

Band Gap Calculations of Bilayer Graphene and Bilayer Armchair Graphene Nanoribbon

E. Sustini¹, Khairurrijal¹, F. A. Noor¹, and R. Syariati¹

¹Physics of Electronics Materials Research Division Faculty of Mathematics and Natural Science, Bandung Institute of Technology

E-mail : euis@fi.itb.ac.id

Abstract. Graphene has a high potential for use in electronic devices because it has a unique characteristic, electrons in massless grasses and has a speed close to the speed of light. Graphene conductivity at temperature space is $40\,000\text{ cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$ in the air. In addition, thermal conductivity can reach $2\,800\text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. The mechanical properties of graphene are very strong and flexible, and optical properties it has a white light transmittance of 95%. Therefore, graphene is suitable for transparent screen and the flexible electrode. The energy band gap of monolayer graphene can be changed by reducing the size, as for the band gap of bilayer graphene was affected by symmetry between two layers. So, it is interesting to research the band gap characteristics of bilayer armchair graphene nanoribbon (AGNR). In this paper, we have calculated the band gap of bilayer graphene and bilayer AGNR in various parameters such as band width and symmetry between two layers. The method used is tight binding method by only taking into account its nearest neighbors only. The results obtained from this simulation show that the band gap will be more open if asymmetry of the structure bilayer graphene is increasing and the band gap of AGNR will be more open if ribbon width decreased, is not affected by asymmetry.

Keywords. Band gap, graphene, and nanoribbon.

1. Introduction

The unique electronic characteristics of graphene make it the potential for applications on the device both for graphene monolayer and bilayer graphene. Monolayer graphene properties are the same as bilayer graphene. At room temperature in the air both materials have a high electrical conductivity that is up to $40\,000\text{ cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$ [1]. While the thermal conductivity of these two materials reaches up to $2\,800\text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ [2]. The mechanical properties are strong and flexible [3] while for optical properties are equally transparent with white light transmittance reaching 95 % [4]. Hence both of these materials have very wide applications including transparent screens and flexible electrodes making them suitable for touch screens.

The graphene monolayer with bilayer graphene differs on the possibility of adjusting the width of the band gap. The band gap of monolayer graphene can be changed by reducing its size to the nanoscale. Graphene in this size is one of them named as graphene nanoribbon (GNR) [5]. There are two types of GNR namely, armchair GNR (AGNR) and zigzag GNR (ZGNR). AGNR is known to have semiconductor properties depending on the big of the width while ZGNR has conductor



properties. Another difference, that energy dispersion of monolayer graphene is linear [5]. The bilayer graphene banding of the bandgap may be accomplished by impurity and gate voltage regulation [6]. In addition, the effective mass of bilayer graphene is nonzero (but can be said to be very small) and the parabolic dispersion energy relationship [7] so that the bandgap profile produced by the bilayer will be different from that of the monolayer. In this research, we calculated the band gap of bilayer graphene and bilayer AGNR with parameter asymmetry and width of the ribbon.

2. Theoretical approach

2.1. Dispersion energy of Bilayer Graphene

In one of bilayer graphene lattice, there are four atoms, A_1 , B_1 , A_2 , and B_2 so that the wave function is defined [1].

$$\Phi_{A_m/B_n}(r) = \frac{1}{\sqrt{N}} \sum_{R_{A_m/B_n}} e^{iKR_{A_m/B_n}} \psi_{A_m/B_n}(r - R_{A_m/B_n}) = e^{iKr} \psi_{A_m/B_n}(r) + e^{iK'r} \psi'_{A_m/B_n}(r), \quad (1)$$

$$m = 1, 2, \quad n = 1, 2,$$

with $R_{A/B}$ representing the atomic position of atoms A and B, N is the number of primitive cells of a lattice, $e^{iKR_{A_m/B_n}}$ representing a periodicity of the lattice, and $\psi_{A_m/B_n}(r - R_{A_m/B_n})$ representing the Bloch function. Physically, electrons can move from one atom to another that is the nearest neighbor of the atom. For example, an electron on A_1 atom can move to atoms B_1 , A_2 , or B_2 . From these conditions, the dispersion energy relationship can be determined by using the Schrödinger equation $H\Phi = E\Phi$ so that the matrix forms are

