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SYSTEMATIC STUDIES OF THE ELECTRONIC TRANSPORT IN REALISTIC EDGE DISORDERD GRAPHENE NANORIBBONS

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Abstract

We have made systematic studies of the electronic transport in realistic edge disordered graphene nanoribbons with, both zigzag and armchair edges. Three different defect topologies were examined. The stone-wales mechanism reconstructs zigzag graphene nanoribbon edges into alternating pentagon-heptagon pairs, while in a armchair it causes two separate armrest hexagons to merge into adjacent heptagons. In realistic defect topologies we first relaxed the atomic geometries using density functional theory. In tight binding parameters for the relaxed geometries from the standard quantum chemical parametization of the extended Huckel model was considered. The calculated conductances revealed strong backward scattering and electron hole symmetry depending upon the edge and defect. An additions defect induced band whose wave function was poorly matched to the propagating states of the pristine ribbon. We found that the electron-electron interactions gave rise to charge redistribution towards the edges of the ribbons when gating shifted the ribbon Fermi energy away from the Dirac point.

Keywords: Nanoribbons; Dirac point, Ribbon Fermi energy.

INTRODUCTION

Dubois etal [1] studied that realistic edge topologies strongly affect electron transport in the armchair graphene nano ribbons. He showed that conductance can be suppressed by orders of magnitude for electrons or holes depending upon the defect geometry. Hawkins etal [2] studied a few defect topologies for armchair and zigzag graphene nanoribbons, they showed that pentagon and heptogon edge reconstructions to have little effect on the ribbon conductance near the Dirac point Fernandez-Rossier etal [3] and Ihnatsenka etal [4] showed that electron-electron interactions modify electron conduction in graphene nanoribbons substantially when the electron Fermi level is not at the charge neutrality point, electrons are predicted to accumulate along the edges of the ribbon. Han etal [5] and Molifor etal [6] reported that the transport gaps measured experimentally in graphene nanoribbons. Evaldson etal [7] and Mucciolo etal [8] studied theoretically the electronic transport properties of graphene nano ribbons. Kobayshi etal [9] and Koskinen etal [10] studied experimentally and characterized individual edge effects by means of Raman spectroscopy, scanning tunneling microscopy or transmission electron microscopy. Song etal [11] and Huang etal [12] reported the high degree of chemical reactivity of graphene edges favoured edge reconstruction with different topologies in ab initio calculations. The obtained results were compared with previously obtained theoretical and experimental results.

METHOD

Ihnatsenka method has been used for the purpose of the work. The space Hartree potential was uses as

$$V^H(\mathrm{r}) = \frac{e^2}{4\pi\varepsilon_0\varepsilon}\int d\mathrm{r}' \sum_k \frac{n_k(\mathrm{r}')}{\sqrt{|r-r'|^2 + b_k^2}}$$

Where $-en_k(r')$ is the *k*th electron charge placed at distance b_k from the graphene layer. The edge reconstruction was introduced as randomly located defects at the edges of the hexagonal graphene lattice. We have used geometry relaxations for the edge reconstruction in graphene nanoribbons using Gaussian 09 software package. The carbon atoms belonging to the defect core as well as several nearest atoms at the edge were allowed to relax freely, the other carbon atoms being held fixed in the standard hexagonal graphene geometry was kept planar. The matrix elements in the Hamiltonian given below

$$H = \sum_i \left(E_i + V_i^H\right) a_i^\dagger a_i - \sum_{(i,j)} t_{ij}\left(a_i^\dagger a_j + H.C.\right)$$

were modified to account for reconstructed topology by calculating the relevant matrix elements within the extended Huckel model. The E_i is the bare atomic orbital energy on atom i, t_{ij} is the matrix element between nearest neighbor atoms V_i^H is the Hartree potential at atom i which results from the coulomb interaction with the uncompensated charge density $(-e_m)$ in the system. The conductance was obtained by the relation as the function of Fermi energy

$$g = \frac{-2e^2}{h}\int dE \sum_{ij} T_{ij}(E) \frac{\partial f\left(E - E_f\right)}{\partial E}$$

