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Theoretical Study of Surface Properties of Polar Semiconductors in Dielectric Medium at Nano Scales

Abstract

Surface Plasma wave (SPW) is sensitive probe of optical properties of cylindrical surfaces of Nanosubstances. The purpose of these reports is to demonstrate the use of SPW to study the reflective, absorptive properties of nano size substances like KF, CsCl and AgCl by deriving the spatial dispersion relation for three modes coupling with the help of computational methods for different radius. This study is important in electronic communication, medical sciences and computer applications.

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Introduction

Localized Plasmon's modes are responsible for the variation of reflective and absorptive properties of substances [1,2] and propagating surface Plasmon's modes in the intersurfaces are the cause of strong angular dependence of the films reflective when measured under specific conditions [3]. Also nano material films shows an enhanced optical transmission due to the excitation of surface Plasmon modes [4]. Carbon nanotubes have remarkable electrical and mechanical properties. Collective electron excitation in a carbon nano tubes can provide important information about their structural and electronic properties. Using electron energy loss spectroscopy, Pichler et al [5] experimentally studied the electron excitations in single walled carbon nanotube and measured the Plasmon energies. In recent years, many experimental and theoretical workers have been done to study high frequencies excitation by Fetter [6] used a simple Hydrodynamic model. Wei and Wang [7] studied the dispersion relation quantum ion acoustic wave oscillations in single walled carbon nanotubes with modified hydrodynamic model which was developed by Hassetal [8, 9]. There are many auther[12-18] who have working on Plasmon intreraction on condenced materials and find various surprising results on Plasmon resonance effects.

Hydrodynamical Model

The modified Bloch's equation for the semiconductor [12] may be written as-

$$m\frac{D\bar{v}}{Dt} = -e\left[\bar{E} + \frac{1}{c}\left(\bar{\nabla}\times\bar{B}\right) - mv\bar{\nabla} - \bar{\nabla}\int_0^{n(\bar{r},t)}\frac{d\rho(n')}{n'}\right] \quad (1)$$

$$\bar{\nabla}\times\bar{B} = \frac{4\pi}{c}\bar{J} + \frac{1}{c}\frac{\partial\bar{D}}{\partial t} \quad (2)$$

$$\frac{\partial n}{\partial t} = -\bar{\nabla}.(n\bar{v}) \quad (3)$$

$$\bar{\nabla}.\bar{E} = \frac{4\pi e}{E}\left[N_+(\bar{r}) - n(\bar{r},t)\right] \quad (4)$$

Equation (1) is the Euler's equation of motion. The operator $\frac{D}{Dt}$ is co-moving time derivative given by-

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + V_x\frac{\partial}{\partial x} + V_y\frac{\partial}{\partial y} + V_z\frac{\partial}{\partial z} \quad (5)$$

Where V_x, V_y and V_z are the components of velocity $\bar{V}(r,t)$ in x, y and z directions respectively. $\frac{Dv}{Dt}$ gives the acceleration of an electron in the fluid and may be written with the help of equation (5) as-

$$\frac{Dv}{Dt} = \frac{\partial v}{\partial t} + (v.\bar{\nabla})v \qquad (6)$$

The first term on the right hand side of equations (1) is force exerted on a free electron by the electromagnetic field which is produced due to the density of fluctuations of the electron gas. The electric and magnetic fields may be written in terms of scalar and vector potential as-

$$\bar{E} = -\bar{\nabla}\Phi - \frac{1}{c}\frac{\partial \bar{A}}{\partial t} \qquad (7)$$

$$\bar{B} = \bar{\nabla} \times \bar{A} \qquad (8)$$

The second term of equation (1) is the restoring force due to the short range interactions with the background i.e. the interaction of the electrons with lattice vibrations. υ Represents the collision frequency and is assumed to be constant. The last term represents the force due to pressure 'P' and an electron in the mass of the fluid. The pressure is taken to be of Fermi type assuming that the electrons are totally free i.e.

$$P(n) = \frac{\hbar^2 (3\pi^2)^{2/3} n^{5/3}}{5m} = \xi n^{5/3} \qquad (9)$$

And
$$\xi = \frac{\hbar^2 (3\pi^2)^{2/3}}{5m} \qquad (10)$$

With these substitutions eqn. (1) reduces to

$$m\frac{\partial \bar{v}}{\partial t} = e\left[\left(\frac{1}{c}\frac{\partial \bar{A}}{\partial t} + \bar{\nabla}\phi\right) - \frac{e}{c} v \times (\bar{\nabla} \times \bar{A}) - m(v.V)v - mvV - \nabla \int_0^{n(r,t)} \frac{d\rho(n')}{n'}\right] \qquad (11)$$

Where 'm' and 'e' represent the mass and charge of a free electron and $n(\bar{r},t)$ is the instantaneous electronic concentration at a position $\bar{r}$.

