

Hypersound Absorption of Acoustic Phonons in a degenerate Carbon Nanotube

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Abstract

Absorption of acoustic phonons was studied in degenerate Carbon Nanotube (i.e. where the electrons are found close to the Fermi level). The calculation of the hypersound absorption coefficient (Γ) was done in the regime where $ql \gg 1$ (q is the acoustic phonon number and l is the electron mean free path). At $T = 10K$ and $\theta > 0$ (θ being scattering angle), the dependence of Γ on acoustic wave number (\vec{q}), frequency (ω_q), and $\gamma = 1 - \frac{V_D}{V_s}$, (V_s and V_D being the speed of sound and the drift velocity respectively) were analysed numerically at $n = 0, \pm 1, \pm 2$ (where n is an integer) and presented graphically. It was observed that when $\gamma < 0$, the maximum amplification was attained at $V_D = 1.1V_s$ which occurred at $E = 51.7Vcm^{-1}$. In the second harmonics, ($n = \pm 2$), the absorption obtained was compared to experimental measurement of acoustoelectric current via the Weinreich relation and the results qualitatively agreed with each other.

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Introduction

Carbon Nanotubes (CNT) are graphite sheets seamlessly wrapped into cylinders characterised by a chiral index (m,n) , with m and n being two integers, which specify the carbon nanotube uniquely [1, 2, 3]. This has recently attracted lot of interest for use in many semiconductor devices due to its remarkable electrical [6], mechanical [7], and thermal [8, 9, 10, 11] properties which are mainly attributed to its unusual band structures [12]. The π -bonding and anti-bonding (π^*) energy band of CNT crosses at the Fermi level in a linear manner [12]. In the linear regime, electron-phonon interactions in CNT at low temperatures leads to the emission of large number of coherent acoustic phonons [8, 9, 10]. Studies of the effect of phonons on thermal transport [11, 12], on Raman scattering [13] and on electrical transport [14] in CNT is an active area of research. Also, the speed of electrons in the linear region is extremely high. This makes CNT a good candidate for application of high frequency electronic systems such as field effect transistors (FET's) [15], single electron memories [16] and chemical sensors [17]. Another important investigation in the linear regime is interaction of acoustic phonons with drift charges in CNT. It is well known that when acoustic phonons interact with charge carriers, it is accompanied by energy and momentum exchange which give rise to the following effects: Absorption (Amplification) of acoustic phonons [18, 19]; Acoustoelectric Effect (AE) [20, 21, 22, 23, 24, 25]; Acoustomagnetolectric Effect (AME) [26, 27, 28, 29, 30]; Acoustothermal Effect [31] and Acoustomagnetoacoustic Effect [31]. The idea of acoustic wave amplification in bulk material was theoretically predicted by Tolpygo (1956), Uritskii [32], and Weinreich [33] and in N-Ge by Pomerantz [34]. In Super-

lattices, the effect of hypersound absorption/amplification was extensively studied by Mensah et. al [35, 36, 37, 38, 39], Vyazovsky et. al. [40], Bau et. al [41], while Shmelev and Zung [42] calculated the absorption coefficient and renormalization of the short-wave sound velocity. Azizyan [43] calculated the absorption coefficient in a quantized electric field. Furthermore, Acoustic wave absorption/amplification in Graphenes [44, 45, 46], Cylindrical quantum wires [47], and quantum dots [48, 49] have all received attention. On the concept of Acoustoelectric effect (AE) in bulk [50] and low-dimensional materials [51], much research has been comprehensively done both theoretically and experimentally. Acoustoelectric effect in CNT's is now receiving attention with few experimental work done on it. Ebbecke et. al. [52] studied the AE current transport in a single walled CNT, whilst Reulet et. al [53] studied AE in CNT. But in all these research there is no theoretical studies of AE in CNT. In this paper, the absorption (amplification) of hypersound in CNT in the regime $ql \gg 1$ (q is the acoustic wave number and l is the electron mean free path) is considered where the acoustic wave is considered as a flow of monochromatic phonons of frequency (ω_q).

It is worthy to note that the mechanism of absorption (amplification) is due to Cerenkov effect. For practical use of the Cerenkov acoustic-phonon emission, the material must have high drift velocities and large densities of electrons [19]. Carbon Nanotubes (CNT) has electron mobility of 10^5 cm^2/Vs at room temperature. At low temperatures ($T = 10\text{K}$), CNT exhibit good AE effect, which indicates that Cerenkov emission can take place in it [54]. The paper is organised as follows: In section 2, the kinetic theory based on the linear approximation for the phonon distribution function is

setup, where, the rate of growth of the phonon distribution is deduced and the absorption coefficient (Γ) is obtained. In section 3, the final equation is analysed numerically in a graphical form at various harmonics where the absorption obtained are related to the acoustoelectric current via the Wienrich relation [33]. Lastly the conclusion is presented in section 4.

