# **Guided Waves in the Optical Carbon Nanotube Wave Guide**

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#### ABSTRACT

The cylindrical carbon nanotube is an optical wave guide in which the monochromatic guided wave propagates and formulated by Maxwell's wave equations that described by the components of the electric and magnetic fields with different modes. The roots of wave equation are obtained as Bessel's functions that explain the characteristics of guided wave in the carbon nanotube with phase components. The transverse electric and magnetic fields in linearly polarized waves are parallel and orthogonal over cross section. The normalized propagation function is found with the normalized frequency parameters for the lower order of modes. The guided mode as linearly polarized modes of electromagnetic wave with the axial conductivity and the propagation frequency in the carbon nanotube.

Keywords: Caron Nanotube, Maxwell's equation, Bessel's function, Guided wave, Normalize Propagation function.

#### 1. Introduction:

First time the carbon nanotube was discovered on rolling up of graphene i.e., single sheet of graphite [1]. It is formed by CVD method. The structure of carbon nanotubes is discussed in the References [2,4 and 16] that explained about chiral, zigzag, and armchair carbon nanotube, radius of carbon nanotube and metallic characteristics with analyzing propagation of the surface Plasmon wave determined by the numerical results [2].Measuring of optical absorption spectra is investigated with the large absorption bands optically transitions [3]. In energy region, an excitation is of metallic phase experimentally. The optical properties are demonstrated [4] with optical absorption spectra (OAS) using arc method showing the peaks of metallic density of state that explains optical spectra. The density of state peaks split due to a trigonal warping effect for metallic carbon nanotube (MCNT). In (3n, 0) zigzag MCNT, the splitting width is maximum and in armchair MCNT, it is zero.

The polymer coating carbon nanotubes give electromagnetic response at low frequency range up to 10<sup>7</sup> Hz in infrared region that verified by experiment [5]. An application of polymer carbon nanotube is determined with tetra-hertz regime for dielectric that expressed polymer carbon nanotube permittivity. The frequency 3THz is used. The polymer coating single wall carbon nanotube is analyzed with electromagnetic characteristic and dielectric property in 25 Hz to 100 Hz range of frequency. The effective conductivity has been calculated by Waterman – Truell Approach for low frequency peak. The electrical conductivity has been described using the Drude model [6] that associate signal propagation of slow surface wave as the Plasmon resonance experimentally and theoretically.

The electronic structure of carbon nanotubes expressed with quantum optic application. The optical properties of carbon nanotube vary fluorescence energies with equal structure. Nakanishi and Ando studied about optical response of carbon nanotubes for finite length [7] and it is calculated with induced edge charges that excited of Plasmon mode with the wave vector  $Q(=\pi/I)$  in dirty tubes and arise strong electric field due to edge charge.

Using the equivalent multishell approach, the antenna efficiency and characteristics of propagation of electromagnetic waves is expressed for identical finite length metallic carbon nanotube for guided waves with slow – wave coefficients [8]. The theoretically investigation of propagation of electromagnetic wave in the double wall carbon nanotube is described the propagation frequency of electromagnetic wave within material parameter and wave number [9]. Kumar and Shuba have analyzed the symmetric guided wave propagation through finite length multiwalled carbon nanotubes with gold core as the antenna and attenuation coefficient in 10 to 100 GHz frequency range that represents high attenuation of propagation of surface wave [10, 11]. The optical interband didn't occur in the low frequency regime and the guided wave can be propagated in the multiwall carbon nanotube at low or high attenuation with axial surface conductivity depending material characteristics. The plane transverse monochromatic wave propagates through the single walled carbon nanotube as speed of light and is described by Gaussian wave and solution of Helmholtz partial differential equation [12]. Kumar has been also described the behavior of single wall carbon nanotube as wave guide with Helmholtz equation and used the electric hertz potential for propagation of electromagnetic wave through carbon nanotubes [13].

Victor described electromagnetic field in wave guide with Helmholtz equation using spectral parameter power series method and obtains dispersion for wave guide that leads group velocity [9] and propagation

constant by using numerical approach with Fourier transform and found asymptotic formula for TE wave and TM wave [14].

