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Influence of Correction Factor on Nearest Neighbour Hopping Parameterin Energy Dispersion Relation of Graphene Nanoribbon

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Abstract

We investigated on energy dispersion relation (E-KR) of graphenenanoribbon (GNR) considering its two prototypical shapes but only of AGNR in nearest neighbor interactions. Two parts $\frac{\Delta}{2}$ and $(\hbar\gamma_s)^2$ of E-KR relation have different characteristics independently expresses their importance. A correction factor $Ä_{ã_1}$ is used for hopping between two edge carbon atoms to count edge relaxation. Influence of this factor on hopping parameter exemplifies the edge bond relaxation effect in AGNR.

Keywords: Energy dispersion relation; Graphene nanoribbon; Nearest neighbor interactions; Ballistic performance; Correction factor, Edge bond relaxation

Introduction

Carbon nanomaterial reveals different outstanding properties subject to their geometrical structures. Nanoscale strips of single layer graphene named as GNRs have recently been the focus on widespread efforts in theoretical and practical field [1]. There is a confinement of carriers in two directions so GNRs are a one dimension (1D) structure with [2] GNRs are expected to have electronic properties as like as in those of Carbon nanotubes (CNTs) that can be unwrapped into GNRs as there is structural similarity with compared to CNTs and effects in quantum confinement [3]. Today's theoretical statistics indicates that characteristics such like metallic or semiconducting behavior in GNRs unlike from that in CNTs [4,5]. Two prototypical edge shapes are formed by cutting graphene sheet along a straight line named as the armchair edge and the zigzag edge between the two edge orientations with a difference of 30° in the axial direction [6]. Either one of these two "ideal" shapes or more complex geometries composed of a mixture of armchair and zigzag shaped fragments is formed depending on the cutting direction, the edges of the GNRs [7]. GNRs are classified by the number of dimer lines (zigzag lines) named as armchair (zigzag) edges on both sides across the ribbon width [8,9]. GNRs are semiconducting due to the edge effects for all sub-10 nm make more attractive for electronic device applications [10]. The electronic band structure of AGNRs are found to play an important role in the edge bond relaxation and the 3NN interactions [11-14] that are not prominent in CNTs. Using the NEGF formalism atomistic simulations of GNRFETs have also been described [15-18]. But they are expensive so we have examined by MATLAB simulation of the influence of correction factor on nearest neighbor of hopping parameter in AGNR. GNRs semiconducting properties can be guessed through its geometrical nature where width is [19-22] rely on N [21,23] in which this properties occur in GNRs when m=3p or m=3p+1, where p is an integer [24]. At first we have calculated the main energy dispersion than without considering the correction factor we measured the energy dispersion from which we calculate the percentage of deviation or error on energy.

Approach

With a view to following the standard GNR literature convention —"armchair" and —"zigzag" denote to the shape of the edge in the transport direction of the GNR and, that is contrasting to the CNT convention [25]. An armchair ribbon is cut so that the edge looks as if it consists of repeated armchairs. The width of an armchair ribbon can be defined in terms of the number of dimer lines (N): [26]

$$W_{ac} = (\text{m-1})\frac{\sqrt{3}}{2}\text{a} \tag{1}$$

Again we can write from the above equation

$$\text{m} = \frac{2w_{ac} + 2\sqrt{3}a}{\sqrt{3}a} \tag{2}$$

Where a=1.42 the nearest neighbor distance and m=3p or m=3p+1 or m=3p+2.

Now to observe the ballistic performance along with the band structures in the energy range of interest of AGNR where

E-k dispersion parameter is given by [10]:

$$\frac{\Delta}{2} = \tilde{a}_1(2s\cos\frac{p\pi}{m+1}+1) + \tilde{a}_3(2s\cos\frac{2p\pi}{m+1}+1) + 4(\frac{\tilde{a}_1+\Delta_{\gamma_1}}{m+1})\sin^2\frac{p\pi}{m+1} \tag{3}$$

Where p=m/3 or (m-1)/3 or (m-2)/3 and s=0.129 indicates overlapping integral.