Theory

We will proceed following the works of [50, 51] where the kinetic equation for the phonon distribution is given as

$$\frac{\partial N_{\vec{q}}}{\partial t} = \frac{2\pi}{\hbar} \sum_p |C_{\vec{q}}|^2 \{ [N_{\vec{q}}(t) + 1] f_{\vec{p}}(1 - f_{\vec{p}'}) \delta(\varepsilon_{\vec{p}'} - \varepsilon_{\vec{p}} + \hbar\omega_{\vec{q}}) - N_{\vec{q}}(t) f_{\vec{p}'}(1 - f_{\vec{p}}) \delta(\varepsilon_{\vec{p}'} - \varepsilon_{\vec{p}} + \hbar\omega_{\vec{q}}) \} \quad (1)$$

where $N_{\vec{q}}(t)$ represent the number of phonons with 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 $f_{\vec{p}}(1 - f_{\vec{p}'})$ represent the probability that the initial \vec{p} state is occupied and the final electron state \vec{p}' is empty whilst the factor $N_{\vec{q}}f_{\vec{p}'}(1 - f_{\vec{p}})$ is that of the boson and fermion statistics. The unperturbed electron distribution function is given by the shifted Fermi-Dirac function as

$$f_{\vec{p}} = [\exp(-\beta(\varepsilon(\vec{p} - mv_D) - \mu))]^{-1} \quad (2)$$

where $f_{\vec{p}}$ is the Fermi-Dirac equilibrium function, with μ being the chemical potential, \vec{p} is momentum of the electron, $\beta = 1/kT$, k is the Boltzmann constant and V_D is the net drift velocity relative to the ion lattice site. In a

more convenient form, Eqn(1) can be written as

$$\frac{\partial N_{\vec{q}}(t)}{\partial t} = 2\pi|C_{\vec{q}}|^2 \left[\frac{N_{\vec{q}}(t) + 1}{1 - \exp(-\beta(\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D))} + \frac{N_{\vec{q}}}{1 - \exp(-\beta(\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D))} \right] \times \sum_{\vec{p}} (f_{\vec{p}} - f_{\vec{p}'}) \delta(\varepsilon_{\vec{p}'} - \varepsilon_{\vec{p}} + \hbar\omega_{\vec{q}}) \quad (3)$$

To simplify Eqn.(3), the following were utilised

$$Q = \sum_{\vec{p}} \frac{f_{\vec{p}} - f_{\vec{p}'}}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}'} - \hbar\omega_{\vec{q}} - i\delta} \quad (4)$$

$$f_{\vec{p}} = [\exp(-\beta(\varepsilon_{\vec{p}} - \mu)) + 1]^{-1} \quad (5)$$

Given that

$$\Gamma_{\vec{q}} = -2|C_{\vec{q}}|^2 \text{Im}Q(\hbar\vec{q}, \hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D) \quad (6)$$

the phonon generation rate simplifies to

$$\Gamma_{\vec{q}} = 2\pi|C_{\vec{q}}|^2 \sum_{\vec{p}} (f_{\vec{p}} - f_{\vec{p}'}) \delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}'} - (\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D)) \quad (7)$$

In Eqn.(7), $f_{\vec{p}} > f_{\vec{p}'}$ if $\varepsilon_{\vec{p}} < \varepsilon_{\vec{p}'}$. When $\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D > 0$, the system would return to its equilibrium configuration when perturbed where

$$N_{\vec{q}}^0 = [\exp(-\beta(\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D) - 1)]^{-1}$$

But $\hbar\omega_{\vec{q}} - \hbar\vec{q} \cdot V_D < 0$ leads to the Cerenkov condition of phonon instability (amplification). The linear energy dispersion $\varepsilon(\vec{p})$ relation for the CNT is given as [55]

$$\varepsilon(\vec{p}) = \varepsilon_0 \pm \frac{\sqrt{3}}{2\hbar} \gamma_0 b(\vec{p} - \vec{p}_0) \quad (8)$$

The ε_0 is the electron energy in the Brillouin zone at momentum p_0 , b is the lattice constant, γ_0 is the tight binding overlap integral ($\gamma_0 = 2.54\text{eV}$). The

\pm sign indicates that in the vicinity of the tangent point, the bands exhibit mirror symmetry with respect to each point. The phonon and the electric field are directed along the CNT axis therefore $\vec{p}' = (\vec{p} + \hbar\vec{q})\cos(\theta)$. Where θ is the scattering angle. At low temperature, the $kT \ll 1$, Eqn.(5) reduces to

$$f_{\vec{p}} = \exp(-\beta(\varepsilon(p) - \mu)) \quad (9)$$

Inserting Eqn.(8 and 9) into Eqn.(7), and after some cumbersome calculations yield

$$\Gamma = \frac{4\hbar\pi|C_{\vec{q}}|^2 \exp(-\beta(\varepsilon_0 - \chi\vec{p}_0))}{\gamma_0 b \sqrt{3}(1 - \cos(\theta))} \{ \exp(-\beta\chi(\eta + \hbar\vec{q})\cos(\theta)) - \exp(-\beta\chi\eta) \} \quad (10)$$

where $\chi = \sqrt{3}\gamma_0 b/2\hbar$, and

$$\eta = \frac{2\hbar^2\omega_{\vec{q}}(1 - \frac{V_D}{V_s}) + \gamma_0 b \sqrt{3}\hbar\vec{q}\cos(\theta)}{\gamma_0 b \sqrt{3}(1 - \cos(\theta))}$$

