Ab-initio study of edge defects in Graphene Nanoribbon

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Introduction

Graphene is studied widely for its potential applications of nanoscale electronic/photonic/ spintronic devices [1]. All the superior properties of graphene encourage us to downscale graphene devices. Unnecessarily, edge irregularities/defects are created in the geometrically constricted regions during electron/ion beam exposure in the device fabrication process. These defects strongly affect the electronic properties of the device and consequently its transport characteristics are also affected.

Model and Calculation method

The GNR channel sandwiched between semi-infinite graphene electrodes (shown in Fig. 1) was used for the quantum transport calculations. The electronic states were calculated by using the density functional theory (DFT). The quantum transport was calculated by using the non-equilibrium Green's function (NEGF) method which is implemented in the OpenMX package [2]. The edges of the GNR and the horizontal edges of the electrodes are terminated by hydrogen atoms.

Results and Discussion

At first one single vacancy defect is created in the GNR channel as shown in Fig. 2. This structure was geometrically optimized to realize the stable structure. After the geometrical optimization, the defect region is rearranged to the structure shown in Fig. 3. Carbon atoms in the defected region self-organized to form dangling bond-less structure, which is inherent property of the graphene.

To study the electronics and transmission properties of the geometrically optimized single vacancy defect channel, Density of States (DOS) calculation and transmission analysis was done. Fig. 4 and Fig. 5 show the DOS and the transmission spectrum of the GNR device with geometrically optimized channel, respectively. From the DOS plot inception of mid-gap states near the fermi-energy level can be clearly noticed. By comparing the DOS and transmission spectrum plots, it can be clearly understood that mid-gap states are not contributing to transmission of electrons across the electrodes. Moreover, the values of transmission coefficients are lower compared to the pristine GNR channel at a given energy (Fig. 6). This is due to scattering introduced by edge irregularities. Even though there is no dangling bond present in the channel, the self-assembled defect region leads to scattering of the electrons. This indicates that edge irregularities play a very important role in the carrier transport.

To study the impact of increase in the number of defects at the edge, we have simulated one, two, and three defects channel. Its transmission spectra are given in Fig. 6. From this result, we can clearly see the increase in the scattering with the increase in the defects. On the positive side, the widening of the transport bandgap can be clearly notice from this result. This helps us to realize wider bandgap in the Graphene. In the conference, results of zigzag GNR will also be presented.

References

[1] Geim, A. K. & Novoselov, K. S. The rise of graphene. Nature Mater. 6, 183–191 (2007).
[2] http://www.openmx-square.org/

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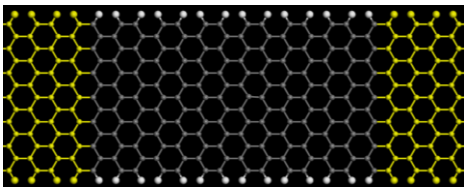

Fig. 1. Structure of the GNR channel sandwiched between semi-infinite graphene left and right electrodes (yellow coloured atoms).

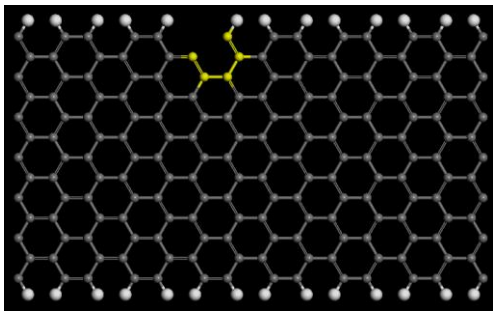

Fig. 2. GNR channel with single edge defect. The yellow bonds indicate the region of defect.

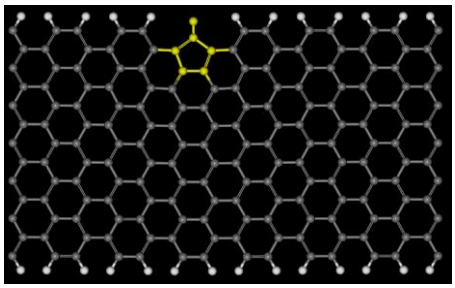

Fig. 3. Rearranged Single edge defect of the GNR channel after the geometrical optimization of the channel region.

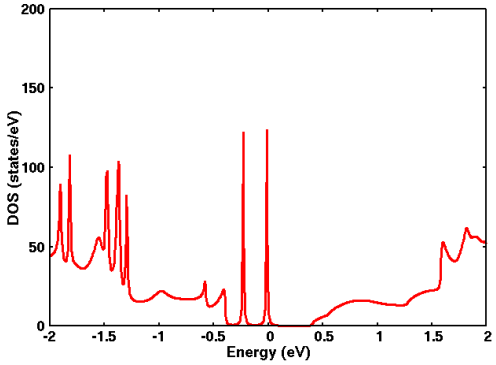

Fig. 4. Density of states of the geometrically optimized single edge defected GNR channel.

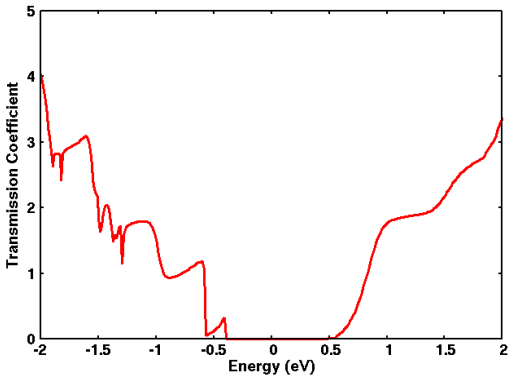

Fig. 5. Transmission spectrum of the geometrically optimized single edge defected GNR channel.

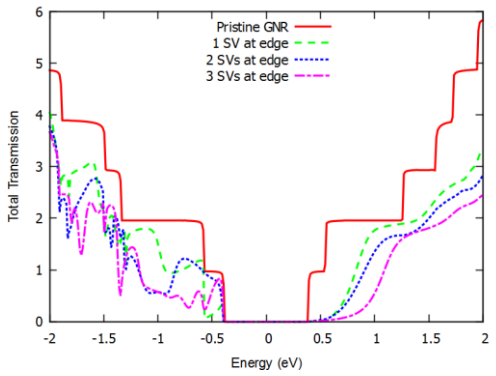

Fig. 6. Transmission spectra of the pristine GNR, and the GNR device with one, two, and three edge defects.