Theoretical Study of a Zigzag Graphene Nanoribbon Field Effect Transistor

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Abstract

Graphene nanoribbons with zigzag edges show metallic behavior and are thus considered not appropriate for transistor applications. However, we show that by engineering line defects and using positive substrate impurities one can obtain a suitable effective transport gap at least for analog applications. The transfer and output characteristics of these structures are investigated employing quantum mechanical simulations and tight-binding model for the electronic structures.

Approach and Results

Graphene has received much attention for possible applications in nanoelectronics due to its excellent transport properties. However, as a zero band-gap material, graphene is not suitable for transistor applications. Graphene nanoribbons (GNRs) , on the other hand, are thin strips of graphene, whose electronic properties depend on the chirality of their edges and their width. Zigzag GNRs (ZGNRs) show metallic behavior, whereas armchair GNRs (AGNRs) are semiconductors with a band-gap inversely proportional to their width [1]. Therefore, AGNRs have been suggested recently as a channel material for transistors. For an optimal performance, the width (W) of the ribbons must be scaled down to 1-2 nm with an atomic edge precision. However, line-edge roughness and substrate impurities can significantly degrade their transport properties [2].

Although pristine ZGNRs are a zero band-gap material, as opposed to AGNRs, their ballistic transport can even be sustained in the presence of line edge roughness [3]. A bandgap, however needs to be achieved for transistor applications. In this work, we show that an “effective transport gap” can be opened up in ZGNRs in the presence of positive substrate impurities. It is even possible to increase the gap by embedding an extended line defect (ELD) as shown in Fig. 1. Here we note the ELD ribbon geometry by ELD-ZGNR(n,m), where n is the number of zigzag edges above and m the number below the line defect. Such ELD-ZGNR structures have been experimentally realized in Ref. [4]. The achievable gap can provide current saturation (Fig. 2a), and small but adequate I_{on}/I_{off} ratios for long channel analog transistor applications.

The electronic structure is described by a first nearest-neighbor tight-binding model. This model has been recently used to describe the electronic band structure of ELD-ZGNRs and the results are in good agreement with first-principles calculations [5]. For transport, the non-equilibrium Green's functions method is employed. The system geometry consists of two semi-infinite contacts and a channel of length L, as shown in Fig. 1. We consider rough edges, with the roughness extending up to four layers on each side of the ribbon.

By embedding an extended line defect, the transmission of electrons near the Fermi energy increases from one to two, whereas the transmission of holes remains at one. In addition, positive impurities in the substrate constitute a repulsive potential for holes (a barrier for holes but a well for electrons) and degrade the hole transport more than that of electrons. The presence of edge roughness and positive substrate impurities, therefore, induces an asymmetry between electron and hole transport, which acts as an “effective transport gap”, which can result in I_D-V_D saturation as shown in Fig. 2a. In addition, large transconductance can be achieved in these channels as shown in Fig. 2b, which is larger than values achieved in state-of-the-art III-V short channel transistors [6]. Such high transconductance indicate that EDL-ZGNRs could be candidates for analog transistor applications.

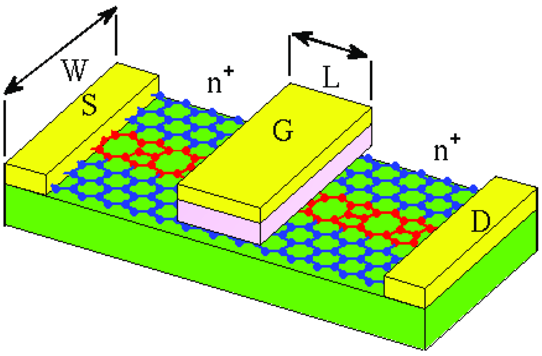

Fig. 1: Schematic of the device geometry. The extended line defect is shown in red. S, G, and D stand on the source, gate, and drain electrodes, respectively.

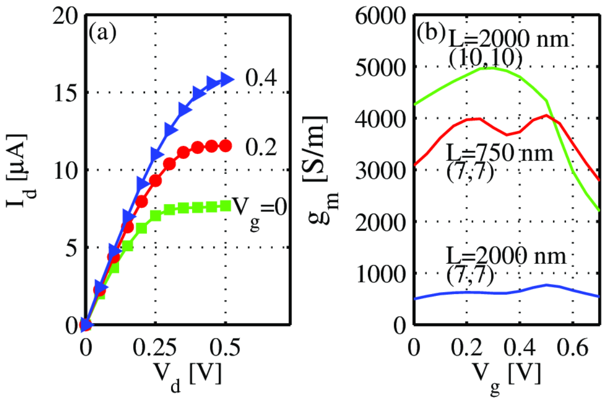

Fig. 2: (a)The output characteristic of the ELD-ZGNR(10,10) with L=2000nm and W=4.4nm. (b) The transconductance of ELD-ZGNRs with different widths and lengths. The Fermi level of the contacts is assumed to be 0.3 eV.

Conclusion

We show that an effective transport gap can be achieved in ZGNRs in the presence of positive substrate impurities and extended line defects. Our results indicate a transconductance in excess of 4500 S/m, a much larger value that the one achieved in state-of-the-art analog devices.

Acknowledgment

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