Numerical analysis

Considering the finite electron concentration, the matrix element can be modified as

$$|C_{\vec{q}}|^2 \rightarrow \frac{|C_q|^2}{|\aleph^{(el)}(\vec{q})|^2} \quad (11)$$

where $\aleph^{(el)}(\vec{q})$ is the electron permittivity [50]. However, for acoustic phonons, $|C_{\vec{q}}| = \sqrt{\Lambda^2\hbar\vec{q}/2\rho V_s}$, where Λ is the deformation potential constant and ρ is the density of the material. From Eq.(10), taking $\varepsilon_0 = \vec{p}_0 = 0$, the Eqn.(10) finally reduces to

$$\Gamma = \frac{|\Lambda|^2\hbar^3 q^2 \exp(-\beta\chi\eta)}{2\pi\hbar\omega_q \gamma_0 b \sqrt{3}(1 - \cos(\theta))} \left\{ \sum_{n=-\infty}^{\infty} \frac{\exp(-n(\theta + \beta\chi\eta))}{I_n(\beta\chi(\eta + \hbar\vec{q}))} - 1 \right\} \quad (12)$$

where $I_n(x)$ is the modified Bessel function. The parameters used in the numerical evaluation of Eqn(12) are: $|\Lambda| = 9\text{eV}$, $b = 1.42\text{nm}$, $q = 10^7 \text{ cm}^{-1}$, $\omega_q = 10^{12}\text{s}^{-1}$, $V_s = 4.7 \times 10^5 \text{ cm s}^{-1}$, $T = 10\text{K}$, and $\theta > 0$. The dependence of the absorption coefficient (Γ) on the acoustic wave number (\vec{q}), the frequency (ω_q) and (γ) at various harmonics ($n = 0, \pm 1, \pm 2$) are presented below. For $n = 0$, the graph of Γ versus \vec{q} at varying frequencies and that of Γ versus ω_q for various acoustic wave numbers are shown in Figure 1(a and b). In Figure 1a, an amplification curve was observed, where the minimum value increases by increasing ω_q but above $\omega_q = 1.6 \times 10^{12}\text{s}^{-1}$, an absorption was obtained. In Figure 1b, it was observed that absorption switched over to amplification when the \vec{q} values were increased. For $n = \pm 1$ (first harmonics), in Figure 2a, it was observed that absorption exceed amplification and the peaks shift to the right. A further increase in ω_q values caused an inversion of the graph where amplification exceeds absorption (see Figure 2b). A similar observation was seen in Figure 3 (a and b), where, the peak values shift to the right and decreases with increasing \vec{q} values (see Figure 3a) but in Figure 3b, an inversion of the graph occurred for increasing values of \vec{q} . Figure 4 (a and b), shows the dependence of Γ on γ by varying either ω_q or \vec{q} . In both graphs, when $\gamma < 0$, produce non-linear graphs which satisfy the Cerenkov condition, but at $\gamma > 0$, the graph returns to zero. The observed peaks in Figure 4a, shift to the left by increasing ω_q whilst in Figure 4b, shift to the right by increasing \vec{q} . For further elucidation, a 3D graph of Γ versus ω_q and γ or Γ versus \vec{q} and γ are presented in Figure 5 (a and b). In both graphs, when $\gamma = -0.10$, a maximum amplification was obtained. For $n = \pm 2$ (Second harmonics), the dependence of the absorption coefficient Γ on ω_q is presented

