Bulletin of Pure and Applied Sciences.
Vol.39 D (Physics), No.2,
July-December 2020 P.135-139
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: 10.5958/2320-3218.2020.00020.2
Available online at www.bpasjournals.com

Transport Properties in Chemically Doped Metallic Nanotubes

Anand Kumar Singh*, Ashok Kumar

Author's Affiliations:

Anand Kumar Singh
Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, Bihar 852128, India.
E-mail: tryanandkumarsingh@gmail.com

Ashok Kumar
University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, Bihar 852128, India.
E-mail: ashokabnu@gmail.com

***Corresponding author:**
Anand Kumar Singh
Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, Bihar 852128, India.
E-mail: tryanandkumarsingh@gmail.com

Received on 09.04.2020
Accepted on 10.10.2020

ABSTRACT

We have studied the transport properties in periodic chemically nitrogen doped metallic nanotubes. We have found that the ballistic properties of carbon nanotubes remained for some doping configurations. It was also found that the resonant effect associated with specific symmetry of the wave function was close to the Fermilevel. We have shown that both axial and screw periodicities gave rise to such a behavior and that specific but realistic disorder preserved this ballistic transport in doped metallic carbon nanotube. The properties which were four found during investigation are related to long range correlation effects predicted for the electronic properties and the quantum transport of nitrogen doped graphene when chemical dopic effects only one of the two sublattices of graphene. For the purpose of research paper we have used Green's formalism in the framework of the tight binding approach. We have found that conductance response was unchanged because one of the two conductance channels remained open for symmetry reasons. It was also found that the energy of the quasibound states depend on the specific local modification but not based on the symmetry of the quasibound states. The bound properties remained true for both armchair and chiral nanotubes. The obtained results were in good agreement with previously obtained results.

KEYWORDS Transport, periodic, doped, metallic, nanotube, ballistic, symmetry.

INTRODUCTION

Lin et al.[1] had observed the local electronic perturbation of a single nitrogen substitution by electron energy loss spectroscopy and scanning tunnel microscopy but macroscopic samples are mainly characterized by a disordered distribution of defects with different atomic structures as confirmed by transport measurements[2] photoemission spectroscopy[3]. Latil et al.[4] predicted that a small amount of dopants nearly 0.5% with random distribution drastically affects the quantum conductance of the nanotube at the required energy. At this energy the quantum resistance increases exponentially with the system length as a clear consequence of the Anderson localization phenomenon[5]. This localization effect has been numerically simulated for substitutional chemical defects[6] and verified experimentally

for different types of topological defects[7]. Biel et al.[8] predicted anomalous doping effects for chemically doped carbon nanoribbons. Applications as diverse as nanoelectronics, sensors, medical imaging, flexible electronics, and photovoltics have been proposed by Jorio et al.[9]. Poor control of growth mechanism has curved the development of devices with adjusted intrinsic properties, even if post synthesis chirality sorting is improving[10]. Chemical doping and functionalization have been investigated to overcome this limitation and to tailor the electronic and structural properties of carbon nanotubes, nitrogen and Boron chemical substitutions are popular since they only slightly modify the atomic structure of the carbon network[11]. Choi et al.[12] studied the effects of an isolated nitrogen or boron atom on the transport properties of an armchair carbon nanotube have been examined revealing a drop of conductance from the ballistic at the specific quasibound states energy located at about 0.5eV above the Fermi level. Tison. Y et al. studied tunnel spectroscopy[13]. The obtained results were compared with previously obtained results.

METHOD

For the purpose of our work we have used Gaussian law. The onsite effective parameters of the carbon atoms are modified around the defect up to a distance $d_c \approx 7.5\text{Å}$ along the surface of the tube. Then

$$\varepsilon(d) = \varepsilon_c - |U| \exp\left(\frac{-0.5d^2}{\sigma^2}\right).$$

Where ε_c is the asymptotic on site energy of carbon, U and σ are the depth and width of the potential well induced by the nitrogen atom. Fitting on the ab initio calculations,

$|U| \approx 6e\text{V}$ and $\sigma = 15\text{Å}$.

