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Comparison the structural, electronic and transport properties of (5, 0) zigzag GaN nanotube with BN nanotube: DFT theoretical calculation

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Abstract—The structural, electronic and transport properties of zig-zag (5, 0) GaN nanotube and BN nanotube have been studied using Density Functional Theory (DFT). Comparing GaN nanotube with BN nanotube, we have obtained distinguishing features of GaN nanotube. The band structure, density of state, band gap and current-voltage (I-V) characteristics of two these structures were studied under low-bias conditions. The obtained results demonstrate and indicate that the GaN nanotube has a very good electronic and transport properties than the BN nanotube, which is highly promising in future optoelectronic device applications.

Index Terms—Gallium nitride nanotube; Boron Nitride nanotube; DFT; I-V character; TranSiesta.

I. INTRODUCTION

Nanotubes are intensely studied and considered to have a huge potential application in all sorts of nanoscale devices, nanostructured materials or instrumentations containing nanoscale components, include computational and experimental nanoscience, theoretical and applied nanotechnology and molecular engineering, theoretical, computational and experimental condensed matter physics and chemistry, and many other fields [1-9]. Due to the advanced application of carbon nanotubes, researchers are also trying for other materials nanotubes [10]. As an important III-V semiconductor, gallium nitride (GaN) is of great importance due to its high thermal, mechanical stability and optoelectronic properties [11- 14]. Gallium Nitride nanotubes were successfully synthesized by using epitaxial casting method [15]. GaN is a wide-band-gap semiconductor of interest for high brightness, blue light-emitting diodes, laser, Transistor and flat panel displays [16-19]. The properties of bulk Boron Nitride (BN) are similar to those of diamond, for example, excellent thermal conductivity, high chemical resistance and high melting point [20, 21]. In addition, since BN is a piezoelectric material, its tubular structure is a candidate for applications in nanometer-scale sensors [22]. Boron Nitride nanotube has been synthesized mainly by methods that have been well documented earlier for CNT fabrication including arc discharge, chemical vapor deposition and laser ablation [23]. BN nanotubes offer new opportunities for spin-based electronic devices (Spintronic) [24]. Also they were recently being used for applications in digital switches and tunneling Field Effect Transistors when functionalized with metallic quantum dots [25, 26]. In this paper the structural, electronic and transport properties of (5, 0) zigzag GaN and BN nanotubes were compared.

II. COMPUTATIONAL METHOD

In this study we have taken a zigzag (5, 0) GaN and BN nanotube with 60 atoms its central region (scattering region) for the charge transfer. The on tube device consists of tree part i.e., left electrode, channel region and right electrode that the two proposed nanotubes as the channel region, illustrated in Figure 1. These tubes were located on the bulk gold electrodes. Two gold (Au) (100) electrodes are used as a nanotube contact metal.

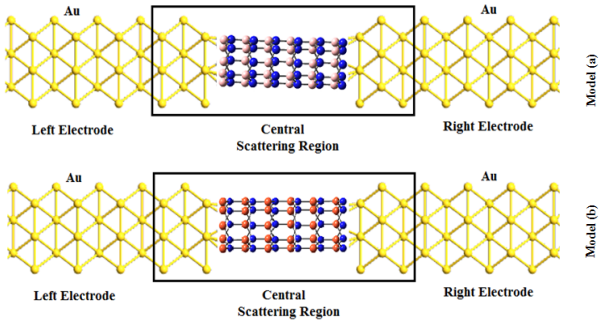

Fig. 1. Device structures of (a) model of BN nanotube (b) model of GaN nanotube as the scattering region. Pink, blue and orange spheres indicate Boron, Nitrogen and Gallium atoms respectively.

