

Excitation of Carbon Molecule in CNT Due to External Electromagnetic Wave

Abstract

Carbon nanotube is a well-known tube. Surface Plasmon oscillation has been studied on surface of carbon atoms of CNT after incident of em waves of different radius of CNT by theoretical study. This study is done by special dispersion relation of two mode coupling on surface of CNT.

Keywords: Surface, Plasmon, Hydrodynamical Model, Surface Polariton, Chiralvector.

Introduction

Graphene are quasi one-dimensional material which could be regarded as a rolled-up graphics layer (i.e. one atom thick layer of graphene in the cylindrical form. It has a radius of a few nano meters and length up to centimeters. A graphene layer is a semi metallic material. Nevertheless, when a graphene layer is rolled up it may become either metallic or semi-conducting, depending on its geometry.

Aim of the Study

The author has interest to study the properties of different atoms of CNT of different radius of tubes. These research papers contain new investigation in semiconductors and give relevant idea of surface properties of materials. The author investigates the properties of condensed substances at nanoscale in presence of Plasmon oscillations

Review of Literature

Collective excitations in the single and multi-walled carbon nanotubes have been studied by several authors [1-3]. Hydro dynamical model [4] have been found an important method to study the properties of nanotubes. Plasma wave which propagate on the surface of nanotubes of different radius in dielectric medium are studied theoretically [5]. This investigation shows that frequencies of Plasmon can be change with respect to radius of nanotubes and surrounding dielectric mediums. The explicit of Plasmon dispersion relations between propagation constant of em waves and frequencies of Plasmon shows the attenuation properties of nanotubes of different substances.

Excitation of Carbon Molecule in CNT

The geometric structure of graphite sheets is uniquely determined by the chiral vector $R=ma_1+na_2 \equiv (m, n)$, where m and n are integers and a_1 & a_2 are the elementary vectors of the dimensional graphene lattice. The radius of the graphene is given by:

$$r_e = \frac{a_o}{2\pi} \sqrt{m^2 + mn + n^2}$$

Where $a_o = \sqrt{3} b_o$, is the lattice constant of the graphite sheet and $b_o=1.42 \text{ \AA}$ is the distance the nearest neighboring carbon atoms. A graphene is metallic of $m-n=3q$ where $q=0, 1, 2$, Thus, arm chair nano tubes are always metallic, whereas zig-zag nano tubes are metallic only if $m=3q$ with $q = 1, 2 \dots$

Now it is assumed that both zig-zag $(m, 0)$ and arm chair (m, n) nano-tubes as infinitesimally thin and infinitely long cylindrical shells of radius r_c with its axis along the z-direction and regard the Semiconductors to consist of π -electrons super imposed with equilibrium densities (per unit area) n_o . In equilibrium the π -electron fluid has no velocity and n is the perturbed density (per unit area) of fluid, produced by the π -electron themselves under the action of the electric field generated by the fixed positive ions of the lattice. Hydrodynamic theory has been used to describe



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electronic motion of electrons on the surface of condensed materials in terms of two dynamical variables, namely the electron-density functions, next and 4 (x, t) = 4φ, 4₂). The basic equations in this linearized Hydro dynamic model are the equations of motion, the equations of continuity -

$$\frac{\partial u(x,t)}{\partial t} = -n_0 \nabla_{11} u(x,t)$$

$$n_0 \frac{\partial u(x,t)}{\partial t} = -\alpha \nabla_{11} n(x,t) -$$

$$e \frac{n_0}{m_{\text{eff}}} E_{11}(x,t) - \gamma n_0 u(x,t)$$

The dispersion relation can be written approximately as:

$$\omega^2 = \alpha k^2 + \frac{e^2 v_F}{\xi \pi^2 \hbar} \frac{K}{r_c} \quad (1)$$

The right hand side of eqn. (1) depends strongly on the radius of the nano tube.

