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Remarking
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Energy Band Effect on the Dispersion Relation of Surface Plasmon Wave in Single Walled Carbon Nano Tubes

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Abstract

It is studied the energy band effects on the dispersion relation of the surface Plasmon waves in single walled carbon nano tubes of metallic character, by using the semi classical kinetic theory of electro dynamics. The conduction electrons of the system are modeled by an infinitesimally thin layer of free-electron gas which is described by means of the semi classical kinetic theory of the electron dynamics. The effects of the energy band structure is taken into account and a more accurate dispersion relation for surface Plasmon oscillation in the zigzag and armchair nano tubes of metallic character is obtained.

Keywords: Carbon Nano Tubes, Plasma Oscillations, Dispersion Relation

Introduction

Carbon nano tubes were first synthesized in 1991 by Iijima [1] as graphitic carbon needles, ranging from 4 to 30 nm in diameter and up to 1 m in length. CNT_S have remarkable electrical and mechanical properties. Collective electron in carbon nano tubes, so called Plasmon modes, can provide important information about their structural and electronic properties. Using electron-energy-loss spectroscopy, Pichler [2] experimentally studied the electron excitations in single walled carbon nano tubes and measured the Plasmon energies. Metallic CNTs are considered suitable candidates in the field of Plasmonic as new Plasmonic waveguides [3-13].These new Plasmonic waveguides can be built by some simple and well-known methods such as CVD [13].

By using the classical electrodynamics and semi classical kinetic theory, Slepyan [3], derived the dispersion relation of surface waves in single walled carbon nano tubes($SWCT_S$) and suggested that CNT_S can be used as a nano wave guide for controlling electromagnetic wave propagation in specified frequency range(i.e. infrared and optical). In particular by solving Maxwell and hydrodynamic equations, the propagation of electromagnetic waves in $SWCNT_S$ is studied [5, 6] and has been shown that dispersion behaviors of the plasma waves with TM and TE modes are quite similar.

$SWCNT_S$ are quasi one dimensional material, which could be regarded as rolled-up grapheme layer in cylindrical form. When a grapheme layer is rolled up it may become either metallic or semi conducting, depending on its geometry. The geometric structure of a $SWCNT_S$ is uniquely determined by the chiral vector $R=ma_1+ na_2\equiv(m,n)$, where m and n are integers, and a_1 and a_2 are the elementary vectors of the dimensional grapheme lattice. The tube radius of CNT is given by

$$r_c = a_0/2\pi \sqrt{(m^2 + mn + n^2)}$$

Where $a_0 = \sqrt{3b_0}$ is the lattice constant of graphite sheet and b_0= 1.42 A^0 is the distance between the nearest-neighboring carbon atoms. A $SWCNT_S$ is metallic if m-n= 3q, where q=0, 1, 2…thus, armchair nanotubes are always metallic, where as zig zag nano tubes are metallic if m=3q with q=1, 2, 3...

It is studied the energy band effects on the dispersion relation of surface Plasmon waves in $SWCNT_S$ of metallic character, by using the semi classical kinetic theory of electron dynamics. In comparison with previous investigations [5, 6] that focus on Plasmon wave oscillations in cylindrical electron gas as a simple model of metallic tubes, stress on more exact analysis of geometrical effects, including the radius and chiral angle of the nanotube.

Aim of Study

Energy band effect is applicablre in medical sciences and technology and information.

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Theoritical Study

Now it is assumed that both zig-zag (m, o) 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 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 describes electronic motion in terms of two dynamical variables, namely the electron-density functions. The basic equations in this linear Hydro dynamic model are the equations of motion, the equations of continuity -

$$\frac{\partial u(x,t)}{\partial t} = - n_o \nabla_{11} u(x, t) \qquad (1)$$

No $\frac{\partial u(x,t)}{\partial t} = - \alpha \nabla_{11} n (x, t)\ e \frac{no}{m_{eff}} E_{11}(x,t) - \gamma n_o u(x,t)$ (2)

Where E_{11} (x, t) = E_z e_z + E_ϕ e_ϕ is the tangential component of electro magnetic field, e is the element charge, m_{eff} is the effective mass of the π-electron and $\nabla_{11} = e_z \left(\frac{\partial}{\partial 2}\right) + a^{-1} e_\phi \left(\frac{\partial}{\partial_\phi}\right)$ differentiates only tangentially to the nano tubes surface. In the right hand side of equ. (2), the first term arise from the internal interaction force in the fluid with $\alpha = \left(\frac{v_F^2}{2}\right)$, i.e. the square of the speed of propagation of density disturbances in a uniform 2D homogenous electron fluid. The second term is the force on π-electron fluid due to the tangential component of the electric field, evaluated at the nano tube surface r=r_c and the last term represents the effects of the scattering of the electrons with the positive charge background, where γ being the friction coefficient.