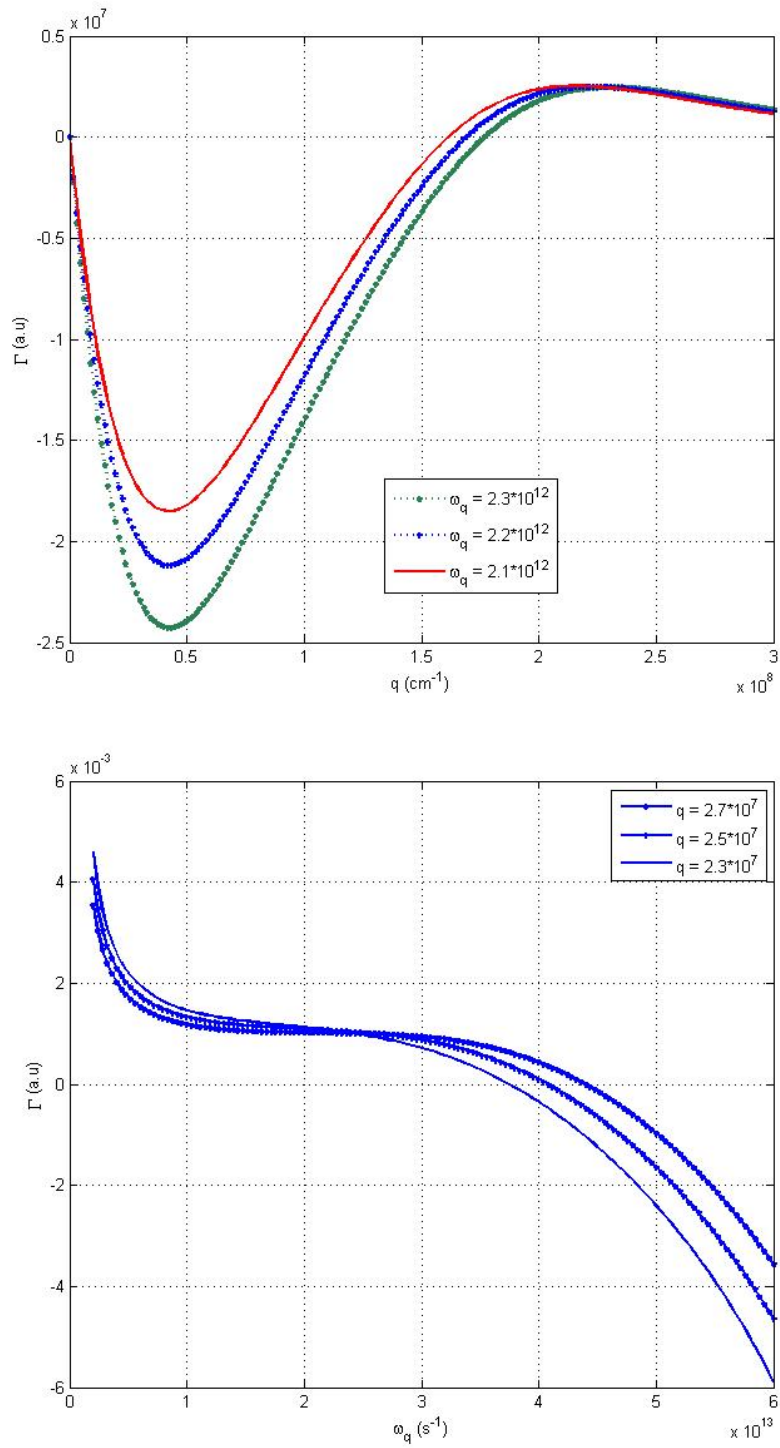


Figure 1: (a) Dependence of Γ on q for varying ω_q at $V_D = 1.2V_s$ (b) Γ on ω_q for varying \bar{q} at $V_D = 1.2V_s$.

