

On the amplification of acoustic phonons in carbon nanotube

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Abstract

We present a theoretical study of acoustic phonons amplification in Carbon Nanotubes (CNT). The phenomenon is via Cerenkov emission (CE) of acoustic phonons using intraband transitions proposed by Mensah et. al., [1] in Semiconductor Superlattices (SSL) and confirmed in [2]. From this, an asymmetric graph of Γ^{CNT} on $\frac{V_d}{V_s}$ and $\Omega\tau$ were obtained where amplification (Γ_{amp}^{CNT}) \gg absorption (Γ_{abs}^{CNT}). The ratio, $\frac{|\Gamma_{amp}^{CNT}|}{|\Gamma_{abs}^{CNT}|} \approx 3.5$, at $V_d = 1.02V_s$, $\omega_q = 3.0$ THz and $T = 85$ K for scattering angle $\theta > 0$. A threshold field at which Γ_{abs}^{CNT} switches over to Γ_{amp}^{CNT} was calculated to be $E_z^{dc} = 6.2 \times 10^3$ V/m. This field is far less than that deduced using Bloch-Type Oscillation (BTO) [3] which is $E_{BTO}^{dc} = 3.0 \times 10^5$ V/m. The obtained Γ_{amp}^{CNT} would enable the use of CNT for the production of SASER.

Keywords: Amplification, Carbon Nanotubes, acoustic phonon, hypersound

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Introduction

The study of amplification of acoustic phonons propagated along the axes of low-dimensional and bulk materials such as Semiconductor Superlattices (SL) [4, 5, 6, 7], 2D-Graphene sheet [8, 9], Quantum Wells (QW) [10, 11], and Carbon Nanotubes (CNT) [12, 13] are actively pursued recently using microscopic theory of electron - phonon interactions. This is due to the electronic and optoelectronic applications including the production of SASER (Sound Amplification by Stimulated Emission of Radiation), for dynamic storage of light in quantum wells and acoustic wave induced carrier transport [9]. When a non-quantizing electric field is applied to these material, and the drift velocity $V_d > V_s$ (V_s is sound velocity) an amplification of acoustic phonons occurs but in the reverse when $V_d < V_s$ it lead to absorption of acoustic phonons. The nature of this phenomenon is related to Cerenkov's emission of phonons by moving carriers [14, 15]. In SSL, amplification of acoustic phonons via Cerenkov's emission was proposed theoretically by Mensah et. al., [1]. The Mensah formalism of intra-miniband transitions via deformation potential (dp) in SSL has been confirmed experimentally by Shinokita [2] to amplify over 200% of acoustic phonons. Recently, a series of related studies in Graphene and CNT with degenerate energy dispersion has been conducted (theoretically) in the hypersound regime $ql \gg 1$ (q is the acoustic wavenumber, l is the mean free path). The results obtained qualitatively agreed with an experimentally obtained results [12, 19]. In multilayer-graphene-based system, Yurchenko et. al., [16] obtained amplification in the hydrodynamic regime $ql \ll 1$ in a collisionless system with condition $2V_D > V_S$. Dagher, et. al., [4] utilised the Boltzmann transport equation (BTE) to investigate the

amplification of travelling waves in metallic CNT biased by a dc field. The amplification attained was as a result of Bloch-Type Oscillations (BTO). In CNT, the π -bonding and anti-bonding (π^*) energy band crosses at the Fermi level in a linear manner [17] where, intra-band scattering process depends on the phonon modes. These modes are the Longitudinal acoustic (LA), Transverse acoustic (TA) and the Radial Breathing Mode (RBM) which is the weakest scattering mode. For each phonon branch, an electron can be scattered either by zone center phonon, or by a zone boundary phonon. The energy dispersion $\varepsilon(p_z)$ is near the Fermi level therefore, at low temperatures, conduction occurs through well separated discrete electron states. This leads to the emission of large number of coherent acoustic phonons [14, 15, 18]. The extreme electron mobilities makes CNT, a good candidate for the amplification of acoustic phonons. Till date, few studies [3, 18] has been conducted to understand amplification in CNT. In this paper, we utilised the theory proposed by [1] and verified experimentally by [2] to study amplification of acoustic phonons in CNT. 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 amplification is obtained. In section 3, the final equation is analysed numerically in a graphical form at the harmonic. Lastly the conclusion is presented in section 4.