$$\begin{bmatrix} E_{A_1} & -\gamma_0 f(k) & \gamma_4 f(k) & -\gamma_3 f^*(k) \\ -\gamma_0 f^*(k) & E_{B_1} & \gamma_1 & \gamma_4 f(k) \\ \gamma_4 f^*(k) & \gamma_1 & E_{A_2} & -\gamma_0 f(k) \\ -\gamma_3 f(k) & \gamma_4 f^*(k) & -\gamma_0 f^*(k) & E_{B_2} \end{bmatrix} \begin{bmatrix} \Phi_{A_1} \\ \Phi_{B_1} \\ \Phi_{A_2} \\ \Phi_{B_2} \end{bmatrix} = \varepsilon_\alpha \begin{bmatrix} 1 & s_0 f(k) & 0 & 0 \\ s_0 f^*(k) & 1 & s_1 & 0 \\ 0 & s_1 & 1 & s_0 f(k) \\ 0 & 0 & s_0 f^*(k) & 1 \end{bmatrix} \begin{bmatrix} \Phi_{A_1} \\ \Phi_{B_1} \\ \Phi_{A_2} \\ \Phi_{B_2} \end{bmatrix} \quad (2)$$

With E_{A_1} , E_{B_1} , E_{A_2} , and E_{B_2} is the initial energy of the electrons in each atom while $f(k)$ describes the geometrical factor of the position of the neighboring atom. As γ_1 is illustrating the parameters coupled between the pair of orbital dimer (identical) electrons of atoms A_2 and B_1 . In this parameter, there is no $f(k)$ as it is a vertically coupled pair. γ_3 , explain about the coupling pair of electron orbitals of the non-dimer atoms of A_1 and B_2 . In addition, in the second equation, there exists γ_4 a parameter of the interlayer electron orbitals between the dimer and non-dimer pairs of the A_1 and A_2 or B_1 and B_2 atoms. The last parameter for the left-hand side of Equation 2 is that γ_0 it is physically a parameter of an electron jump from one atom to the nearest neighbor atom on one layer. Visually, the role of these parameters can be seen in Figure 1.

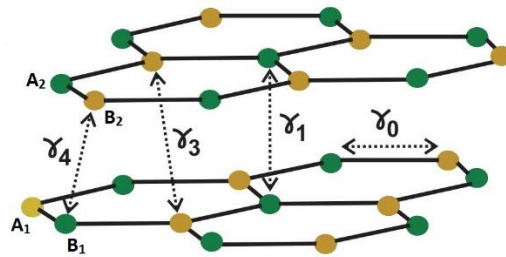


Figure 1. Bilayer graphene structure with parameters of electron leap

The wave number $k = K + p$, K is the point at which the conduction band and the valence band meet, whereas p is the vector shift. Assuming the overlap parameter s_0 and s_1 zero, with $v_0 = 3a\gamma_0/2\hbar$, $v_3 = 3a\gamma_3/2\hbar$, $v_4 = 3a\gamma_4/2\hbar$ and taking into account the condition of the asymmetry bilayer graphene, γ_4 will be zero, the value $E_{A_1} = E_{B_1} = -U/2$, and $E_{A_2} = E_{B_2} = U/2$ (U potential energy) so will be obtained

$$\varepsilon_\alpha = \pm \sqrt{\frac{\gamma_1^2}{2} + \frac{U^2}{4} + \left(v_0^2 + \frac{v_3^2}{2}\right)p^2 + (-1)^\alpha \sqrt{\frac{1}{4}(\gamma_1^2 - v_3^2 p^2)^2 + v_0^2 p^2 (\gamma_1^2 + U^2 + v_3^2 p^2) + 2\gamma_1 v_3 v_0^2 p^3 \cos 3\varphi}}.$$

The form of p is the resultant vector of p_x and p_y which can be written mathematically $p = \sqrt{p_x^2 + p_y^2}$, φ , is the angle between p_x and p_y , and the constant α is degeneration of the bilayer graphene gap having a value of 1 and -1. As for the \pm sign, describes the conduction band and the valence band. From these parameters, bandgap can be searched by calculating the difference between the energy contained in the conduction band and the valence band.