The qunantum conductance and the density of states are computed in the framework of the Green's formalism. Propagating media is embedded between two semi infinite perfect structures as left and right leads. The corresponding Hamiltonian H_C , H_L, H_R and the hopping matrices l_{LC}, h_{CR} are constructed and the Green's function of the device is obtained.

$$gc = \left(\varepsilon - H_C - \Sigma_L + \Sigma_R\right)^{-1}$$

$\Sigma_L = h_{LC}^{+} g_L h_{LC}$ and $\Sigma_R = h_{RC} g_R h_{RC}^{+}$ are the left and right self energies while $g_{L,R} = \left(\varepsilon - H_{L,R}\right)^{-1}$ are the Green's functions of the left and right leads. The conductance response G is obtained from

$$G = Tr\left[\Gamma_L g_c^r \Gamma_R g_C^a\right]\frac{2e^2}{h},$$

Where $T_{L,R} = i\left[\Sigma_{L,R}^r - \Sigma_{L,R}^a\right]$ are the coupling matrics at the interfaces $\frac{C}{R}$ and $\frac{C}{L}$. $\Sigma_{L,R}^a$ and $\Sigma_{L,R}^r$ are Hamiltonian conjugates. The *r* and *a* superscripts correspond to the retarded and advanced Green's functions. The density of states per spin is obtained from

$$\text{dos}(E) = \frac{1}{\pi}\text{Im}\left\{\text{Tr}\left[gc(E)\right]\right\}.$$

Tr is the trace of the matrix and Im is the imaginary part.

RESULTS AND DISCUSSION

Figure 1 shows the effect of two successive cavities with different sizes d_1 and d_2 is shown for constant $d_1 + d_2 = 30d_0$. The conductance plateau G_0 is preserved around the quasibound energy Ed when d_1 and d_2 the sized of super cells are both multiples of $3d_0$ even if they are different. This indicated that one conduction channel remains open even if the dopants are not periodically positioned along the tube axis as long as the distance between them is related to the periodicity of the wave function. The cavity effect for longer systems is shown in Figure 2(b). Figure 2(b) also shows the averaged electronic density of states and the transmission coefficient are present for a periodic arrangement of the nitrogen dopant, for a system with random axial position of the nitrogen dopant and for a system with pseudorandom axial position such that each $d_{N\text{-}N}$ is always a multiple of $3d_0$. For totally random $d_{N\text{-}N}$ the propagatiog electron waves are fully backscattered around Ed and no conductivity is observed. The propagating media behave like and Anderson insulator in this energy domain. High density of states is also observed in the last two cases associated with the Anderson localization process for one of the conduction channels while the other channel remains open. A difference between the periodic configuration and the random $3nd_0$ is observed at other energies. We also studied the conductance of doped nanotubes with a screw periodicity of the defect positions. Both ordered and disordered cases were examined for the same systems characterized by $d = 15d_0$ and $n = 8$ supercells. The transport properties are not modified if we introduce a circular disorder in the doping scheme as long as the dopants remain on the same lattice. Other rotational disorders close to the remaining conduction channel and lead to an electronic transport gap around E_d. We have further studied metallic nanotubes on the Bloch like behavior of electronic transport in disordered chemically doped systems. The rotational disorder was examined for the nitrogen doped, we found that a rotation $\Delta\phi$ around the tube axis of the second i.e central nitrogen atom does not qualitatively modified the conductance if it corresponds to the threshold axis of the nanotube while other rotation angles open a conduction gap.

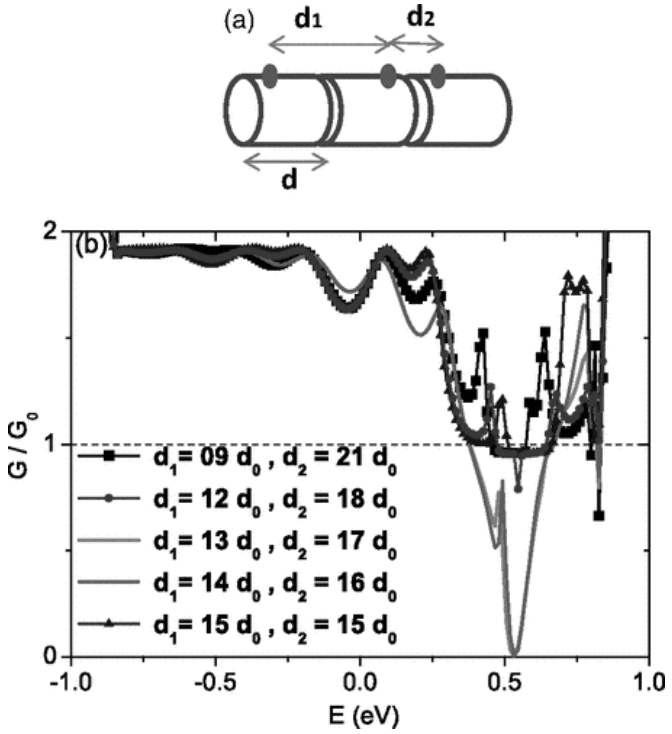

Figure 1: Conductance of a (10, 10) CNT with three nitrogen atoms, separated by distances d_1 and d_2. The total distance $d_1 + d_2$ is kept at $30d_0$(d_0 = 2.46Å).

