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The Effect of Stone-Wales Defect on the Geometrical Parameters and Electronic Properties of ACNTs (14, 14)

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Abstract

In this work, we intend to investigate the effect of Stone–Wales defect (SW defect) in armchair (14, 14) carbon nanotubes (ACNTs (14, 14)) and how it perturbs the energy states near the Fermi level. The SW defect may occur in graphene, carbon nanotubes (CNTs), and similar carbon frameworks, in which the four adjacent six-membered rings of a pyrene-like region turn into two five-membered rings and two seven-membered rings when the bond uniting two of the adjacent rings rotate. Our calculations indicate that ACNTs (14, 14) with SW defect have semiconducting behavior, although the armchair CNTs are expected to be metal. The band-gap of ACNTS (14, 14) with SW defect is 0.11 eV. In addition, the obtained results show that the density of states of ACNTs (14, 14) with SW defect reaches its zenith at 13 eV. The results show that the C–C bond lengths and diameter of ACNTs (14, 14) with SW defect are 1.40 Å and 18.74 Å, respectively.

1. Introduction

A Stone-Wales (SW) defect is a crystallographic deformity that includes the change of connectivity of two π-bonded carbon atoms, resulting in their rotation by 90° with respect to the midpoint of their bond [1-3]. The SW defect may occur in carbon nanotubes (CNTs)~~,~~ and graphene, in which the four adjacent six-membered rings of a pyrene-like region turn into two seven-membered rings and two five-membered rings when the bond uniting two of the adjacent rings rotates. The rearrangement in the crystal lattice is supposed to have significant implications for the thermal [4], mechanical, electrical, and chemical properties of these materials [5].

CNTs were discovered by Sumio Iijima in 1991 [6]. Single walled carbon nanotubes (SWCNTs) usually have a length of several micrometers and a diameter of 1-2 nm. This ratio makes them nearly ideal one-dimensional (1-D) objects. As a result, SWCNTs are expected to have unique properties [7-10]. The cylinder structure of a graphene layer of these nanostructures is the main reason for their special electronic and other physical properties [11-14]. Investigating the geometry and electronic properties of CNTs is an applicable method to learn more about their essence. The formation kinetics of SW defects have been reported by Kabir et al. [15]. Moreover, Ertekin et al. have computed the formation energies of SW defects in CNTs [16]. Zhou et al. studied the formation energy of SW defects in CNTs [5].

In this work, we intend to investigate the effect of SW defect in armchair (14, 14) carbon nanotubes (ACNTs (14, 14))and how it perturbs the energy states near the Fermi level.

2. Materials and Methods

2.1 *Computational details*

CNTs are hollow cylinders composed of one or more concentric graphene layers in a honeycomb lattice arrangement. We have simulated the effect of SW defects on the electronic properties and geometrical parameters of ACNTs (14, 14) in this work. The simulated lattice of CNT with SW defect has been shown in Figure 1.

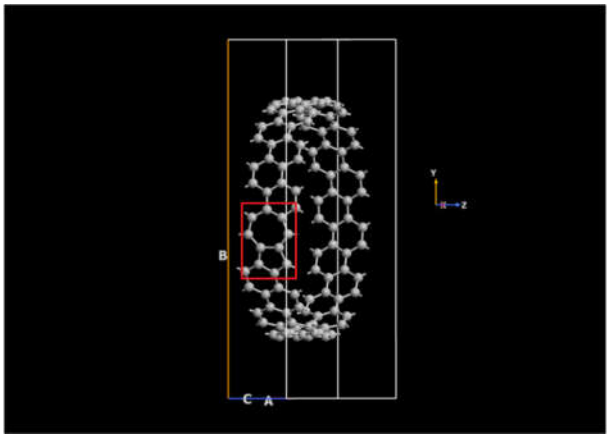

Figure 1. ACNTs (14, 14) with SW defect

The tight-binding (TB) or linear combination of atomic orbitals (LCAO) method is a semi-empirical method that is primarily used to calculate the band structure and single-particle Bloch states of a material. The semi-empirical TB method is simple and computationally very fast. The screw symmetry of the nanotubes permits the construction of a TB model that is based on a two-atom unit cell, rather than on the translational unit cell with NC two-atom unit cells [17, 18]. This TB model has advantages regarding the computational time and the accuracy of the outputs. Our model parameters are given by $V_{ss\sigma}$= 4.76 eV, $V_{sp\sigma}$=4.33 eV, $V_{pp\pi}$=−2.77 eV, $V_{pp}\sigma$= 4.37 eV [19]. The other two parameters, $V_{s*p\sigma}$, $V_{s*s*\sigma}$, can be obtained from Table 1 in reference [20].

3. Results and Discussion

3.1 *Electronic parameters*

The band structure and DOS of ACNTs (14, 14) with SW defect are represented in Figures 2 and 3, respectively. The graphs indicate the simulated nanotube has semiconducting behavior. The band-gap of ACNTS (14, 14) with SW defect is 0.11 eV. Compared to ZCNTs (5, 0) [21] with SW defect (E_g=0.319) and ZCNTs (10, 0) [22] with SW defect (E_g=0. 19), ACNTS (14, 14) with SW defect has a smaller band-gap. The main reason is that the curvature effects and the p-orbitals overlap in the smaller nanotubes (ZCNTs (5, 0) and ZCNTs (10, 0)) eventuate in filling the energy states near the Fermi levels.