The electric field vector E(x,t) can be expanded in the following Fourier forms as :-

$$E(x,t) = \sum_{m=-r}^{+r} \int_{-x}^{+x} dq\ E_m(r_1, q)\ exp\ [i(m\phi + qz - wt)] \qquad (3)$$

For the TM modes, the field components can be expressed in terms of E_{zm},

$$\frac{1}{r} \frac{d}{dr}\left(r \frac{d}{dr} E_{zm}\right) - \left(K^2 + \frac{m^2}{r^2}\right) E_{zm} = 0, \qquad (4)$$

Where $K^2 = q^2 - W^2/c^2$ and c is velocity of light. The parameter K is a real quantity in the region

$$\frac{W}{q} < c \qquad (5)$$

This means that it is the slow transverse magnetic waves. By eliminating the velocity field u (x, t), one can obtain the following equation from eqns (1) and (2) as :

$$\left(\frac{\partial^2}{\partial t^2} + r\frac{\partial}{\partial t}\right) n(x,t) = \alpha \nabla_{11}^2 n(x,t) + e \frac{n_0}{M_{eff}} \nabla_{11} E_{11}(x,t) \qquad (6)$$

solving eqn. (6) by means of the space-time fourier transforms for the induced density n(x,t) on the cylindrical surface, we find that :

$$n(x,t) = \sum_{m=-r}^{+r} \int_{-x}^{+x} dq\ N_m(q)\ exp.[i\ (m\phi + q_z - w_t] \qquad (7)$$

Where, $N_m = - \frac{i.e.}{\Omega_m} \frac{\eta_o}{m_{eff}} \left(qE_z + \frac{m}{r_c} E\phi\right)$ (8)

and $\Omega m = (\omega + i\gamma)\ \omega - \alpha\ (q^2 + m^2/ r_c^2)$. Now, we use the appropriate boundary condition, we have

$E_{rm}(r_c)\ I_{r>rc}$ - E_{rm} (r_c) $I_{r<rc}$ = $\frac{-e}{\varepsilon_o}$ N_m (9)

Where ε_o is the permittivity of free space and the radial component E_{rm} and the azimuthal component $E_{\phi m}$ of the electric field, are given as :

$$E_{rm}(r) = - i \frac{q}{k^2} \frac{d\ E_{2m}(r)}{dr} \qquad (10)$$

$$E_{\phi m}(r) = \frac{mq}{k^2 r} E_{2m}(r) \qquad (11)$$

On the other hand, the relevant solution of eqn. (5) is :

$E_{1m}(r) = E_{01} K_m(k r_c) I_m(k r)$ $(r < r_c)$ (12)

and $E_{2m}(r) = E_{02} I_m(k r_c) K_m(k r)$ $(r > r_c)$ (13)

Where $I_m(x)$ and $K_m(x)$ are the modified Bersel functions. Substituting eqns. (12) and (13) with boundary condition eqn. (9), by using eqn. (8); for q>> w/c, one can obtain the dispersion equation as:

$$w_r + iw_\gamma = \alpha\left(k^2 + \frac{m^2}{r_c 2}\right) + W_c^2 \left(k^2 + \frac{m^2}{r_c 2}\right) I_m(k_{rc})\ K_m(k_{rc}) \qquad (14)$$

where $\omega_p = (e^2 n_o/\varepsilon_o r_c m_{eff})^{1/2}$ is the eight frequency of the π - electron gas layer in metallic graphine. The solution of eqn. (14) yield complex frequencies $\omega = \omega_{rt} + i\ \omega_i$. It may be observed that the imaginary part ω_i will be given by - $\gamma/2$. In fact, by writing $\omega = \omega_r + i\gamma/2$, the solution for finite damping will be of the form:

$$\omega = \left\{\alpha\left(k^2 + \frac{m^2}{r_c 2}\right) + \omega_p^2 r_c^2 \left(k^2 + \frac{m^2}{r_c 2}\right) I_m(kr_c) K_m(kr_c) - \frac{\gamma^2}{4}\right\}^{1/2} - i\frac{\gamma}{2} \qquad (15)$$

This friction coefficient is the inverse of the electron relaxation timeτ. Using above equation the frequency of lattice vibration can be calculated. Hence the dispersion characteristics of the surface waves in the system are dependent on nano tube geometry, the wave number, the angular momentum, and the friction coefficient. However, it is easy to find that by increasing friction coefficient, the dispersion curves shift to lower frequencies.

