Original Article

Bulletin of Pure and Applied Sciences.
Vol.37 D (Physics), No.1, 2018: P.7-10
Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: 10.5958/2320-3218.2018.00002.7

Resonant Features in Bilayer Nanoribbons in a Single Mode Regime with a Short Range Defect

Gautam Kumar Sinha[1], Om Prakash Singh[2]

Author's Affiliations:
[1]Research Scholar, University Deptt. of Physics, J.P. University, Chapra, Bihar, India, 841301
[2]University Department of Physics, J.P. University, Chapra, Bihar, India, 841301

Corresponding author:
Gautam Kumar Sinha
Research Scholar,
University Deptt. of Physics,
J.P. University, Chapra, Bihar, India, 841301

E-mail: gautamkumarsinha@gmail.com

Received on 17.02.2018,
Accepted on 26.03.2018

Abstract

We have studied resonant features in bilayer nanoribbon in a single mode regime with a short range defect. We have found the effect of edge disorder on the transport properties of a graphene nanoribbons and bilayer graphene nano-ribbons. We have developed an analytical approach that provides the exact results for the transmission coefficients of graphene nanoribbons. We have considered the case of bilayer graphene nanoribbons with zigzag and armchair edges. We have found that for the case of zigzag edge bilayer nanoribbon remain practically insensitive to the disorder situated close to the edges. This behavior is not related to the chiral edge state residing at the zigzg boundary, as this behavior persist into the few mode regime as well. It is related to the effective boundary condition at the zigzag edge which does not couple valleys, thus hindering the intervally scattering due to the edge disorder. The armchair edge mixes the valleys and it is found that the conductance of a graphene nanoribbons and a bilayer graphene nanoribbons is strongly affected by a small defect concentration. We have calculated the conductance in bilayer graphene nanoribbons with many defects on the basis of tight binding recursive Green's function technique.

Keywords: Resonant, bilayer, nanoribbon, defect, disorder, transport, graphene, transmission, chiral edge, scattering, conductance, Green function.

1. INTRODUCTION

Han et al [1] and Lin et al [2] presented pronounced feature of transport experiments in graphene nanoribbons is the absence of conductance quantization. This effect was observed in conventional

semiconductor quantum wires and quantum point contact systems. Novoselov et al [3] studied the electronic and transport properties of nanoribbons. A number of various techniques have been developed to fabricate graphene nanoribbons. Molitor et al [4] presented electron beam lithography and etching technique for this purpose. Cai et al [5] used bottom-up approach to study the transport properties of bilayer nano ribbons. Areshkin et al [6] and Wurm et al [7] theoretically studied the effect of disorder in graphene nanoribbons in many different context including the transport gap formation, suppression of quantization, symmetries, and localization, Meyer et al [8] showed the effect of disorder in the bulk of graphene nano-ribbons such as charged coulomb impurities can be reduced by using suspended samples. Schedin et al [9] presented that vacancies and defects have a small concentration in high quality exfoliated samples. Evaldsson et al [10] and Mucciolo et al [11] demonstrated that edge disorder is largely responsible for the formation of the transport gap and the suppression of the conductance quantization. Zig zag and armchair edges probed by scanning tunneling spectroscopy exhibit different features of the standing wave patterns were presented by Park et al [12] and Chen et al [13]. Wakabayashi et al [14] demonstrated remarkable property of graphene nano ribbon attributed to the single valley transport caused by the existence of a chiral mode propagating at the edge of the graphene nanoribbons.

2. METHOD

We have used the standard nearest neighbor p-orbital electron tight binding Hamiltonian of the form $H = H_0 + V_0$, where H0 is the kinetic energy operator and V_0 describes the electron scattering on defects. Bilayer graphene is considered in the form of Bernal stacking. The kinetic energy operator has the form

$$H_o = -\gamma_0 \sum \left(a_{l,i}^{\dagger} b_{l,i+\Delta} + \text{H.c.} \right) - \gamma_1 \sum_i \left(a_{1,i}^{\dagger} a_{2,i} + \text{H.c} \right) - \gamma_3 \sum_i \left(b_{1,i}^{\dagger} b_{2,i} + \text{H.c} \right) \quad \ldots (1)$$

where $a_{l,i}^{\dagger}\left(a_{l,i}\right)$ and $b_{l,i}^{\dagger}\left(b_{l,i}\right)$ are the creation (annihilation) operators for sublattices A and B in the layer l = 1, 2 in the unit cell i. γ_0 is the nearest-neighbor hopping energy within one layer ($\gamma_0 \approx 3.16$ eV). For Bilayer graphene nanoribbons we have assumed $\gamma_1 = \frac{0.39}{3.16}\left[\gamma 0\right]$ and γ_3 = 0, we have considered the minimal low-energy model. The sublattices A_1 and A_2 are situated on the top of each other, where as sites belonging to B_1 and B_2 are displaced. The scattering on defects is written as