This coupling SP-SOP mode depends upon frequency and wave vector of carbon and other nano materials on the cylindrical surfaces [10, 11, and 12]. The another derived spatial dispersion relation for three modes coupling (surface Plasmon, polariton and phonon) at cylindrical surfaces at nano size radius is given as-

$$RX_l^{'}(\gamma kr)\left[\varepsilon_\infty(k\omega)\Omega^2 - \varepsilon_0(k\omega)\frac{\omega_t^2}{\omega_p^2}\right] \times$$
$$\bar{\varepsilon}(k\omega)\left[\Omega^2 - \frac{\omega_t^2}{\omega_p^2} - \left(\varepsilon_\infty(k\omega)\Omega^2\right) - \varepsilon_0(k\omega)\frac{\omega_t^2}{\omega_p^2}\Omega^2\right] \times$$
$$y_l(\alpha kR).(RZ_l(\delta kR))^{'} + \left(\Omega^2 - \frac{\omega_t^2}{\omega_p^2}\right)\Omega^2 \varepsilon_B\left[(Ry_l(\alpha kR))^{'} Z_l(\delta kR)\right]$$
$$-\left(\Omega^2 - \frac{\omega_t^2}{\omega_p^2}\right) l^2 \bar{\varepsilon}(k\omega)\varepsilon_B(k\omega) X_l(\gamma kR) y_l(\alpha kR).Z_l(\delta kR) = 0 \qquad (12)$$

Where X_l, Y_l & Z_l are solutions of Bessel's differential equations and X_l^1, Y_l^1 & Z_l^1 are derivatives of X_l, Y_l & Z_l which is function of α, β, γ, δ and radius of cylinders ω_t & ω_p are frequencies of transverse wave (phonons) & Plasmon on the surface of cylinders, Ω is frequency ratio of transverse wave and Polariton waves, ε_0 ε_∞ & ε_B are the dielectric constants for lower frequency, higher frequency and Bulk dielectric medium respectively and $\mathcal{E} = (\mathcal{E}_0 + \varepsilon_\infty)/2$ is average medium between interfaces .Now if radius of cylinder is taken as infinity then eq. (12) become as

$$\Omega^6 \left(\frac{\omega_p}{\omega_t}\right)^2 \varepsilon_\infty - \left[\varepsilon_0 + \left\{\bar{\varepsilon} + (1+\varepsilon_\infty)k^2\right\}\left(\frac{\omega_p}{\omega_t}\right)^2\right]\Omega^4 + \left[\left\{(1+\varepsilon_0) + \bar{\varepsilon}\left(\frac{\omega_p}{\omega_t}\right)^2\right\}k^2 + \bar{\varepsilon}\right]\Omega^2 - \bar{\varepsilon}k^2 = 0 \qquad (13)$$

Eq.(2) is cubic in Ω^2, and when omega vs. k is plotted for different radius , specified conditions are considered by taking ω_t =0 and k→0 ,so that the dispersion relation (13) reduces to :

$$\Omega = \sqrt{\frac{\bar{\varepsilon}}{(1+\varepsilon_\infty)}} \qquad (14)$$

Similarly, the pure surface optical phonon mode is obtained by taking ω_P=0 and k→infinite, so that eq. (13) reduces to:

$$\Omega = \sqrt{\frac{(1+\varepsilon_0)}{(1+\varepsilon_\infty)}\left(\frac{\omega_t}{\omega_p}\right)} \qquad (15)$$

Pure photon mode is obtained by ω_P=0, as well as ω_t =0, and is given by:

$$\Omega = \sqrt{\frac{(1+\varepsilon_\infty)}{\varepsilon_\infty}}k \qquad (16)$$

Table - 1
for AgCl of ω_{sp}/ω_t (radius)

K	R=1Å	R=2 Å	R=4 Å	R=8 Å	R=16 Å
11	0.731606	0.615327	0.320792	0.248437	0.242957
12	1.192797	1.056934	1.001527	0.997161	0.996888
13	1.690038	1.609697	1.598266	1.597522	1.597475
14	2.214776	2.178956	2.175835	2.175640	2.175628
15	2.761879	2.746706	2.745623	2.745556	2.745552
16	3.318774	3.311976	3.311528	3.311150	3.311498
17	3.878741	3.875435	3.875224	3.875211	3.875210
18	4.439395	4.437656	4.437547	4.437540	4.437539
19	4.999995	4.999017	4.998956	4.998953	4.998952
20	5.560347	5.559765	5.559729	5.559727	5.559727