Here for convenient to understand say m=3p or 3p+1 or3p+2. Also [10].

$$(\hbar\gamma_s)^2 = (3d)^2\left\{\begin{array}{l} -\frac{1}{2}\gamma_1 s\cos\frac{p\pi}{m+1}\text{X}\left[\gamma_1+\gamma_3(2\cos\frac{2p\pi}{m+1}+1)+4(\frac{\gamma_3+\Delta_{\gamma_1}}{m+1})\sin^2\frac{p\pi}{m+1}\right] \\ -\gamma_3(\gamma_1+2\gamma_3\cos\frac{2p\pi}{m+1}+4\left(\frac{\gamma_3+\Delta_{\gamma_1}}{m+1}\right)\sin^2\frac{p\pi}{m+1}) \end{array}\right\}$$

Where γ_1=-3.2 eV indicates first nearest neighbor hopping parameters,

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γ_3=-0.3 eV third nearest neighbor hopping parameters and Δ_{γ_1} =-0.2 eV is the correction of γ_1 for the bonds due to the edge bond relaxation and ħ is the reduced Planck constant [11].

The main goal of our investigation is the 'term' which causes an error of correction factor in energy dispersion relation is

$$\frac{\Delta_e}{2} = \gamma_1(2s\cos\frac{p\pi}{m+1}+1) + \gamma_3(2s\cos\frac{2p\pi}{m+1}+1)$$

$$(\hbar\gamma_s)^2 = (3d)^2\left\{-\frac{1}{2}\gamma_1 s\cos\frac{p\pi}{m+1}\mathrm{X}\left[\gamma_1+\gamma_3(2\cos\frac{2p\pi}{m+1}+1)\right]-\gamma_3(\gamma_1+2\gamma_3\cos\frac{2p\pi}{m+1})\right\} \quad (6)$$

So the final energy dispersion equation become which has ± value denoted as [10]

$$\mathrm{E} = \sqrt{((\frac{\Delta}{2})^2 - (\hbar\gamma_s k)^2)} \quad (7)$$

$$\mathrm{E}_e = \sqrt{((\frac{\Delta_e}{2})^2 - (\hbar\gamma_s k)^2)} \quad (8) \text{ or}$$

$$\mathrm{E}_e = \sqrt{((\frac{\Delta}{2})^2 - (\hbar\gamma_s k)^2{}_e)} \quad (9) \text{Or}$$

$$\mathrm{E}_e = \sqrt{((\frac{\Delta_e}{2})^2 - (\hbar\gamma_s k)^2{}_e)} \quad (10)$$

To check the influence of correction factor of γ1 we have omitted the Δ_{ce} term from equation (3), (4) for this corresponding value of E is obtained as E_e. Based on this value the percentage of error can be calculated.

$$e_r = \frac{\text{actual value of E- error value of E}(\mathrm{E_e}))}{\text{actual value of } E}\ \mathrm{X}\ 100\% \quad (11)$$

Results and Discussion

The energy dispersion relation is the exact solution of observing the edge bond relaxation of AGNR which is obtained for varying with k state of energy band.

We have seen that -39.8694i, -39.8695i, -39.8696i eV energy is found for successively m=3p, 3p+1, 3p+2 values where width of our device is w=2.46nm. Again real value of E is observed in -1.8153, -1.8153, -1.8154 eV and then after three values complex energy value is found.

Now our main objectives is on % of error value says that how the correction factor influence on energy dispersion in nearest neighbor hopping parameters.

The deviation is negligible as the minimum % of error is fixed and maximum % of error is getting decreased.

Conclusion

In this paper, we have neglected the correction factor but we avoid totally the Δ_{ce} term in equation (3), (4) which results error although in nanoscale especially for AGNR not sensitive. So the value is changed after four faction point. However we have tried to demonstrate the response of correction factor on nearest neighbor hopping parameters which indicates the edge bond relaxation in AGNR at nanoscale which can be neglected as the % of error also found after four fraction point but in large scale device it is more sensitive.

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