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ANALYTICAL COMPUTATION OF BAND STRUCTURE AND DENSITY OF STATES OF ZIGZAG SINGLE-WALL CARBON NANOTUBE FOR DIFFERENT STRUCTURAL PARAMETERS

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ABSTRACT
Band structure and electron density of states of single-wall zigzag carbon nanotube are analytically computed using nearest neighbor tight binding (NNTB) approximation and theory of linear combination of atomic orbitals (LCAO). DOS is calculated by varying cylindrical dimension, lattice index and neighboring atomic distance. Results show that magnitude of peak of DOS increases with decreasing radius of the tube, lowering bandgap and decreasing of nearest neighbor distance. Wave-vector dependent Hamiltonian is calculated by solving time-independent Schrödinger equation to study band structure. Bandgap is also computed for the two lowest modes only as a function of nearest neighbor distance for different semiconducting tubes. With increase of distance between neighboring atoms and decreasing lattice index, bandgap of semiconducting nanotube linearly increases. For higher order mode, bandgap increases with significant rate compared to the lowest mode. Results can be utilized in developing zigzag CNT-based devices and circuits.
Keywords: Zigzag nanotube, Nearest neighbor tight binding approximation, Linear combination of atomic orbitals, Density of states, Band structure, Wave-vector dependent Hamiltonian

I. INTRODUCTION

Band structure and density of states of a quantum structure are the fundamental properties in describing the electrical characteristics of the devices based on the nanostructure, and henceforth near-accurate computation of these properties is performed by several theoretical researchers over the last two decades for various low-dimensional structures. Carbon nanotube is one promising candidate in this area which provides unique opportunity where computational approaches on atomistic based modeling can be verified exactly with experimental results [1], paving the way of accurate device design [2]. Since the invention of CNT [3], significant progress is achieved to understand physics of the device and their possible applications in electronic [4-5] and photonic [6] domains. Single [7] and multi-wall [8] nanotubes are already experimentally made, among which SWCNT is already preferred due to their enhanced stability

[9]. Armchair and zigzag are the two types thoroughly investigated [10-11] in the last decade with different geometrical parameters, and various numerical approaches are used [12-14] to study the basic device physics. Different materials other than carbon [15-16] are also used by experimental researchers to explore novel properties for various electronic applications.

Density of states profile of carbon nanotube has a set of peaks, which is symmetric w.r.t Fermi level [17]. This is verified by several experimental techniques [18-20], which provides the dependency of DOS and band structure on wave-vector. In this paper, DOS and band structure are analytically calculated using nearest neighbor tight binding approximation and theory of linear combination of atomic orbitals as function of circular periodicity, lattice index and nearest neighbor distance. Time-independent Schrödinger equation is solved for estimating wave-vector dependent Hamiltonian, and from the results, bandgap is computed for two lowest order modes. Results are important for designing zigzag SWCNT-based transistors.

II. MATHEMATICAL MODELING

Using tight binding approximation for two identical points, Bloch theorem is applicable which can be written as:

$$\psi(\vec{r}+\vec{R}) = \exp(\vec{k}.\vec{r})\psi(\vec{r}) \ . \tag{1}$$

Wave function satisfies Bloch theorem can be written as

$$\psi_j(k.\vec{r}) = \frac{1}{N}\sum_{\vec{R}}^{N} \exp(\vec{k}.\vec{r})\psi_j(\vec{r}-\vec{R}) \ . \tag{2}$$

According to the theory of LCAO, total wave-function of the molecule is given by

$$|\psi_{mol}>=\sum_k C_k|\psi_{atom} \ . \tag{3}$$

Then the usual Hamiltonian eigen equation

$$H\psi = E\psi \tag{4}$$

can be written in the following manner

$$(H-OE)\psi = 0 \ . \tag{5}$$

where ‘O’ is the overlap matrix. In order to calculate eigen values, we consider that the levels involving 2s, $2p_x$, $2p_y$ orbitals are decoupled from those involving $2p_z$ orbitals and they are far away from Fermi energy [21], so conduction and valence bands are formed due to $2p_z$ orbitals. Henceforth, electrons in the π bonds contribute to the conductance of CNT, so the dispersion relation can be determined by only considering these electrons into calculation using NNTB approximation.

