Simulation Field Effect Transistor Bipolar Graphene Nano-Ribbon

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Abstract

The purpose of this paper is to use software package ATK-SE package, in combination with virtual Nano-Lab (VNL), can be used to investigate a Nano-scale transistor. For the transistor structure we will use a graphene junction device, where ATK is used to investigate the properties of a similar system. The effect of various parameters on the structure of graphene Nano-ribbon checked. It consists of 3 regions and forms a metal-semiconductor-metal junction. By applying a gate potential to the central region, the system can function as a field effect transistor, which is able to calculate properties, Transmission spectrum, Temperature dependent conductance, Conductance and Current as function of gate potential and temperature. So in this paper, the device design and simulation parameters are associated with improved performance.

1. Introduction

Nano-technology consists of creating useful materials, pieces, and systems, and controlling them in linear Nano-meter scale and creating an ideal arrangement of molecules and atoms in order to produce new materials with desirable properties. Nano-structures have high surface volume ratio and as they are very small they can be used in creating the systems which have higher element density in comparison to other different scales. Thus, smaller electronic devices, faster instruments, more complicated functionalities, and very low energy consuming can be achieved simultaneously by controlling the reaction and complexity of Nano-structure. In the meantime, because of

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unique electrical and mechanical proper Nanotubes and graphene are attractive materials for making field effect transistors in Nano scale and have captured attention of a lot of scientists. Graphene are two-dimensional sheets of carbon atoms in a hexagonal configuration in which the atoms are jointed together by SP² hybrid. Graphene is called the magical material of 21st century. A unique material with a carbon-based and high atom density, it is the firmest material ever studied and with the highest electrical conductance among the known materials is a substitution for silicon. The unusual combination of its properties such as high mechanical solidity, adjustable high electrical and thermal conductance, with high optical and surficial properties by chemical functionalizing has received special attention of researchers. The fact that it is hard for chemists to find a substitution for graphene caused its abundant usage in Nano-electrics, solar batteries, and super condensers. The final goal of promoting transistors using high stimulatory of Carriers is for functioning in the output of 0.3-3 THz which has not been achieved yet. In this case, graphene which has a two-dimensional structure received attention and studied. Graphene’s measured high stimulatory, which is one of necessary prerequisites for quick transistors, can be used for small scaled transistors with higher functioning speed than common transistors. Lack of energy gap in graphene increases minimum current and decreases on/off current ratio noticeably. Nano-ribbons of graphene are used to create energy gap and proper on/off current ratio. Nano-ribbons of graphene are introduced as a detached ribbon, cut of a graphene sheet. The way of cutting graphene for producing Nano-ribbons of graphene is defined by a chirality vector. Nano-ribbons of graphene don’t have fit alternative marginal conditions, which the Nano-tubes have. Therefore, band structure of Nano-ribbons of graphene doesn’t have a solution for closed state and it should be calculated numerically. Advantages of devices designed by Nano-ribbons of graphene over other devices based on carbon are:

- GNRs with different width and edges can also be connected without failure.
- GNRs can properly be connected to other devices, especially to metallic GNRs with low connect resistance.
- Free edges in GNRs can be used to impure them.

Nano-ribbons of graphene have two kinds of armchair and zigzag according to the arrangement of carbon atoms. For creating a device with graphene connections which functions as a field effect transistor, we used Nano-ribbons of graphene connection as zigzag-armchair-zigzag. Metallic zigzag Nano-ribbons of graphene with six atoms in width and four times longitudinal repetition are as source and drain electrodes and the central part consists of Nano-ribbons of graphene of semi-conductor armchair with four atoms in width and five longitudinal repetition is as the channel of device. For this device, the lengths of the electrodes are selected 7.3 Angstrom. In this phase, a de-electric area under the central area is needed. Transforming the spatial area into a de-electric area with proportional de-electric co-efficiency of 4, and adding a second spatial and metallic area, applying -1V voltage, the GNRFET is created according to Fig. 1. Among the properties of this structure, we can point that it doesn’t need the entrance of impurity in source and drain electrodes because of their metallic properties.

![Fig. 1. The device system considered in this tutorial consists of a z-shaped graphene Nano-ribbon, on top of a dielectric and controlled by a metallic gate. The contour plot illustrates the electrostatic potential through the system.](image)

It consists of 3 regions and forms a metal-semiconductor-metal junction. By applying a gate potential to the central region, the system can function as a field effect transistor. We will calculate the following properties of the system.
2. Simulation

2.1. Bipolar property of GNRFET

Bipolar property in Z-A-Z structure means the passing of current by electrons in a range of gate voltage and by holes in another range of gate voltage. Fig. 2 shows bipolar conductance in device with 20 nanometer channel length and 0.1 V drain source voltage. It means that by increasing source gate voltage from minus amount to about half of drain source voltage, the role of hole carriers in conducting the current decreases gradually; and by increasing voltage to more than half of drain source voltage electrons function as major carriers in transmission of current, Tian et al. (2010). Band structure of graphene nanoribbons armchair semiconductor (7, 0) is shown in Fig. 2, for example.

Fig. 2. (a) Bipolar conductance in GNRFET; (b) GNR Band Structure of armchair GNRs (7, 0).