#### 2. Theoretical Methods

## 2.1 Carbon Nanotube (CNT):

Rolled up of graphene sheet called carbon nanotube in cylindrical form behaves as wave guide and that formed by CVD method. The structure of carbon nanotubes described by the chiral vector,  $\vec{C}_h = ma_1 + na_2 \equiv (m, n)$ , and the radius of the tube,  $R_c = \frac{\sqrt{3} b}{2\pi} \sqrt{m^2 + mn + n^2}$ ,  $b = \frac{a}{\sqrt{3}} = 1.42 \text{ A}^\circ$ . It is metallic if |m - n| = 3q, q = 0,1,2,3,...



Figure 1: Graphene structure for armchair, chiral and zigzag carbon nanotubes with chiral vector.

#### 2.2 Optical characteristics:

The optical nature of carbon nanotubes is quasi one-dimensional properties [3, 4] of chiral and it may disappear if carbon nanotubes become larger and larger and used in optical devices. The optical density spectra are represented using the Electric Arc process. The purified nanotube represents the optical absorption at 4.5eV that corresponds to  $\pi$  – Plasmon in loss energy spectrum that is not seen clearly in as – prepared tube.

The axial conductivity described by Antonio and et.al, in an optical range that depends on chirality is given as

$$\sigma_{zz}(\omega) = -\frac{ie^2\omega}{\pi^2\hbar R_c} \left\{ \frac{1}{\omega(\omega + \frac{i}{\tau})} \sum_{s=1}^m \int_{1^{st}BZ}^{\square} \frac{\partial F_c}{\partial p_z} \frac{\partial \epsilon_c}{\partial p_z} dp_z - 2\sum_{s=1}^m \int_{1^{st}BZ}^{\square} \epsilon_c |R_{vc}|^2 \frac{F_c - F_v}{\hbar^2 \omega^2(\omega + \frac{i}{\tau}) - 4\epsilon_c^2} dp_z \right\}$$
(1)

Where, *e* represents electron charge,  $\hbar$  represents normalized Plank's constant,  $p_z$  shows the axial projection of quasi momentum of electron,  $\omega$  is the angular frequency,  $F_c$  and  $F_v$  are the Fermi distribution function that described as  $F(\epsilon^{\pm}) = \frac{1}{e^{\left(\frac{\epsilon^{\pm}}{K_B T_0}\right)_{+1}}}$ ,  $T_o(= 235K)$  shows the absolute temperature. In equation (1), second term

of right side explains the transitions between valence and conductive bands and the interaband motion of  $\pi$ -electrons are described by first term of right side. The optical interband transition [12] does not occur at the low frequency regime. The conductivity,  $\tilde{\sigma}_{zz}$ , may be evaluated for chiral metallic carbon nanotube of radius,  $R_c = \frac{\sqrt{3}mb}{2\pi}$ , as  $\tilde{\sigma}_{zz} = i \frac{3e^2 b \gamma}{\pi^2 h^2 R_c} \frac{1}{\omega + iv}$ , Where, vare collision frequency and equal to  $v_z/\lambda$  and  $\lambda$  being the mean free path of electrons! It is possible that  $\tilde{\sigma}_{zz} \rightarrow \sigma_{\infty}$  when,  $R_c \rightarrow \infty$  or  $m \rightarrow \infty$ . The band gap depending on chirality around the Fermi energy and electric field distribution of finite length CNTs calculated. Many body works on axial conductivity and describes many ways as for chiral, zigzag,  $\left(\tilde{\sigma}_{zz} = i \frac{2\sqrt{3}e^2 \gamma}{m\pi\hbar^2} \frac{1}{\omega + iv}\right)$ , armchair carbon nanotubes etc. and all are based on Boltzmann conductivity. The experimental evidence [7] describes the optical density spectra (ODS) representing the tetra – hertz peaks and Plasmon nature that explained by peak in ODS to lower values for longer carbon nanotubes. If carbon nanotubes are metallic, it contributes in to tetra – hertz peak to antenna or Plasmon resonance. The absorption spectrum of single wall carbon nanotube is for metallic single wall carbon nanotube of the first allowed transition and it shows the peak at 650nm for metallic carbon nanotube. The frequency dependence [5] optical density spectra and conductivity are with peaks of tetra – hertz.