2.2. Dispersion energy of Bilayer Graphene

To obtain the dispersion energy relation of the bilayer AGNR, the first thing to do is to assume that one of the lengths of the bilayer graphene is made on a nanometer scale. In this simulation, it is assumed the size in the x-direction is restricted. Physically, the restriction will make the wave number in the x-direction has a unique value. This condition leads to a boundary condition that has a range $r=0$ and $r = w_{ac} + \sqrt{3}a$ is illustrated in Figure 2. With this boundary condition, the wave function in Equation 1 applies

$$\Phi_{A_{1/2}}(r=0) = \Phi_{B_{1/2}}(r=0) = \Phi_{A_{1/2}}(r = w_{ac} + \sqrt{3}a) = \Phi_{B_{1/2}}(r = w_{ac} + \sqrt{3}a) = 0. \quad (3)$$

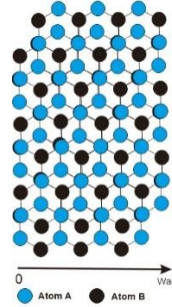


Figure 2. Bilayer AGNR Structure

The solution form for ψ_{A_m/B_n} and ψ'_{A_m/B_n} in Equation 1 by Ansatz is given sinusoidal form which is written as follows [5]

$$\begin{aligned} \psi_{A_m/B_n} &= A e^{ip_x x} + B e^{-ip_x x}, \\ \psi'_{A_m/B_n} &= C e^{ip_x x} + D e^{-ip_x x}. \end{aligned}$$

Here A , B , C , and D are constants. By using the boundary conditions in Equation 3 it will be obtained

$$A + B + C + D = 0,$$

$$A e^{i(p_x + K)(w_{ac} + \sqrt{3}a)} + D e^{-i(p_x + K)(w_{ac} + \sqrt{3}a)} + B e^{-i(p_x - K)(w_{ac} + \sqrt{3}a)} + C e^{i(p_x - K)(w_{ac} + \sqrt{3}a)} = 0.$$

The condition of the boundary conditions is met if $B = -C$ and $A = D = 0$ and $\sin[(p_x - K)(w_{ac} + \sqrt{3})] = 0$ produces. So, the wave number for the x-direction is written to be

$$p_x = \frac{n\pi}{w_{ac} + \sqrt{3}a} + \frac{2\pi}{3\sqrt{3}a}.$$

With w_{ac} is the width of the AGNR bilayer.

$$\varepsilon_a = \pm \sqrt{\frac{\gamma_1^2}{2} + \frac{U^2}{4} + \left(v_0^2 + \frac{v_3^2}{2}\right)p^2 + (-1)^a \sqrt{\frac{1}{4}(\gamma_1^2 - v_3^2 p^2)^2 + v_0^2 p^2 (\gamma_1^2 + U^2 + v_3^2 p^2) + 2\gamma_1 v_3 v_0 p^3 \left(\left(\frac{p_x}{p}\right)^3 - 3\frac{p_y^2 p_x}{p^3}\right)}}.$$

3. Results and discussion

Figure 3 (a) shows the bandgap of the bilayer graphene under normal conditions and when there is a high asymmetry called the Mexican Hat Effect. From the picture, it is seen that the bandgap of bilayer graphene actually has zero band gap. However, when the arrangement of its high asymmetry structure the band gap was becoming open. This phenomenon occurs because when the bilayer graphene structure in that state the value of Δ parameter equals with γ_1 [7]