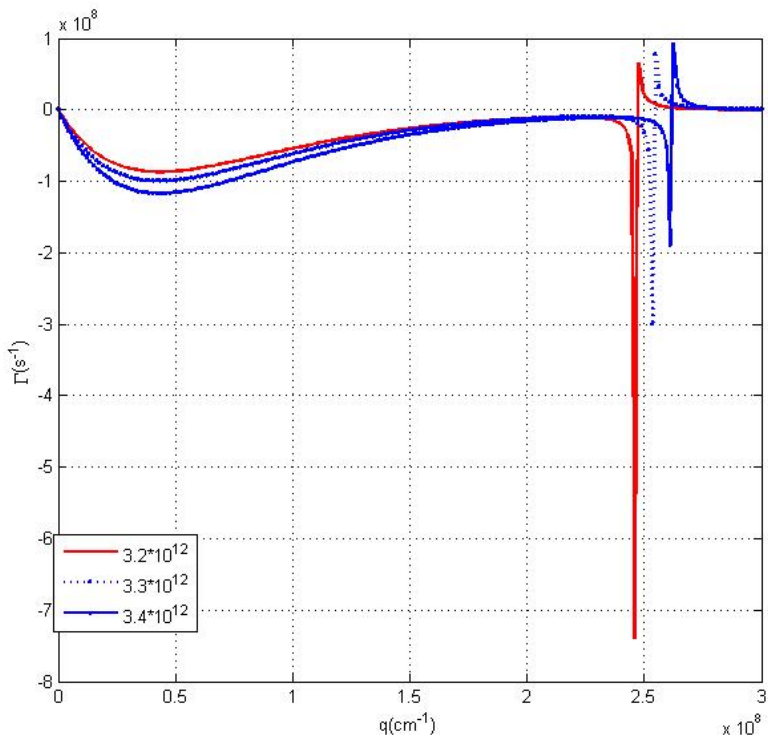
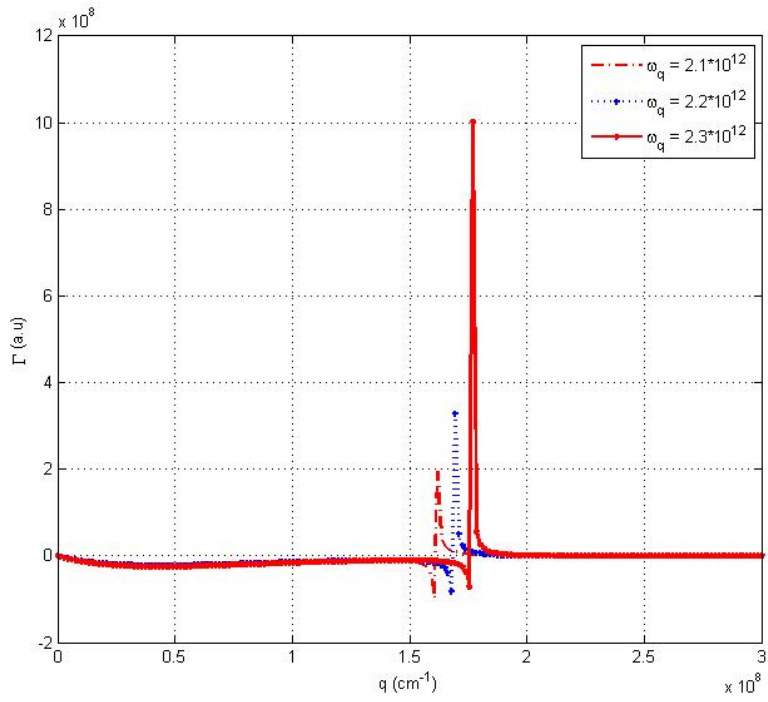
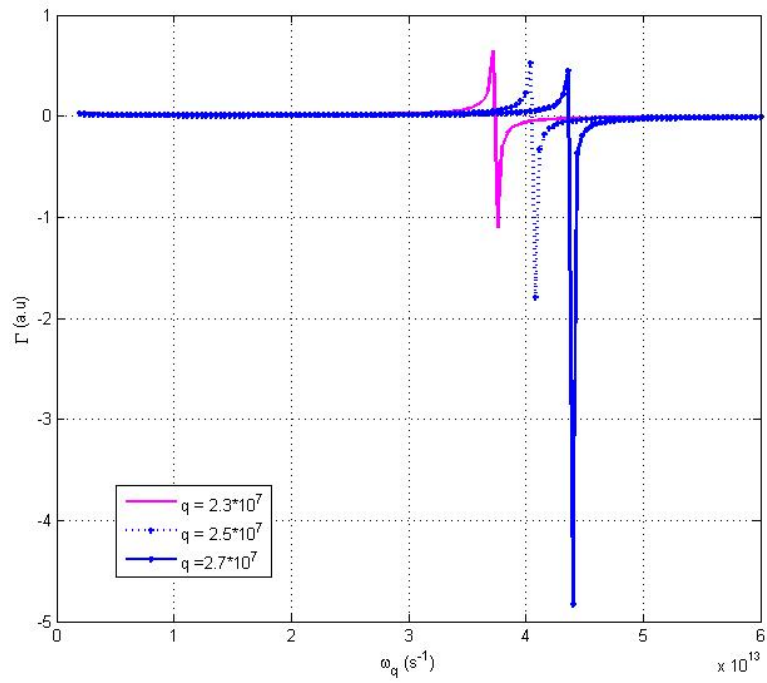
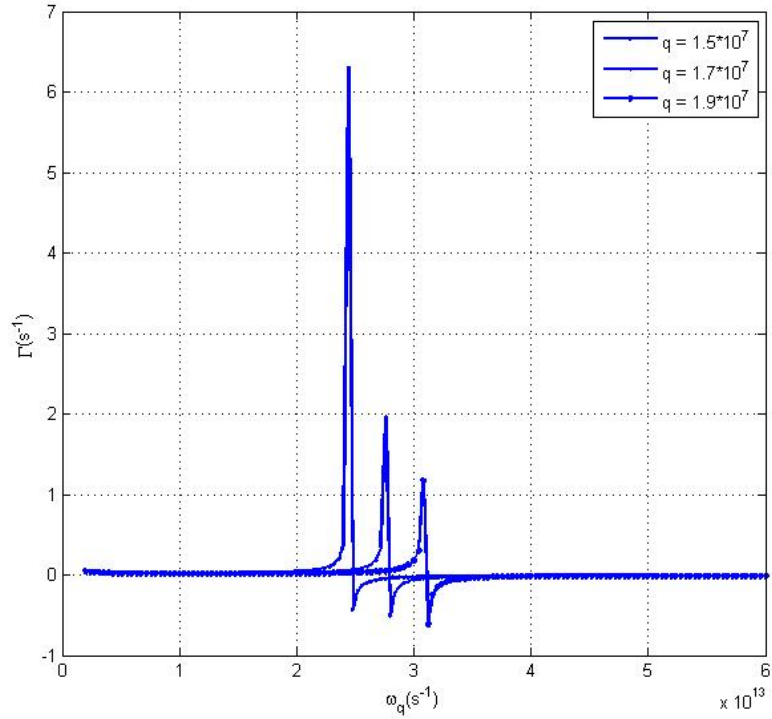


Figure 2: Dependence of Γ on \vec{q} at $V_D = 1.2V_s$ showing (a) Absorption exceeds Amplification (b) Amplification exceeds Absorption.



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Figure 3: Dependence of Γ on ω_q (a) Absorption exceeds Amplification (b) Amplification exceeds Absorption.