Theory

We will proceed following the works of [18, 19, 20] where the kinetic equation for the phonon distribution is given as

$$\begin{aligned} \frac{\partial N_q}{\partial t} &= \frac{2\pi}{\hbar} \sum_p |C_q|^2 \{ [N_q(t) + 1] f_p (1 - f_{p'}) \delta(\varepsilon_{p'} - \varepsilon_p + \hbar\omega_p) \\ &\quad - N_q(t) f_{p'} (1 - f_p) \delta(\varepsilon_{p'} - \varepsilon_p + \hbar\omega_q) \} - \gamma N_q(t) \end{aligned} \quad (1)$$

where $N_q(t)$ represent the number of phonons with wave vector q at time t . The factor $N_q + 1$ accounts for the presence of N_q phonons in the system when the additional phonon is emitted. The $f_p(1 - f_{p'})$ represent the probability that the initial p state is occupied and the final electron state p' is empty whilst the factor $N_q f_{p'}(1 - f_p)$ is that of the boson and fermion statistics. γ denotes phonon losses which includes phonon scattering or phonon absorption due to non-electronic mechanisms, phonon decay due to anharmonicity of the lattice. In a more convenient form, Eqn. (1) can be written as

$$\begin{aligned} \frac{\partial N_q(t)}{\partial t} &= 2\pi |C_{-q}|^2 \left[\frac{N_q(t) + 1}{1 - \exp(\beta(\hbar\omega_q - \hbar\vec{q} \cdot V_D))} + \frac{N_q}{1 - \exp(-\beta(\hbar\omega_q - \hbar\vec{q} \cdot V_D))} \right] \\ &\quad \times \sum_p (f_p - f_{p'}) \delta(\varepsilon_{p'} - \varepsilon_p + \hbar\omega_q) \end{aligned} \quad (2)$$

$\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the absolute temperature. Here, phonon losses were ignored and the lowest order in the electron-phonon coupling is approximated by f_p and

$$N_q = [\exp(-\beta(\hbar\omega_q - \hbar\vec{q} \cdot V_D)) - 1]^{-1}$$

Eqn.(2) can further be expressed as

$$\begin{aligned} \frac{\partial N_q(t)}{\partial t} &= 2\pi |C_q|^2 \left[N_q(t) - \frac{1}{1 - \exp(\hbar\omega_q - \hbar q \cdot V_D) - 1} \right] \\ &\quad \times \text{Im}Q(q, \hbar\omega_q - q \cdot V_D) \end{aligned} \quad (3)$$

where

$$Q = \sum_p \frac{f_p - f_{p'}}{\varepsilon_p - \varepsilon_{p'} - \hbar\omega_q - i\delta} \quad (4)$$

and

$$f_p = [\exp(-\beta(\varepsilon_p - \mu)) + 1]^{-1} \quad (5)$$

From Eqn. (3) the phonon generation rate is given as

$$\Gamma_q = -2|C_q|^2 \text{Im}Q(\hbar\vec{q}, \hbar\omega_q - \hbar\vec{q} \cdot V_D) \quad (6)$$

this simplifies to the phonon transition as

$$\Gamma_q = 2\pi|C_q|^2 \sum_p (f_p - f_{p'}) \delta(\varepsilon_p - \varepsilon_{p'} - (\hbar\omega_q - \hbar\vec{q} \cdot V_D)) \quad (7)$$

the total rate of absorption and emission of phonon is obtained by the summation over all the initial and final electrons states. In Eqn.(7), $f_p > f_{p'}$ if $\varepsilon_p < \varepsilon_{p'}$. When $\hbar\omega_q - \hbar\vec{q} \cdot V_D > 0$, the system would return to its equilibrium configuration when perturbed but $\hbar\omega_q - \hbar\vec{q} \cdot V_D < 0$ leads to the Cerenkov condition of phonon instability (amplification). From perturbation theory, the transition probability per unit time from the initial state $|p\rangle$, consisting of electron having momentum p_z , to the final state $|p'\rangle$, which consists of an electron with momentum p'_z and a phonon with wave vector q . The phonon and the electric field are directed along the CNT axis therefore $p'_z = (p + \hbar q)\cos(\theta)$ where θ is the scattering angle. In CNT, the linear energy dispersion $\varepsilon(p)$ relation is given as [13]

$$\varepsilon(p_z) = \varepsilon_0 \pm \frac{\sqrt{3}}{2\hbar} \gamma_0 b (p_z - p_0) \quad (8)$$

