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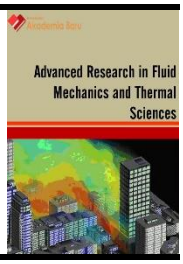

Polarizability and Band Gap of Boron Nitrite Nanotubes for Different Length and Diameter

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ABSTRACT

The electronic and optimized structure of boron-nitrite nanotube (BNNT) has been generated by the nanotube modeler program and analyzed using the PM3 semi-empirical quantum computational method. The electronic structure of BNNT generated for various diameters and lengths. Calculation of band-gap which obtained from the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular orbital (LUMO) levels exhibit clear oscillation that depends on the length and diameter of the tube due to the positions of the periodic ions. Polarizability for various length and diameters were computed, using HyperChem and MOPAC programs. The result shows that the polarizability sharply increased up to $4x10^5$ A^3 at electric field 0.002 au then decayed while by varying n which is related to diameter the polarizability increases up to $7x10^6$ A^3 when n=14, and at m=11.

1. Introduction

Nanotubes have been given significant attention over the last decade since the carbon nanotubes (CNTs) were identified [1]. BN nanotubes (BNNTs) are structural analogs of CNTs where C atoms are substituted by alternating Boron and nitrogen atoms. BNNTs were predicted theoretically in 1994 and then a year after synthesized by arc discharge. BN nanotubes have a structure similar to that of carbon nanotubes (CNT), except the CNT can be conducting or superconducting depending on the rolling direction and radius, while the BNNTs are electrical insulator with a wide band gap of about 5.5eV and independent of the tube chirality and morphology [2,3]. while carbon nanotube may be either metallic or semiconductor depending on their indices (*l*, m) [4]. Also, Meunier and coworkers show that for BN/C nanotubes system, the valence and conduction band offsets are spatially direct with values of 0.82 ev and -2.09 ev respectively [5], BNNT consists of an equal number of boron and nitrogen atoms and similarly structured as carbon, thus exists in various crystalline forms. It has great potential and interest in nanotechnology. Due to the effective phonon heat transfer, BNNTs are good

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thermal conductors as reveals by theoretical and experimental studies made by several researchers. A layered BN structure is more thermally and chemically stable than the graphitic carbon structure. Also, it displays a stable wide band gap, excellent mechanical strength, high thermal conductivity UV light emission; therefore, BNNTs are used as nanofillers for composites [6].

As a binary chemical compound, Boron nitride is consisting of equal proportions of boron and nitrogen composition BNNT [7,8]. Structurally; it is similar to carbon and takes a similar physical form i.e. a Graphite-like one, and a diamond-like one. The latter is the only material nearly as hard as diamond. Boron nitride is stable in the air to approx. 1000°C, and under reduced conditions or inert gases it can be used up to 1800°C [7].

Boron is one to the left on the periodic table from carbon and nitrogen is one to the right. Therefore, it is not surprising that a graphene-like lattice can be synthesized from alternating boron and nitrogen atoms.

Boron nitride is far more resistant to oxidation than carbon and therefore, suited for high-temperature applications in which carbon nanostructures would burn. Moreover, BN nanotubes electronic properties are independent of tube diameter and the number of layers, unlike tubes made of carbon, making BN nanotubes much more amenable. By doing these tubes, it is conceivable to have devices on single BN tubes which have diameters on the order of nanometers and lengths on the order of microns.

The range of applications (e.g., in optoelectronic devices) of these boron nitride nanotubes would be greatly extended if their band gap can be tuned to desired values in a controlled way. Another way to modify the band gap of the nanotube is to apply an external electrical field as reported by Kim *et al.,* [8,9]. Practically, a nanotube on an insulating substrate can be subjected to a strong transverse electric field through an applied gate voltage. Such systems are prototype nanoscale field-effect transistors.