Considering one $2p_z$ orbital per carbon atom, resultant matrix can be written as

$$h(k)=\begin{bmatrix}0 & -t\\ -t & 0\end{bmatrix}+\begin{bmatrix}0 & -t\exp(i\vec{k}.\vec{a}_1)\\ 0 & 0\end{bmatrix}+\begin{bmatrix}0 & -t\exp(i\vec{k}.\vec{a}_2)\\ 0 & 0\end{bmatrix}+\begin{bmatrix}0 & 0\\ -t\exp(i\vec{k}.\vec{a}_1) & 0\end{bmatrix}+\begin{bmatrix}0 & 0\\ -t\exp(i\vec{k}.\vec{a}_2) & 0\end{bmatrix} \quad (6)$$

where '*t*' is the distance between the matrix elements of neighboring C atoms, a_1 and a_2 are lattice vectors corresponding to lattice indices '*m*' and '*n*'. h(k) is the 2×2 matrix which is written down by summing over any unit cell and all its four neighboring unit cells. Henceforth, h(k) may be re-written as

$$h(k)=\begin{bmatrix}0 & h_0\\ h_0 & 0\end{bmatrix} \quad (7)$$

where

$$h_0=-t[1+\exp(i\vec{k}.\vec{a}_1)+\exp(i\vec{k}.\vec{a}_2)] \quad (8)$$

h_0 is the element of h(k) matrix. Every point on a periodic lattice formed by unit cell can be described by a set of integers (p,q,r) where

$R=p\vec{a}_1+q\vec{a}_2+r\vec{a}_3$

with $\vec{a}_1=\hat{x}a+\hat{y}b$, $\vec{a}_2=\hat{x}a-\hat{y}b$, $\vec{a}_3=\hat{z}c$

where $a=\frac{\sqrt{3}a_0}{2}$, $b=\frac{\sqrt{3}b_0}{2}$.

The expression of energy can be written in the following form

$$E(k)=\pm|h_0|=\pm|t|\sqrt{1+4\cos k_y b_0\cos k_x a_0+4\cos 2k_y b_0} \quad (9)$$

where we considered a nanotube with circumferential vector along the Y-direction, so that we can write the magnitude of the vector as $2bkm\hat{y}$. Due to the periodic boundary condition, allowed k-values which are perpendicular to kx axis is $2\pi\nu$ for νth subband. Hence, we can equate them as

$2bmk\,\hat{y}=2\pi\upsilon\,\hat{y}$

which gives

$$k=\frac{\pi\upsilon}{bm} \quad (10)$$

where $3\upsilon=(m-n)$, *m* and *n* are the lattice indices. Using this relation, expression of energy as a function of momentum vector may be written in the following form

$$E(k) = \pm \frac{3ta_0}{2} \sqrt{k_x^{\,2} + \left[\frac{2\pi}{3b} \left(\frac{3\upsilon}{2m} - 1 \right) \right]^2} \quad . \tag{11}$$

Density of states contributed by the lowest subband of metallic CNT is given by

$$D(E) = 2 \times 2 \times \frac{1}{L} \sum_{k_t} \delta[E - E(\Delta k_t)] = \frac{8}{3\pi a_0 t} \quad . \tag{12}$$

Density of states contributed by the lowest subband of semiconducting CNT is given by

$$D(E) = 2 \times 2 \times \frac{1}{L} \sum_{k_t} \delta[E - E(\Delta k_t)] = \frac{8}{3\pi a_c t} \frac{E}{\sqrt{E^2 - (E_\upsilon / 2)^2}} \Theta(|E| - (E_\upsilon / 2)) \tag{13}$$

here E_v is the energy of v^{th} subband.

