iJRASET
International Journal For Research in Applied Science and Engineering Technology



INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 9 **Issue:** XII **Month of publication:** December 2021

DOI: https://doi.org/10.22214/ijraset.2021.39562

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International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.538
Volume 9 Issue XII Dec 2021- Available at www.ijraset.com

Amplification and Attenuation of Acoustic Phonons in Graphenelike Silicene

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Abstract: ***Because of unique physical properties, graphene, a 2D honeycomb arrangement of carbon atoms, has attracted tremendous attention. Silicene, the graphene equivalent for silicon, could follow this trend, opening new perspectives for applications, especially due to its compatibility with Si-based electronics. Silicene has been theoretically predicted as a buckled honeycomb arrangement of Si atoms and having an electronic dispersion resembling that of relativistic Dirac fermions. We calculate theoretically in this article, the amplification and attenuation of acoustic phonons due to an external temperature gradient in Silicene at temperature T =77K in the hypersound regime. The dependence of normalized amplification or attenuation on the frequency wasnumerically evaluated. It is observed from our calculations that when the temperature gradient is zero, absorption of acoustic phonons occurs and when temperature gradient is greater than zero, absorption switches to amplification of acoustic phonons.***

Keywords: Silicene, Amplification, Attenuation, Acoustic phonons, Temperature gradient.

I. INTRODUCTION

Silicene and graphene have similar electronic structures. Both have a Dirac cone and linear electronic dispersion around the Dirac points. Both also have a quantum spin Hall effect. Both are expected to have the characteristics of massless Dirac fermions that carry charge, but this is only predicted for silicene and has not been observed, likely because it is expected to only occur with free-standing silicene which has not been synthesized. It is believed that the substrate on which the silicene is made has a substantial effect on its electronic properties. Two-dimensional (2D) materials are promising candidates for future electronic devices [1-3]. Examples of three such materials are a monolayer of graphene, its silicon-based counterpart silicene, and monolayer MoS_2. In such systems, two-dimensionality allows very precise control of the carrier density by a gate which enables tuning of the electron-phonon interaction. Electron-phonon interaction in graphene has been studied previously [4,5], but with the recent advances in fabrication of devices based on other 2D materials, like the first demonstration of a silicene transistor [6], further studies of interaction phenomena in 2D materials are necessary.

When comparing the electrical performance of devices one often considers the carrier mobility of the materials. Mobility is a key parameter for the semiconductor industry describing the motion of electrons when an electric field is applied. Experiments can approach the “intrinsic” phonon-limited mobility by several means. One experiment combines defect-free edge contacting [7] of gate-tunable graphene electrodes with MoS_2encapsulated in hexagonal boron nitride layers [8].

The silicon equivalent of graphene was first mentioned in a theoretical study by Takeda and Shiraishi [9] in 1994 and then reinvestigated by Guzman-Verri et al., in 2007 who named it as Silicene [10]. However, silicene does not seem to exist in nature nor is there any solid phase of silicon similar to graphite. Silicene is predicted to be stable up to 1500 K, after which it formed a three-dimensional amorphous structure.35 Defects have been found to reduce the thermal stability of silicene by as much as 30% [11]. Passivating the defects improved the stability. The thermal conductivity of silicene has been well studied and assumed to be mainly due to phonon transport. An inplane thermal conductivity of 20 W/m K has been calculated using equilibrium MD simulation at 300 K, [12] compared to a value of 3000–5000 W/m K for suspended graphene [13] and 150–200 W/m K for silicon. The reduction has been attributed to two main causes. One is the lowering of the partial density of states (PDOS) for frequencies below 20 THz (phonon softening), and the other is due to the blueshift in the PDOS to higher frequencies (phonon stiffening). The result is a reduction in the phonon modes present for heat conduction at low temperatures. The temperature dependence of j has been computed over $0 < T < 400$ K [13], with a maximum value of about 100 W/m K near 100 K, compared to around 1000 W/m K for bulk Si [14] and 3000–5000 W/m K for graphene.