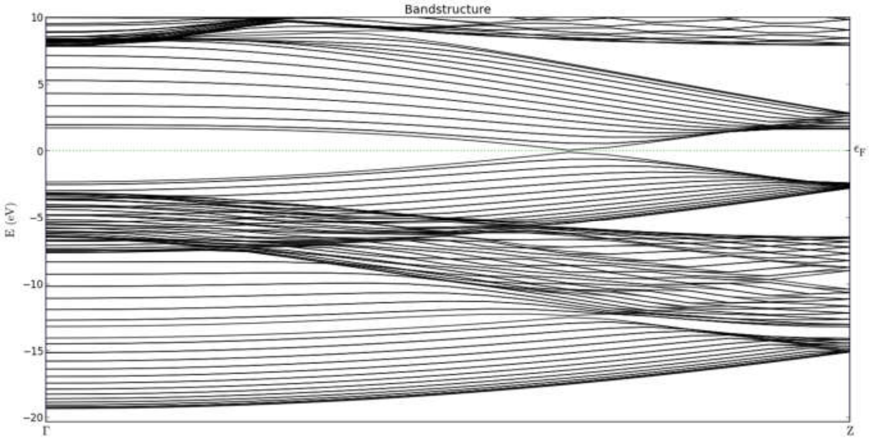

Figure 2. Electronic band structure of ACNTs (14, 14)

Figure 3 shows that the density of states of ACNTs (14, 14) with SW defect reaches its zenith at 13 eV. For ZCNTs (10, 0) with SW defect, the maximum of the density of states in -2 eV to 2 eV is located at 2 eV. It is worth mentioning that there is no more available data to compare our results with.

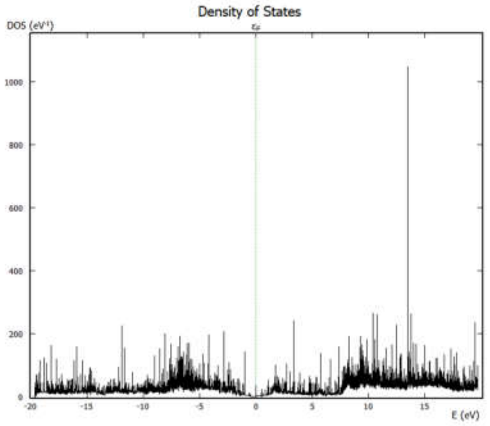

Figure 3. electronic band structure of ACNTs (14, 14)

3.2 *Geometrical parameters*

CNTs are chemically bonded with sp2 bonds, a highly strong form of molecular interaction. This feature combined with CNTs' natural inclination to rope together via van der Waals forces, supplies the probability to develop low-weight and ultra-high strength materials with highly conductive thermal and electrical properties. This makes them highly attractive for numerous applications.

Each CNT has a specific chirality and geometry. Bertoni [11], Mori et al. [23], and Movlarooy [24] have confirmed that the physical properties of CNTs depend on their geometrical parameters and chirality. According to Ref [25], the rotation operation, ψ, of ACNTs (14, 14) is $\pi/14$ radians. In this study, the effect of SW defect on the geometrical parameters of ACNTs (14, 14) has been calculated, and the results are shown in Table 1. The results show that the C–C bond lengths and diameter of ACNTs (14, 14) with SW defect are 1.40 Å and 18.74 Å, respectively. The other calculated parameters have not been reported yet to assess the accuracy of the data.

Table 1. Simulated geometrical parameters of ACNT (14, 14) with SW defect using the TB method

Symbol	**Name**	**Value**	**Experiment results (Å)**
$a_{C\text{-}C}$	Carbon–Carbon distance	1.40 Å	1.42 [26]
a	Length of unit vector	2.40 Å	-
L	Circumference of CNT	58.51 Å	-
d_R	Diameter of CNT	18.74 Å	-
T	Length of T	5.43 Å	-
θ	Chiral angle	30°	-
N	Number of hexagons per 1D unit cell	62	-
-	Number of atoms per 1D unit cell	124	-

4. Conclusions

The TB method has been exploited to simulate the effect of SW defects on the electronic properties and geometrical parameters of ACNTs (14, 14). The screw symmetry of the nanotubes permits the construction of a TB model that is based on a two-atom unit cell, rather than on the translational unit cell with NC two-atom unit cells. This TB model has advantages regarding the computational time and the accuracy of the outputs. Our model parameters are given by $V_{ss\sigma}= 4.76$ eV, $V_{sp\sigma}=4.33$ eV, $V_{pp\pi}=-2.77$ eV, $V_{pp}\sigma= 4.37$ eV. The results show that ACNTs (14, 14) with SW defect have semiconducting behavior, although the ACNTs are expected to be metal. The results suggest that the C–C bond lengths and diameter of ACNTs (14, 14) with SW defect are 1.40 Å and 18.74 Å, respectively.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding this article.

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