#### 2.3 Numerical Approach:

We have the standard form of Maxwell's equations given as  $\nabla^2 \vec{E} = \mu \varepsilon \frac{\delta^2 \vec{E}}{\delta t^2}$ 

$$\nabla^2 \vec{H} = \mu \varepsilon \frac{\delta^2 \vec{H}}{\delta t^2} \tag{3}$$

Let us consider the cylindrical co-ordinate system  $(r, \phi, z)$  and the z-axis is along the axis of the carbon nanotube waveguide. The cylindrical co-ordinates are expressed with the Cartesian co-ordinates shown in Figure 2.



Figure 2: Cylindrical co-ordinate of carbon nanotube (CNT) with Cartesian co-ordinate.

The wave equation is expressed as

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$$\frac{\delta^2 E_Z}{\delta r^2} + \frac{1}{r} \frac{\delta E_Z}{\delta r} + \frac{1}{r^2} \frac{\delta^2 E_Z}{\delta \phi^2} + k_c^2 E_Z = 0$$
(4)

And 
$$\frac{\delta^2 H_Z}{\delta r^2} + \frac{1}{r} \frac{\delta H_Z}{\delta r} + \frac{1}{r^2} \frac{\delta^2 H_Z}{\delta \phi^2} + k_c^2 H_Z = 0$$
(5)

Where,  $k_c^2 = \omega^2 \mu \varepsilon - \beta^2 = k^2 - \beta^2$  and  $k^2 = \omega^2 \mu \varepsilon$ . These equations are obtained by taking the z-component of wave equations (2) and (3) and replacing  $\delta^2 / \delta t^2$  and  $\delta^2 / \delta z^2$  operator by  $-\omega^2$  and  $-\beta^2$  respectively. The roots of equations (4) and (5) for plane monochromatic wave [14] expressed as  $E_z = e^{i\vec{k}\cdot\vec{r}}\hat{e}_z$  and  $H_z = e^{i\vec{k}\cdot\vec{r}}\hat{e}_z$ that give the characteristic of transverse wave propagating through the carbon nanotube. The electromagnetic wave is confined within a cylindrical metallic carbon nanotube wave guide and it propagates either in TM or TE mode. In TE and TM modes, the electric field vector and the magnetic field vector lies in transverse plane i.e., right angle to the z-direction. Under this condition, we have two things, first  $E_z = 0$  that  $H_z$  is finite and second  $H_z = 0$  that  $E_z$  is finite. We have the complete solution of equation (4) and (5) expressed as

$$E_z = [PJ_n(k_c r) + QK_n(k_c r)]Fe^{in\phi}$$
(6)

And 
$$H_z = [LJ_n(k_c r) + MK_n(k_c r)]Fe^{in\phi}$$
(7)

Here, *F*, *P*, *Q*, *L* and *M* are all arbitrary constants.  $J_n(k_c r)$  is the Bessel's function and  $K_n(k_c r)$  is the modified Bessel's function that all infinite at origin (r = 0). The functions  $J_n(k_c r)$  and  $K_n(k_c r)$  are with  $k_c r$  for the value of n = 0, 1, 2, 3, .... The arbitrary constant *Q* and *M* must be equal to zero if  $E_z$  and  $H_z$  is finite at (r = 0). Now we use the common designation  $J_n(ur)$  and  $E_z$  and  $H_z$  including phase components expressed as

$$E_z = A_1 J_n(ur) e^{jn\phi} e^{j(\omega t - \beta z)}$$
(8)

And 
$$H_z = B_1 J_n(ur) e^{jn\phi} e^{j(\omega t - \beta z)}$$
(9)

Where,  $A_1 = PF$ ,  $B_1 = LF$  and  $ur = k_c r$ . The Eigen value equation for  $\beta$  expressed as

$$(I_n + K_n)(K_1^2 I_n + K_2^2 K_n) = \left(\frac{\beta n}{r}\right)^2 \left(\frac{1}{u^2} + \frac{1}{s^2}\right)^2$$
(10)