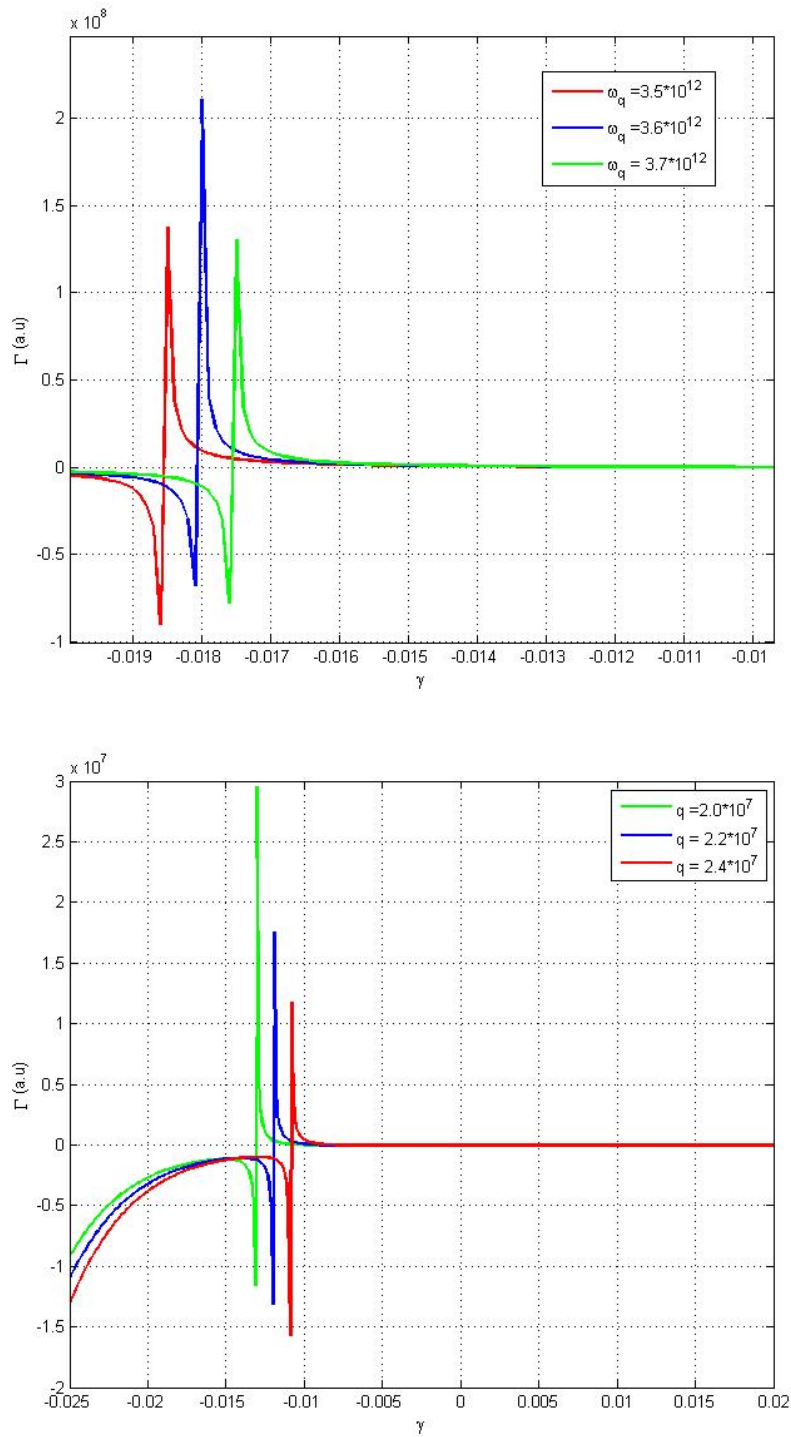
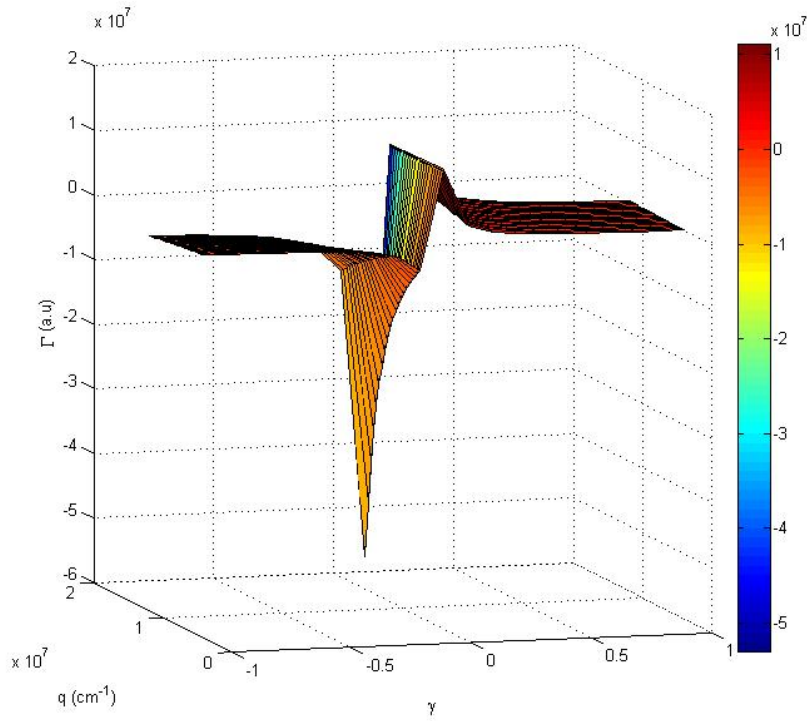
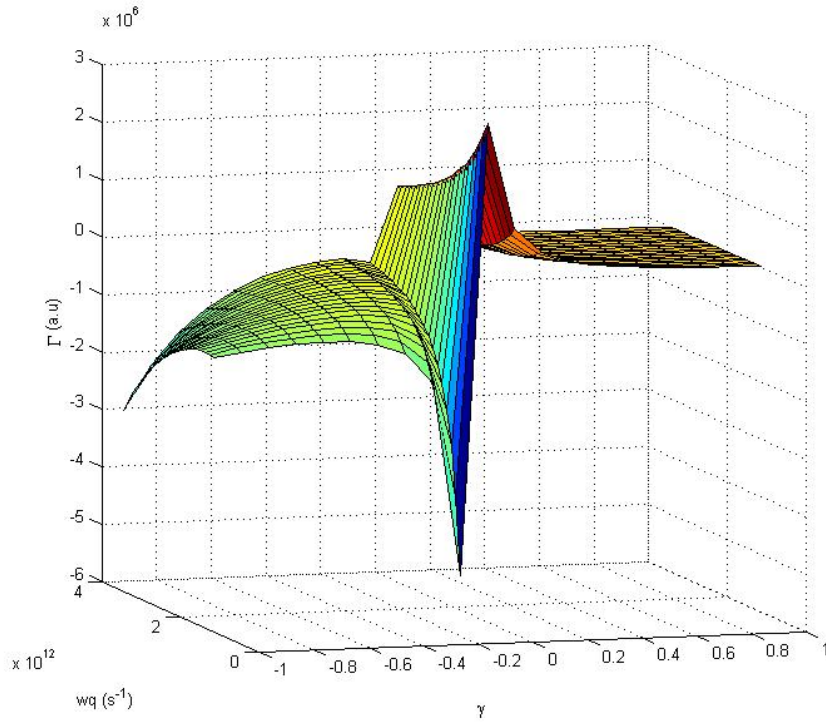