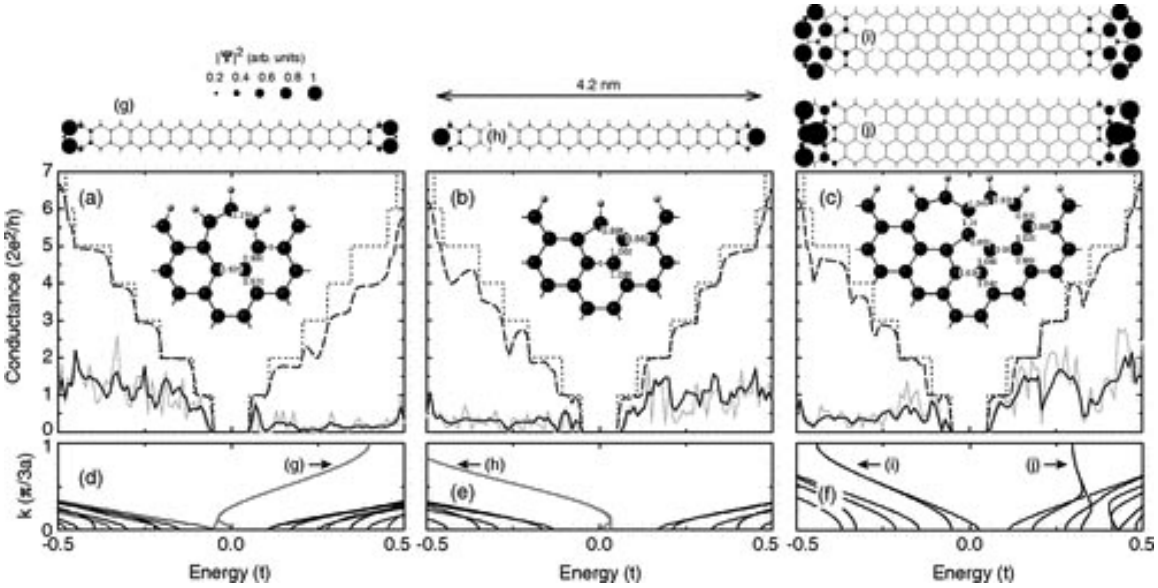
RESULTS AND DISCUSSION

We have studied transport properties in realistic edge disordered graphene nanoribbons. Graph (1) shows the conductances of graphene ribbons with heptagon edge defects. The conductance for a single relaxed heptagon developed stronger back scattering for higher electron subbands. When the defect concentration grows the conductance becomes suppressed more strongly with pronounced oscillations due to quantum wave interference in the case of armchair ribbons. For sufficiently large defect concentrations the electron transport mechanism undergoes a transition from ballistic transport to Anderson localization. We found that if the heptagon defect is repeated periodically along the edges of the ribbon an additional electron subband appears in the graphene nanoribbon spectrum mainly at positive energies. This additional subbands is poorly matched to the Blochstates propagating in the pristine graphene nano ribbon leads and results in strong electron backscattering in the positive energy range. For heptagon defects randomly distributed along the graphene nano ribbons edges this additional electron subband breaks up into electron defect states that also mediate electron backscattering giving rise to the much stronger suppression of electron conductance than hole conductance.