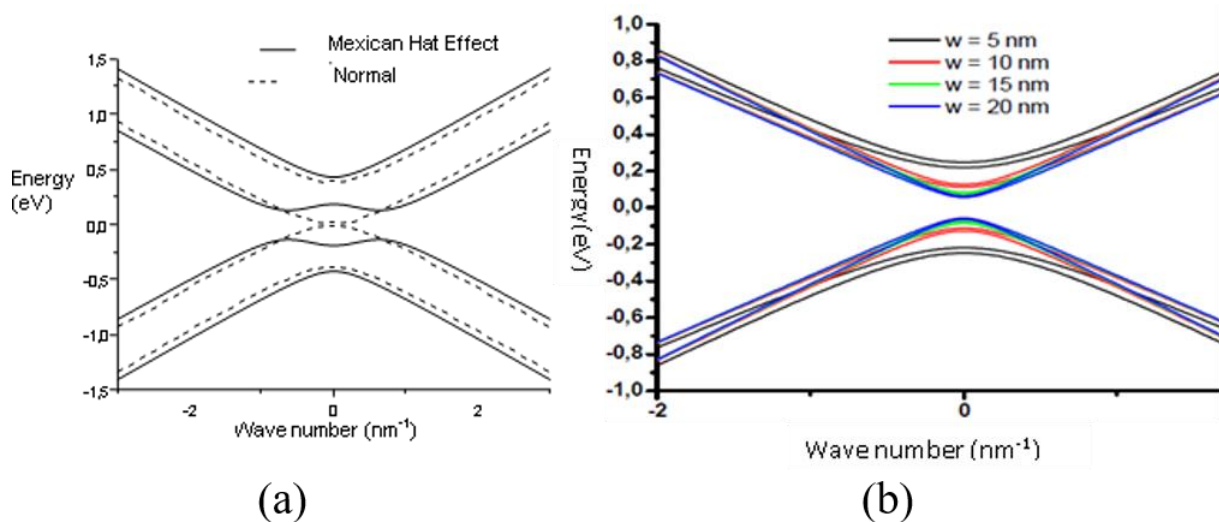


Figure 3. The band gap energy of (a) bilayer graphene based on asymmetry (b) bilayer AGNR

Figure 3(b) describes the band gap of the bilayer AGNR seen at point K with four variations of the ribbon width. The picture shows that the larger the ribbon width value of the bilayer AGNR, the resulting bandgap getting smaller. In the figure, it is also seen that with the increase of AGNR ribbon width, the band gap degeneration approaches the lowest energy level. Another thing that can be discussed about the absence of Mexican Hat Effect despite high asymmetry. This condition arises because of the influence of the limited value of wave numbers in the x-direction, due to limited size width. In addition, the effective Hamiltonian role of the bilayer AGNR provides the effect of band gap changes in terms of degeneration, asymmetric structure, or in the opening of the bandgap due to changing values γ_1 , γ_3 , and γ_4 .

4. Conclusions

By using tight binding method (TB) has been found dispersion energy relation of bilayer graphene and bilayer AGNR graphene. The difference between these two materials is seen in several ways. In the bilayer graphene, there is a Mexican Hat Effect that makes the bilayer graphene energy gap affected

by the asymmetry structure while in the AGNR bilayer there is no Mexican Hat Effect and the band gap is only influenced by the bandwidth.

Acknowledgments

This research was financially supported by “PTUPT DIKTI” Research grand in the fiscal year of 2017

References

- [1] Dean C R 2010 Boron nitride substrates for high-quality graphene electronics *Nat. Nanotech.* **5** pp 722–726
- [2] Novoselov K S 2004 Electric field effect in atomically thin carbon films *Science*. **306** pp 666–669
- [3] Neek-Amal M and Peeters F M 2010 Nano indentation of a circular sheet of bilayer graphene *Phys. Rev. B*. **81** p 235421
- [4] Nair R R 2008 Fine structure constant defines visual transparency of graphene *Science*. **320** pp 1308–1311
- [5] Castro Neto A H 2009 The electronic properties of graphene *Rev. Mod. Phys.* **81** pp 109–162
- [6] McCann E and Fal’ko V I 2006 Landau-Level degeneracy and quantum Hall effect in a graphite bilayer *Phys. Rev. Lett.* **96** pp 086805
- [7] McCann E and Koshino M 2013 The electronic properties of bilayer graphene **76** pp 056503