Limit $k_{rc} \rightarrow 0$, where the phase velocity of the surface Plasmon is comparable to the velocity of light, the surface Plasmon oscillations couple with the

electromagnetic wave and radiation effects are present. The expression of Bessel functions, can be written as

$$I_m(x) = \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m$$

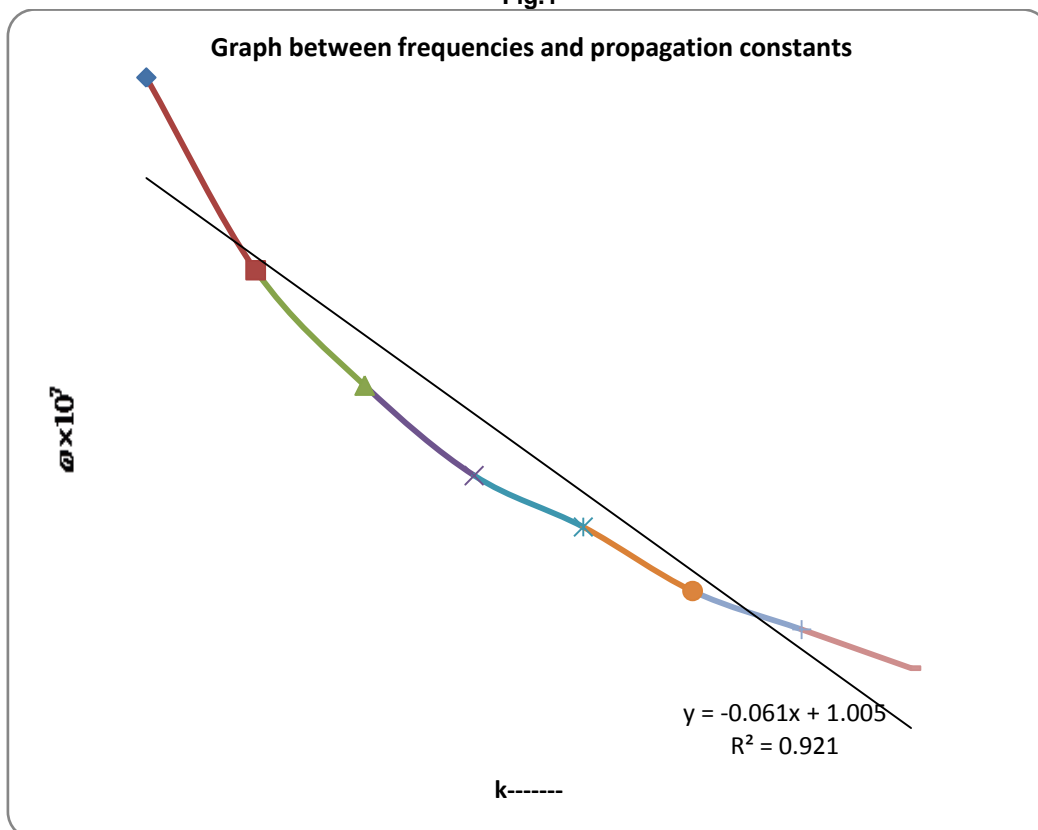
$$K_m(x) = \frac{\Gamma(m)}{2} \left(\frac{2}{x}\right)^m \quad (\text{for } m \neq 0) \text{ and } K_0(x)$$

$$= \frac{\ln 1.123}{x} \quad (\text{for } m = 0)$$

$$\omega(m=0, K \approx 0) \approx \left[\frac{4e^2 v_F}{\epsilon_0 \pi^2 \hbar} \ln \left(\frac{1.123}{K_{rc}} \right) \right]^{1/2} K \quad (2)$$

This is also quite sensitive to the geometric of the nanotube of graphene. Comparing the long-wavelength and short wavelength limits, it can be seen that the energy band structure play an important role in the dispersion relation, for all values of wavelength. The graph has been plotted for different positions of atoms of carbon at nanoscale.

