

# Calculation and Analysis of Graphene Nanoribbons Field Effect Transistor Structure and Characteristics

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**Abstract.** Because there is no gap between conduction band and valence band of graphene, it is difficult to achieve switching characteristics when transistors are fabricated. In order to open the graphene band gap, researchers have explored many methods, such as tailoring Shi Mocheng quantum dots, nanobelts, nano grids or laying graphene on a special substrate, one of the feasible ways is to regulate the electrical properties of graphene by doping. Through the analysis on the structure and properties of graphene band calculation, with the help of computer aided simulation, the ID and VG characteristics analysis of the Schottky barrier graphene field effect transistor (SBFET) and MOS structure of graphene field effect transistor (MOSFET) are investigated in this study. The results are of high reference value for the study of the structure and properties of graphene nanoribbons.

## 1. Introduction

Graphene is a two-dimensional film with only one carbon atom thickness, which is composed of carbon atoms with hybridized orbits and six angle honeycomb lattices. The graphene material is very thin, but the hardness is very high, very good transparency is very low, the light absorption, good thermal conductivity, the thermal conductivity than diamond and carbon nanotube; the graphene material has high mobility and low resistivity, mobility than carbon nanotubes and silicon the high resistivity of copper and silver materials is lower, the minimum resistivity material; the resistivity of graphene is low, the conduction speed is very fast, so it can be the development of ultra-thin electronic components and electric liquid crystal materials, has a very good application prospect.

## 2. Graphene and its application

With the continuous rise of graphene materials, graphene has more extensive applications, including sensors, solar battery materials, lithium ion battery materials, semiconductor and thin film crystal and composite materials, are described in detail in the four main areas of application.

### 2.1. Sensor applications

The small volume of graphene but a large surface area, high sensitivity and its application in sensor materials, can obtain higher sensitivity than conventional sensors, such as Singapore, Nanyang Technology University developed a graphene material optical sensing sensor, Its sensitivity is 1000 times stronger than that of ordinary graphene sensors.

### 2.2. Energy storage and new type display



The electrical conductivity of graphene and the transmission performance is very good, the light can be used in the storage battery and the display screen, touch screen using indium tin oxide materials most of the graphene has very good prospects, it is likely to replace indium tin oxide used in touch screen for future production, Samsung Toshiba and many other well-known mobile phone manufacturers have been locked in this type of material, and focus on the layout of development, I believe that in the near future will develop a new type of touch screen is higher than ordinary screen sensitivity.

### 2.3. Semiconductor materials

Most of the siliceous material of semiconductor material and semiconductor device at present, strong manufacturing enterprises and research institutions have begun to carry out research and development of graphene, such as the Columbia University has developed a graphene - silicon optoelectronic chip, IBM researchers have developed a graphene field-effect transistor, its performance to manufacturing silicon semiconductor devices compared with the traditional good material.

### 2.4. Biomedical applications

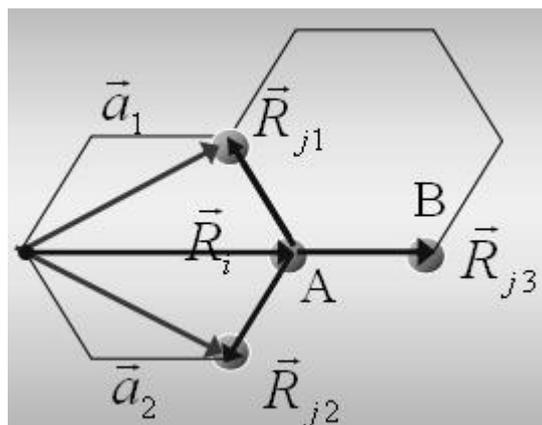
Graphene nano materials have been applied to the biomedical field. As the carrier of nano drug, biological imaging and detection, it can be used for bacterial analysis, DNA and protein detection, such as the University of Pennsylvania to develop graphene nano hole equipment, greatly improving the detection speed of DNA sequence.