Chun-Wei Chen and coworkers reported that the electronic structures of carbon (C) and boron nitride (BN) nanotubes under a transverse electric field were investigated through the first-principles pseudopotential density-functional theory (DFT) calculations and found that band gap modifications occur both in the semiconducting C and BN nanotubes under an external electric field by inducing a semiconductor–metal transition. The variations of the band gap sizes with transverse electric fields are very different between C and BN nanotubes. In the semiconducting C nanotube, a sharp semiconductor–metal transition does not occur until a threshold electric field is achieved; the BN nanotubes, on the other hand, shows a gradual reduction of the band gap size once an external electric field is applied due to the larger ionic bonds of BN. Besides, the semiconductor–metal transition in both C and BN nanotubes occurs at a lower value of the electric field with increasing diameter. The ability to tune the band gap in both C and BN nanotubes by an external electric field provides the possibility for future electronic and electro-optic nanodevice applications [10].

Boron nitride can be doped to p-type with beryllium and to n-type with sulfur, silicon, or if co-doped with carbon and nitrogen. Both hexagonal and cubic BN are wide-gap semiconductors with a band-gap energy corresponding to the UV region. If a voltage is applied to h-BN or c-BN, it emits UV light in the range 215-250 nm and therefore can potentially be used as light-emitting diodes (LEDs) or lasers [7]. Also, calculations on BN nanotubes in the presence of a transverse electric field were performed and it has been found that these systems exhibit a dramatic decrease in band gap when subject to strong fields. This effect should be realizable experimentally for the 5 nm or more diameter BN nanotubes, and it may be very important for tuning the band gap of BN nanotubes for practical applications [7].

The BNNTs have an exceptional stiffness, with a young's modulus of about 1.2TPa. Therefore, they are promising for the reinforcement of polymeric composites and ceramics. This will lead to

applications in lighter, faster, and affordable transportation, as well as lightweight armors. Also, the unique nature of BNNTs is associated with the nature of their partial ionic bonds, makes it preferable to CNTs for hydrogen storage because ionic B-N bonds induce a dipole moment between hydrogen and the nanotubes for stronger binding [11,12]. The wide band gap is substantial for BNNTs applications in the electronic industry [13]. On the other hand, many researchers had synthesized and studied BN nanotubes such as Singhal and his coworkers [14] who used a simple chemical method. Miandal *et al.,* [15] investigated the dependence of annealing temperature on the optical and structural of the films. The results showed that there is a modification in the absorption spectrum of PTAA thin films as the annealed layers where there is an increase in the absorptive with the increase in annealing temperature and the estimated band gap within 3.05-3.14 eV. Abu Bakar *et al.,* [16,17] was successfully deposited $CuGaO_2$ thin film on glass substrate by using RF puttering deposition method in a controlled Argon atmosphere. the results showed that the crystallinity of the thin film is increase with increasing annealing temperature and annealing duration.

In this study, BN nanotubes are generated by the nanotube modeler program and the polarizability and band gaps are obtained using hyberchem and Mopac programs. An example of these nanotubes is shown in Figure 1.