$$V_0 = U \sum_{i:l=1,2} \left(a_{l,i}^{\dagger} a_{l,i} + b_{l,i}^{\dagger} b_{l,i} \right) \quad \ldots . (2)$$

where the summation runs over defected sites with the on-site potential U. All energies in the unit of strong hopping energy γ_0 for bilayer graphene. We have used a model of the strong short range scattering setting U=100 in numerical calculations and setting $U \to \infty$ in analytical ones. For bilayer graphene nanoribbons calculations were performed numerically on the basis of the recursive Green's function technique. Green's functions of every slice in the scattering region were calculated and recursiovely coupled by the Dyson equation to obtain the Green's function of the whole scattering region. The surface Green's functions of the Bloch states of the infinite leads. The transmission and the conductance at zero temperature is provided by the Landau formula.

$$G = \frac{2e^2}{\hbar} \sum_{\alpha,\beta} T_{\beta,\alpha}, T_{\beta,\alpha} = \left| t_{\beta,\alpha} \right|^2 \quad \ldots . (3)$$

Where $T_{\beta,\alpha}$ and $t_{\beta,\alpha}$ are the transmission coefficient and transmission amplitude from the incoming state α in the left lead to the outgoing state β in the right lead. We have calculated the local density of state of graphene nanoribbons with defect.

3. RESULTS AND DISCUSSION

We have presented the results for the conductance of nanoribbons with single mode defects. The calculations have been performed for bilayer graphene nano-ribbons of width, 23.71nm and armchair bilayer graphene nanoribbons of width 23.73nm. We have considered zigzag and armchair nanoribbons with a single defect at the edge. Resonant features are shown in fig 1(c) and 1(d). The transmission of the bilayer graphene nano-ribbons as shown in fig 1(c) and 1(d) is practically unaffected by the defect and exhibits a narrow resonance when the defect is on sublattice. The ribbon's transmission is more suppressed in comparision to the case of graphene nano-ribbons and shows a broad dip in the energy region of the first propagating mode. The transmission of bilayer graphene nanoribbons is affected very little when the defect is on sublattice. Graph (1) shows that the transmission depends on the defect positions across a nanoribbon in the energy interval of the first propagation mode. The transmission of graphene nanoribbons and bilayer graphene nanoribbons for certain defect position is unaffected by the presence of defect as shown in graph (1) (b) and (1) (d) corresponding to T=1, because in these positions the wave function of armchair ribbons vanishes. If defect situated sufficiently close to the edge of bilayer graphene nanoribbons, the transmission in the first code and in the few mode regime remains unaffected when T□1. When the defect is moved from the ribbon's edge the influence of the edge diminishes and the backscattering becomes possible. Which is shown in graph (1) (a) where the transmission coefficient decreases from its value T=1 when the distance from the edge increases. This allows the back scattering by the short range defects regardless of their distance from the edge. This holds true regardless of number of propagating modes in the ribbon as shown in the graph (1)(b). A single defect in an infinite graphene sheet accommodates a localized quasibound state with the energy E=0. The wave function of this state vanishes at the sublattice hosting the defect and is localized around the defect at another sublattice. The observed resonant dips in the transmission of nanoribbons represent Fano resonances that originate from the interference of an extended state in the ribbon with a weakly coupled quasibound state residing at the defect.