Where,  $I_n = \frac{J'_n(ur)}{uJ_n(ur)}$  and  $K_n = K'_n = \frac{K'_n(sr)}{sK_n(sr)}$ . The discrete values of  $\beta$  restricted to the range  $K_2 \le \beta \le K_1$ . The modified second kind Bessel function  $K_n(sr)$  for large values of r is given as  $K_n(sr) = \frac{e^{-sr}}{\sqrt{sr}}$  and  $K_n(sr) \to 0$  as  $sr \to \infty$  provides s is a positive real quantity. The right side of equation (10) vanishes and we have

$$I_0 + K_0 = 0 (11)$$

And 
$$\frac{J'_a(ur)}{uJ_0(ur)} + \frac{K'_n(sr)}{sK_0(sr)} = 0$$
 (11a)

Again  $J'_0(ur) = -J_1(ur)$  and  $K'_0(sr) = -K_1(sr)$  so,

$$\frac{J_1(ur)}{uJ_0(ur)} + \frac{K_1(sr)}{sK_0(sr)} = 0$$
(12)

That corresponds to transverse magnetic mode TM<sub>op</sub> (E<sub>z</sub>=0) and

$$K_1^2 I_0 + K_2^2 K_0^2 = 0 (13)$$

Or, 
$$\frac{K_1^2 J_1(ur)}{u J_0(ur)} + \frac{K_2^2 K_1(sr)}{s K_0(sr)} = 0$$
 (14)

That corresponds to transverse electric mode  $TE_{op}$  (H<sub>z</sub>=0). The parameter associated with the cutoff condition and referred to V-number or V-parameter is given as

$$V^2 = r^2(u^2 + s^2) \tag{15}$$

The number of modes exists in waveguide function of V that represented by the normalized propagation function 'b' from equation (15) as

$$\frac{V^2 - r^2 u^2}{V^2} = \frac{r^2 s^2}{V^2} = b \tag{16}$$

The V – parameter is related to number of modes M expressed as  $M = \frac{v^2}{2}$ . The mode (n, p) is derived by adding (n – 1) and (n + 1) solutions in the core given by

$$E_{z} = E_{0}\{J_{n-1}(ur)\cos(n-1)\phi + J_{n+1}(ur)\cos(n+1)\phi\}$$
(17)

$$H_{z} = H_{0}\{J_{n-1}(ur)\cos(n-1)\phi + J_{n+1}(ur)\cos(n+1)\phi\}$$
(18)

So, the Bessel function as

$$J_{n-1}(ur) + J_{n+1}(ur) = \frac{2n}{ur} J_n(ur)$$
(19)

From equation (17) and (18) we have

$$\frac{H_z}{E_z} = \frac{H_0}{E_0} \tag{20}$$

We know the amplitude of E and B as  $\frac{B_0}{E_0} = \sqrt{\epsilon \mu \sqrt{1 + \left(\frac{\sigma}{\epsilon \omega}\right)^2}}$  then we can calculate  $\frac{H_z}{E_z}$  as

$$\left(\frac{H_z}{E_z}\right)^4 = \left(\frac{\mu}{\mu_0^2}\right)^2 \left\{\varepsilon + \left(\frac{\sigma}{\omega}\right)^2\right\}$$
(21)

The frequency of propagation of electromagnetic wave,  $\omega$ , is calculated by the relationship for m = 0, and m  $\neq$  0 respectively and may written as

$$\omega^2 = \frac{4e^2 v_F}{\varepsilon_0 \pi^2 \hbar} \ln\left(\frac{1.123}{kR_c}\right) k \tag{22}$$

And

# $\omega = \frac{1}{R_c} \sqrt{m \left( \alpha \, m + \frac{e^2 v_F}{\varepsilon_0 \pi^2 \hbar} \right)} \tag{23}$

# 3. Results and Discussion:

The guided electromagnetic energy travels in carbon nanotube waveguide if mode is away from cutoff frequency. The electromagnetic field patterns and propagation constant for modes are similar. For (n, p) = (0, 1) and (2, 1), the differences with pair modes  $TE_{01}$  and  $TM_{01}$  reduces to zero i.e., limit of weakly guiding shown in Figure 3. We have found that the components of longitudinal field as  $E_z$  and  $H_z$  are smaller than that

of the main transverse components of the guided wave solutions. Transverse electric and magnetic fields are parallel and orthogonal over cross-section in the linearly polarized (LP) modes ( $LP_{11} = TE_{01}, TM_{01}$ ) of waves.



