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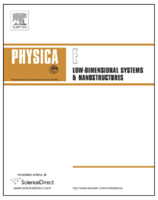

Band structure of deformed armchair nanoribbon with bond alternation

Nguyen Ngoc Hieu [a,*], Le Cong Nhan [b]

[a] *Institute of Research and Development, Duy Tan University, Da Nang, Vietnam*
[b] *Department of Environmental Science, Saigon University, Ho Chi Minh city, Vietnam*

HIGHLIGHTS

- In the presence of bond alternation all armchair GNRs are semiconducting.
- Slope of dependency of the energy gap on its stress depends on tension direction.
- We can control the band gap of nanoribbon by its strain.

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ABSTRACT

Electronic energy band structure of deformed armchair graphene nanoribbons with bond alternation is studied by the tight-binding approximation. In the presence of bond alternation, all armchair graphene nanoribbons become semiconducting with small band gap opened at center of the Brillouin zone. Under tensional strain, armchair graphene nanoribbons can become metallic at the critical values of deformation and we can control the band gap of nanoribbon by its strain.

1. Introduction

Graphene is a single layer of carbon atoms packed in a honeycomb lattice [1]. Besides carbon nanotubes (CNTs), another one-dimensional carbon nanostructures, graphene nanoribbons (GNRs) can be obtained by cutting a graphene sheet along a certain direction in the form of a quasi-one dimensional wire. Due to edge structures, GNRs have extraordinary electronic properties which open many ways for applications in nanoelectronic devices.

Generally, the electronic properties of carbon low-dimensional systems are particularly sensitive to structural perfection, size, and geometry [2,3]. For example, the electronic properties of CNTs are determined by their diameter and chirality. Because of the Peierls transition, armchair CNTs become semiconducting at low temperature and Peierls distortions lead to the Kekule structure with two essentially different C–C bond lengths and a triple translational period [4]. The ground state of the (6, 0) CNT is found to have a Kekule structure with four types of bonds and difference between lengths of long and short bonds of about 0.005 nm [5]. Due to the presence of dimerization structure, the semiconductor–metal transitions in CNTs are actual in connection with perspectives of their applications in nanoelectronic and nanoelectromechanical devices.

Studies of structure and elastic properties of GNRs are also of fundamental interest. Many works have studied the electronic properties of both pristine and deformed GNRs [6–10]. Although the lattice distortion leading to appearance of dimerization structure (bond alternation) GNRs has also been studied by the tight-binding model at very early [11], however, up to date, GNRs with bond alternation seem to remain unclear and less understood. In this paper, we study the electronic band structure of armchair GNRs with bond alternation under strain using the simple tight-binding model. The dependence of band gap on the magnitude of tension and the bond lengths is also considered.

2. Deformed graphene with bond alternation

Under stress ε, in the framework of the elasticity theory, the position vector of carbon atoms is given by the following relationship [12]

$$\mathbf{R}_i = (1+\overline{\varepsilon})\mathbf{R}_{0i}, \tag{1}$$

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[*] Corresponding author. Tel.: +84 511 3827111; fax: +84 511 3650443.
E-mail address: hieunn@duytan.edu.vn (N.N. Hieu).

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where $\mathbf{R}_{0i}$ and $\mathbf{R}_i$ are the position vectors of carbon atoms before and after stress, $\bar{\varepsilon}$ is the strain tensor in the graphene plane.

x, y coordinates are shown in Fig. 1 and the strain tensor is given by Ref. [12]

$$\bar{\varepsilon} = \varepsilon\begin{pmatrix} \sin^2\theta - \sigma\cos^2\theta & (1+\sigma)\cos\theta\sin\theta \\ (1+\sigma)\cos\theta\sin\theta & \cos^2\theta - \sigma\sin^2\theta \end{pmatrix}, \tag{2}$$

where σ is Poisson's ratio and θ is defined as the angle between the applied tension vector and axis Ox. The axis Ox is parallel to the armchair direction of graphene lattice. This implies that tension along the armchair (Ox) and zigzag (Oy) directions corresponds to $\theta = 0$ and $\theta = \pi/2$, respectively.