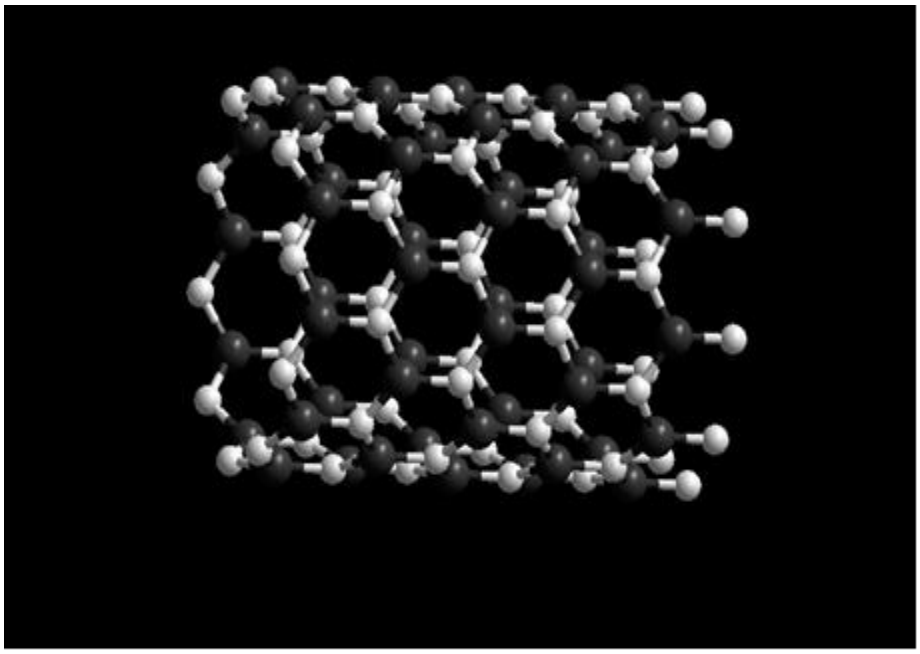


Fig. 1. (10,0) zigzag BN nanotubes

2. Evaluation Methods

In the present work, First, an SWBN nanotube (n=10, m=0) is designed using Nanotube Modeler Software, as an example of these nanotubes is shown in figure 1, We chose zigzag-type (n,n) nanotubes to study, the electronic properties.

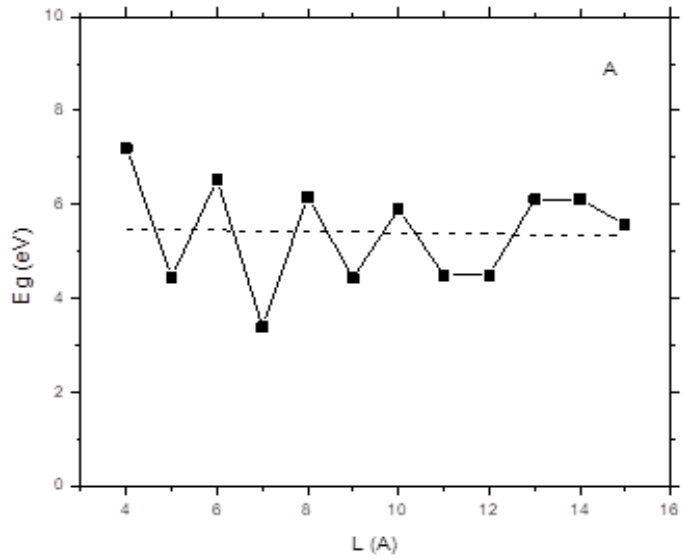
Different types of BN NT (i.e. different lengths and diameters) are generated to study the electronic properties by evaluating the energy gap obtained from the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular orbital (LUMO) levels, and the polarizability, which computed for different BNNT lengths and diameters using MOPAC2016 [18] and HyperCHem programs.

3. Results and Discussion

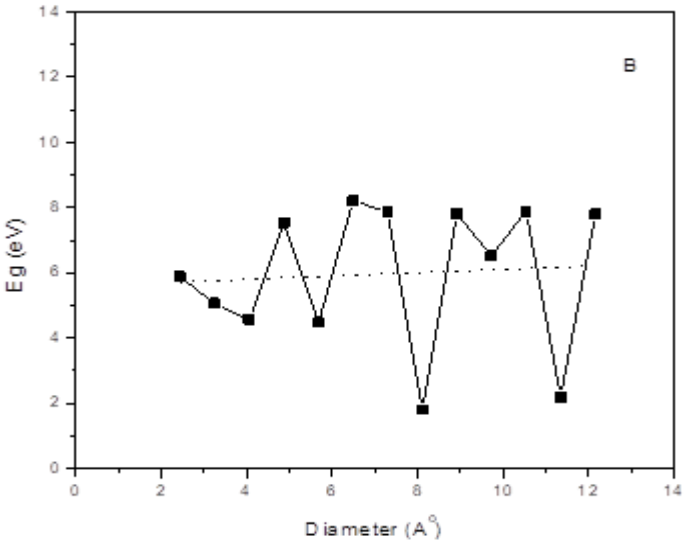
It has been found that the band gap of BNNT is independent of the length and diameter of nanotubes as shown in Figure 2. The oscillation shown in the graph is probably due to the periodic potential of the B and N atoms. The band gap was determined from the HOMO and LUMO energy levels as

$Eg = E_{Homo} - E_{Lumo}$,

while the polarizability was calculated by the simulation program using PM3 approximation.



(a)



(b)

Fig. 2. Band gap variations with the (a) length and (b) diameter of the nanotubes

The polarizability variation of BN nanotubes for length and diameter variations has been studied and found that it increases with the increase of diameter as shown in Figure 3 and with the increase of length as shown in Figure 4. For both figures, the polarizability increases with increasing length

and diameter, and maximum values have been recorded at high values of diameter and length. The study was made for increasing diameter alone for different lengths of nanotube and varying the length for different diameters. Figure 5 shows polarizability variation with n for the zigzag structure of BN nanotubes BN (6, 0).

