Bulletin of Pure and Applied Science
Physics, Vol.43D No.1,
January-June 2024 P.19-24
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: https://doi.org/10.52710/bpas-phy.4
Available online at www.bpasjournals.com

Electronic Transistions in Incommensurate Double Walled Carbon Nantoubes and Analysis of Band Structure

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ABSTRACT

The study of intertube electronic transitions and band structure of incommensurate double walled carbon nanotubes were made. It was possible in the case of double walled carbon nanotubes with super imposed extended Brillouin zones corresponding to constituent of single walled carbon nanotubes. The selection reules allowed the intertube transitions which were geometric and permittd to determine the transitions and band structure of double walled carbon nanotubes. This was powerful tool with Rayleigh spectroscopy used for structural identification. All existing methods for optical spectra of double walled carbon nanotubes used the number of transitions as an input parameter which was equal to the number of transitions in pristine single walled carbon nanotubes in the measured spectral range. It was found that the intertube transition was doubled due to symmetry breaking with respect to the electron hole permutation. The analysis predicted the splitting and values of dipole matrix elements for possible intertube transitions. We have used the nearest neighbor tight binding approximation for analyzing band structure of double walled carbon nanotubes. It was found that unconventional electronic transitions in double walled carbon nanotubes with much greater structural diversity. The expressions found for energy dispersions contained additional terms which corresponded to cross band interaction and increased the accuracy of calculations. We have calculated more compact and more accurate expressions for the energies of optical transitions. We have also used effective Hamiltonian for analyzing band structure of incommensurate double walled carbon nanotubes. The obtained results were found in good agreement with previously obtained results.

KEYWORDS

Electronic Transition, Band Structure, Incommensurate, Carbon Nanotube, Transition, Symmetry Breaking, Tight Binding, Interaction.

How to cite this article: Kumari M. and Kumar N. (2024). Electronic Transistions in Incommensurate Double Walled Carbon Nantoubes and Analysis of Band Structure. *Bulletin of Pure and Applied Sciences-Physics,* 43D (1), 19-24.

INTRODUCTION

Liu et al. [1], Zhao et al. [2] and Levshov et al. [3] studied theoretically the electronic properties of double walled carbon nanotubes. Tran et al. [4] and Rochal et al. [5] also studied theoretically the structure of double walled carbon nanotubes in the case of incommensurate system. Yu et al. [6] and Chen et al. [7] showed the incommensurability with the curved geometry and structural diversity of double walled carbon nanotubes of electronic properties and their various applications. Liu et al. [8] presented optical spectrum a superposition of spectra of single walled carbon nanotubes formed the double walled carbon nanotube with a small shift of peaks caused by weak Vander wals interaction between the inner and outer layers. The electronic transitions in incommensurate double walled carbon nanotubes using theoretical model based on perturbation theory [9-15]. Koshino et al. [16] made a alternative approach to calculate a small region of the band structure in incommensurate double walled carbon nantotueb. Zhao et al. [17] presented an optical spectrum rearrangement experimentally in the double walled carbon nanotube and found that the measured Rayleigh spectrum and optical transitions originated from the inner and outer single walled carbon nanotubes contained a few additional one. It was also found that both inner and outer tubes were nearly armchair and their chirality angles were approximately equal. Bristrizer et al. [18] and Trambly et al. [19] studied that the structural organization demonstrated moiré patterns and electronic band structure opened up new possibilities for altering their electronic properties. Li et al. [20] and Kim et al. [21] showed that by varying the angle between the layers in twisted bilayer graphene changed the position of the Von Hove singularities in the density of electronic states of the twisted bilayer graphene. Cao et al. [22] and Po et al. [23] presented that when the Von Hole singularity was close to the Fermi energy the electronic instabilities arised in the bilayer superlattice which resulted in new states of superconducting and Mott insulating [24]. The twisted bilayer graphene was found a few systems where fractal structure of electronic spectrum in the magnetic field was found which was called Hofstadfer butterfly [25]. Saito et al. [26] and Reich et al [27] used the nearest neighbor tight binding approximation for the study which was convenient tool for analyzing the band structure of double walled carbon nanotubes. In this geometric selection rules allowed the intertube transitions.