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. At low temperature, when, $k_B T \ll 1$, Eqn.(5) reduces to

$$f_p = \exp(-\beta(\varepsilon(p_z) - \mu)) \quad (9)$$

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

$$\Gamma^{CNT} = \frac{4\hbar\pi|C_q|^2 \exp(-\beta(\varepsilon_0 - \chi p_0))}{\gamma_0 b \sqrt{3}(1 - \cos(\theta))} \{ \exp(-\beta\chi(\eta + \hbar q)\cos(\theta)) - \exp(-\beta\chi\eta) \} \quad (10)$$

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

$$\eta = \frac{2\hbar^2\omega_q(1 - \frac{V_d}{V_s}) + \gamma_0 b \sqrt{3}\hbar q \cos(\theta)}{\gamma_0 b \sqrt{3}(1 - \cos(\theta))} \quad (11)$$

Analysis

In the formulation, we utilise a perturbation theory of electron transition where, electrons are assumed to drift relative to the lattice ions. The wavelength of the phonon is short compared with the screening length for the electrons. Electron-electron interactions and phonon losses are ignored but the electron-phonon interaction C_q is assumed to be weak and treated as perturbation. In Eqn. (1), the quantum-mechanical matrix element describing the electron-phonon coupling for a highly excited (intense acoustic wave) phonon is $|C_{-q}|^2 \approx |C_q|^2$. Considering the finite electron concentration, the matrix element can be modified as

$$|C_q|^2 \rightarrow \frac{|C_q|^2}{|N^{(el)}(q)|^2} \quad (12)$$

where $\aleph^{(el)}(q)$ is the electron permittivity. However, for acoustic phonons, $|C_q| = \sqrt{\Lambda^2 \hbar q / 2\rho V_s}$, where Λ is the deformation potential constant and ρ is the density of the material. From Eq.(10), taking $\varepsilon_0 = p_0 = \mu = 0$, the Eqn.(10) finally reduces to

$$\Gamma^{CNT} = \frac{|\Lambda|^2 \hbar^3 q^2 \exp(-\beta\chi\eta)}{2\pi \hbar \omega_q \gamma_0 b \sqrt{3}(1 - \cos(\theta))} \left\{ \sum_{n=-\infty}^{\infty} \frac{\exp(-n(\theta) + \beta\chi\eta)}{I_n(\beta\chi(\eta + \hbar q))} - 1 \right\} \quad (13)$$

where $I_n(x)$ is the modified Bessel function. When the scattering angle $\theta = 0$, $\Gamma = \infty$ whereas for $\theta > 0$ and $V_d > V_s$, Γ^{CNT} changes sign from positive (+) to (-) and amplification is obtained. To analyse Eqn. (15), the following parameters were used: $|\Lambda| = 9\text{eV}$, $b = 1.42 \times 10^{-9}\text{m}$, $q = 10^4 \text{ m}^{-1}$, $\omega_q = 10^{12}\text{s}^{-1}$, $V_s = 4.7 \times 10^3 \text{ m s}^{-1}$, $T = 85 \text{ K}$, and $\theta > 0$. The choice of these parameters especially that of the acoustic wavenumber is based on our previous studies [18]. The dependence of Γ^{CNT} on $\frac{V_d}{V_s}$ at $n = 1$ is presented below (see Figure 1a). From the graph, there is absorption (Γ_{abs}^{CNT}) when $V_d < V_s$ but when $V_d > V_s$ it switches over to amplification (Γ_{amp}^{CNT}). This satisfy the Cerenkov condition for acoustic phonon emission. The maximum Γ_{amp}^{CNT} occurred at $V_d = 1.02V_s$. The amplification obtained far exceed the absorption. The ratio of the amplification to absorption

$$\frac{|\Gamma_{amp}^{CNT}|}{|\Gamma_{abs}^{CNT}|} \approx 3.5 \quad (14)$$

To determine the threshold field at which Γ_{abs}^{CNT} switches to Γ_{amp}^{CNT} , we calculated and found the V_d to be

$$V_d = \frac{8\gamma_0}{\sqrt{3}\hbar b m} \sum_{r=1}^{\infty} \frac{r^2 \Omega \tau}{1 + (r\Omega\tau)^2} \sum_{s=1}^m F_{rs} E_{rs} \quad (15)$$