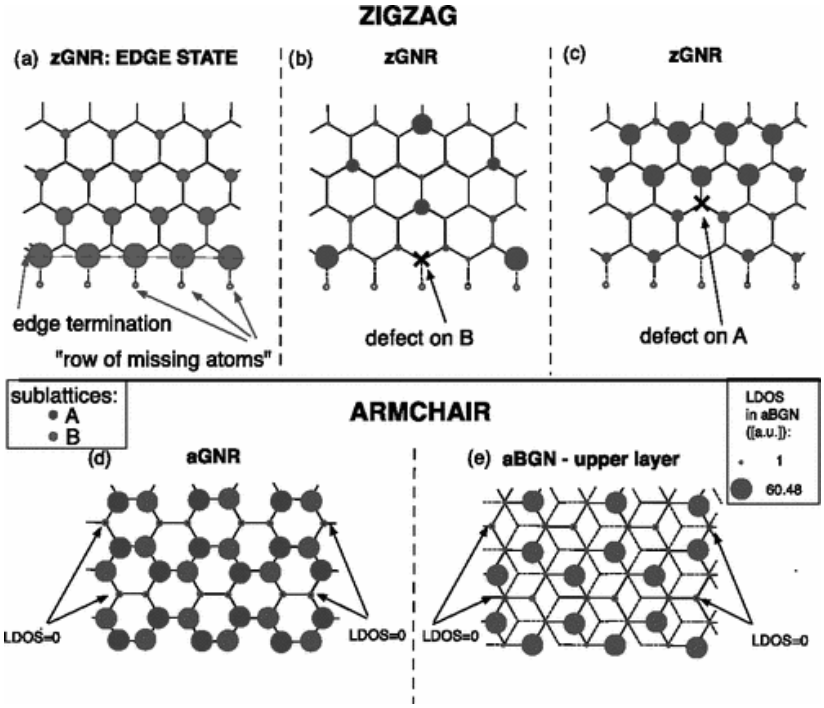
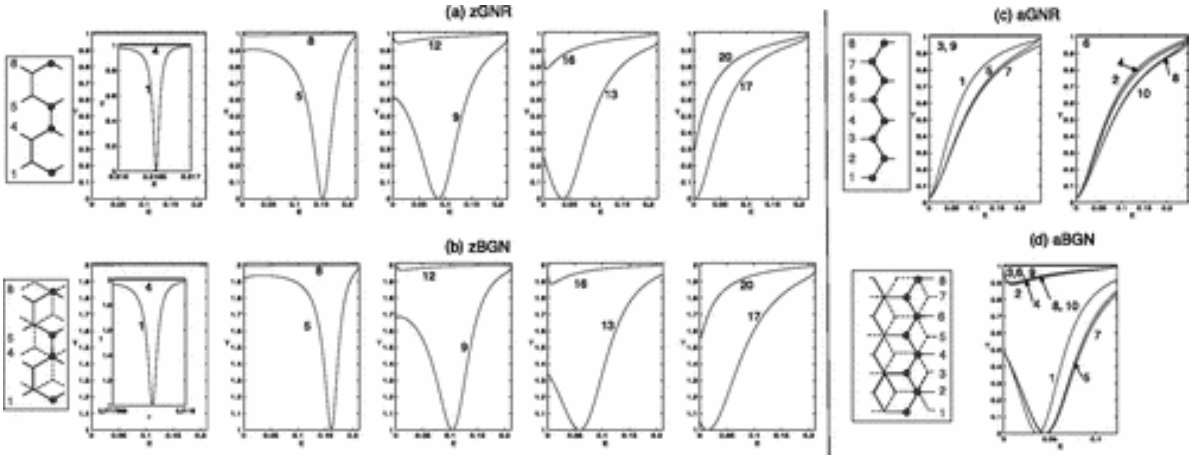


Fig 1: LDOS for bilayer zigzag and armchair nanoribbons in the energy interval corresponding to the first propagating mode.



Graph 1: Resonant dips in the transmission of a (a) zGNR, (b) zBGN, (c) aGNR, and (d) BGN with a single defect situated at different distances from the ribbon's edge.

4. CONCLUSION

We have calculated an analysed the local density of state of a ribbon with defect for the resonance features. The wave function is localized at sublattice. The wave function of the quasi bound state of such a defect is strongly affected by the presence of the edge. The resonant state cannot be localized in the immediate vicinity of the defect sublattice, because the edge strongly suppresses the wave function and the wae function has to vanish at the neighboring row of missing atoms. The quasibound state of a defect in bilayer graphene is localized in the layer where the defect is situated and has the same structure as the localized state in monolayer graphene. Calculations for bilayergraphene nanoribbons were performed numerically on the basis of the tight binding recursive Green's function technique. Bilayer nanoribbons with a short range defect show resonance features in the lowest energy mode. For high energies the armchair and zigzag ribbons becomes equally sensitive to the edge disorder. For the disorder preserving the edge topology, the conductance of bilayer graphene nano ribbon is a single mode regime remains unchanged in comparison to the ideal case.

REFERENCES

1. Han. M.Y. ozyilmaz. B, Zhaug. Y and Kim. P., (2007), Phys. Rev. Lett, 98, 206805.
2. Lin, Y. M., Perebeinos. V, Chen. Z and Avouris. P., (2008), Phys. Rev. B., 78, 161409.
3. Novoselov. K.S., Geim. A.K, et al (2004), Science, 306, 666.
4. Molitor. F, et al (2009), Phys. Rev. B., 79, 075426.
5. Cai. J. et al (2010), Nature (London), 466, 470.
6. Areshkin. D.A., Gunlyeke. D, and White. C.T. (2007), Nano Lett. 7, 204.
7. Wurm. J, Wimmer. M and Richter. K, (2012), Phys. Rev. B., 85, 245418.
8. Meyer. J.C., et al (2007), Nature (London), 446, 60.
9. Schedin. F, et al (2007), Nat. Mater, 6, 652.
10. Evaldsson. M, Zozoulenko. I.V., Xu.H. and Heizel. T., (2008), Phys. Rev. B., 78, 161407.
11. Mucciolo. ER, Castro Neto. A.H., and Lewenkopf. CH. (2009), Phys. Rev. B, 79, 075407.
12. Park. C. et al (2011), Acad. Sci, (U.S.A), 108, 18622.
13. Chen. X. et al (2011), ibid, 98, 093111.
14. Wakabayashi. K. Fujita. M, Ajiki. H. and Sigrist. M. (1999), Phys. Rev. B., 59, 8271.