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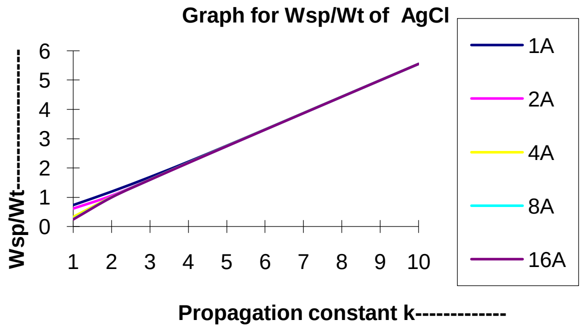


Table 2
For CsCl (radius)

K	R=1Å	R=2 Å	R=4 Å	R=8 Å	R=16 Å
1	0.731606	0.615327	0.320792	0.248437	0.242957
2	1.192797	1.056934	1.001527	0.997161	0.996888
3	1.690038	1.609697	1.598266	1.597522	1.597475
4	2.214776	2.178956	2.175835	2.175640	2.175628
5	2.761879	2.746706	2.745623	2.745556	2.745552
6	3.318774	3.311976	3.311528	3.311150	3.311498
7	3.878741	3.875435	3.875224	3.875211	3.875210
8	4.439395	4.437656	4.437547	4.437540	4.437539
9	4.999995	4.999017	4.998956	4.998953	4.998952
10	5.560347	5.559765	5.559729	5.559727	5.559727

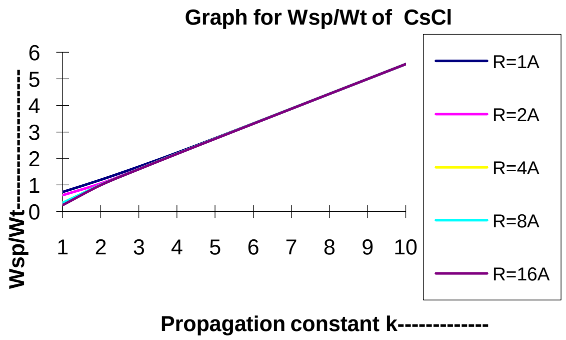
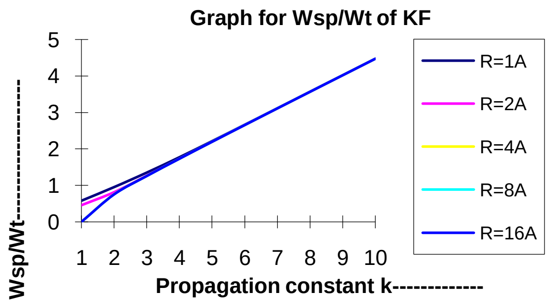


Table - 3
for KF (radius)

K	R=1Å	R=2 Å	R=4 Å	R=8 Å	R=16 Å
1	0.576112	0.458197	-	-	-
2	0.949571	0.814658	0.758192	0.753698	0.753417
3	1.347832	1.268568	1.257262	1.256526	1.256480
4	1.768659	1.733666	1.730612	1.730420	1.730408
5	2.210058	2.195285	2.194229	2.194164	2.194160
6	2.660146	2.653540	2.653105	2.653078	2.653076
7	3.112725	3.109517	3.109312	3.109299	3.109299
8	3.565661	3.563975	3.563869	3.563863	3.563862
9	4.018341	4.017393	4.017334	4.017330	4.017330
10	4.470637	4.470073	4.470038	4.470036	4.470036



Explanation of surface Plasmon frequency (ω_{sp}/ω_t) with respect to propagation constant k for different radius of cylindrical surface of AgCl, CsCl and KF from graphs.

Conclusion

The author observes that –

1. The variation of surface plasmon frequencies(ω_{sp}/ω_t) with respect to propagation constant K for 1 Å is very sharp.
2. For small value of k (1 Å- 2 Å), the frequency has large variation for different radii of surface of CsCl and AgCl.
3. Thus, the surface plasmon frequency is very large for smaller radii R=1 Å and very small for larger radii of surface of CsCl and AgCl.
4. The slope of curve is very large for larger radii R= 16 Å and small for R=1Å.for curved surface of CsCl and AgCl.
5. The variation of (ω_{sp}/ω_t) with respect to K for 2 Å is sharp.
6. For K=1Å, surface Plasmon does not exist above 1Å, as there is no required cluster of Plasmon at the surface.
7. The surface plasmas frequencies vary linearly with k, above 1Å to 16Å vary sharply but surface Plasmon frequency is very large for 1Å and very small for 16Å and above it.
8. The slope of curve is very large for larger value of R=16Å and very small for R=1Å for the surface of KF.

Thus author observe that as radius of curved surface increases the Plasmon frequency decreases in the range (k=1Å- 10Å), for all type of materials CsCl, AgCl and KF. The frequency of surface Plasmon has very small variation in KF compared to CsCl and AgCl with respect to radius and propagation constant. The reason is that KF is not a good conductor and it behaves like semiconductor. This study is important in electronic communication and nanotechnology in Physical world.

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