Fig.1



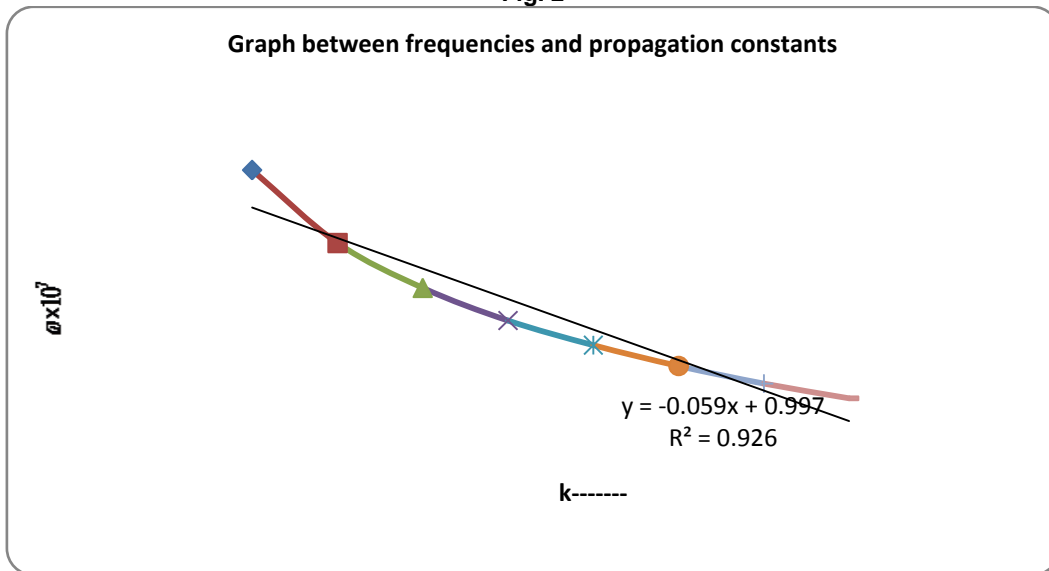
It is clear from fig. 1 that for zero mode of lattice vibration, the frequency of lattice vibration decreases exponentially with increasing the

propagation constant k, for armchair $a_0=2.459\text{\AA}$ and $b_0=1.42\text{\AA}$ with radius $r_c=3.9\text{\AA}$ for position atom $m=10$ and $n=0$. It is also clear that for propagation constant

range 0.4 to 0.6, the frequency of lattice vibration slightly increases and then slows down but the linearity of the graph shows that the propagation constant as increases the frequency of lattice vibration almost becomes constant. At higher value of propagation constant the lattice frequency becomes almost constant but low frequency of atom at high value of propagation constant of electromagnetic

waves. This shows that frequency of Lattice vibration changes as variation of propagation constant of external sources, thus it is clear that larger wavelength em wave, Plasmon frequency become low but lattice frequency be high. It vibrate only at its position and no motion of Plasmon, so low Plasmon frequency. Thus it is clear that k increases lattice frequency decreases