## 3. Structural properties and energy band calculation of graphene

The electronic band structure of graphene can affect the characteristics of the larger, the whole structure is to separate carbon atoms as the base, the perturbation is generated by the surrounding carbon atoms, the energy level distribution of graphene can be analyzed by matrix calculation, using approximate two quantized Hamiltonian can be expressed in graphite electron tight binding model, such as Formula (1) shown.

$$H = \varepsilon_{2pz} \sum_i (a_i^+ a_i + b_i^+ b_i) - t \sum_{\langle i, j \rangle} (a_i^+ b_j + h.c) \quad (1)$$

The influence of electron spin is neglected in Formula (1), where  $\langle i, j \rangle$  is the sum of the electron transitions to the neighboring lattice, and  $\varepsilon_{2pz}$  is the energy of the single electron  $2pz$  orbit.



**Figure 1.** Schematic diagram of adjacent atomic reference atoms

As shown in Figure 1, the graphite lattice can be represented by the two neighboring carbon atoms A, B, the geometrical environment of these two carbon atoms is not equivalent. The A atom is chosen as the reference atom, whose vector is  $\vec{R}_i$ , and the vectors of the neighboring B atoms are  $\vec{R}_{j1}$ ,  $\vec{R}_{j2}$  and  $\vec{R}_{j3}$ . Suppose that  $a_i^+(b_j)$  is generating or destroying operators of electronics at  $\vec{R}_i(\vec{R}_j)$ . In

Formula (1), this symbol can be expressed as an electron produced by  $a_i^+$  at  $\vec{R}_i$  after  $b_j$  destroyed an electron at  $\vec{R}_j$ . It can also be seen as electron transition from  $\vec{R}_j$  to nearest neighbor  $\vec{R}_i$ , the transition energy is  $t = 2.8eV$ . By Fourier transformation we can get that

$$a_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{R}_i} \hat{a}_{\vec{k}} \quad (2)$$

$$b_j = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{R}_j} \hat{b}_{\vec{k}} \quad (3)$$

$$\begin{vmatrix} \varepsilon_{2pz} - E & -t(1 + e^{-i\vec{k} \cdot \vec{a}_1} + e^{-i\vec{k} \cdot \vec{a}_2}) \\ -t(1 + e^{i\vec{k} \cdot \vec{a}_1} + e^{i\vec{k} \cdot \vec{a}_2}) & \varepsilon_{2pz} - E \end{vmatrix} = 0 \quad (4)$$

In the case of ideal structure model, graphene can select atomic orbital energy level  $\varepsilon_{2pz} = 0$  as the reference point of  $\pi$  band energy  $E(k)$ , and the energy band of graphene atom can be obtained by unfolding the above formula.

$$\begin{aligned} E^2 &= t^2(1 + e^{i\vec{k} \cdot \vec{a}_1} + e^{i\vec{k} \cdot \vec{a}_2})(1 + e^{-i\vec{k} \cdot \vec{a}_1} + e^{-i\vec{k} \cdot \vec{a}_2}) \\ &= t^2\{3 + 2\cos(\vec{k} \cdot \vec{a}_1) + 2\cos(\vec{k} \cdot \vec{a}_2) + 2\cos[\vec{k} \cdot (\vec{a}_1 - \vec{a}_2)]\} \end{aligned} \quad (5)$$

In Formula (5),

$$\vec{k} \cdot \vec{a}_1 = (k_x, k_y) \left( \frac{3a}{2}, \frac{\sqrt{3}a}{2} \right) = \frac{3a}{2} k_x + \frac{\sqrt{3}a}{2} k_y \quad (6)$$

$$\vec{k} \cdot \vec{a}_2 = \frac{3a}{2} k_x - \frac{\sqrt{3}a}{2} k_y \quad (7)$$

$$\vec{k} \cdot (\vec{a}_1 - \vec{a}_2) = \sqrt{3}ak_y \quad (8)$$

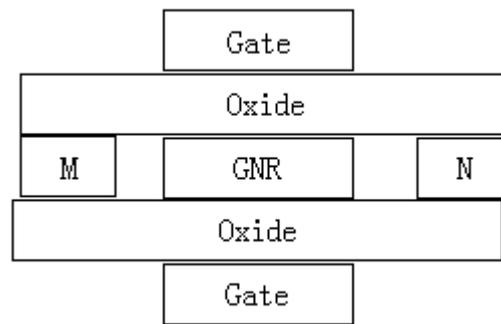
After elementary trigonometric function and difference operations, graphene band can be got as shown in formula (9).

