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Consequence of Quantum Confinement of Electrons in Carbon Nano Tubes

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ABSTRACT:

The distinction of Nano materials with other bulk materials lies in dimensionality of the systems. For instance, we cite the field of carbon nano tubes and other nano materials have in recent days been a promising and emerging area of research due to its dimensionality .When the particular dimension of a bulk matter is comparable or smaller than de-Broglie wave length of the electron, and then electrons and holes are confined along this direction. As a result of the quantum confinement in conducting nano tubes, on solving Schrödinger equation for one dimensional square potential well of infinite depth, we will have quantized result for electronic energy with which we can show size dependent drift velocity and current density with which we can show size dependent kinetic energy and de-Broglie wave length of the electron.

KEYWORDS: CNT, de-Broglie Wavelength, Heisenberg uncertainty, Potential well, quantum well.

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INTRODUCTION:

It has been so far found See, for instance ref [1,2] electrical and mechanical properties of carbon nano tubes depend on the structure of carbon nano tubes. When CNT is extremely narrow (Thin) *i.e* for a very thin carbon Nano conductor for which $A^{1/2} << L$ [1]where the diameter of the tube is a few nano meter. Heisenberg uncertainty principle tells us that if we confine a particle of mass m to a very small region of length say ΔZ, then we may introduce its uncertainty in its momentum [3] $\Delta P_Z \approx \frac{h}{\Delta Z}$,the confinement of the electron in the Z direction thus introduces additional kinetic energy of magnitude

$$E_{Con} \approx \frac{(P_Z)^2}{2m} \frac{\hbar^2}{2m(\Delta Z)^2} \geq \frac{1}{2} K_B T \text{ -----------(i)}$$

K_B is Boltzman constant

Equation (i) gives us the idea that size dependent quantum confinement effect will be important if

$$\Delta Z \approx \sqrt{\frac{\hbar^2}{mK_B T}} = \sqrt{\frac{4\hbar^2}{m^2 v^2}} = \frac{2h}{2\pi mv} \square \frac{h}{\pi p_z} \text{ ....(ii)}$$

But, $$\lambda_{d.B} = \frac{h}{P} \therefore \Delta Z \approx \lambda_{d,B} \text{ ....(iii)}$$

Then the de-Broglie wave length of the electrons may be assumed to be comparable with the diameter,*i.e* $\lambda_{d.B} \approx d$ hence energy associated with transverse dimension is quantized [3] due to the quantum confinement of the electrons. Well, we start with an ideal one dimensional potential well of infinite depth and of length 'L',in which eletron moves almost freely *i.e*

Assuming infinite depth of the well, then the well known unnormalized wave function

$$\psi_n(x) = A\text{Sin}\frac{n\pi x}{L}, \quad n = 1,2,3............$$

In deriving the result total quantized energy we could normalise the wave function of the electron by solving the schroodinger wave equation, which for an electron turns out to be

$$\psi_n(x) = \sqrt{\frac{2}{L}}\,\text{Sin}(\frac{n\pi x}{L}), \quad n = 1,2,3........$$

Hence , the total quantized energy is given by[4, 5]

$$E_n = \frac{n^2 h^2}{8mL^2} \text{----------------(iv)}$$

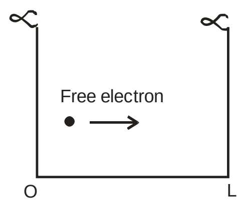

Figure-01

Now, since the electron spatial density in the nano tube varies directly with the probability density of the electron, that is we can write $N_\rho(x) = C\sum_{1}^{N_0} \left|\psi_{n_i}\right|^2$,

Velocity of the electron $v_n = \frac{nh}{2ml}$ ---------------------*(v)*

Note the carbon nano tubes with armchair wrapping have been produced so far which exhibit metallic or conducting nature with helicity indices *(m,n) with m=n* or m-n/3 is an integer

Introducing transit time of the electron in nano tube[6] $\tau_n = \int_0^L \frac{dX}{V_n} = \frac{L}{v_n}$

$$\tau_n = 2m\frac{L^2}{nh} - - - - \text{-(vi)}$$

With the aid of equation (2), (3) & (4) it has been so far established theoretically

$$\sigma_n = \frac{2Le^2}{Anh} \text{……………………….(vii)}$$

MATERIALS AND METHODS:

For dealing with our problem we consider previous model[5] of CNT with the one dimensional approach of carbon nano tubes in which electron is within the well of infinite depth ,so that electron is completely free to to move within the well .That means electron is confined from transverse directions in the tube that results in the quantized nature of the total energy[1].Hence one dimensional box model with single electron constitute the starting point for fruitful approach to find the quantized drift velocity and current density. Then, we theoretically simulate the kinetic energy and de-Broglie wave length of the electron.