Figure 4: Dependence of Γ on γ at $\theta = 80^\circ$ (a) By increasing ω_a (b) By increasing q



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Figure 5: (a) Dependence of Γ on ω_q and γ and (b) Dependence of Γ on \vec{q} and γ .

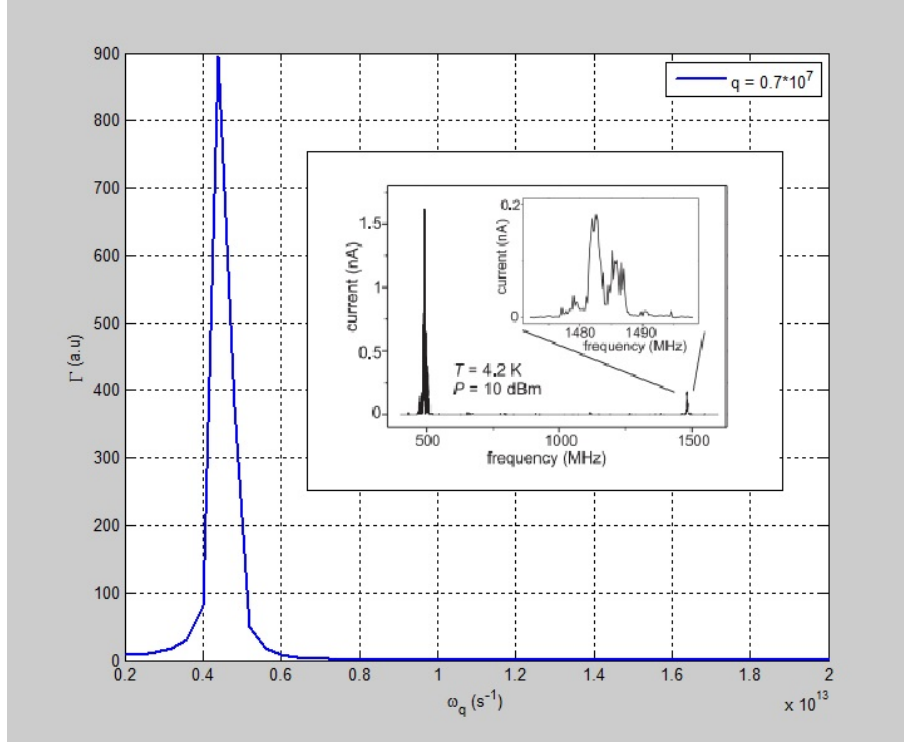


Figure 6: Second harmonic graph of the dependence of Γ on ω_q . Insert shows the experimental graph for acoustoelectric current versus frequency [52]

in $2D$ and $3D$ form as shown in Figure 6 and 7. In Figure 6, an absorption graph was obtained. The insert shown is an experimental results obtained for the Acoustoelectric current in Single walled Carbon Nanotube [52]. Figure 7 (*a* and *b*) is the $3D$ representation of the absorption in second harmonics. From Weinreich relation [33], the absorption coefficient is directly related to the acoustoelectric current, therefore from Figure 6, the results obtained for the absorption coefficient qualitatively agrees with the experimental results presented (see insert). In the $3D$ graphs, the maximum amplification and absorption occurred at $\gamma = -0.1$ which is equivalent to $V_D = 1.1V_s$. With the electric field $E = \frac{V_D}{\mu}$ gives $E = 51.7V/cm$.

