Bulletin of Pure and Applied Science
Physics, Vol.45D No.1,
January-June 2026 P.29-34
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
Available online at www.bpasjournals.com

Collapsed Semiconducting Nanotubes Having Degenerate Band at Fermi Level Due to Broken Axial Symmetry

[1]Md. Arman Ali* and [2]Anil Kumar

Author's Affiliations:
[1]Research Scholar, Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India.
E-mail: armanalimdp@gmail.com
[2]Department of Physics, R. J. M. College, Saharsa, Bihar, India.
E-mail:– kanil1961@gmail.com

***Corresponding author:**
Md. Arman Ali
Research Scholar, Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India.
E-mail: armanalimdp@gmail.com

ABSTRACT

Full collapsed semiconducting nanotubes became metallic, having singly degenerate band at Fermi level due to broken symmetry. It was found that wave function used was mismatched, which leaded to higher contact resistance in respect of ideal contact. A new method was used for degeneracy lifting due to interaction among π-orbitals on sidewalls of collapsed nanotube produced larger magnitudes of bands and were splitted in fully collapsed carbon nanotubes. A continuum model was considered for explanation of carbon atoms in carbon nanotubes with metal. For this purpose a semiatomistic model was used for description of positions of carbon atoms in the presence of metal and substrate. Carbon nanotube interatomic interactions were explained by valence force model considering stiffness opposite to misalignment of neighboring π-orbitals for reduction of bending stiffness. Substrate was planar and rigid but metal was isotropic. Deformations on electronic structures were created due to effect of metal induced nanotube. Band gap reduction was found in deformed carbon nanotubes and increased metal induced doping of nanotube, which reduced the resistance by means of conduction channels, mismatched function and scattering at contact.

KEYWORDS

Collapse, degenerate, symmetry breaking, mismatched, carbon nanotube, deformation.

Received on 27.03.2025, Revised on 14.05.2026, Accepted on 10.06.2026

How to cite this article: Ali A. and Kumar A. Collapsed Semiconducting Nanotubes Having Degenerate Band at Fermi Level Due to Broken Axial Symmetry. *Bulletin of Pure and Applied Sciences- Physics,* 2026;45D (1): 29-34.

INTRODUCTION

Effect of deformations on electronic structure and contact resistance between metal deformation and round positions of nanotube was studied. Smalley et al. studied electrical properties of carbon nanotubes by using many technologies. For this purpose semiconducting single walled carbon nanotube field effect transistors were considered. High performance

channels were used for study of increase in contact resistance due to decrease in size. Which scaled the devices as channel transport and formed ballistic property [1]. Baimova et al. studied that carbon atoms are capable of providing numerous structures as monoatomic crystalline layer of grapheme [2]. So nano materials of structure of mechanical and thermal properties were considered for study [3]. Graphene was grown on a substrate in a carbon rich environment. Lui et al. studied that these defects were created by means of roughness of substrate and difference between thermal expansion coefficients of graphene and substrate [4]. These defects changed the properties of graphene as electrical conductivity [5], thermal conductivity and electricity. Wang et al. and Zhao et al. studied and found that deformations in graphene were created by thermal compression of substrate at cooling stage [6,7]. Defects were also found during the procedure of graphene sheet transfer [8]. Aljedani et al., Cox et al. , Zhang et al. used quasi analytical models based on calculus of variations, continuum mechanics modes with finite element method and all atom models utilizing molecular dynamics for explanation of wrinkles folds [9, 10, 11]. These modes permitted to explain appearance of folds of wrinkles during uniaxial compression continuum mechanics treatment was considered for uniaxial and biaxial compression of sufficiently large graphene sheet study [12]. Elliott et al; Gadagkar et al., Umeno et al., Magnin et al. and Hu et al. studied the effect of external hydrostatic pressure on shape of wrinkles. It was found that at critical pressure wrinkle was flattered or collapsed into denser from vertical two layer fold. Study of collapse of hollow carbon nanotubes under pressure was also studied. Stability of a flat compressed sheet state was analysed and was found that structures of wrinkles were formed during uniaxial and biaxial compression of sheet [13, 14, 15, 16, 17]. Savin and Klinov studied wrinkles in graphene suspended on flat substrate and in case of structure collapse under hydrostatic pressure [18]. Alexander et al. used method of molecular dynamics and molecular mechanics for simulation of wrinkle formation for a system due to compression of graphene sheet lying on flat solid substrate. It was found that due to uniaxial compression nanosheet produced transition into stable wrinkle states for a finite length. It was also found that wrinkles were completely flattered [19].