The semi-empirical pm3 calculation reveals that the energy gap of zigzag nanotube has an oscillatory behavior depending on the number of sections along the tube and does not affect the amplitudes.

The tubular diameter of nanotube influences the HOMO-LUMO and hence band gap slightly decreased with an increase of diameter which is represented by (n).

The HOMO has a bonding character and the LUMO has an anti-bonding character along the tubular axis which leads to the high bandgap. The polarizability shows an increase with (n) after (n=10) as shown in Figure 5, while in n<10, there is no change is noticed due to the close distances between the alternating B and N ions positions which help to diminish the effect of potential effects.

Figure 6 shows the polarizability increases sharply and then decreases exponentially with increasing the external electrical field. Also, the figure indicates that the effects of the axial and transverse electrical fields are the same when exerted on the BN nanotubes. The charity n is used instead of diameter due to the proportionality of the diameter of nanotubes with respect to n.

In other words, Figure 6 shows the sharp increase of polarazibity with the increase of the external applied electric field then after the exponential decrease. There is no big difference between a traverse (solid squares) and the axial (circles) fields if applied. The external field causes band gap modification and charge redistribution in the nanotube. When the field is applied the state charges are mostly located at a certain atom i.e. N atom due to its electron affinity, and the degree of the charge redistribution is sensitive to the external electric field due to high ionicity of BN bonds, which restrict the movement of the dipoles and that cause the polarazability decrease after the sharp increase. Due to this modification in polarizability and hence in band gap, the BN nanotube may undergo band gap opening and closing mode when subjected to a traverse electric field as mentioned by Kim and his coworkers [19]. The charity n is used instead of diameter due to the proportionality of the diameter of nanotubes with respect to n.

