21] Balandin AA. Thermal properties of graphene and nanostructured carbon materials. Nat Mat 2011;10(8):56981

[22] Sharma, S. and Singh, S. P., J. Appl Phys. 10 46656-1 (1974)

[23] Epstein E.M. Fiz. Tekh. Poluprov. 8 1584-7 (1975)

[24] Mensah, S. Y., and G. K. Kangah. ”Amplification of acoustic waves due to an external temperature gradient in superlattices.” Journal of Physics: Condensed Matter 3, no. 22 (1991): 4105.

[25] Sankeshwar, N. S., S. S. Kubakaddi, and B. G. Mulimani. ”Thermoelectric power in graphene.” Intech 9 (2013): 1-56.