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Transport properties of zigzag graphene nanoribbons in the confined region of potential well

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ZGNR (zigzag graphene nanoribbon)
CNT (carbon nanotube)

A B S T R A C T

We report and adduced bandstructure by applying an external electrostatic potential inside the potential well or confined region, also outside the potential well. We study the electronic transport in ZGNR structures. We have utilized the non-equilibrium Green's function to calculate the Local Density of States (LDOS) and the transmission in the tight-binding framework. We want to study the confined (bound) states of an electron trapped inside the quantum well. We have studied the single subband in our system and calculated Transmission as well as the LDOS and charge distribution. The nearest neighbour tight binding model based on p_z orbital forms the Hamiltonian in our case. Transmission curves show oscillations with the increase of layers of unit cell in the confined region, as it used to happen in Fabry-Perot resonances. Charge distribution for the case of bound states has been discussed.

1. Introduction

Quantum Transport in mesoscopic devices is becoming a topic of great research. We are interested in ZGNR, since experimental-wise the zigzag GNR are relatively very easy to produce and their edges are very much favorable to form bonds with other atoms and as well with compounds [1–3]. Advancements in the field of Nanoscale technologies have resulted in the fabrication of GNR and CNT-based devices. These novel devices may dominate the future of electronics and computer industries. Hence, it becomes extremely important to study Physics and the modelling of these GNR and CNT based devices. The most important thing that one should study first is conductance of these novel materials, which will take the role of the channel in the futuristic nanoscale devices. Nano electronics and spintronic are becoming emerging fields day by day, and researchers have determined current corresponding to even single molecule [4]. This is due to its application in diverse fields, so that our devices can become more efficient and powerful. Graphene layers have honeycomb lattice of covalent-bond carbon atoms. As shown in Fig. 1 that number of unit cells are shown in the rectangular shape, can be called as slices of unit cells (M) and N should be multiple of 4. It can be treated as two different sub-lattices, which can be labelled A and B. Graphite-related materials have been a subject of interest. Graphene has superb electrical properties as well as thermal properties. In case of GNR [5], researchers have observed band gap, which was not there in case of graphene sheet. It can be used for device purposes, since we know that band gap is inversely proportional to width of GNR [1]. Edge states of ZGNR have been discussed in this work, since finite graphite systems having a zigzag edge exhibit a special edge states [6]. Researchers

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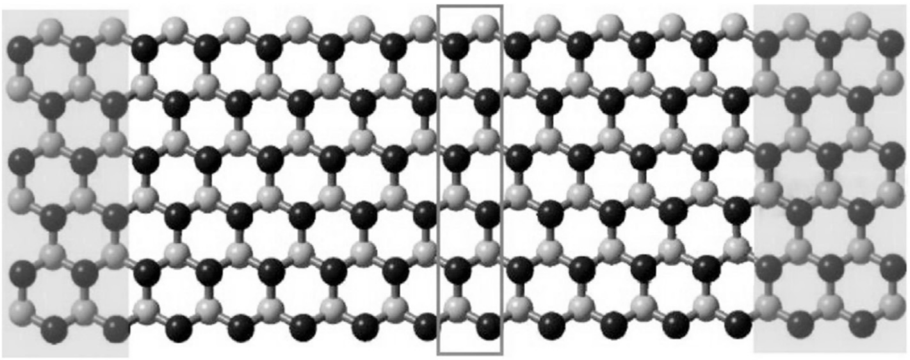

Fig. 1. Schematics of the transport channel connected to two semi-infinite Zigzag nanoribbons (shaded regions), in unit cell as shown in rectangle [16], having number of atoms per unit cells 12.

have investigated the microscopic understanding of the conductance reduction [7]. Due to special band structure, it has not high mobility, but also a lot of other extraordinary properties. It has opened a new possibility in the fields of microelectronics, semiconductor and other novel applications. The object investigation is ZGNR of finite length or ZGNR based quantum dot. In this work, we study the transport across a quantum dot created electrostatically by external potential as shown in Fig. 2. The red line indicates the constant energy given to create finite potential well and not the Fermi level (chemical potential) of the system. We have obtained this bandstructure in the first Brillouin Zone. We obtained band structure by diagonalizing Hamiltonian and plotted energies in terms of k. The object of investigation is to study the transport properties of ZGNR of finite length/ZGNR based quantum dot. The difference is that such structure is created electrostatically and which in principle is tunable.

Similar work has been done by applying gate voltage, where electric conductance of graphite ribbon with locally applied gate voltage has been studied using Landauer approach. Nanographite ribbon with zigzag boundaries exhibits the single electronic transport channel due to the edge states. Transmission probability is 1, i.e. perfect transmission. In this work, region sandwiched by the barriers plays the role of a quantum dot, while in our work, we have created potential well by fixing constant energy with red line Fig. 2 [8]. Researchers have studied GNR as Bulk Modes (BM), which are the basis solutions to the Schrodinger's equation. They have established a complete set of BM for graphene ribbons at arbitrary energy and demonstrate BMs for graphene ribbons at arbitrary energy. They demonstrate BMs uses in efficient electronic transport simulation of graphene based electronic devices with in the mode-matching method as well as Green's function method. They obtained complete sets of BMs for graphene and graphene ribbons for both ZGNR and armchair graphene ribbons at arbitrary energy [9]. We have shown in this Fig. 2, how the QW has been created and it is shown with red line that pictorially may cut some bands, will determine the value of k and also band number and transverse modes. It has nothing to do with edge states presented in Figs. 3 and 4. Researchers have also applied mode-matching approach to current blocking effect in GNR and shown that the randomness of the interface tilting destroys the parity effect. If the spread of tilting parameter is larger than the lattice constant, while we have not studied this effect in our work [10]. Our main motive behind this work is to show that GNR shows the metallic behaviour inside the confined region of potential well. Zigzag GNRs are metallic structures

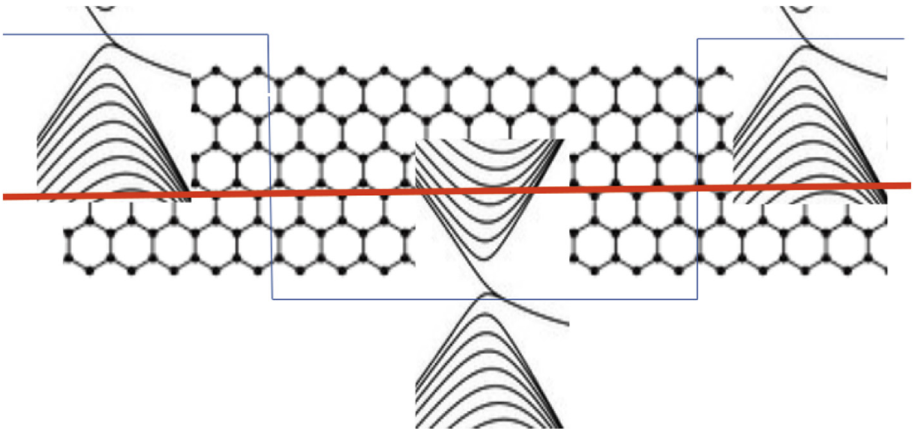

Fig. 2. Potential well created by applying an external potential, where red line shows the fixed energy. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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