METHOD

Molecular dynamics and molecular mechanics were used for simulation of study of collapsed carbon nanotubes and calculation of results numerically for a system lying on rigid substrate under uniaxial and biaxial compression. Atomic position were obtained by minimizing the total energy of the system is given by

$$E = E_{bending} + \sum_{i,j} U_{cc}(i,j) + \sum_{i} \int U_{sc}(i)\, ds_s + \sum_{i} \int U_{MC}(i)\, ds_M + \gamma \int dS_M + \iint U_{MS}\, dS_M\, dS_S$$

Where i and j run over carbon atoms for carbon nanotube, U_{CC}, U_{MC} and U_{SC} are Vander Waals interactions. Minimum energy were calculated for electronic structure using density function theory. Perdew-Burke-Ernzerhof generalized gradient approximation was used for exchange correlation energy. Study of effect of metal induced nanotube deformations on electronic structure and electrical contact resistance at interface between deformed and round portions of a tube were made and explained. Reduction of deformed carbon nanotubes were studied by increasing number of conduction channels and mismatch of wave function with scattering at the contact. Leading of mismatch for higher contact resistances were studied. A new mechanism was used for degeneracy lifting created from interaction among π-orbital on adjacent sidewalls of collapsed nanotubes were studied. Rectangular graphene sheet was considered for which contained chains of valence bonds along x-axis consisted zigzag structure and along y-axis consisted armchair structure. Periodic boundary conditions at the edge of sheet were applied. Hamiltonian for nano sheet is given by the relation

$$H = \sum_{n=1}^{N} \left[\frac{1}{2} M(u_n, \hat{u}_n) + Q_n + W_n + Z(u_n) \right]$$

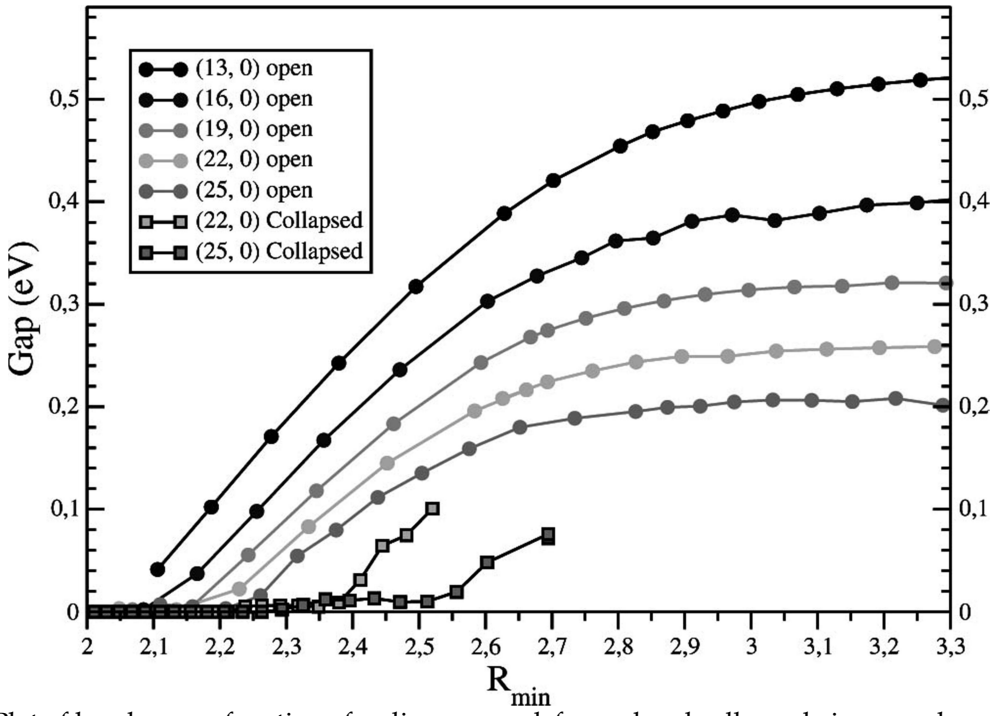
Where M is the mass of carbon atom, $u_n = x_n(t), y_n(t), z_n(t)$ is a vector represented the position of *n*th atom at time t, Q_n is the valent interaction for neighboring carbon atoms, a relation is given by

