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# Band Gap Mechanism for Armchair Single Walled Carbon Nanotubes and Metal Semiconductor Transition for Symmetry Breaking

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**ABSTRACT**

We have studied structures of single walled carbon nanotubes and metal semiconductor transition for the symmetric breaking. It was found that band gap existed for metallic armchair single walled carbon nanotubes. Calculations were made to analyse the meta-stability of the corrugated structures of armchair single walled carbon nanotubes. The corrugated single walled carbon nanotube structures are always lower in energy than the non corrugated nanotubes. The curvature effect was that the corrugated structure breaks the local symmetry between different carbon atoms. A true gap is created which does not vanish even when an external magnetic field is swept. The corrugation length and band gap gaps are decaying functions of the nanotubes radius and approached zero for carbon nanotube such as graphene. This was also true for zigzag and chiral single wall carbon nanotubes. The obtained results were found in good agreement with previously obtained results.

**KEYWORDS**

Structure, Single Walled Carbon Nanotube, Metal Semiconductor, Transition Symmetry, Band Gap, Corrugation, Armchair, Zigzag, Chiral.

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## INTRODUCTION

A single wall carbon nanotube is viewed as a quasi one dimensional cylindrical tube rolled up from a graphene sheet [1]. It is specified uniquely by a pair of integer (*n*,*m*) called chirality index [2-4] and its electronic property sensitively depends on the chirality and diameter of nanotubes. For an ideal graphene the valence and conduction bands are classified as $\sigma$ and $\pi-$orbitals characters. Six $\sigma$ bands lie either deep below or high above the Fermi energy and are responsible for the structural bonding. The curvature effects and dependence on large diameter was presented by some investigators [5-7], the small diameter cases were also presented by them. The discrepancy, a curvature induced $\pi$ - $\sigma$ hybridization effect was proposed by several investigators [8-10]. The renormalized hopping integral became

anisotropic with respect to the axial and circumferential directions, which effectively shifted the Dirac points. A hybridization effect does not change the allowed sets of wave vectors in a circumferential direction for armchair single walled carbon nanotubes. Armchair single walled carbon nanotube remains metallic and are protected from such a curvature effect [11]. Ajiki and Ando [12] studied that true band gap does not vanish as the external magnetic field varied. The band gap opening mechanism is suitable process for the study of our present work. Deshpandeya et al [13-15] presented the semiconducting single walled carbon nanotubes as the Mott insulators. The structural deformation is a common phenomenon in low dimensional systems, the structural twist and strain models have been investigated from very early on several groups [16-17]. The phenomenological calculations showed that band gaps be created by twist distortions in armchair single walled carbon nanotubes but the estimated structural transition temperature differed by two orders of magnitude due to the poor material parameters [18-19]. Harigaya et al [20] and Viet et al [21]studied in plane Kekule structures which created band gaps did not create true band gaps. So corrugated structures were called for the study. Sahin et al [22] studied that Silicon and germanium formed a monolayer honeycomb lattice but with a corrugated stay in different planes separated by a corrugation length. Blasé et al [23] presented a stable structure when graphene is rolled up into nanotubes. Such corrugated structures have been verified by *abinitio* calculations in boron nitride nanotubes. So such a scenario has been proposed for carbon nanotubes for study.

## METHOD

Electronic structure and total energy calculations using Vaspetal package. This package was implemented of a highly accurate full potential project augmented wave method suggested by Blochl. The generalized gradient approximation of Perdew and Wang was adopted for the exchange correlation potential. In the band structure calculation of nanotubes a basic building block of a nanotube was chosen as a unit cell and provided boundary conditions were implemented both along the nanotube's axis and lateral directions. In the case of armchair with chiral index (*n*,*m*), the basic building block included 4*n* carbon atoms. It was arranged in a hexagonal lattice with an intertube separation of at least 20Å to avoid the interaction between neighbouring single walled carbon nanotubes. In the self consistent field potential and total energy calculations a set of $(1\times1\times11)$ *K*-point sampling was used for Brillouin zone integration in *k*-space. The *k*-point mesh was generated by the Monkhorst pack scheme, a kinetic energy cut off for a plane wave basis set was taken as 500eV. The obtained results were compared with previously obtained results.

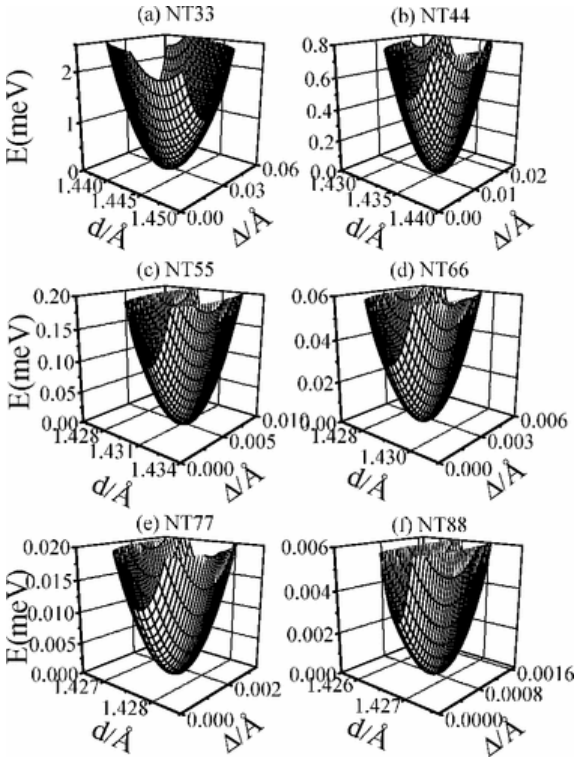
## RESULTS AND DISCUSSION

Graph (1) shows the normalized energy per carbon atom for the six armchair single walled carbon nanotubes were potted in $(d,\Delta)$ parameter space with respect to the local minimum. The chiral index was from *n*=3 to *n*=8 and the radius of single walled carbon nanotubes ranged from 2 to 5.5Å. The total minima have been demonstrated for single walled carbon nanotubes and corrugated structures of single walled carbon nanotubes. The local minima energy have been calculated by the relation.