Structural relaxation of all models is calculated using the SIESTA-3.2 [27] package based on pseudopotential DFT calculations. All calculation have been performed within the framework of Local Density Approximation (LDA) using the exchange-correlation functional of Perdew-Zunger (PZ) [28] and the norm-conserving Troullier-Martins pseudopotentials [29] are used for the core-valance interactions. We employed a double-ζ polarized (DZP) basis set for all atoms. Relaxed geometries are obtained by minimization of the total energy using Hellmann-Feynman forces including Pulay-like corrections. A mesh cutoff 350 Ry was used for the computation of the electron densities and potentials. The proposed structures optimized until all forces acting on atoms are less than 0.01 eV/A°. Then in order to investigate the structural, electronic and transport properties of these structures, the band structure (BS), density of state (DOS) and I-V characteristics are calculated.

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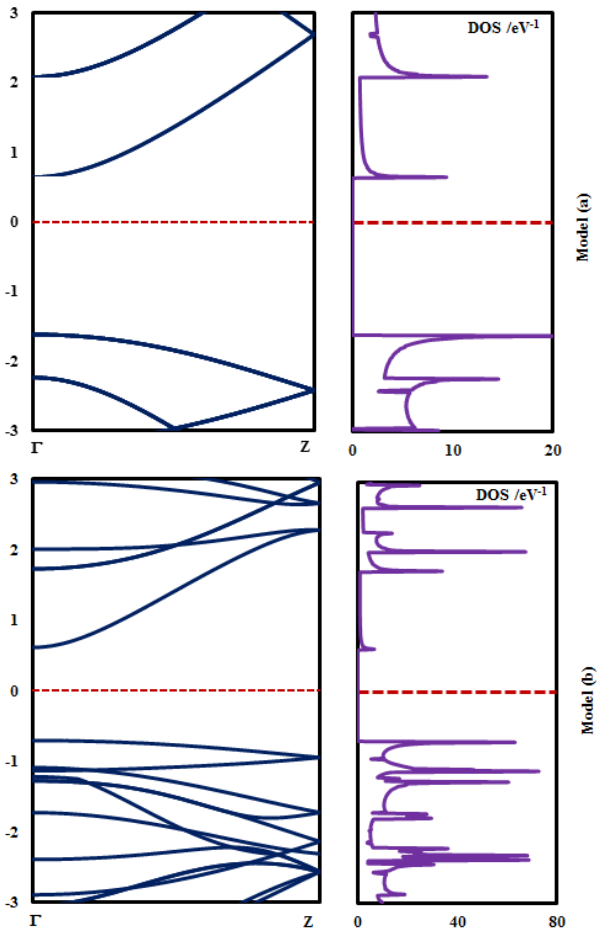

Fig. 2. Electronic band structures and density of states (DOS) of nanotube of (a) BN (b) GaN. The dash lines indicate the Fermi level.

III. DENSITY OF STATE (DOS) AND BAND STRUCTURE (BS)

It is essential to understand the conductance behavior of the proposed structure thus electronic band structure (BS) and density of state (DOS) of the considered structures are calculated. The electronic band structure and density of state diagrams of these models are shown in Figure 2. The band structures diagram shows these two nanotubes are semiconducting. It can be clearly seen that the band gap for the GaN nanotube is smaller than the BN nanotube. The bandgap of these tubes are 1.324 eV and 2.263 eV respectively. Table 1 shows the result of gap energies of both structures obtained using DFT calculations. As well as on observing DOS diagrams for both nanotubes, no peak has been found at their Fermi level, evident of their semiconducting behaviour, however dispersed peak can be seen in conduction band and valance band with one of them reaching the maxima. The DOS profile of the GaN nanotube is shown the highest value of the electron density than the BN nanotube.