$$Q = \sum_{\Omega_1} U_1 + \sum_{\Omega_2} U_2 + \sum_{\Omega_3} U_3 + \sum_{\Omega_4} U_4 + \sum_{\Omega_5} U_5$$

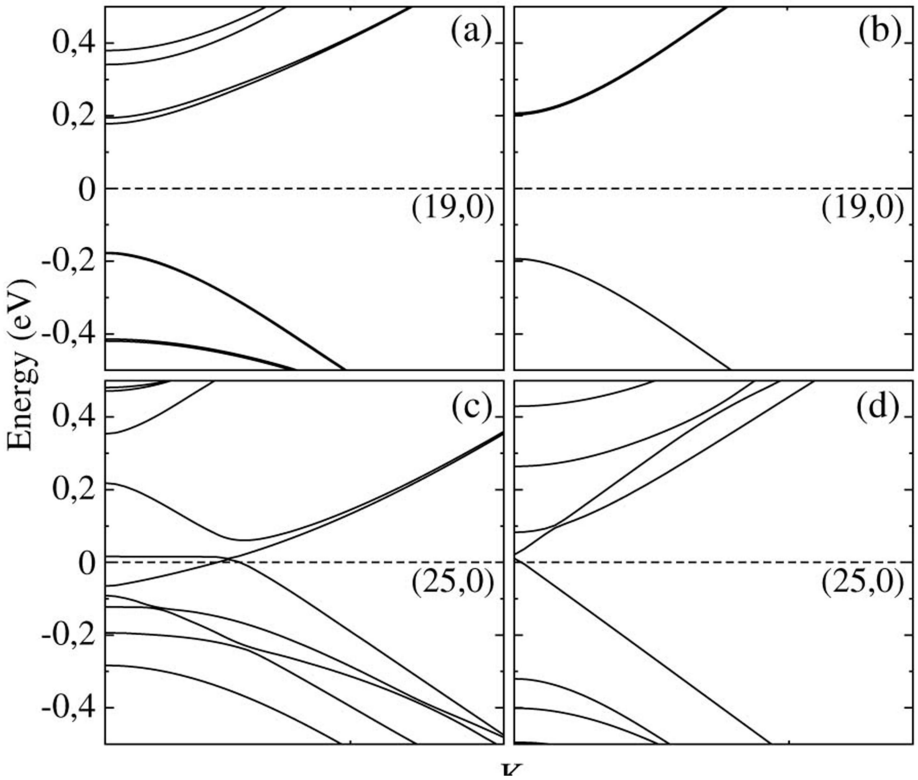
Where Ω_i is the set of configuration $i = 1,2,3,4,5$.