Figure 3: Corresponding modes TE and TM in CNT waveguide with linearly polarized modes (LP).

There are equivalent roots with the reversed field polarities for each LP modes with degenerate solutions. The weak guide approximation relative to the boundary condition given as

$$u_{np}\frac{J_{n-1}(u_{np}r)}{J_n(u_{np}r)} = -s_{np}\frac{s_{n-1}(s_{np}r)}{s_n(s_{np}r)}$$
(24)

So, we have  $u_{np}$  and  $s_{np}$  with numerical solution and  $\beta_{np}$  for guided mode may be determined.

The variation between  $\left(\frac{H_z}{E_z}\right)^2$  and  $\left(\frac{\sigma}{\omega}\right)$  is parabola shown in Figure 4 and represents increasing the fields or conductivity. The quasi transverse structures of electromagnetic guided waves are characterized with low attenuation.



Figure 4: Plot the square of fraction of magnetic field and electric field along z – direction to the fraction of conductivity and propagation frequency. As soon as increasing the  $\left(\frac{\sigma}{\omega}\right)$ ,  $\left(\frac{H_z}{E_z}\right)^2$  will increase. Therefore, the electromagnetic field depends on the conductivity as well as propagation frequency.

Equation (22) is quasi-acoustic mode and equation (23) is sensitive for geometry of nanotube and they represent when R<sub>c</sub> increases,  $\omega$  decreases see Figure 5. The parameter k in region  $\omega/q < c$  (speed of light),  $k^2 = q^2 - \omega^2/c^2$  it means we have the slow TM wave. Consider  $\omega = vq$  and we have the speed lines of the three electron beams expressed by Figure 6. We have maximum phase and group velocity for the maximum propagation frequency and vice-versa by the expression,  $v_p = v_g = \frac{\delta \omega}{\delta k}$  and  $v_p \cdot v_g = v^2$ .



Figure 5: Variation of propagation frequency,  $\omega$ , with the radius, R<sub>c</sub>, of carbon nanotube.



Figure 6: The velocity of electron beams in different CNTs for m = 0 (a), 1(b). As increasing the electromagnetic wave frequency, decreasing the radial penetration depth for TM surface. The range of velocities is  $0.93 \times 10^6$  to  $4 \times 10^6$  m/s [2].

The propagation function 'b' as a function of 'V' for the lower order of modes is shown in Figure7. All modes can exist for values of 'V' that exceeds the limit value. The value of V(ur) = 2.405 is the first root lower order Bessel function  $J_0(ur) = 0$ . If  $V \le 2.4$  as 2.356 for wavelength = 0.8µm, the propagation is possible. So, the guided wave can propagate through optical carbon nanotube wave guide.



Figure 7: b – the normalized propagation function as the function of V – parameter and the curves of  $TE_{0p}$ and  $TM_{0p}$  modes for (0,1).

# 4. Conclusions:

We have discussed about the guided waves in the optical carbon nanotube wave guide. The optical characteristics of carbon nanotube are described by optical density spectra and optical range of axial conductivity. The roots of Maxwell's equations for cylindrical carbon nanotube have been given the Bessel's functions that explain the nature of propagation of electromagnetic waves in TE and TM modes in carbon nanotube as guided waves. We have found the normalized propagation function 'b' and the number of modes within V – parameter. Both the electric and magnetic fields are parallel and orthogonal in linearly polarized waves showing by Cartesian components. The variations of square of fraction of magnetic field and electric field along z – direction are to the fraction of axial conductivity and the propagation frequency. The electromagnetic wave is higher. As increasing the radius of carbon nanotube, decreasing the propagation frequency i.e., for small radius, we have found the higher frequency. The velocity of electron beam in optical carbon nanotube wave guide is of range  $10^6$ .

As results, the guided waves in optical carbon nanotube wave guide is verified by normalized propagation function with V – parameter and described by Bessel's function and orthogonal linearly polarized wave in TE and TM modes. The velocity of guided wave is explained with phase velocity and group velocity as the speed of electron beam in carbon nanotube wave guide with the electromagnetic propagation frequency. So, we have maximum phase and group velocity for the maximum propagation frequency and vice-versa. We have concluded that the electromagnetic wave travels with maximum velocity and maximum frequency through the small radius carbon nanotube wave guide.

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