III. RESULTS AND DISCUSSION

Using Eq. (12) and Eq. (13), density of states function of zigzag SWCNT is computed and plotted as a function of energy with various geometrical parameters. Fig 1 shows the DOS profile with three different values of lattice index. From the plot, it may be seen that for when the lattice index (*m*) becomes a multiple of three (3), magnitude of the peaks increases. This is due to the fact that the criterion gives metallic character, for which conductivity increases rapidly. With decrease of '*m*', magnitude of peak sharply decreases which speaks for its semiconducting behavior. When comparative study is made between two semiconducting nanotube, it is observed that position of peak shifts left for higher conductivity. This speaks in favor of low bias application. Also number of peaks decreases when metallic property is exhibited.

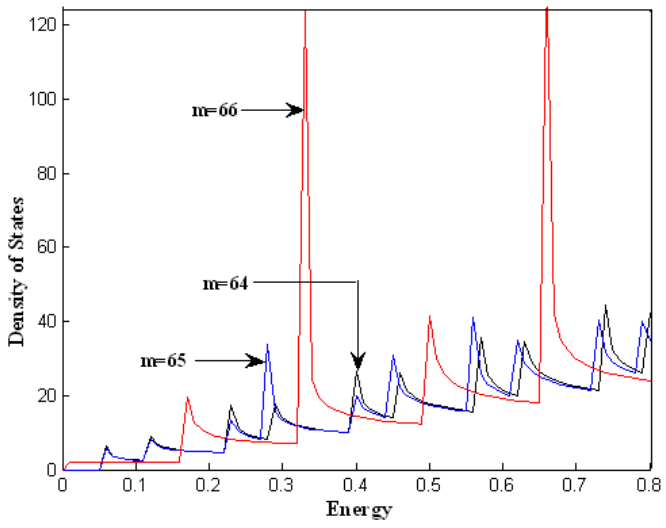

Fig 1: Density of states with energy for zigzag CNT with three different lattice indices having 0.1 nm radius

By varying the radius of the nanotube, it is observed that density of states increases with decreasing dimension. This is plotted in Fig 2. This is due to the fact that with increasing diameter, quantum confinement decreases, which reduces DOS. But because of the periodicity of

the structure, position of the peak remains unchanged with changing dimension. Relative magnitude of the peak may better be observed with higher energy value.

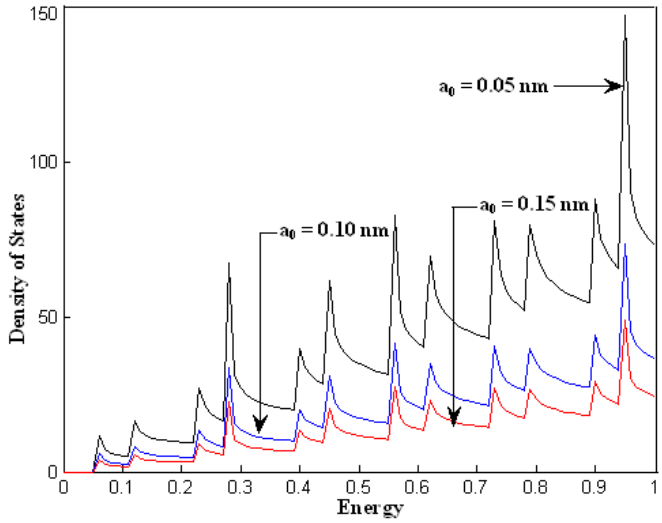

Fig 2: Density of states with energy for zigzag semiconducting carbon nanotube with three different radii

For metallic and semiconducting nanotubes, propagation vector is plotted with energy for both along X and Y axes. In Fig 3, band structure may be visualized because for m=66 (metallic), there exists no energy gap, whereas for semiconducting nanotube, bandgap exists. The plot is made for lowest subband only to understand the conductivity. By varying the nearest neighbor distance, propagation vector along Y axis is computed and plotted as a function of energy, shown in Fig 4. Symmetric nature is maintained throughout the energy spectrum, but the energy gap increases at the center with increase of atomic distance.