RESULTS AND DISCUSSION

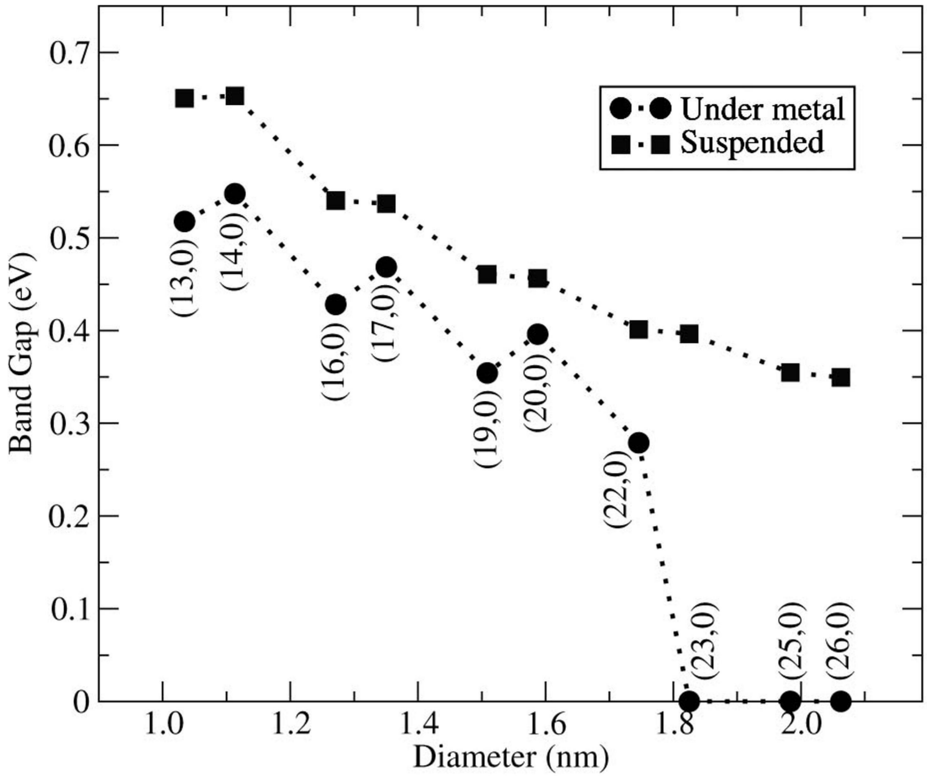
Molecular dynamics and molecular mechanics were used for the study of collapsed semiconducting nano materials having singly degenerate band at Fermi level means of broken axial symmetry. Magnitude of degeneracy lifting were larger than room temperature was obtained. In this study wave function mismatched leaded higher contact resistance were compared with ideal contact. For fully collapsed carbon nanotube the self consistent Fermi energy of round carbon nanotube in metal corresponding to on state resistance were studied and explained. Tight binding approach was used for the study of electronic structure and calculations of results. Calculation of contact resistance was also done by this approximation. Graph (1) shows that band gaps gradually decreased with decreasing radius of curvature and became zero at critical value. It was found that when total energy was minimized, stabilized collapsed carbon nanotubes and band gaps became zero larger than critical values which is shown in Graph (1). It was also found that band gaps in collapsed carbon nanotubes were smaller than in comparison to open carbon nanotubes by means of π-π interaction between orbitals on adjacent side walls separated at Vander Waals distance in collapsed carbon nanotubes and provided stronger electronic structure. Changes in electronic structure due to deformations provided contact resistance at interface between round and deformed positions of nanotube. Graph (2) shows the plot of band structure of metal deformed and collapsed nanotubes. For collapsed carbon nanotubes an additional long range action between carbons were found for different layers. Band structure due to four orbital tight binding model were found for curvature induced mixing of π and σ orbitals. Graph (3) shows the plot of band gaps of round and metal deformed versus carbon nanotubes as function of carbon nanotube diameter. It also shows that density functional theory band gaps in suspended carbon nanotube i.e. round carbon nanotubes without substrate and metal and in metal deformed carbon nanotubes. It was found that electronic structure was modified and resulted deformed carbon nanotube structures in continuum model due to increase in metal surface energy and Vander Waals attraction between side walls. Uniaxial compression was applied to nano sheet for transition in to many stable wrinkled states having infinite length. Higher energy states of wrinkles of finite length aligned along their ends were partially overlapped. Effect of external hydrostatic pressure on the shape was also studied. It was found that for critical pressure wrinkle collapsed into vertical two layer fold i.e. completely flattered.



Graph 1: Plot of band gap as function of radius versus deformed and collapsed zigzag carbon nanotubes.



Graph 2: Plot of band structures of metal deformed and collapsed nanotubes.



Graph 3: Plot of band gaps of round and metal deformed versus carbon nanotubes as function of carbon nanotube diameter.