Silicene has recently attracted strong theoretical attention [15-17]. For example, Cahangirov et al [17], using density functional theory, have shown that a silicon quasi 2-dimensional structure is stable (without of any imaginary vibrational frequency) only if a low buckling (LB), 0.044 nm, is allowed. They also report that for this LB structure, the Si-Si nearest-neighbour distance is reduced

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ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.538
Volume 9 Issue XII Dec 2021- Available at www.ijraset.com

to 0.225 nm from that of the bulk, and that the electronic density of states indicates the system is ambipolar. Their calculated band structures exhibit a crossing at K and K' points (reflecting the semi-metallic character of silicene) and a linear dependency near the crossing (reflecting a mass-less Dirac fermion character). The same authors find that silicene nano-ribbons (NRs) exhibit electronic and magnetic properties likewise very similar to those of graphene. Theoretical work has focused on the interesting physical properties of silicene. For example, it has been found that silicene possesses a band structure that is similar to that of graphene, with massless Dirac-fermion charge carriers [18]. An energy gap can be opened and tuned by either applying an external perpendicular electric field [19] or alkali-atom adsorption [20]. Also, silicene has pronounced spin-orbit coupling, which led to the prediction that the quantum spin-Hall effect [21] and the quantum anomalous Hall Effect [22] would be detectable. In addition, silicene-based van der Waals heterostructures are predicted to have fascinating physical properties. The graphene-silicene vertical heterostructure is predicted to be a promising candidate as anode material [23, 24] and nanocapacitor, [25] and the silicene-arsenene vertical heterostructure is predicted to be useful in nanoelectronic and optoelectronic devices [26].

In this present work, a theory for normalized amplification and attenuation of acoustic phonons in Silicene has been studied numerically as a function of frequency and temperature gradient.

II. THEORY

The basic Boltzmann Transport Equation (BTE) for the population of acoustic phonons $N_q(t)$ is given by [27]

$$\frac{dN_q(t)}{dt} = \frac{2\pi}{\hbar} g_s g_v \sum_{k,k'} |M_q|^2 \{[N_q(t)+1] f_k (1-f_{k'}) \delta(E_{k'} - E_k + \hbar\omega_q) - N_q(t) f_{k'} (1-f_k) \delta(E_{k'} - E_k - \hbar\omega_q)\} \delta_{k,k'+q}, \quad (1)$$

where $g_s = g_v = 2$ representing respectively the spin and valley degeneracy. $N_q(t)$ account for the number of phonons with a wave vector q at time t. $[N_q(t)+1]$ accounts for the presence of N_q phonons in the system when an additional phonon is emitted. The $f_k(1-f_{k'})$ represent the probability that the initial k state is occupied and final electron state k' is empty while the factor $N_q(t) f_{k'}(1-f_k)$ is that of the Fermi statistics. In the above equation (1), the summation over k and k' can be transformed into integrals by

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

with A be the area of the sample, and assuming that $N_q(t) \gg 1$, yields

$$\frac{dN_q(t)}{dt} = \alpha_q N_q \quad (2)$$

where

$$\alpha_q = \frac{AD^2}{(2\pi)^3 \hbar v_f \rho v_s} \int_0^\infty k dk \int_0^\infty k' \, dk' \int_0^{2\pi} d\varphi \int_0^{2\pi} d\theta \left\{ [f(k) - f(k')] \delta\left(k - k' - \frac{1}{\hbar v_f}(\hbar\omega_q)\right) \right\} \quad (3)$$

having $k' = k - \frac{1}{\hbar v_f}(\hbar\omega_q)$. $D$is the acoustic deformation potential constant, ρ is the density of silicene, v_f is the Fermi velocity, v_s is the sound velocity, and $f(k)$ is the Fermi-Dirac distribution function. Here the acoustic wave will be considered as phonons of frequency ω_q in the short-wave region $ql \gg 1$ (with q being acoustic phonon wave vector and l is the electron mean free path). From equation (3), the linear approximation of the distribution function is given as

$$f(k) = f_0\{E(k) + q f_1(E(k))\} \quad (4)$$

At low temperature, $k_B T \ll 1$, the Fermi-Dirac distribution function becomes

$$f_0(E(k)) = e^{-\beta(E(k))} \quad (5)$$

From equation (4), $f_1(E(k))$ is derived from Boltzmann transport equation as

$$f_1(E(k)) = \tau \left[(E(k) - \xi)\frac{\nabla T}{T}\right] \frac{df_o(p)}{dE} \upsilon(k) \quad (6)$$