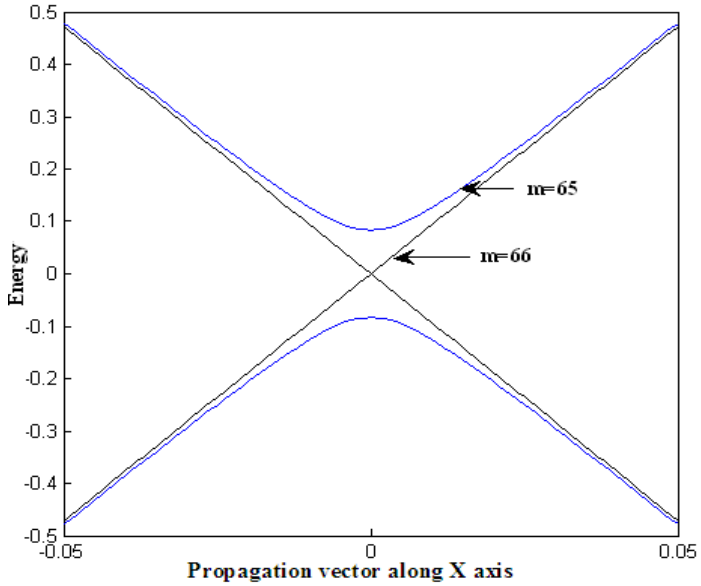

Fig 3: Band structure for lowest subband of metallic and semiconducting carbon nanotube

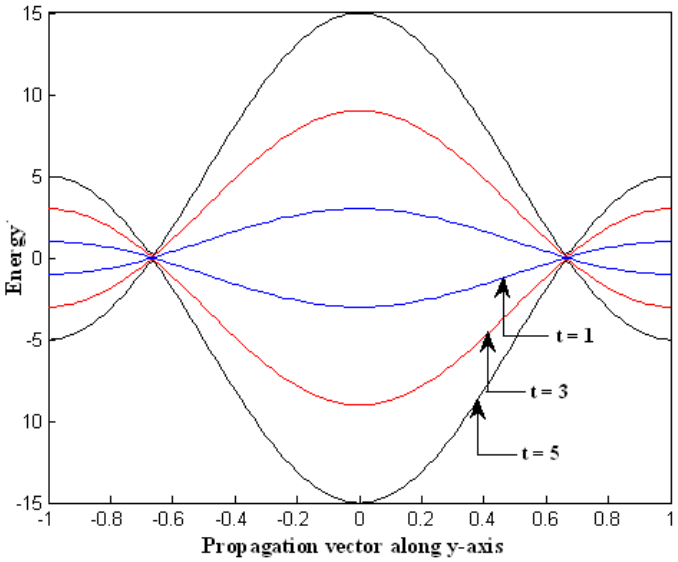

Fig 4: Band structure for semiconducting nanotube with radius 0.1 nm for different values of matrix elements between neighboring carbon atoms

Density of states is also plotted with energy for different nearest neighbor distance, shown in Fig 5. From the plot, it may be seen that with increasing distance, magnitude of peaks decreases. This is because closed packed unit cell provides better confinement. This computation is possible for NNTB approximation. Also due to the closeness, number of peaks increases according to the theory of LCAO. Henceforth, choice of technique is justified.

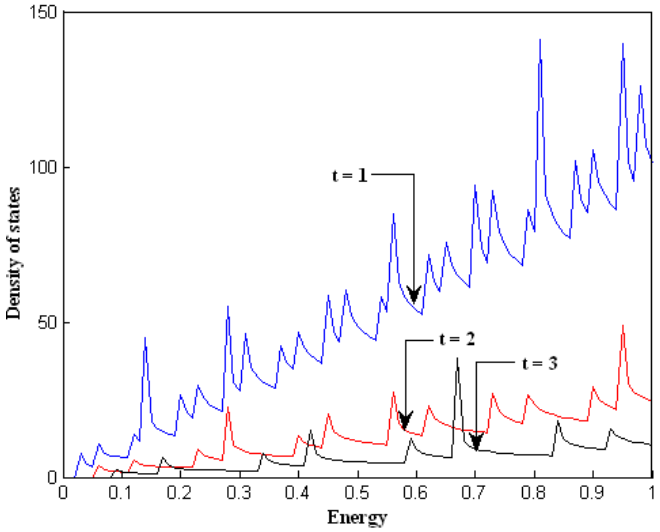

Fig 5: Density of states with energy for semiconducting SWCNT with radius 0.1 nm for different values of matrix element between neighboring carbon atoms