CONCLUSION

Study of collapsed semiconducting nanotubes of singly degenerate band at Fermi level by means of broken symmetry was made. Vander Waals forces affected the properties of carbon nanotubes to deform or collapsed in metal contacts by the use of abinitio band structure calculations and was found that band gap was reduced by means of deformations and fully collapsed nanotubes became metallic. Mismatch of wave functions between collapsed and round portions of carbon nanotube provided higher contact resistance. Band splitting affected transport at room temperature. Effect of metal induced nanotube deformations on electronic structure and electrical contact resistance at interface between deformed and round portions of nanotube were found. Band gap decrease in deformed carbon nanotubes enhanced metal induced doping of nanotube and decreased the resistance due to conduction channel.

REFERENCES

1. Smalley RE, Dresselhaus MS, Dresselhaus G, Avouris P, editors. *Carbon nanotubes: synthesis, structure, properties, and applications*. Vol. 80. Berlin: Springer; 2003.
2. Baimova JA, Korznikova EA, Dmitriev SV, Liu B, Zhou K. Review on crumpled graphene: unique mechanical properties. **Rev Adv Mater Sci.** 2014;39:69-83.
3. Liu Y, Hu C, Huang J, Sumpter BG, Qiao R. Tuning interfacial thermal conductance of graphene embedded in soft materials by vacancy defects. **J Chem Phys.** 2015;142:244703.
4. Lui CH, Liu H, Mak KF, et al. Ultraflat graphene. **Nature.** 2009;462:339-341.
5. Guan Y, Yazyev OV. Electronic transport in graphene with out-of-plane disorder. **npj 2D Mater Appl.** 2024;8:1.
6. Wang M, Huang M, Luo D, et al. Single-crystal, large-area, fold-free monolayer graphene. **Nature.** 2021;596:519-524.

7. Zhao C, Shan L, Sun R, Wang X, Ding F. Wrinkle formation in synthesized graphene and 2D materials. **Mater Today.** 2024;81:104-125.
8. Lanza M, Wang Y, et al. Tuning graphene morphology by substrate toward wrinkle-free devices: experiment and simulation. **J Appl Phys.** 2013;113:104301.
9. Aljedani J, Chen MJ, Cox BJ. Variational model for collapsed graphene wrinkles. **Appl Phys A.** 2021;127:886.
10. Cox BJ, Dyer T, Thamwattana N. A variational model for conformation of graphene wrinkles formed on a shrinking solid metal substrate. **Mater Res Express.** 2020;7:085001.
11. Zhang Y, Wei N, Zhao J, Gong J, Rabezuk T. Quasi-analytical solution for the stable system of multilayer folded graphene wrinkles. **J Appl Phys.** 2013;114:063511.
12. Zhang K, Arroyo M. Adhesion and friction control localized folding in supported graphene. **J Appl Phys.** 2013;113:193501.
13. Elliott JA, Sandler JKW, Windle AH, Young RJ, Shaffer MSP. Collapse of single-wall carbon nanotubes is diameter dependent. **Phys Rev Lett.** 2004;92:095501.
14. Gadagkar V, Maiti PK, Lansac Y, Jagota A, Sood AK. Collapse of double-walled carbon nanotube bundles under hydrostatic pressure. **Phys Rev B.** 2006;73:085402.
15. Umeno Y, Yachi Y, Sato Y, Shima H. On the atomistic energetics of carbon nanotube collapse from AIREBO potential. **Physica E.** 2019;106:319-326.
16. Magnin Y, Rondepierre F, Cui W, Dunstan DJ, San-Miguel A. Collapse phase diagram of carbon nanotubes with arbitrary number of walls: collapse modes and macroscopic analog. **Carbon.** 2021;178:552-560.
17. Hu C, Chen J, Zhou X, Xi Y, Huang X, Wu Z, Ma S, et al. Collapse of carbon nanotubes due to local high pressure from van der Waals encapsulation. **Nat Commun.** 2024;15:3486.
18. Savin AV, Klinov AP. Supplementary materials for the article "Wrinkles in graphene suspended on flat substrates: structure and collapse under hydrostatic pressure" [Internet]. Zenodo; 2025. Available from: https://doi.org/10.5281/zenodo.15481045
19. Savin AV, Klinov AP. Wrinkles in graphene suspended on flat substrates: structure and collapse under hydrostatic pressure. **Phys Rev B.** 2025;111:245403.