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Here $\upsilon(k) = \frac{\delta E(k)}{\hbar \delta k}$ is the electron velocity, ξ is the chemical potential, τ is the relaxation time and ∇T is the temperature difference. Substituting equations (4) - (6) in equation (3) and expressing further gives

$$\alpha = \frac{q\hbar AD^2}{(2\pi)^3 v_F \rho v_s}\int_0^\infty \left(k^2 - \frac{k\hbar\omega_q}{\hbar v_f}\right)\left\{e^{(-\beta(\hbar v_f k))} - \beta\hbar q\tau(\hbar v_f k)\frac{\nabla T}{\hbar T}e^{(-\beta\hbar v_f k)} - e^{(-\beta\hbar v_f(k-\frac{\hbar\omega_q}{\hbar v_f}))} - \beta\hbar v_f q\tau(\hbar v_f(k - \frac{\hbar\omega_q}{\hbar v_f}))\frac{\nabla T}{\hbar T}e^{(-(\beta\hbar v_f(k-\frac{\hbar\omega_q}{\hbar v_f})))}\right\} \quad (7)$$

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

$$\alpha = \alpha_0\left\{(2-\beta\hbar\omega_q)(1-e^{(-\beta\hbar\omega_q)}) - q\tau v_f\left[6(1+e^{(\beta\hbar\omega_q)}) - \beta\hbar\omega_q(2+\beta\hbar\omega_q e^{(\beta\hbar\omega_q)})\right]\frac{\nabla T}{T}\right\} \quad (8)$$

where $\alpha_0 = \frac{2AD^2 q}{2\pi\beta^3\hbar^3 v_f^4 \rho v_s}$ (9)

III. RESULTS AND DISCUSSION

To understand the complex equation for the amplification and attenuation, equation (8) is numerically analyzed using the following Silicene characteristic material parameters, D =3.2eV, v_s = 6.3x10^2 m/s, v_f = 5.8x10^5 m/s, τ = 10^{-12} sec, q =10^8 m^{-1} and T = 77K.

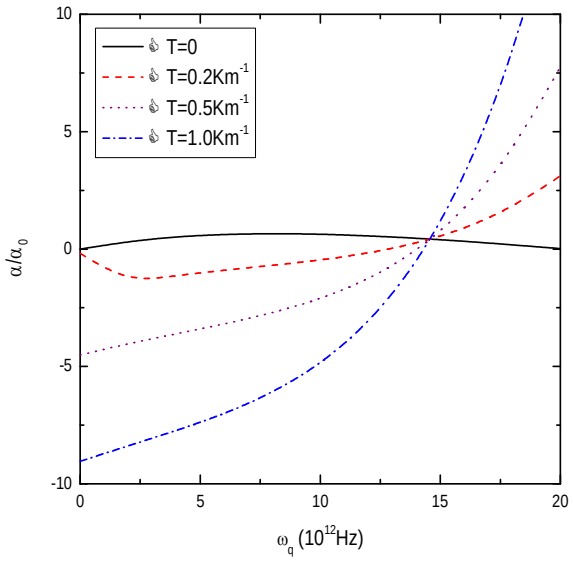


Figure 1: Normalized graph of $\frac{\alpha}{\alpha_0}$ on ω_q for different ∇T.

In figure 1, a normalized graph of $\frac{\alpha}{\alpha_0}$ on ω_q for different ∇T is plotted. It is observed that, when ∇T = 0, attenuation//absorption of acoustic phonons $\frac{\alpha}{\alpha_0} > 0$ is obtained. When $\nabla T > 0$, the magnitude of attenuation reduces and switches to amplification of acoustic phonons upto ω_q =15 THz. After reaching this critical value of frequency 15THz, now attenuation/absorption of phonons can be observed. This is in agreement with theory of thermoelectric amplification of phonons. Absorption of phonons takes place when the temperature gradient is zero (∇T = 0) because the first term is dominant in equation (8), which represents the absorption part of the phonons. When the temperature gradient is greater than zero ($\nabla T > 0$), the second term in equation (8) dominates which causes the amplification of phonons.

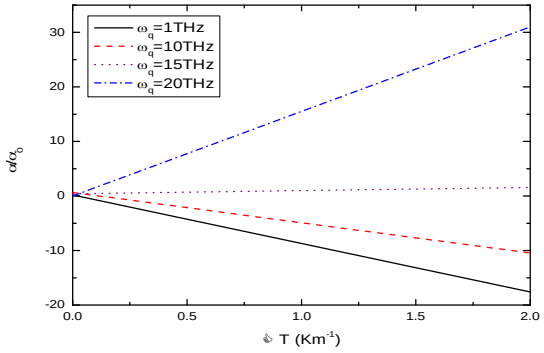


Figure 2: Normalized graph of $\frac{\alpha}{\alpha_0}$ on ∇T for different ω_q.

