Transport Gap Engineering in Zigzag Graphene Nanoribbons

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Graphene, a recently discovered form of carbon, has received much attention over the past few years due to its excellent electrical, optical, and thermal properties [1]. With an extraordinary carrier mobility and high current density [2], graphene's application in electronic devices is promising. As a zero band-gap material, pristine graphene cannot be used as a semi-conducting channel in transistors. However, there are several proposed schemes for opening up a band gap [3,4]. Graphene nanoribbons (GNRs) are thin strips of graphene, where the band gap depends on the chirality of the edge and the width of the ribbon. Zigzag GNRs (ZGNRs) show metallic behavior, whereas armchair GNRs (AGNRs) are semiconductors [3]. In recent years, AGNRs have been extensively studied as channel materials and ZGNRs as metalic electrodes in electronic devices [5,6].

The band-gap of AGNRs is inversely proportional to their width [3]. To obtain a band-gap of nearly 0.5 eV, the width of the ribbon should be around 2nm. On the other hand, it has been shown that line edge roughness and substrate impurities can significantly degrade the ballistic transmission in AGNRs [7]. The effect of these scattering mechanisms is more deteriorative in narrower ribbons. Therefore, high performance AGNR-based transistors can not be achieved. In this work, we suggest a new scheme to open up a transport gap in ZGNRs. In this approach, line edge roughness and substrate impurities are used as mechanisms for band-gap opening.

Ballistic transport through ZGNRs is sustained in the presence of line edge roughness and substrate impurities [8]. Very recently, transport properties of ZGNRs with extended line defects along the ribbon's length (ELD-ZGNR) has been studied [8]. In this work, we investigate the transport properties of this structure in the presence of line edge roughness and long-range substrate impurities. This structure is represented by two parameters (n_1,n_2), where n_1 is the index of ZGNR above the line defect and n_2 is the index below the line defect. In addition, we consider another topology of this defect, (see Fig.1-a), where two line defects parallel to the edges are presented in the ribbons, 2ELD-ZGNR, and represent this structure with three parameters (n_1,n_2,n_3).

To study the transport properties of electrons the non-equilibrium Green functions are used. The electronic Hamiltonian matrix is described by the first nearest-neighbor tight-binding model with a hopping parameter of −2.7 eV and the on site potential is shifted to zero so that the Fermi level remains at 0 eV. The band structure of ELD-ZGNR(10,10) and 2ELD-ZGNR(8,4,8) are shown in Fig.1-c and Fig.1-d. For comparison, the folded band structure of ZGNR(20) is also presented in Fig.1-b. The main differences between the band structures of ELD-ZGNR(10,10) and 2ELD-ZGNR(8,4,8) with the original band structure of ZGNR(20) are: i) the asymmetry between electrons and holes around the Fermi level with respect to the extra conduction subbands corresponding to the extended line defects and ii) band folding because of a larger unit cell in ELD-ZGNR and 2ELD-ZGNR. In contrast to ZGNRs, the first subband of ELD-ZGNRs and 2ELD-ZGNR are also sensitive to the long-rang defects because of band folding. However, as shown in Fig.2, the electron current density is confined around the line defects. In fact, a line defect behaves like a quantum wire in the middle of the ribbon. Therefore, the conduction bands corresponding to the line defects, indicated by dashed line in Fig.1, are less sensitive to the line edge roughness. As a result, it is possible to suppress transport of carriers through the first valence band and maintain transport along the first conduction band.

The average electron transmission probability over many samples is shown in Fig.3 for ELD-ZGNRs(5,5), ELD-ZGNR(10,10), and 2ELD-ZGNR(8,4,8). The mean free path of electrons in the conduction subbands is higher than that of holes in the valence subband because the quantum wire conduction takes place around the line defect which is far from the edges. Therefore, by increasing the length a transport gap is opened up. As expected, the mean free path is longer in wider ribbons. As a result, ELD-ZGNRs of (5,5) and (10,10), and 2ELD-ZGNR(8,4,8) need a length of around 250 nm, 2 μm, and 2 μm, respectively, to get an transport gap of nearly 0.2 eV.