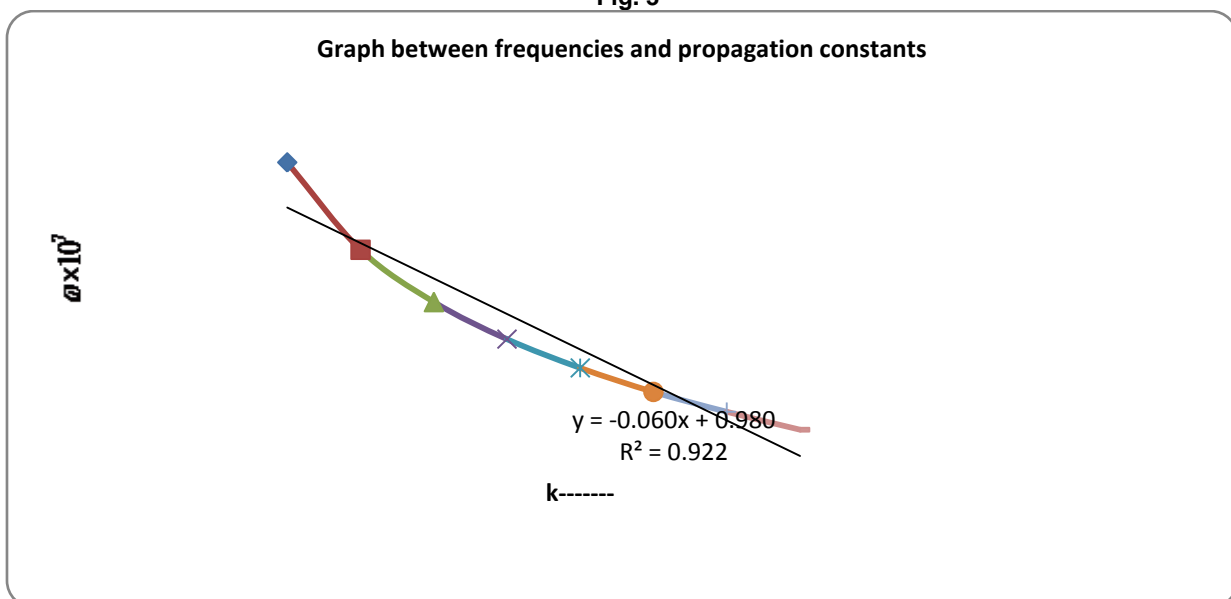
Fig. 2



As seen from above fig. 2 that for zero mode of lattice vibration and for chiral vectors $a_0=2.459\text{\AA}$, $b_0=1.42\text{\AA}$, radius $r_c=5.40\text{\AA}$ and for position atom $m=8=n$, the frequency of lattice vibration decreases exponentially with increasing the propagation constant k . It is also seen that for propagation constant range from 0.1 to 0.3, the frequency of lattice vibration decreases rapidly. At higher value of propagation constant the frequency of lattice vibration becomes

small but not constant. Here the atom is different as atom taken previous case because chiral vector are same but radius is different with position of atom is different i.e. $m=n=8$. The lattice frequencies are less than the lattice frequency of inner tube of CNT with different position of atoms. It is clearly seen that the graph of fig. 1 is more linear than fig. 2.

Fig. 3



It is clear from fig. 3 that for zero mode of lattice vibration and for position atom $m=30$, $n=0$ with

$r_c=11.7\text{\AA}$, the frequency of lattice vibration decreases exponentially with increasing the propagation constant

k and finally becomes almost constant at higher value of propagation constant. It should be noted here that the frequency decreases rapidly in the region of propagation constant from 0.1 to 0.2. The also graph shows that for large radius of CNT the lattice

frequency is lesser that smaller radius of CNT and slop of curve is .0604 of radius 11.7A which is slightly more than 0.059 for radius 5.40A. This is due to more effective than other position of atoms of CNT.