METHOD

We have developed the concept of intertube electronic transitions and explained the mechanism of the phenomenon. The weak Vander Waals interlayer coupling in double walled carbon nanotubes changed the band structure of pristine single walled carbon nanotubes corresponding different nanotubes became possible. The nearest neighbor tight binding approximation to make convenient tool for analyzing the band structure of double walled carbon nanotubes. We have obtained expressions for energy dispersions contained additional terms which corresponded to cross band interaction and increased the accuracy of calculations. We have considered the effective Hamiltonian which was used to analyse the band structure of incommensurate double walled carbon nanotubes. We have calculated the dipole matrix element for intertube transitions. The Hamiltonian of an individual single walled carbon nanotube is written as

$$H = \begin{pmatrix} 0 & f(q) \\ f^{*}(q) & 0 \end{pmatrix},$$

Where

$$f(q) = Y\left[\exp\left\{\frac{-i(a_1+a_2)}{3}.q\right\} + \exp\left\{\frac{i(2a_1-a_2)}{3}\right\} + \exp\left\{\frac{i(-a_1+2a_2)}{3}.q\right\}\right]$$

is the matrix element describing the interaction between the graphene sublattices, Y is the hopping coefficient, a_1 and a_2 are the graphene's primitive transitions expressed in a cylindrical coordinate system of single walled carbon nanotube, where the first and second components corresponds to the projections on the circumference and the longitudinal axis of the tube, $q = (\mu, k)$ is the wave vector. The first integer component μ numbers the cutting lines and second component *k* is the wave vector

projection along them. The Eigen energies of the Hamiltonian $E^{\pm} = \pm\left| f\left(\mu,k\right)\right|$, while eigenvectors is

$$\left|\psi^{\pm}\right\rangle = \left|\psi_A\right\rangle \pm e^{i\psi}\left|\psi_B\right\rangle$$

Where $\left|\psi_A\right\rangle$ and $\left|\psi_B\right\rangle$ are the Bloch wave function of the sublattice, the positive and negative signs correspond to the states in the conduction band and valence band, $\varphi = Arg\left(\frac{|f|}{f}\right)$ is the phase shift between the sublattices. The electronic states in single walled carbon nanotubes was classified using the vector $\left(\mu,k\right)$ and the number $\sigma = \pm$, indexing the conduction $\left(+\right)$ and valence $\left(-1\right)$ bands. In a double walled carbon nanotube an electronic state of one tube strongly interacted with several states of the other tube. We have also considered the interaction between two electronic states $\left(q,\sigma\right)$ and $\left(q',\sigma'\right)$ of the inner and outer single walled carbon nanotubes. Using the matrix representation the effective double walled carbon nanotube Hamiltonian was suitable to describe such pair interaction as

$$H_{DW} = \begin{pmatrix} H_{in} & V \\ V^{*} & H_{out} \end{pmatrix}$$

Where H_{in} and H_{out} are the Hamiltonian of the inner and outer single walled carbon nanotube with V is the interlayer coupling matrix.

$$V = \begin{pmatrix} V_{A,A'} & V_{A,B'} \\ V_{B,A'} & V_{B,B'} \end{pmatrix}$$

$V_{\alpha,\beta} = \left\langle \psi^{in}_{(a)} \middle| \hat{V} \middle| \psi^{out}_{(\beta)} \right\rangle$ are the matrix elements of the interlayer coupling operator $\hat{V}$, describing the interaction between the sublattice of the inner $\left(\alpha = A,B\right)$ and outer $\left(B = A',B'\right)$ nanotubes.

In incommensurate double walled carbon nanotubes when we consider two arbitrarily electronic states $\left(q,\sigma\right)$ and $\left(q',\sigma'\right)$ of the inner and outer tubes the matrix element $V_{\alpha,\beta}$ was averaged over spatial coordinates, vanished due to oscillating phase. For strongly coupled electronic states this was not possible. The strong coupling is for the modes with $q' = q$. The coupling strength decayed exponentially with increasing distance between q and τ points. Due to incommensurability of inner and outer nanotubes, matrix elements $V_{\alpha,\beta}$ are practically real and independent on indices α and β. For the inner tube the shifts of conduction bad and valence band energies was obtained as the sum over three wave vectors and the total energy shift ΔE_{tot} for the in tube electronic transition at the point q was as