The unit vectors of the deformed graphene with bond alternation are defined by $\mathbf{a}_1 = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{a}_2 = \mathbf{r}_1 - \mathbf{r}_3$, where $\mathbf{r}_i$ is the deformed bond vectors defined by Eq. (1). Then, the unit vectors become

$$\begin{aligned} \mathbf{a}_1 &= (a_{1x}, a_{1y}), \\ \mathbf{a}_2 &= (a_{2x}, a_{2y}), \end{aligned} \tag{3}$$

where

$$\begin{aligned} a_{1x} &= \left(a + \frac{b}{2}\right)(1+\varepsilon_{11}) - \frac{b\sqrt{3}}{2}\varepsilon_{21}, \\ a_{1y} &= -\frac{b\sqrt{3}}{2}\left(1 + \varepsilon_{22} - \frac{1}{\sqrt{3}}\varepsilon_{12}\right) + a\varepsilon_{12}, \\ a_{2x} &= \left(a + \frac{b}{2}\right)(1+\varepsilon_{11}) + \frac{b\sqrt{3}}{2}\varepsilon_{21}, \\ a_{2y} &= \frac{b\sqrt{3}}{2}\left(1 + \varepsilon_{22} + \frac{1}{\sqrt{3}}\varepsilon_{12}\right) + a\varepsilon_{12}. \end{aligned}$$

Here a and b are the C–C bond length and ε_{ij} are the components of the strain tensor.

In the nearest-neighbor tight-binding model, the Hamiltonian can be expressed by

$$\mathcal{H} = -\sum_{\mathbf{R}_B}\sum_{i=1}^{3} t_i a^{\dagger}_{\mathbf{R}_B+\mathbf{r}_i} b_{\mathbf{R}_B} + \text{H.c.}, \tag{4}$$

where $a^{\dagger}_{\mathbf{R}_A}(b^{\dagger}_{\mathbf{R}_B})$ and $a_{\mathbf{R}_A}(b_{\mathbf{R}_B})$ are, respectively, the create and annihilate operators an electron at $\mathbf{R}_A(\mathbf{R}_B)$ site in sublattice $A(B)$, t_i is the nearest-neighbor hopping parameter. The dependence of the hopping parameter t_i on the deformed bond length r_i can be described by Harrison's formula [13]

$$t_i = t_0\left(\frac{a_0}{r_i}\right)^2, \tag{5}$$

where $a_0 = 1.42$ Å and $t_0 = 2.7$ eV are the parameters for the C–C bond length and hopping of pristine (undimerized) graphene [14].

In the tight-binding approximation, the energy dispersions of the deformed graphite are given by Refs. [15,16]

$$\begin{aligned} E(\mathbf{k}) = \pm\{&t_1^2 + t_2^2 + t_3^2 + 2t_1t_2\cos[\mathbf{k}(\mathbf{r_1} - \mathbf{r_2})] \\ &+ 2t_2t_3\cos[\mathbf{k}(\mathbf{r_2} - \mathbf{r_3})] + 2t_1t_3\cos[\mathbf{k}(\mathbf{r_3} - \mathbf{r_1})]\}^{1/2}, \end{aligned} \tag{6}$$

where $\mathbf{k}$ is the two-dimensional wave vector.