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Figures

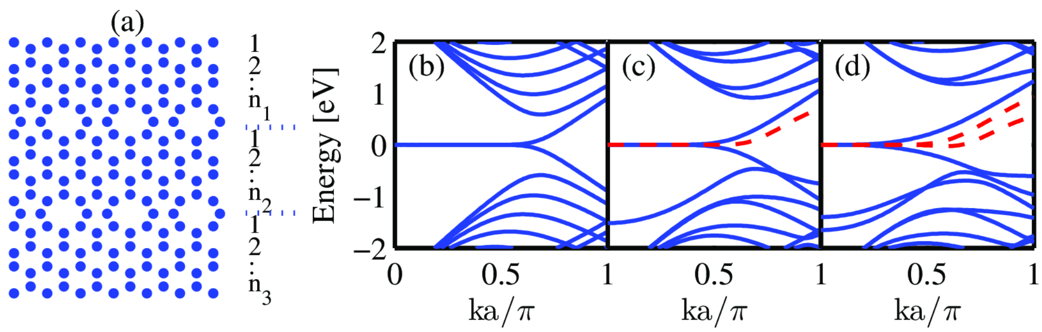

Fig.1: (a) The geometrical structure of ELD-ZGNR and 2ELD-ZGNR. The band structure of (b) ZGNR(20), (c) ELD-ZGNR(10,10), and (d) 2ELD-ZGNR(8,4,8). The band structure of ZGNR(20) is also folded for a better comparison. The bands corresponding to the quantum wires are represented with dashed lines. The translation vector length is a = 0.49 nm.

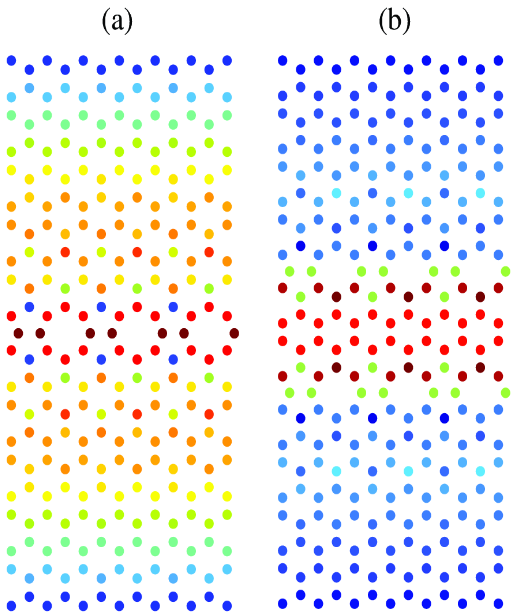

Fig.2: The quantum wire is represented by the current density at E = 0.2 eV for (a) ELD-ZGNR(10,10) and (b) 2ELD-ZGNR(8,4,8).

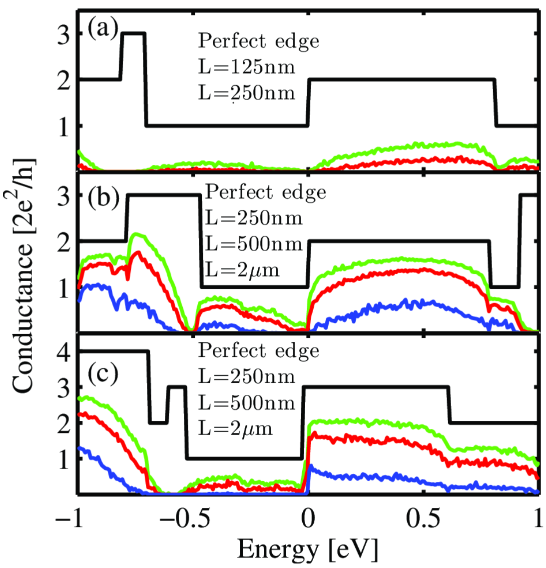

Fig.3: Electrical conductance of (a) ELD-ZGNR(5,5), (b) ELD- ZGNR(10,10), and (d) 2ELD-ZGNR(8,4,8).