The parameter η_o/m_{eff} takes into account the influence of the atomic crystal field. By using the semi-classical model of the π-electron dynamics Migro and Villone obtain the following estimation:-

$$\frac{\eta_0}{m_{eff}} \cong \frac{2v_F}{\pi^2 \hbar} \frac{1}{r_c} \qquad (16)$$

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Where υ_F is the velocity of the electron at the fermi level

$$v_F = \frac{3\upsilon_o\ b_o}{2\hbar}$$

υ_o is a characteristic energy (υ_o = 2.7-3.0ev) of the lattice and it is the Plank's constant; it results that v_F = (0.9-1)x10^6 m/sec. The equation (16) hold good for zig-zag nano tubes with m≅ 3q<60, for arm chair nano tubes with m<50 and for chair vector nano tubes with 2n+m=3q. In the range of validity of eqn. (16) th parameter decreases as the nano tube radius increases.

It is considered that long and short wavelength limits of eqn. (15) for $K_{rc} \to \infty$, by using the well known asymptotic expressions -

$I_m(x) = \frac{e^x}{\sqrt{2\pi x}}$ and $K_m(\chi) = \sqrt{\frac{\pi}{2x}}\ e^{-x}$

with the finite m

The dispersion relation can be written approximately as :

$$\omega^2 = \alpha k^2 + \frac{e^2 v_F}{\xi\pi^2\hbar}\ \frac{K}{r_c} \qquad (17)$$

The right hand side of eqn. (17) depends strongly on the radius of the nano tube.

In the opposite limit $k_{rc} \to o$, 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

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

$Km(x) = \frac{\Gamma(m)}{2}\left(\frac{2}{x}\right)^m$ (for m ≠ 0) and $K_O(x) = \frac{In\ 1.123}{x}$ (for m = 0)

$$\omega\ (m = 0, K \approx 0) \approx \left[\frac{4e^2\ v_F}{\varepsilon_o\pi^2\hbar}\ In\ \left(\frac{1.123}{K_{rc}}\right)\right]^{½} K \quad (18)$$

That is a quasi acoustic mode and for m ≠ 0, then

$$\omega^2 = \frac{\alpha}{r_c^2}\ m^2 + \frac{e^2 v_F}{\varepsilon\pi^2\hbar r_c^2}\ m \qquad (19)$$

This is also quite sensitive to the geometric of the nano tube of graphine. 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.

Table No.1

k (Å^{-1})	ω x10^7 Hz
0.1	1.007
0.2	0.992
0.3	0.983
0.4	0.976
0.5	0.972
0.6	0.967
0.7	0.964
0.8	0.961

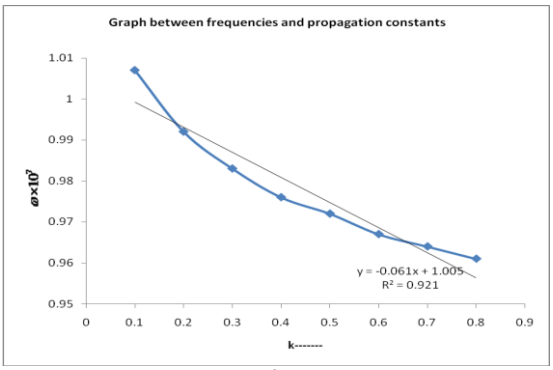

Fig. 1

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=2.459Å and b_0=1.42Å with radius r_c=3.9Å 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 constant.

Table no. 2

k (Å^{-1})	ω x10^7 Hz
0.1	0.9984
0.2	0.9843
0.3	0.9756
0.4	0.9693
0.5	0.9645
0.6	0.9605
0.7	0.9571
0.8	0.9542

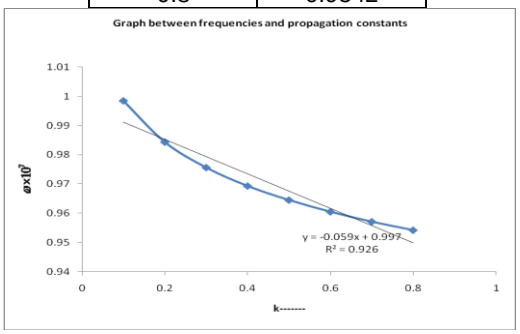

Fig. 2

As seen from above fig. 2 that for zero mode of lattice vibration and for chiral vectors a_0=2.459Å, b_0=1.42Å, radius r_c=5.40Å 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 constant. It is clearly seen that the graph of fig.1 is more linear than fig.2.

Conclusion

A theoretical model based on the classical electrodynamics and hydrodynamic theory is employed to describe the plasmon wave propagation on the surface of the metallic

$SWCNT_S$, where the effect of the energy band structure is taken into account. It has been found that the nanotube geometry play an important role in the dispersion relation of the surface waves, for all values of wavelength. The results obtained make us believe that the hydrodynamical theory in conjection with semiclassical model is available and appropriates for studies of the plasmon wave oscillations in CNT_S , especially for different nanotube geometries.

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