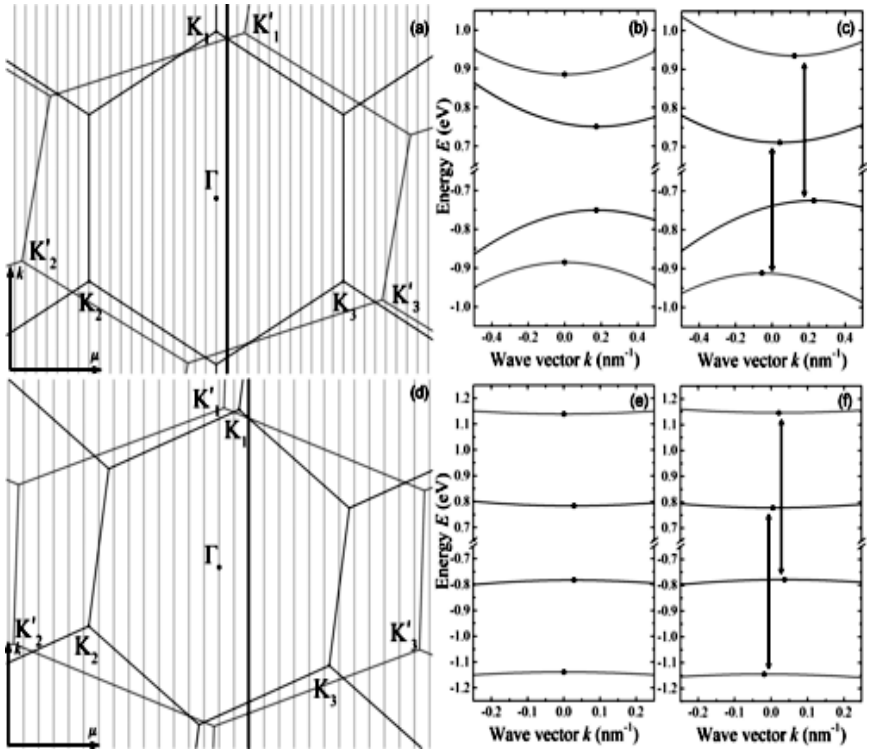
$$\Delta E_{tot}\left(q\right) = \sum_{j=1}^{3} \Delta E_{in}\left(q_j\right)$$

Where wave vectors are expressed as $q_1 = q, q_2 = 2 - b_1, q_3 = q + b_2, b_1$ and b_2 are the basis vectors of the inner tube reciprocal space. The obtained results were compared with previously obtained results.