In the special case, when the tension is along armchair and zigzag directions corresponding to $\theta = 0$ and $\theta = \pi/2$, respectively, the graphene with bond alternation as shown in Fig. 1 has $t_1 = t_0(a_0/r_1)^2$ and $t_2 = t_3 = t_0(a_0/r_2)^2$. Substituting Eq. (1) into Eq. (6) we obtain the energy dispersions of deformed graphene with bond alternation

$$\begin{aligned} E^{t\mathcal{A}}(k_x, k_y) = \pm\Bigg\{&t_1^2 + 4t_1t_2\cos\left[\left(a + \frac{b}{2}\right)(1-\varepsilon\sigma)k_x\right]\cos\left[\frac{b\sqrt{3}}{2}(1+\varepsilon)k_y\right] \\ &+ 4t_2^2\cos^2\left[\frac{b\sqrt{3}}{2}(1+\varepsilon)k_y\right]\Bigg\}^{1/2}, \end{aligned} \tag{7}$$

$$\begin{aligned} E^{t\mathcal{Z}}(k_x, k_y) = \pm\Bigg\{&t_1^2 + 4t_1t_2\cos\left[\left(a + \frac{b}{2}\right)(1+\varepsilon)k_x\right]\cos\left[\frac{b\sqrt{3}}{2}(1-\varepsilon\sigma)k_y\right] \\ &+ 4t_2^2\cos^2\left[\frac{b\sqrt{3}}{2}(1-\varepsilon\sigma)k_y\right]\Bigg\}^{1/2}, \end{aligned} \tag{8}$$

where $t\mathcal{A}(t\mathcal{Z})$ stands for tension along the armchair (zigzag) direction. Sublattice $A(B)$ connects with three sublattices $B(A)$ by one large and two small bonds. In comparison with equilibrium bond length a_0, the two different bonds of the alternation lattice change their lengths by -2δ and δ, where δ can be positive or negative [17]. This assumption is agreement with the quantum chemistry calculations for CNTs [4,5].

The position of the Dirac points of deformed graphene changes due to tension and difference of C–C bond lengths. The shifting of Dirac points can change the electronic properties of CNTs and GNRs because it connects to the parallel k-lines passing or not through Dirac points of the two-dimensional Brillouin zone.

3. Band structure of deformed armchair graphene nanoribbon with bond alternation

An armchair GNRs is strip of graphene that can be obtained by cutting a graphene sheet along the zigzag direction in the form of a quasi-one dimensional wire. Atomic structure of deformed armchair nanoribbon with bond alternation is shown in Fig. 1. All dangling bonds at the edges of graphene nanoribbons will be assumed to be terminated by hydrogen atoms. The width of graphene nanoribbon is defined via a number of dimer N. The unit cell of the armchair GNR contains $2N$ carbon atoms. In this paper we study the applied tension only along armchair and zigzag directions.

The energy spectrum of an GNR can be obtained from that of graphene by applying periodic boundary conditions at both edges of the ribbon. For an armchair GNR as shown in Fig. 1, the periodic boundary condition leads to the discrete transverse wavenumber

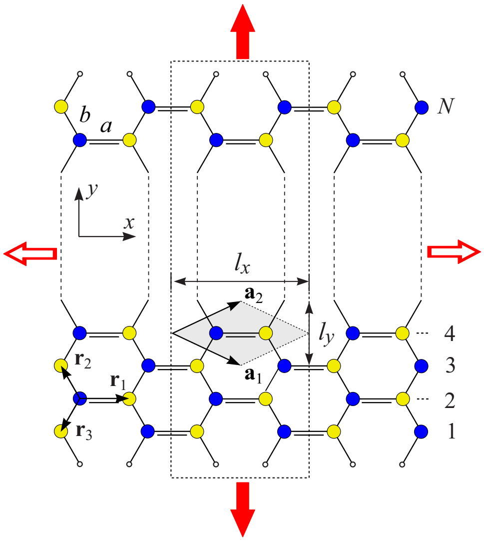

Fig. 1. Atomic structure of graphene with bond alternation. a and b are the C–C bond lengths. The shaded rhombus denotes the primitive cell of the length l_x and the width l_y which contains two carbon atoms (filled circles). The unit cell of armchair graphene nanoribbon is shown as the dashed rectangle. All dangling bonds at the edges are terminated by hydrogen atoms (small empty circles). Filled and empty arrows stand for the tension along zigzag and armchair directions, respectively.