2.2. Transmission spectrum

For simulation and calculating Transmission spectrum ATK-SE: Extended Huckel calculator is used by applying marginal conditions for Poisson equation and applying Dirichlet marginal situation in one direction, and Neumann marginal condition related to 0 electric field in two other directions, with 1,1,50 sampling points and 200 points in energy range and labor energy of -2 to 2 eV, and -1 V gate voltage, the result of simulation is similar to Fig. 3. Note that the transmission spectrum has a low value in the energy range [-0.5, 1.5] eV, corresponding to the energy window within the band gap of the central semi-conducting armchair edge ribbon. The asymmetric position of the electrode Fermi levels relative to the band edges, i.e. the shift of the valence band edge of the central region towards the electrode Fermi levels, Nakada et al. (2005), is due to the applied gate potential of -1 V. To conceive the influence of gate voltage, electro-static potential discrepancy, in 3D state, is similar to Fig. 3.

Fig. 3. (a) Transmission spectrum of the z-a-z-6-6 graphene device structure with a gate potential of -1 V; (b) electrostatic potential discrepancy.

2.3. Calculating the temperature dependent conductance

Transmission spectrum can be used to calculate the conductance of the device as function of the left and right electrode temperatures, $T_L, T_R$. At $T_L = T_R = 0$ the conductance is determined by the transmission coefficient at the Fermi Level, while for finite $T_L$ and $T_R$, the conductance depends on the value of the transmission coefficient in an
energy window around the Fermi level. For $T_L = T_R \neq 0$ the zero bias conductance is given by Equation 1. Where $f'$ is the derivative of the Fermi function. In semiconductors the conductance is often determined by hot electrons or holes propagating within the conduction or valence band, so-called thermionic emission. The hot electrons are located in the energy range of the tails of the Fermi function. Thus, for an accurate determination of the conductance from thermionic emission, it is important that the energy range of the transmission spectrum is such that the tails of Fermi functions are properly sampled. Fig. 3 shows that both the valence and conduction band edges of the central region is within the energy range of the transmission spectrum.

$$\sigma(T_L) = \frac{2e^2}{h} \int T(E) f' \left( \frac{E - E_L^F}{k_B T_R} \right) dE \quad (1)$$

The result of simulation of conductance, according to temperature, is similar to Fig. 4. The temperature dependent conductance for this device is rather atypical for a field effect transistor. Usually the conductance will increase as function of temperature. The decreasing conductance as function of temperature is related to a large conductance at the Fermi level caused by electron tunneling, Tian et al. (2010).

2.4. Effect of the gate potential

We will now change the value in the range [-2, 2] V, and for each value make a new self-consistent calculation and obtain the corresponding transmission spectrum. The results of simulation of conductance in recognition of different gate voltages are according to Fig. 5. The conductance has a minimum for a gate potential of about 0.25 Volt. For this gate potential, the Fermi level is positioned in the mid gap between the valence and conductance band of the central ribbon. Note that there is only a weak dependence of the conductance on the electron temperature, and this illustrates that the transmission is dominated by tunneling. For calculating the linear answer of dependency of gate voltage on conductance, written by script, results in linear answer of conductance as a function of gate voltage. Supposing the effect of gate voltage, a simple change of proportional situation of Fermi level of electrode happens in transmission spectrum. The script in the transmission spectrum begins with a calculation with 0 V gate voltage and by adjusting electrodes voltage of transmission spectrum, electrodes Fermi level relatively move, Tian et al. (2010). Simulation is represented in Fig. 5.

2.5. Calculating the I-V characteristics and self-consistent I-V characteristics

To calculate self-adjusting properties of I-V, effect of changing the external bias in the range [0, 2] Volt. Fig. 6 shows the electro-static potential for a bias of 1 Volt, i.e. -0.5 V on the left electrode and 0.5 Volt on the right electrode, and shows self-consistent current-voltage characteristics of the graphene junction with -1 V gate potential. The results show that how the electro-static potential in the left electrode is closer to the electro-static potential of the gate. Curves are for electrode temperatures 0, 100, 200, ..., 2000 Kelvin. The current shows an increase with the temperature. In obtaining drain source current curve, Poisson equation is used and the charge inside the channel is ignored. We can also use the self-adjusting solution of coupled Schrödinger and Poisson equations in order to take
Fig. 5. Different curves are for different electron temperatures, namely 0, 100, 200, ..., 2000 Kelvin. (a) Conductance as function of the gate potential; (b) Conductance as function of the gate potential calculated using linear response.

Fig. 6. (a) Electrostatic potential of the junction with symmetrically applied bias of 1 Volt and a gate potential of -1 Volt; (b) Self-consistent current-voltage characteristics of the graphene junction with -1 V gate potential.

into account the effect of charge in the channel as the average field. Thus, we will be able to calculate energy distribution function of each carrier in every part of channel by integration of normalized wave function in each point in the channel, Schwierz (2013). The results of simulation is represented in Fig. 7.

Fig. 7. (a) Current voltage characteristic, GNRFET, without considering channel charge (connected lines) and with considering channel charge (dotted lines); (b) normalized energy distribution curve.

3. Conclusions

In this paper, field effect transistor simulation was done by Nano-ribbon of graphene. Using GNR band gap as the channel for GNRFETs is represented as having great importance in measuring high on/off rate. In maximum currents, the channel levels resulting from drain source connections is not noticeable. Designing and simulating Nano-wire field effect transistor with silicon (100) is the future business of this research group.

References