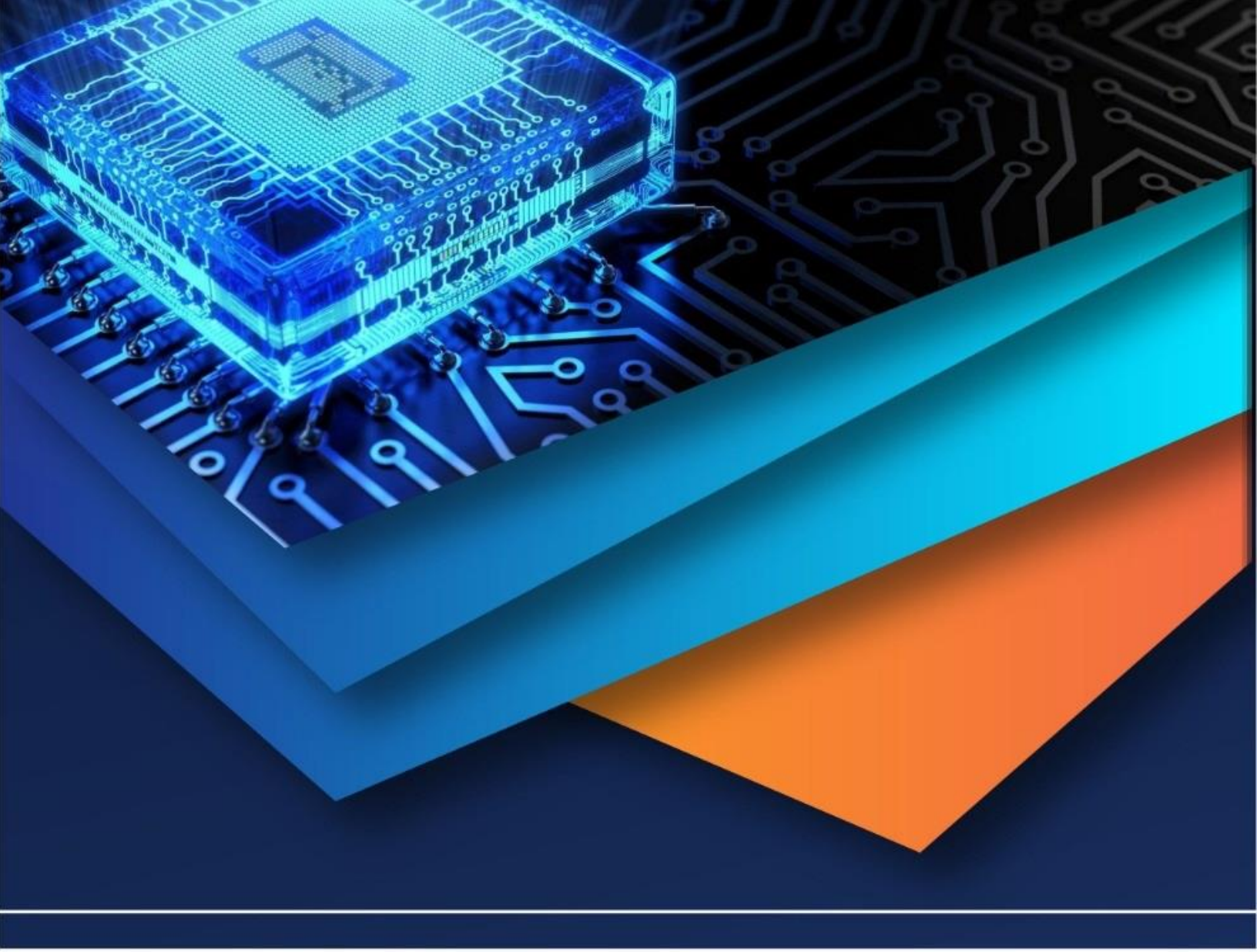
Figure 2 shows the graph of $\frac{\alpha}{\alpha_0}$ on varying ∇T for different ω_q. It is observed from the graph that, for frequencies below 15 THz, amplification of phonons takes place. Also observed that, when the temperature gradient increases $\frac{\alpha}{\alpha_0}$ decreases linearly. When the frequency reaches critical value of 15THz, attenuation of phonons takes place and increases linearly with increase in temperature gradient. This indicates that, when amplification of phonons takes place when $\frac{\alpha}{\alpha_0}$ attains a negative values for phonons having frequency less than 15THz.

IV. CONCLUSIONS

Thermoelectric amplification of acoustic phonons in silicene is studied theoretically. We observed that absorption/attenuation of phonons switches to amplification at values greater than the critical values. The critical value of frequency of phonons observed at T = 77K is 15THz. This makes silicene a much better material for thermoelectric phonon amplification.

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