Fig. 4

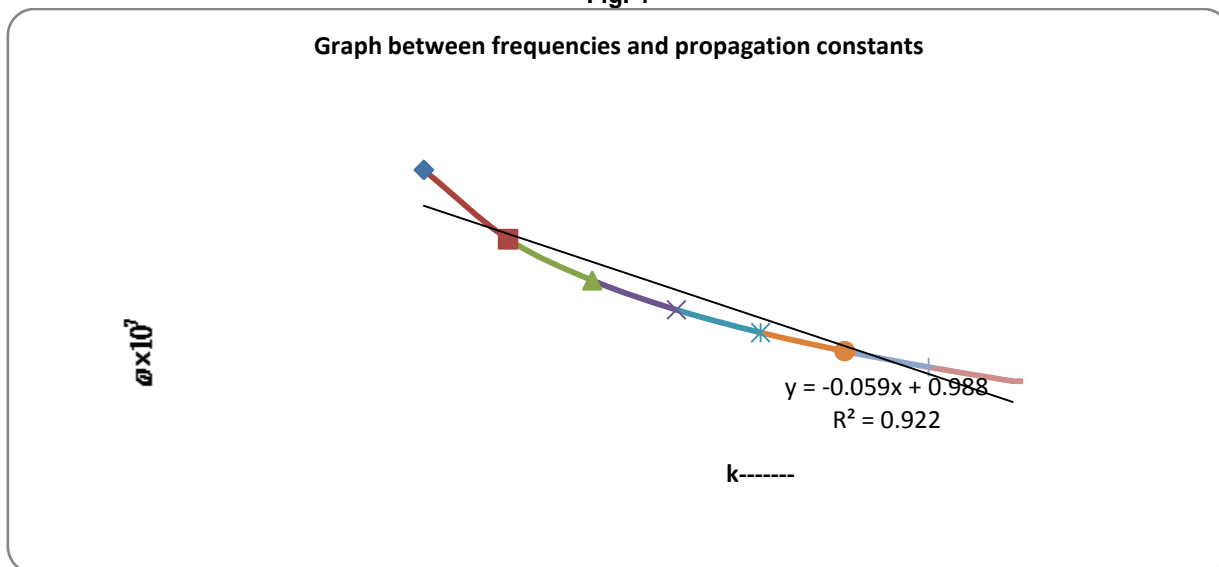
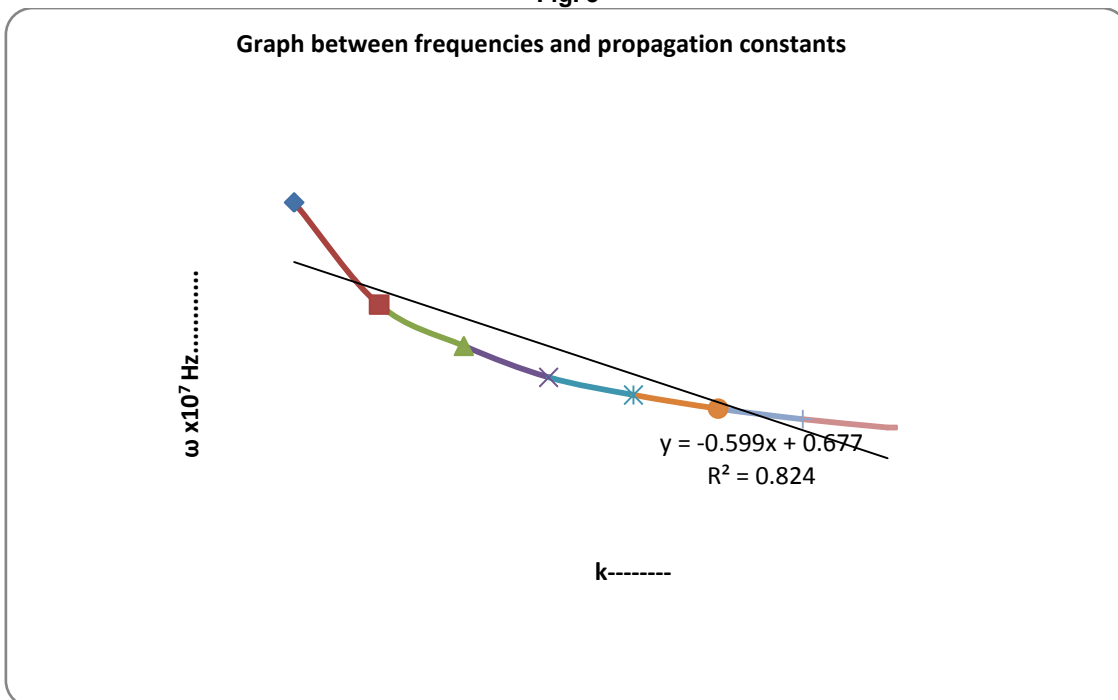


Fig. 4 shows the variation of frequency of lattice vibration with respect to the propagation constant for zero mode of lattice vibration and for $m=12=n$ with radius $r_c=8.106\text{Å}$. It has been seen that the frequency of lattice vibration decreases exponentially with increasing propagation constant k. It is clear from fig. that at propagation constant range

from 0.1 to 0.3, the frequency of lattice vibration decreases gradually. As compare to fig.3, the linearity fig.4 is almost similar. Now as radius is changed with position of molecules, the slope of curve decreases due to external sources of em wave .The Lattice vibration become constant and effective on CNT atoms.