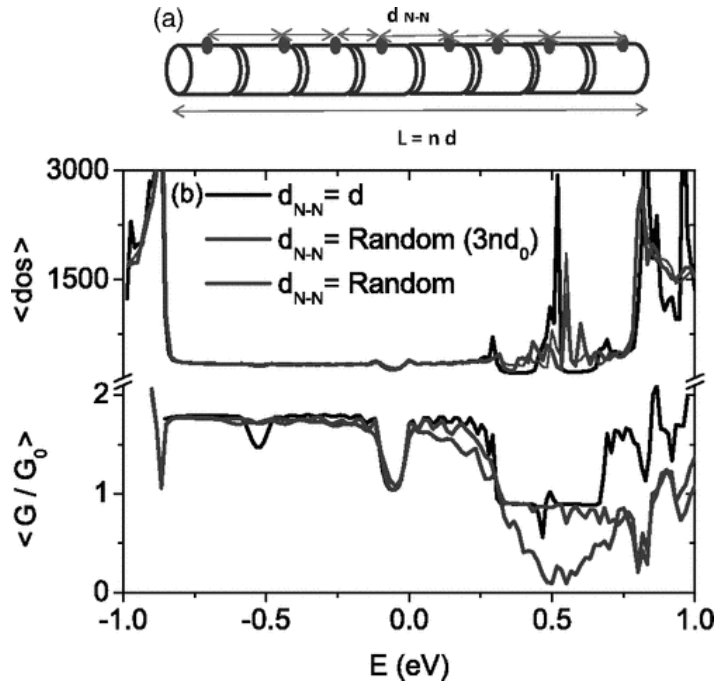

Figure 2: (a) Schematic representation of the random axial disorder $(n=8)$. (b) Averaged conductance $\langle G \rangle$ and averaged density of states $\langle \mathrm{dos} \rangle$ of a nitrogen-doped CNT for different distribution of $d_{N-N}: d_{N-N} = d = 15d_0$ corresponds to order defective case while for the disordered configurations d_{N-N} is a random multiple of $3d_0$ or d_{N-N} takes totally random values.

CONCLUSION

We have studied transport properties in chemically doped metallic nanotubes. We have found that one quantum conductance plateau was settled down around the defect energy only when the period of the structure is a multiple of the Fermi wave length. A conduction gap was also predicted. Resonant electronic transport was observed when the rotational angles fulfill one of the rotational symmetries of perfect nanotube. If correlations between the defects are present delocalized states are obtained. As soon as the defect distribution preserves some symmetry of the original system extended Block- like states were obtained, even for infinite defective systems providing an enhancement of the transport properties for some transmission channels. We also found that both axial and screw periodicities gave rise to such a behavior and that specific disorder preserved ballistic transport in doped metallic carbon nanotube. The obtained results were found in good agreement with previously obtained results of theoretical and experimental works.

REFERENCES

1. Lin. H, Lagoute. J., Chacon. C, Arenal. R, Stephan. O, Repain. V, Gira. Y, Enouz. S, Bresson. L, rousset. S and Loiseau. A, (2008), Phys. Status solidi B, 245, 1986.
2. Ayala. P, Arenal. R, Loiseau. A, Rubio. A, and Pichler. T, (2010), Rev. Mod. Phys. 82, 1843.
3. Kristic. V, Rikken. G. L.J.A., Bernier. P, Roth. S, and Glerup. M, (2007), Europhys. Lett. 77, 37001.
4. Latil. S, Roche. S, Mayou. D and Charlier. J. C., (2005), Phys. Rev. Lett. 92, 256805.
5. Anderson. P. W., Thouless. D. J., Abrahams. E, and Fisher. D. S. (1980), Phys. Rev. B, 22, 3519.
6. Adessi. C, Roche. S, and Blasé. X, (2006), Phys. Rev. B, 73, 125414.
7. Gomez. Navarro. C, Pablo. P. J. De., Gomez.-Herrero. J, Biel.B, Garcia-vidal. F.J, Rubio.A and Flores. F, (2005), Nat. Mater. 4, 534.

8. Biel. B, Blase. X, Triozon. F and Roche. S, (2009), Phys. Rev. Lett. 102, 096803.
9. Jorio. A, Dresselhaus. G, Dresselhaus. M. S, (2008), Carbon Nanotubes : Advanced Topics in the Synthesis, Structure and Applications (Springer, Berling, 2008).
10. Tu.X, Monohar. S, Jagota. Akl and Zheng. M, (2009), Nature, 460, 250.
11. Zheng. B, Hermet. P and Henard. P, (2010), ACS Nano.4, 4165.
12. Choi. H. J., Ihm. J, Louie. S. G and Cohen. M. L, (2000), Phys. Rev. Lett. 84, 2917.
13. Tison. Y, Lin. H, Logoute. J, etal (2013), ACS Nano. 7, 7219.