$$E_{\pm}(k_x, k_y) = \pm t \sqrt{3 + 2\cos(\sqrt{3}k_y a) + 4\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\cos\left(\frac{3k_x a}{2}\right)} \quad (9)$$

The energy band of graphene can be obtained from the calculation formula, and the structure and characteristics of graphene nanoribbons can be analyzed with the help of computer software.

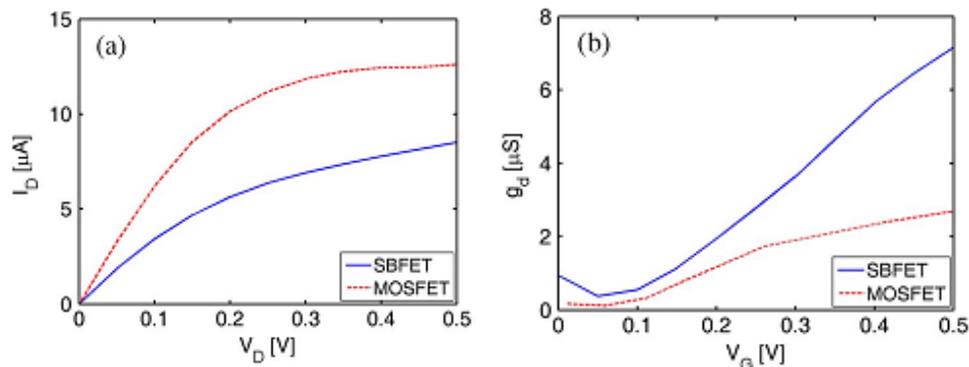
#### 4. Structure and characteristic analysis of graphene nanoribbons

In order to verify the feasibility of graphene band calculation, aided by computer simulation method, the structure and characteristics of graphene nanoribbons has been analyzed, the analytical model can be referred to the ideal Schottky barrier graphene nanoribbons field effect transistor (SBFET) and MOS graphene nanoribbons (MOSFET) with Youngki Yoon et al.,. The parameters of the characteristic analysis are ID and VG characteristics.



**Figure 2.** Schematic diagram of SBFET section

The section of the SBFET is shown in Figure 2, the channel material is graphene nanoribbons, and the source drain is contacted by Schottky. The results of MOSFET and SBFET profiles are similar. The difference is that the source and drain are doped. In the computer aided calculation mode, the SiO<sub>2</sub> gate insulating layer thickness is 1.8nm, the dielectric constant is set to 3.9; the channel material n is set to 12, the length is 18nm, width is 1.38nm, the gap of E<sub>g</sub> is about 0.8eV, the calculation results are shown in Figure 2 is obtained by calculating.



**Figure 3.** ID and VG characteristic curves

Figure 3 shows the VG and ID curve characteristics results obtained by computer aided calculation, the results can be seen from the saturated characteristics of MOSFET showed better characteristics, output from the electrical conductivity, smaller conductance MOSFET, it verified the feasibility of the calculation and analysis of field effect tube of graphene nanoribbons.

## 5. Conclusion

In order to open the band gap of graphene and realize its switching function, it is necessary to control the electrical properties of graphene by doping, which needs to analyze the structural characteristics of graphene. Taking graphene nanoribbons as an example, the ID and VG characteristics of Schottky barrier graphene nanoribbons field effect transistors (SBFET) and MOS graphene nanoribbons (MOSFET) were investigated by computer aided calculation. The analysis results show that MOSFET has more obvious advantages in terms of saturation characteristics and output conductivity. The research of graphene material is not mature, its experimental research is more complex, and the method of calculation and analysis can effectively shorten the research cycle and improve the efficiency of research. Therefore, it is of great practical significance to develop the calculation analysis method with the aid of the auxiliary calculation tools

## 6. Acknowledgements

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