IV. I-V CHARACTERISTICS AND QUANTUM CONDUCTANCE

Transport properties of the proposed models are explored using the TranSIESTA code, which is based on the combination of DFT and NEGF method. We varied the applied bias across two electrodes in the range of 0 to 1V (low bias) and subsequently measured the effective variation in the values of the current and quantum conductance. The current that passes through the central region of the system at a finite bias voltage can be computed using Landauer-Buttiker formalism [30] given by:

$$I(V_b) = \frac{2e^2}{\hbar} \cdot \int T(E, V_b) dE \quad (1)$$

Where $\frac{2e^2}{\hbar}$ is the quantum unit of conductance and $T(E, V_b)$ is the total transmission probability for an incident at an energy E through the device under the applied bias voltages which itself can be calculated as $T(E, V_b) = \sum T_n(E, V_b)$ Here V_b is the applied bias voltage. . For the accuracy of calculations, the electrode temperature has been set to 300 K and for the Brillouin zone integration, a 3 × 3 × 60 Monkhorst-Pack k-point grid has been utilized.

TABLE 1. Gap energy, maximum conductance and applied bias voltage for both proposed models.

Model	BN Nanotube	GaN Nanotube
Energy gap (eV)	1.324	2.263
Maximum conductance (nS)	33	680
Applied voltage Bias (V)	1	0.73

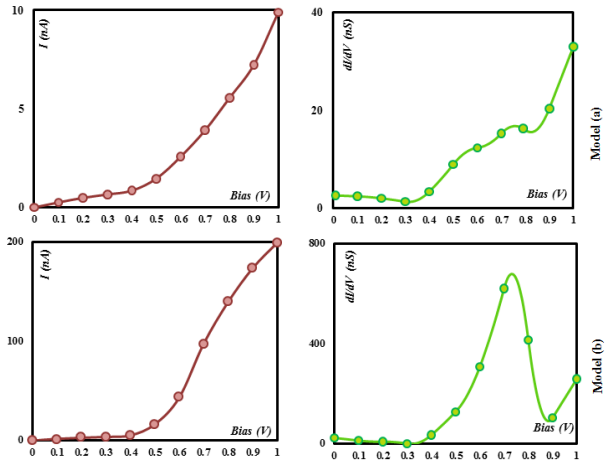

Fig. 3. Current-Voltage characteristics and dI/dV-V curves of a BN nanotube (a) and GaN nanotube (b) contacting two metal Au electrodes.

The transmission spectrum for the two simulated models were analysed by plotting I-V and quantum conductance curves with respect to different applied bias voltages in Figure 3.

In both devices, applied voltages and current flow increase simultaneously. From the I-V characteristics, it can clearly be seen that the electronic conduction is higher for GaN nanotube. We can see from the Figure 3.b that from 0V to 0.4V, the current has a trivial increase then the current increases slowly again with the increase of the bias voltage. For model a, with the increase in the applied voltage, the current flowing through this device increases steadily and reaches a maximum value. In order to gain a clear description, we have shown values of conductance of both the proposed devices at different voltages in table 1.

From the results, it is clear that the GaN device shows enhanced quantum conductance whereas BN device which will find enormous applications in electronic industry. The observed results suggest that the BN nanotube may be an important candidate to design the nano-

molecular diodes and GaN nanotube is helpful as a semiconductor channel for modeling nanotube optoelectronic devices which can be realized with sophisticated modern synthesis technique.

V. CONCLUSION

In this work, DFT calculation were used to investigate and compare the structural, electronic and transport properties of (5, 0) zig-zag GaN with BN nanotube. To obtain information regarding the electronic efficiency of the both nanotube, we have to control several structural property such a density of states, band gap, band structure and I-V characteristic. Among two these structures the GaN nanotube, which indicated a small gap and higher DOS close to Fermi level was considered as the best electronic conductor in comparison to the other studied design structure. Two these devices exhibit a semiconducting character, with a direct band gap at the Γ point, which suggests that these nanotubes may have high potential for full-color display applications. Due to the large band gap of BN nanotube, it is also explored as a tunnel resistance device.

I-V characteristic of two these devices reveal that the proposed structures are a useful semiconducting channel as a nano-molecular diode and nano-molecular transistor for applications in the field of nano-optoelectronic devices and molecular electronics hence GaN and BN at the nanoscale as the nanotube might also be promising candidates for future nano-optoelectronics devices and nanoelectronics-based technologies.

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