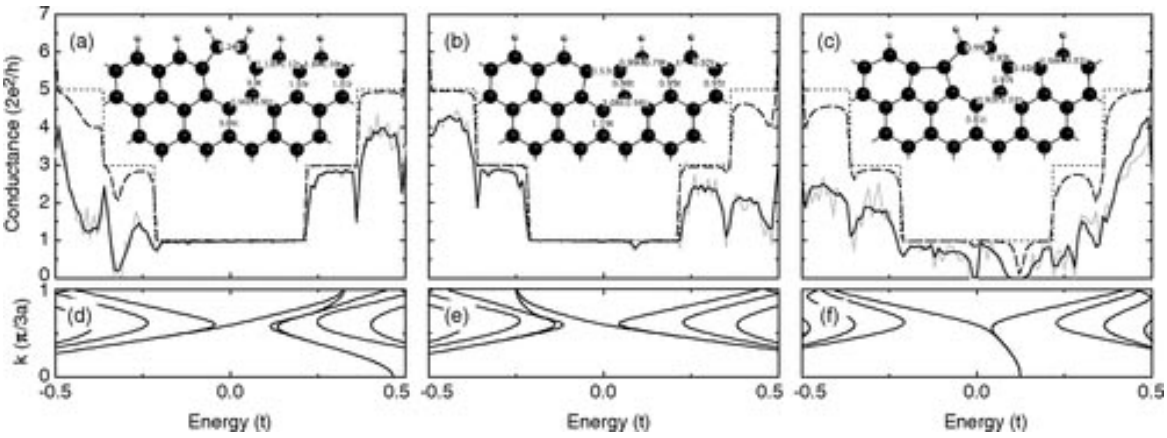
Graph (2) shows edge configuration for the zigzag ribbons. The pristine zigzag graphene nanoribbon supports a zero energy mode whose wave function is localized along the edges. This mode hybridizes with the defect states and no distinct defect bands occur in the band structures. The scattering of the carriers by the defects is generally weaker for the zigzag case. The zigzag 575 defect causes strong conductance suppression near the flat band of the structure with periodically repeated defects as shown in graph (2).

The strong modification of the subband in the previous cases results from the topological properties of the zigzag edge because it supports charge localization at the edges where defect form. Electron-electron interactions result in the redistribution of charge towards the ribbon edges where the edge defects are located. We found that this does not result in stronger electron backscattering by the edge defects in the Hartree approximation than in the noninteracting electron model.

The obtained results demonstrate strong charge scattering by the edge reconstruction defects. The scattering strength being different for electron and holes for both armchair and zigzag ribbons. In electron-hole asymmetry in the conductances of graphene nanoribbons with such defects are found. We also found that the transport gap in the graphene nanoribbon conductance to scale inversely with the ribbon width, it is also seen that edge reconstruction defects is responsible for the gaps observed in previous work. We found strong electron scattering due to reconstructed edge defects. We have seen that our study provided simple and realistic tight binding parameters for edge reconstruction defects and we have calculated the result in the extended Huckel model. When ribbon edges contain several different defects the combined effect on transport appears to be roughly additive. Equal concentrations of heptagon and pentagon defects restore electron-hole conductance symmetry and act to increase the transport gap value. The obtained results were compared with previously obtained results and were found in good agreement.



Graph 1: The conductances (a)-(c) and defect band structures (d)-(f) for armchair graphene nanoribbons with heptagon, pentagon and Stone-wales edge reconstruction defects, respectively.



Graph 2: For zigzag graphene ribbons, the ribbon dimensions W=4.2 nm and L=500 nm correspond to 20 carbon atoms in the cross section and 2033 unit cells along the device.

CONCLUSION

We made systematic studies of the electronic transport in realistic edge disordered graphene nanoribbons with both zig-zag and armchair edges. Three different defect topologies pentagon, heptagon and stone-wales were examined. We calculated conductance revealed strong backscattering and electron hole symmetry depending on the edge and defect. We found that a transport gap to open near the Dirac point. We have seen that electron interactions in two Hartree approximations cause accumulation of charge carriers on the defects. We found that the electron-electron interactions to give rise to charge redistributions towards the edges of the ribbons when gating shifts the ribbon Fermi energy away from the Diarc point. This resulted in enhanced concentrations of the charge carriers on the defects at the edges of the ribbon. Electron-electron interactions play a significant role in transport in graphene ribbons.

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