Fig. 5



Above fig.5 shows the variation of frequency of lattice vibration with respect to the propagation constant k for non-zero mode of lattice vibration and

for $\alpha=0.378 \times 10^{12}$, with radius $r_c=5.40\text{Å}$. It has been seen that the frequency of lattice vibration decreases exponentially with increasing propagation constant k.

It is also seen that there is small increment in the frequency of lattice vibration at propagation constant 0.3. After that the frequency of lattice vibration slows down and finally becomes constant at higher value of propagation constant. The propagation constant k of e m wave is incident on atom of CNT frequency of

Lattice vibration decreases as frequency of e m wave as compare to radius higher radius of CNT and almost fixed for larger frequency of e m waves.

Fig. 6

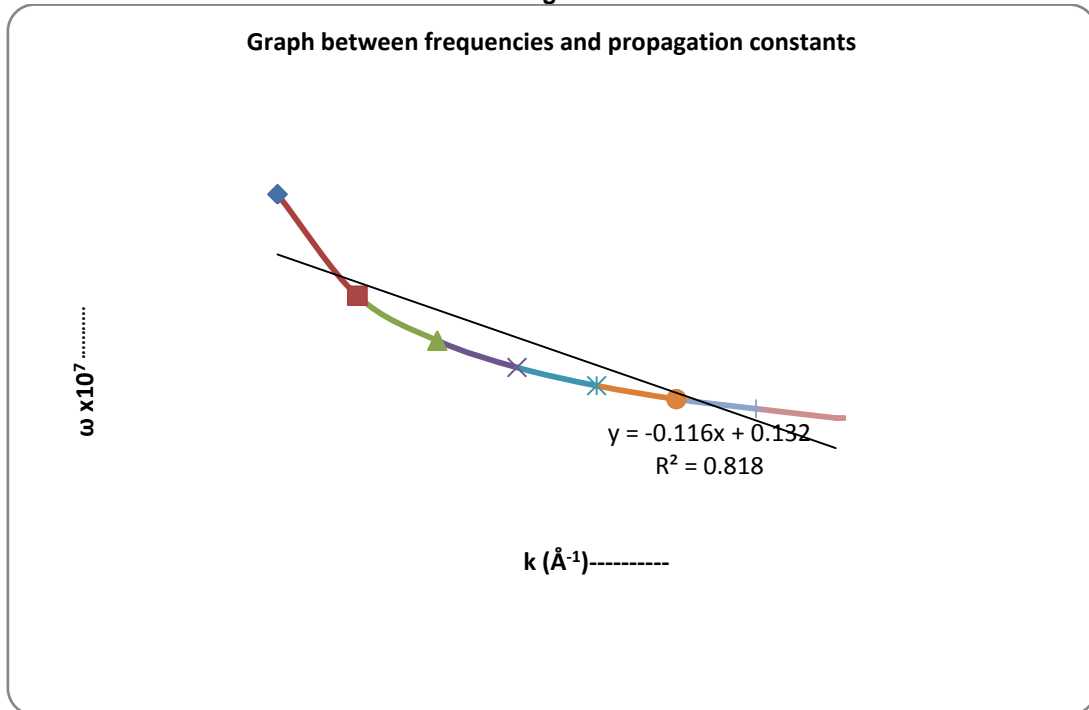


Fig.6 shows the variation of frequency of lattice vibration versus the propagation constant k for non-zero mode of lattice vibration with radius $r_c=11.7\text{\AA}$. It has been seen that the frequency of lattice vibration decreases exponentially with increasing propagation constant k . It is also seen that the frequency of lattice vibration decreases regularly with increasing propagation constant from 0.1 to 0.2. The linearity of fig.6 is more than fig.5. At a sufficient high value of propagation constant the frequency of lattice vibration becomes constant.

Conclusion

The above study is fully theoretical based on computational calculation .This study is applicable on cylindrical hollow shaped CNT and scientific devices.

References

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