Theory: Kinetic energy of the electron $K.E = \frac{1}{2} m v_d^{\,2}$, where v_d is the drift velocity of the electron. To calculate the drift velocity we approach semi classically as follows keeping in mind that the short time for which an electron get accelerated before it under goes a collision is called relaxation time According to free electron model, the electron in a solid move freely. If free time *i.e* time taken between two successive collision be $'\boldsymbol{\tau}'$, $\boldsymbol{mean}$ then, $\boldsymbol{\tau} = \frac{\boldsymbol{\lambda}}{\boldsymbol{v}}$ [5,6] If the applied field on electron of charge $\boldsymbol{-e}$ is $'\vec{\boldsymbol{E}}'$, $\boldsymbol{then\ the\ equation\ of\ motion\ of\ the}$ electron

$$-e\,\vec{E} = m\frac{d^2x}{dt^2}$$

Integrating the above equation, taking magnitude only

, C is the constant of integration

When $'t' = \tau$ then $v = v_{max}$

. *At* $t=0$, $C=0$ as $\dot{x}_0 = 0$, Maximum velocity of electron corresponds to a time duration $'\tau'$[7] as the electron start with a fresh velocity after a collision. since the electron moves with uniform acceleration

$$v_{\max} = \dot{x}_{\max} = e\frac{E}{m}\tau$$

For simplicity this maximum velocity is taken as drift velocity of the electron. If an electron having initial random thermal velocity $\boldsymbol{u_1}$ (Bold letters indicate vectors) get accelerated for a time τ_1,then it will attain a velocity $\boldsymbol{v_1}$,

$$K.E = \frac{1}{2} m v^2{}_d = \frac{1}{2} m\left(\frac{eE}{m}\tau\right)^2 = \frac{1}{2}\frac{(eE\tau)^2}{m}$$

$$= \frac{1}{2}\frac{(eV_{P.D}\tau)^2}{mL^2}$$

$$\mathrm{Since}, \tau_n = \frac{2mL^2}{nh} \therefore K.E == \frac{1}{2}\frac{(eV_{P.D}\,2mL^2)^2}{mn^2h^2L^2} = \frac{2me^2V^2{}_{P.D}L^2}{n^2h^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(viii)$$

Therefore, it is clear that kinetic energy of the electron varies as the square of the quantum state of the electron as a result of its quantum confinement This expression is found to be apparently independent of the area of cross section . However, if drift velocity somehow depends on area of cross section of the tube then obviously kinetic energy is size dependent drift velocity

However, on substituting the size dependent drift velocity[9] in the expression of K.E, we have

$$K.E = \frac{1}{2}mv^2{}_d = \frac{1}{2}m(\frac{V_{P.D}e}{AnhN_n})^2 = \frac{1}{2}m\frac{V^2{}_{PD}e^2}{A^2n^2h^2N^2{}_n} \text{……………………….}(ix)$$

In both the above case we could see $K.E \infty \frac{1}{n^2}$

Since the quantum state depends on the the temperature in CNTs and varies almost linearly in case of ideal one dimensional CNTs, hence it is reasonable to argue that K.E varies almost inversely as the square of the temperature [8,9] That amounts that rise of temperature rapidly decreases the kinetic energy of the electrons in the carbon nano tubes. This results in the reduction of the magnitude of the drift velocity and hence the mean free path decreases.

At this juncture we are a bit interested in estimating the de-Broglie Wave length of the electrons which can be found by using quantum relation

$$\lambda_{d.B} = \frac{h}{mv_d} = \frac{h}{\sqrt{2mK.E}} = \frac{h}{\sqrt{2m\frac{1}{2}m\frac{V^2{}_{PD}e^2}{A^2n^2h^2N^2{}_n}}}$$

$$\lambda_{d.B} = \frac{AnN_nh}{\sqrt{m^2e^2V^2{}_{P.D}}} = \frac{AnhN_n}{meV_{PD}} \text{...}(x)$$

$$\lambda_{d.B}\alpha\ A\ ,\ \lambda_{d.B}\alpha\ n\ ,\ ,\ \lambda_{d.B}\alpha\ N_n$$

$$\lambda_{dB}\alpha\frac{1}{V_{PD}}$$

CONCLUSION

The expression of drift velocity used so far is supposed and expected to be consistent as on using the given expression of drift velocity one may likely achieve current density for n=1(ground state) to be 10^8A/cm^2 for a radius of tube of 15 nm ,with applied voltage of 6 volt which is almost very close to the citation of group of researcher S.Frank[4] and discovered to be 10^7 A/cm^2 .Therefore our findings are more likely be consistent and reliable under defined condition which yield that the that kinetic energy of the electron varies as the square of the quantum state of the electron and hence kinetic energy of the electron of the electrons in the carbon nano tubes. This results in the reduction of the magnitude of the drift velocity as the quantum state rises and hence the mean free path decreases. Further as result of quantum motion of electrons , we find that de-Broglie wave length of the electron varies linearly with the area of the cross section of the tube and the quantum state of the electron. Thus we may expect in case of 1 DCNTs , de-Broglie wave length of electrons depends on the temperature and might vary linearly if $n \infty T$

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