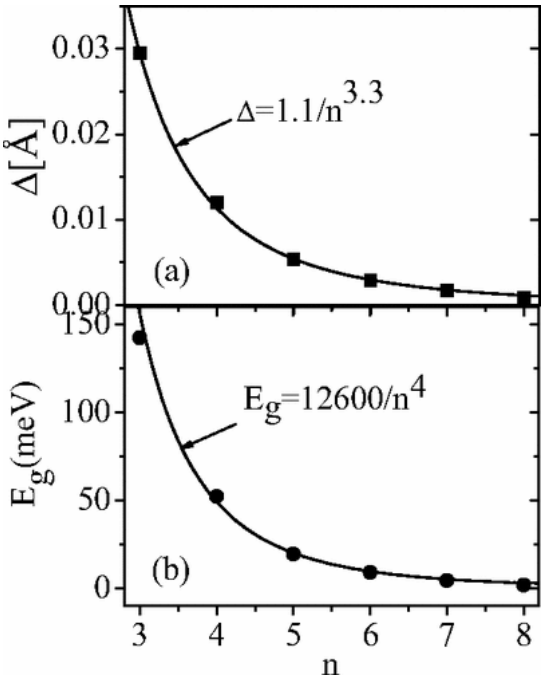
$$E = E_m + B_d\left[\upsilon_1\left(d-d_m\right)+\upsilon_2\left(\Delta-\Delta_m\right)\right]^2 + B_\Delta\left[\upsilon_1\left(\Delta-\Delta_m\right)-\upsilon_2\left(d-d_m\right)\right]^2$$

$E_m$ is the minimum energy per carbon atom at $d_m$ and $\Delta_m$. The corrugated structure was lower per carbon atom by 2 meV for (3,3) and 3 μeV for (8,8) nanotubes $(\upsilon_1,\upsilon_2)$ and $(-\upsilon_2,\upsilon_1)$ are the eigen vectors for two principal axis of elliptical paraboloid. It was found that $E_m$ decreased with the increase of radius which showed that it was possible for metastable structures with respect to graphene. The curvature reduced the bonding strength between carbon atoms and the bond length $d_m$ increased monototically as the radius of the nanotubes was reduced. The stiffness

coefficients were strongly anistropic with an order of magnitude difference and corresponded to soft out of tube distortion mode and hard in tube distortion mode. Graph (2) (a) shows the corrugated structure results from the strong electron-phonon interaction. The corrugation length $\Delta_m$ is a monotonically decreasing function of the nanotube's radius. The largest value of $3\times10^{-2}$ Å for the smallest (3,3) nanotube and $8\times10^{-4}$ Å for a relatively large (8,8) nanotube. Graph (2)(b) shows a true band gap present for all nominally metallic armchair single walled carbon nanotubes. The band gap decreased with radius. The biggest gap of 140 meV was found for the smallest (3,3) single walled carbon nanotube. Corrugated structures are more stable metastable structures of single walled carbon nanotubes which showed the true band gap in nominally metallic armchair single walled carbon nanotubes. The calculated band gaps are large only for very small single walled carbon nanotubes. The difference was caused by the ideal model system and realistic sample. Impurity atoms and electric charges on a substrate created a potential gradient across the single walled carbon nanotube. A hybrid functional approximation to exchange and correlation was used. The corrugated structure was found lower in energy per carbon atom. The stability of corrugated structure under finite temperature was increased. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.




**Graph 1:** The normalized energy distribution as a function of bond length d and corrugation length $\Delta$.




**Graph 2:** Dependencies of corrugation length $\Delta_m$ and band-gap $E_g$ on the armchair index *n*.

## CONCLUSION

We have studied theoretically the structure of corrugated semiconductor having metallic nature. The formation of band gap and transition were studied in the case of metal semiconductor during the symmetric breaking. It was fond that corrugated structures are more stable metastable structure of single walled carbon nanotubes and was able to explain the true band gap in nominally metallic armchair single walled carbon nanotubes. The discrepancy existed for calculated and measured band gaps. The calculated band gap were large only for small single walled carbon nanotube, while measured value demonstrated that they are sizable even for single walled carbon nanotubes with a radius up to nanometer. Impurity atoms and electric charges on a substrate created a potential gradient across the single walled carbon nanotubes. Corrugated structure of single walled carbon nanotube is stable above room temperature while for (8, 8). Single walled carbon nanotube is stable in the Kelvin temperature range. The corrugation broke the local symmetry between two types of carbon sites and a band gap started to develop once graphene sheets were rolled up into nanotubes. The results found were in good agreement of previous results of theoretical and experimental research works.

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