Here,

$$F_{rs} = \frac{a}{2\pi} \int_0^{\frac{2\pi}{a}} \frac{\exp(-iarp_z)}{1 + \exp(\varepsilon(p_z)/k_\beta T)} dp_z \quad (16)$$

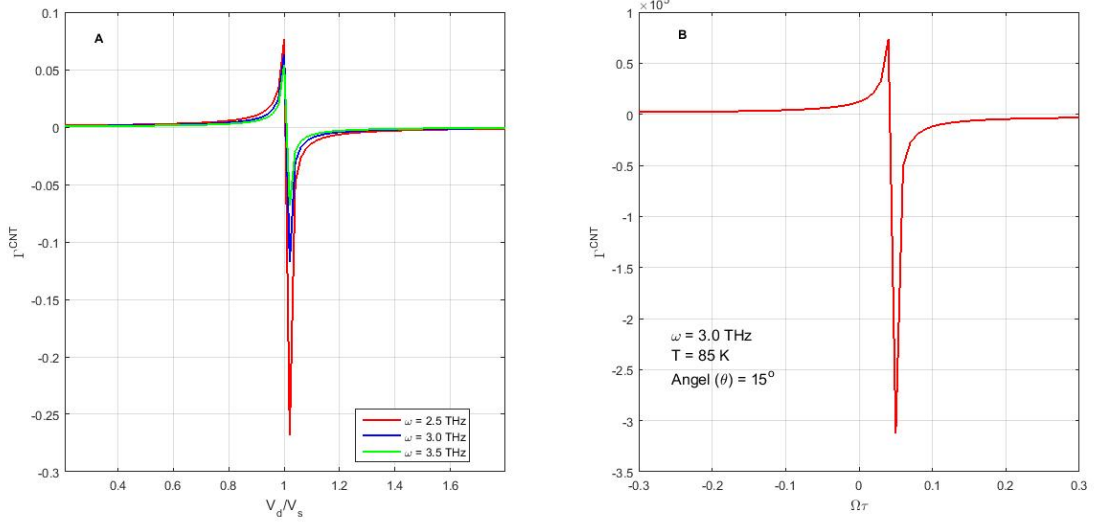


Figure 1: Dependence of Γ^{CNT} on: (a) $\frac{V_d}{V_s}$ at various ω_q (b) $\Omega\tau$ at $T = 85 K$, $\omega_q = 3 THz$ and $\theta = 15^\circ$

and

$$E_{rs} = \frac{a}{2\pi} \int_0^{\frac{2\pi}{a}} \varepsilon(p_z) \exp(-irp_z) dp_z \quad (17)$$

where $\Omega = eaE$ (E is the electric field, r the radius of the CNT, and $a = 3b/2\hbar$). The V_d is solved from the Boltzmann kinetic equation in the τ -approximation [21, 22, 23]. The justification for the τ -approximation can be found in [17]. By substituting Eqn.(15) into Eqn.(11). A graph of Γ^{CNT} against $\Omega\tau$ is plotted in Figure (1b). It can be observed that the threshold field for which Γ_{abs}^{CNT} changes over to Γ_{amp}^{CNT} occurs at $\Omega\tau = 0.04$ which gives $E_z^{dc} = 6.2 \times 10^3 V/m$. This value is far lower than that calculated by Dagher et. al. [4] to be $E_z^{dc} = 3 \times 10^5 V/m$ using Bloch-type oscillations (BTO). This is of the order of 2 which is quite high.

Conclusion

We studied the amplification of acoustic phonon in CNT theoretically in the hypersound regime. The method used involves the Cerenkov emission of acoustic phonons where, when $V_d < V_s$, gave an absorption (Γ_{abs}^{CNT}), but when $V_d > V_s$, an amplification (Γ_{amp}^{CNT}) was obtained. The ratio $\frac{|\Gamma_{amp}^{CNT}|}{|\Gamma_{abs}^{CNT}|} \approx 3.5$, at $V_d = 1.02V_s$, and $\omega = 3.0$ THz. The threshold field at which Γ_{abs}^{CNT} switched over to Γ_{amp}^{CNT} was calculated as $E_z^{dc} = 6.2 \times 10^3$ V/m. This is far lower than that calculated via the BTO to be $E_z^{dc} = 3 \times 10^5$ V/m. We therefore propose the use of Carbon Nanotube as a material for the production of SASER.

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