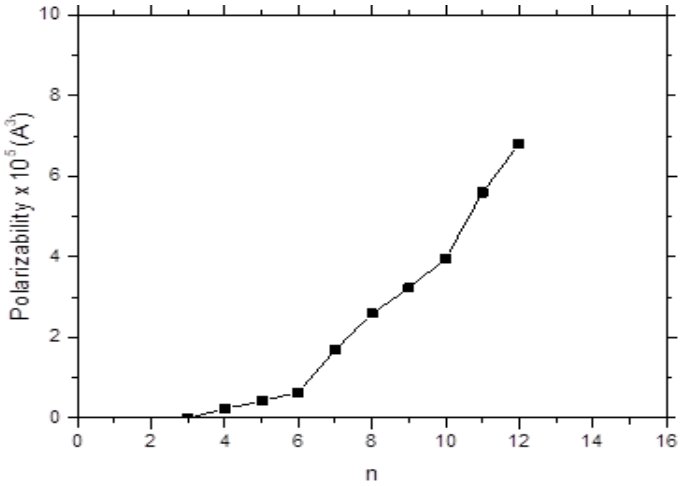


Fig. 3. Ploarizablity vs diameter

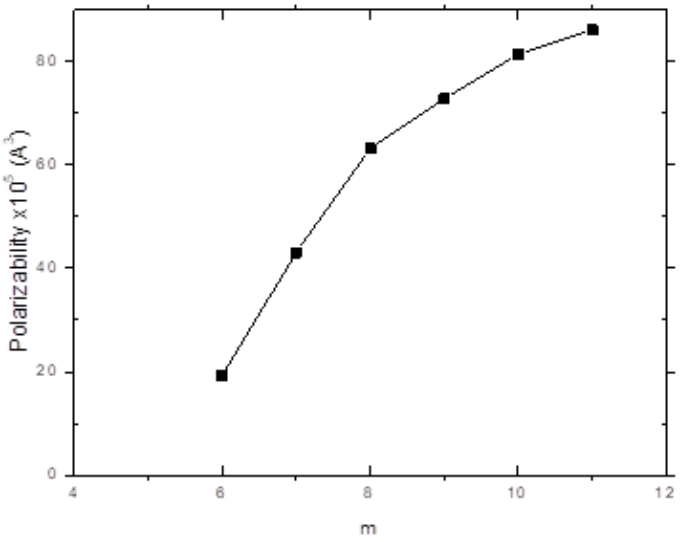


Fig. 4. Polarizability vs length

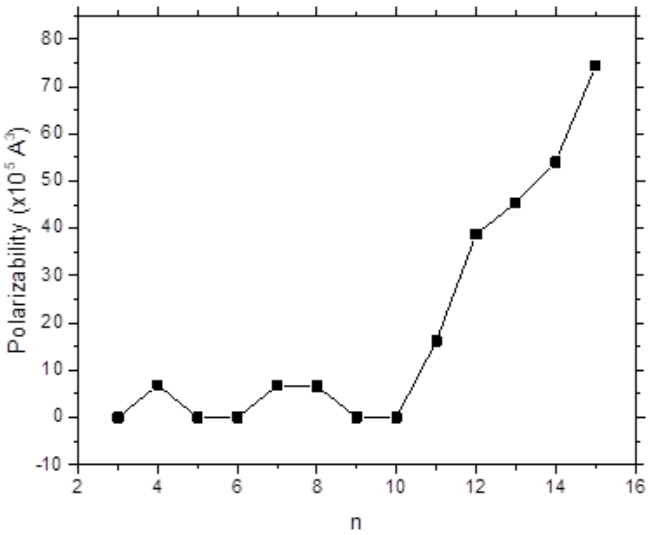


Fig. 5. Polarizablity variation with n for zigzag BN nanotubes

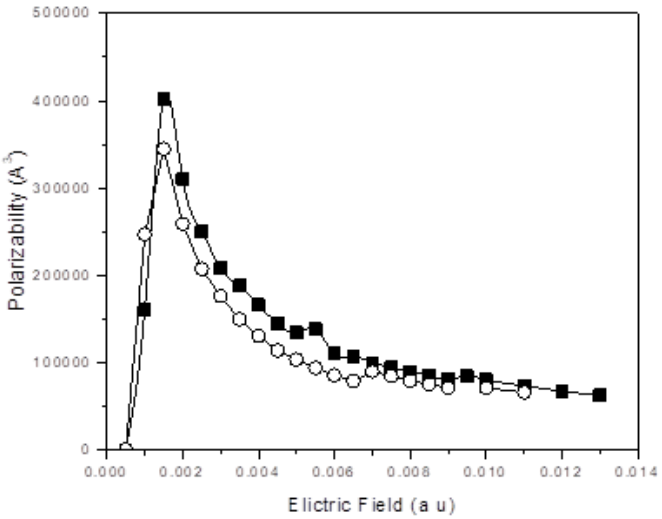


Fig. 6. Polarizability behavior for nanotubes under transverse and axial fields

4. Conclusions

In this work, the Electronic and optimized structure of boron-nitrite nanotube (BNNT) was generated by the nanotube modeler program and analyzed using the PM3 semi-empirical quantum computational method. The results were evaluated the polarizability of various lengths and diameters using HyperChem and MOPAC programs. The key outcomes of the current research can be inferred as follows

i. It has been found in this study the BN nanotube structure has high polarizability which increases with increasing the diameter and length. Due to this behavior, the BN nanotube can be used in many applications that require polarizable structures such as pressure sensors and micro switches. Also, it can be used to capture the poisonous gasses from the environment at the industry due to its affinity.
ii. In some calculations, the polarizability variation shows zigzag lines that possibly due to the periodic variations in the potentials in the structure.
iii. From the calculations on BN nanotubes in the presence of a traverse electric field, it has been found that the structure exhibits a dramatic decrease in band gap when subjected to the strong field which confirms a study made by K.H. Khoo *et al.,* [5], and this effect can be very useful in tuning the band gap of BN nanotubes for certain applications, also it can be used in systems that are prototype nanoscale field-effect transistors.
iv. The BN nanotubes electronic properties are independent of tube diameter and several layers, unlike c-c tubes, which make it more amenable: by doping these tubes, it is conceivable to have devices on single BN tubes which have a diameter on the order of nanometers and lengths on the order of microns.
v. The polarizability sharply increased up to 4x105 A3 at electric field 0.002 au then decayed while by varying n which is related to diameter the polarizability increases up to 7x106 A3 when n=14, and at m=11.

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