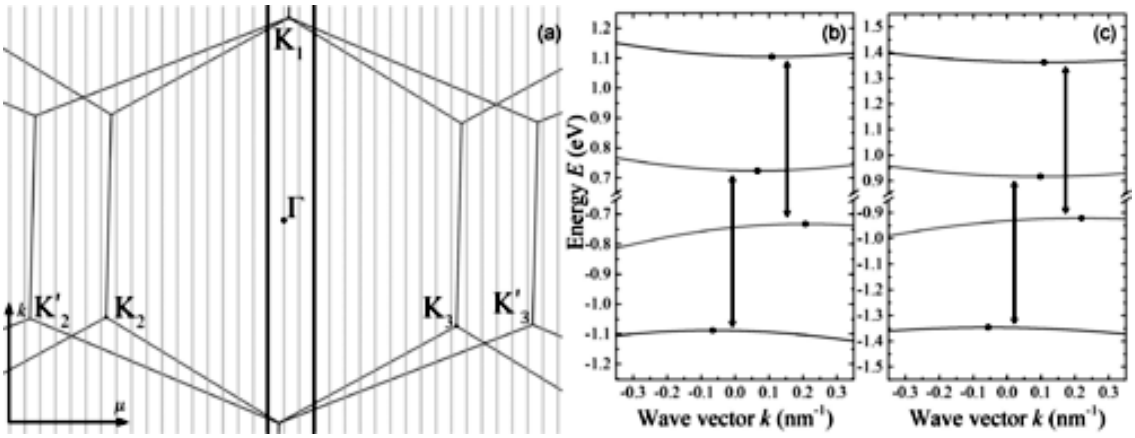
RESULTS AND DISCUSSION

The study of electronic transitions in incommensurate double walled carbon nanotubes and band structure was made. The optical spectra in this case with weak Vander Waal coupling between the layers for small shift of transition energies in comparison with pristine single walled nanotubes were studied. It was found that the spectrum of double walled carbon nanotube contained additional peaks due to interlayer coupling and band structure was modified. Graph (1) (a) shows the superimposed extended Brillouin zones in the reciprocal space. It was found that in the outer nanotube the coupling point in very close to Van Hove singularities of the inner tube. The rare case of situation when both strongly coupled modes in the double walled carbon nanotube are very close to the optical transitions in the spectra of the pristine single walled carbon

nanotubes. In the inner tube the energy bands with $\mu = 1$ are modified due to coupling. The analysis of the interacting modes are carried out within the single Hamiltonian. Using this we have calculated the dispersion curves for the conduction bands and valence bands of the double walled carbon nanotube. The obtained results for dispersions have been shown in graph (1) (c). Graph (1) (b) shows the extrema of the dispersions of the inner and outer tubes which do not found exactly one above the other. The interlayer coupling leaded to rearrangement of the electronic spectrum is shown in graph (1) (c). Which exactly above each other as studied previously and extema of the bands that originated from different single walled carbon nanotubes converged. The wave vector with the coordinates of conduction band bottom and the valence band top of the outer single walled carbon nanotube approximately coincided with the one corresponding of the valence band top of the inner single walled carbon nanotube. Graph (1) (d) shows the superimposed reciprocal spaces of the tubes (10, 6) and (14, 13). Graph (1) (d) shows the calculation of dispersion relations using the Hamiltonian shows a similar spectrum rearrangement as in the case of double walled carbon nanotubes (12,12) and (21,13). The distance between the extrema which originated from the bands of different pristine single walled carbon nanotubes turned out to two times smaller than the distance between Von Hove singularities of conduction band and valence band of the outer single walled carbon nanotubes. The analysis of obtained results of plotted peaks with energies corresponded to transitions with theoretical energies 1.89 and 1.92 eV. Graph (2) (c) shows the transitions with energies 2.35 and 2.37 eV. Graph (2)(a) shows the intertube transitions in the bands with $\mu = 0$ and $\mu = 1$. The energies are found beyond the obtained range and were found close to 1 eV. Analyzation showed that four intertube transitions were found rare. We have found that the obtained results and the energies of possible intertube transitions matched and very close to each other. It was found that intertube optical transitions were present in the spectra of four double walled carbon nanotubes. The calculated double walled carbon nanotube electronic dispersion explained to origin of the transitions. It was found that in intertube transitions occurred which were composed of the tubes with the same handedness. We have developed the theory of intertube optical transitions in double walled carbon nanotubes. We have calculated the band structure of low dimensional system. We have applied the perturbation theory and have considered the effective Hamiltonia (4 × 4) for strongly coupled states of the outer and inner tubes. We have taken the incommensurability of single walled carbon nanotubes in a double walled carbon nanotube and obtained more accurate expression to calculate the energies of the coupled states. The obtained results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: Plot of Brillouin zones in reciprocal space.



Graph 2: Plot of inter tube transitions in double walled carbon nanotubes.

CONCLUSION

We have studied the electronic transitions in incommensurate double walled carbon nanotubes and analysed the band structure. The optical spectra of double walled carbon nanotubes with weak Vander Waals coupling between the layers having small shift of transition energies in comparison to pristine single walled nanotube were studied and analysed. The tight binding approximation was used for the study and calculation of result. It was found that in double walled carbon nanotubes the inter layer coupling modified the band structure of pristine nanotubes. It was found that the intertube electronic transitions occurred in some double walled carbon nanotubes with geometrical shape of super imposed extended Brillouin zones corresponding to constituent of single walled

carbon nanotubes. It was found that selection rules allowed intertube transitions were geometrical and allowed transitions of double walled carbon nanotubes without calculating the band structure. It was also found that Rayleigh spectrum of double walled carbon nanotube contained additional peaks and electronic transitions and additional peaks in double walled carbon nanotubes optical spectrum appeared. The obtained results were found in good agreement with previously obtained results.

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