Energy is plotted as a function of normalized propagation vector (along Y axis) for different nearest neighbor distance in Fig 6. From the graph, it may be seen that energy gap is minimum at

the center and increases as we go away with increasing propagation constant. When this simulation is made, it is assumed that propagation constant is set at zero along X axis.

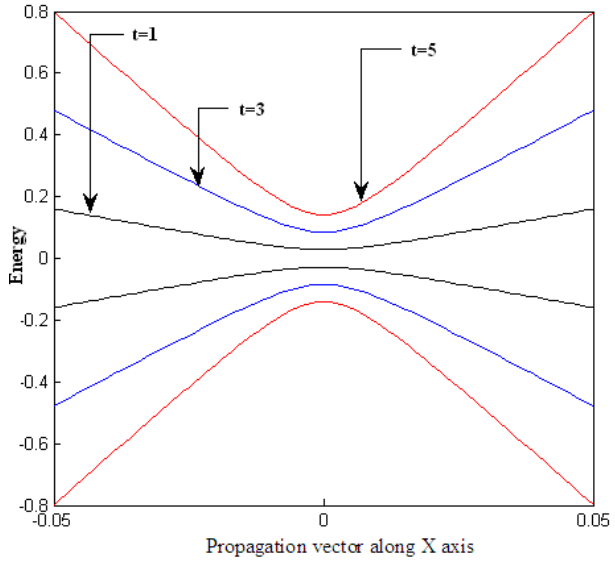

Fig 6: Band structure of semiconducting SWCNT with radius 0.1 nm for different values of matrix element between neighboring carbon atoms

Bandgap for the structure is calculated as a function of nearest neighbor distance for two different semiconducting nanotubes with two lowest order modes. This is plotted in Fig 7. From the plot, it is seen that with increasing the distance between unit cells, conductivity decreases, resulting decrease in bandgap of the structure Computation is made for lowest two modes, and it is observed that bandgap is lower for lowest mode. Also with increase of lattice index, bandgap decreases, as expected from earlier results.

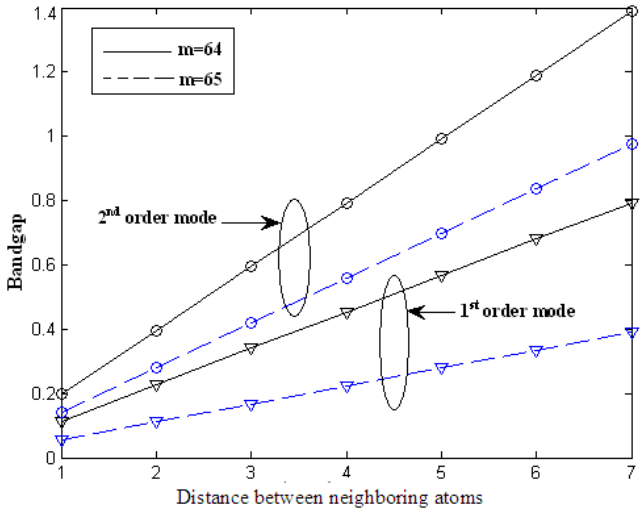

Fig 7: Bandgap with distance between neighboring atoms for two different semiconducting tubes for the lowest two modes

IV. CONCLUSION

In summary, band structure and density of states of zigzag single-wall carbon nanotube are analytically calculated as function of nearest neighbor distance, lattice index (which is directly related with conductivity) and radius of the cylindrical structure. NNTB approximation and theory of LCAO are considered for analytical investigation, and results show the effect of geometrical specifications on electrical performance. Hence a proper choice of design parameters can be made from the available results to design zigzag SWCNT-based electronic or optoelectronic devices.

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