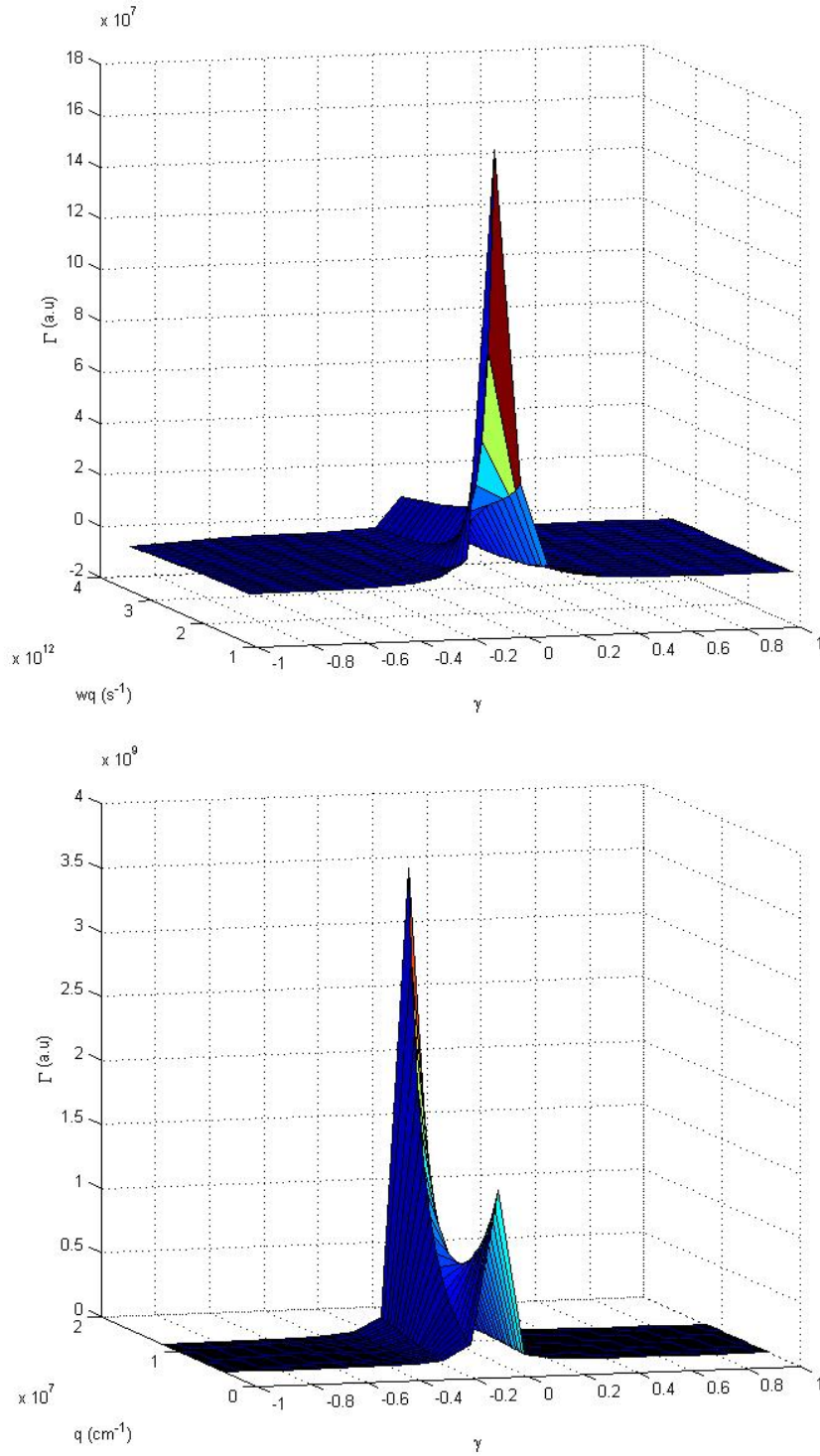


Figure 7: (a) Dependence of Γ on \vec{q} and γ and (b) Dependence of Γ on ω_q and γ .

Conclusion

The expression for Hypersound Absorption of acoustic phonons in a degenerate Carbon Nanotube (CNT) was deduced theoretically and graphically presented. In this work, the acoustic waves were considered to be a flow of monochromatic phonons in the short wave region ($ql \gg 1$). The general expression obtained was analysed numerically for $n = 0, \pm 1, \pm 2$ (where n is an integer). From the graphs, at certain values of ω_q and \vec{q} , an Amplification was observed to exceed Absorption or vice-versa. For $\gamma < 0$, the maximum Amplification was observed at $V_D = 1.1V_s$ which gave us a field of $E = 51.7Vcm^{-1}$. This field is far lower than that observed in superlattice and homogeneous semiconductors permitting the CNT to be a suitable material for hypersound generator (SASER). A similar expression can be seen in the works of Nunes and Fonseca [56].

Very interesting to our work is the qualitative agreement of the absorption graph to an experimental graph resulting from an acoustoelectric current via the Weinreich relation.

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