Investigation of structure and properties of Graphene

Hosseinpour, Mansoureh, Hosseinpour, Maryam
Shahid Beheshti University, Department of Physics, Evin, 1983963113 Tehran, Iran.

E-mail: Hosseinpour.mansoureh@gmail.com

(Received 11 January 2014, accepted 27 June 2014)

Abstract

In this paper, we investigate the Graphene from structural and its properties. We try to show crystal structure of Graphene and a comparison between Graphene and other two-dimensional semiconductors.

Keywords: Thermal conductivity-graphene-chirality.

Resumen

En este trabajo, investigamos estructura y propiedades del grafeno. Tratamos de mostrar la estructura cristalina de grafeno y una comparación entre éste y otros semiconductores de dos dimensiones.

Palabras clave: Conductividad térmica, grafeno, quiralidad.

PACS: 01.40.gb, 01.40.-d **ISSN 1870-9095**

I.INTRODUCTION

Graphite is a three dimensional hexagonal system that has been formed from layers of Carbon atoms. Each of these layers is called graphene. So graphene is single layer graphite. Since the distance between two adjacent layers is about 35/3 A˚ and is so much bigger than the distance between two C-C atoms that is 1/42 A˚, interaction between two adjacent layers in comparison with interaction within in a layer is so petty [1, 2, 3, 4, 5, 6, 7]. Graphene layers are located next to each other in Graphite by the Vanderwaalsy's weak power; while the Carbon atoms in Graphene are next to each other with three Ϭ powerful connection with sp^2 hybridation, and 2pz orbital single electron for each atom, is perpendicular with the Graphene layer making π covalent connection and is the reason for electrical conductivity in Graphene [7].

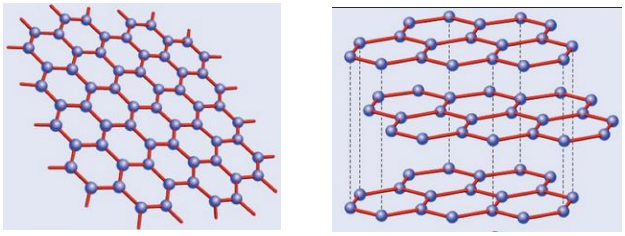

FIGURE 1. Graphene (left), graphite (right).

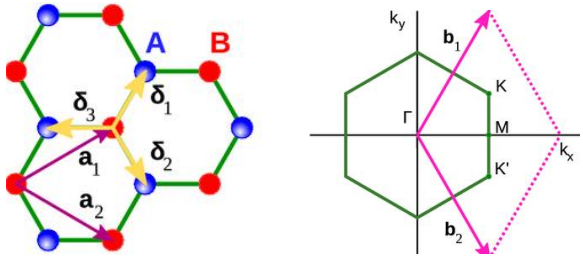

FIGURE 2. First Brilouin region in grapheme.

II.CRYSTAL STRUCTURE OF GRAPHENE

Graphene is a single atomic layer of Carbon atoms in a honeycomb hexagonal structure; in the triangular lattice with two atomic basis in per unit cell. This structure has been made from two sub lattice A and B. Unit cell that has been shown in figure (1) with rhombus, includes two atoms that each of them belongs to one sub lattice. Nearest neighbors distance in Graphine is a≈1/42 A˚. Lattice vectors are as follows:

$$\vec{a}_{1,2} = \frac{a}{2}\left(3, \pm\sqrt{3}\right). \quad (1)$$

Two dimensional graphite lattice vector and rotors are related as follows:

$$\left|\vec{a}_{1,2}\right| = \sqrt{3}a \approx 2/64. \quad (2)$$

Three vectors nearest neighbors as they are shown in figure (1) are as follows:

$$\vec{\delta}_1 = \frac{a}{2}(1,\sqrt{3}) \quad \vec{\delta}_2 = \frac{a}{2}(1,-\sqrt{3}) \quad \vec{\delta}_3 = -a(1,0). \quad (3)$$

In first Brilouin region inverse space, as it's shown in figure (1), it's hexagonal. Basis vectors of inverse lattice are as follows:

$$\vec{b}_{1,2} = \frac{2\pi}{3a}(1,\pm\sqrt{3}). \quad (4)$$

As can be seen, vectors $\vec{b}_1$ and $\vec{b}_2$ in hexagonal inverse lattice are rotated as much as 90° in comparison with vectors $\vec{a}_1$ and $\vec{a}_2$ in real lattice. To obtain basis vectors of inverse lattice as it's common in two dimensional lattices, do as follows:

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\hat{z}}{A} \qquad \vec{b}_2 = 2\pi\frac{\vec{a}_1\times\hat{z}}{A}. \quad (5)$$

A is area of unit cell in real space. Two particular point *k* and *k´* in figure (3) are known as Dirac points. Other points of this hexagon according to the position they have are corresponding to one of these two points. The position of Dirac points in momentum space are as follows:

$$\vec{K} = \left(\frac{2\pi}{3a}, \frac{\pm 2\pi}{3\sqrt{3}a}\right). \quad (6)$$

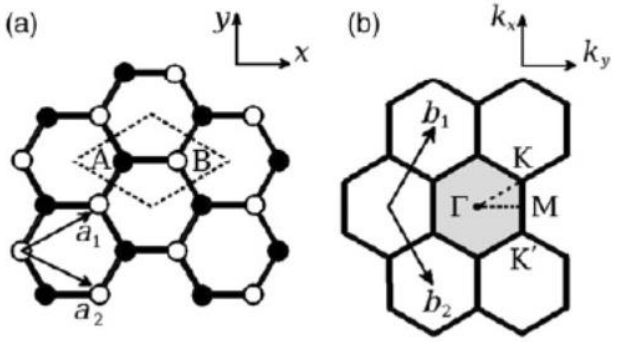

FIGURE 3. Cell diagram of Graphene.

Each atom has been bonded to its own nearest neighbors by σ strong bonds that make 120° angle in graphene page σ results sp^2 hybridization for three capacity electrons of 2s, $2p_x$ and $2p_y$ orbitals. The fourth capacity electron is in orbital $2p_z$ and it is perpendicular to Graphene page. Thus the one weak πbond is formed by overlap of $2p_z$ with other $2p_z$ orbitals. Transport properties of Graphene are determined by these delocalized π electrons.

Graphite crystal structure that includes Graphene layers, is accompanied with within layers strong correlation of Graphene and weak bonds between layers. It seems that the origin of this weak correlation between layers is weak Van Der Waals's interaction. (Distance between the layers is *0/34 nm* that is so much more than the distance between nearest neighbors of a layer $a_{c\text{-}c}$*= 0/142 nm.*) [9].

III.COMPARISON OF GRAPHENE AND OTHER 2-DIMENSIONAL SEMICONDUCTORS

Graphene is a two dimensional semi-conductor with zero band-gap, but there are many quality differences between Graphene and other two dimensional semi-conductors that among them we can mention the following:

1. Two dimensional semi-conductor systems including big band-gap, are usually more than one electron-volt and electrons and holes in them are under examination in the structure with the electron or hole pattern. Graphene is a semi-conductor, lacking band-gap. In this system carriers in Dirac points switch from kind of electronic to hole or vice versa. The result of zero energy-gap in Graphene is acquiring metallic nature and chemical potential is always perched in Valence-band or conduction band against that, two dimensional semi-conductors, turned to insulation below a certain voltage and Fermi level situates in energy-band.

2. Graphene systems are chiral but there is no chirality in two dimensional semi-conductors and the wave function of system is non-chiral and is in $\psi(r.z) \sim e^{iq.r}\xi(z)$ form.q and r respectively are wave vector and position vector and ξ (z) is wave vector that is limited in order to z. chirality in Graphene results special transport behavior in structure[15].

3. Dispersion relation of energy in single layer graphene is changed linear with momentum while the dispersion relation of energy is square for two dimensional semi-conductor with momentum [8]. This difference results fundamental differences in transport properties of both systems.

4. Graphene is an ideal two dimensional system, it means since the Graphene layers have the thickness of an atom, carriers are limited in two dimensions but in the structures of two dimensional semi-conductors, by the effect of applied limitation with electric field, dynamics quantum considered, two dimensional. So the result of two dimensional semi-conductors is quasi-two dimensional system. And the average thickness is always from 5nm to 50nm [14].

5. Graphene has a high thermal conductivity and special electronic and mechanical properties. Graphene itself is a semi-conductor but in comparison with the other semi-conductor, is an alternative for silicon because of its special properties and will be used as an ideal material in electronic. As electronic components got smaller, local heating is more important problem and silicon specially will have problem. Materials like Graphene has higher thermal conductivity and can effectively remove this wasted heat.

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