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Structural and transport properties of SWGaNNTs: Theoretical study

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ABSTRACT: In the present study, the structural and transport properties of single wall gallium nitride nanotubes (SWGaNNTS) were theoretically studied by using ab-initio calculations under density functional theory (DFT) with TranSIESTA code employing norm-conserving pseudopotential. During the calculation, the tetragonal supercell geometry has been chosen and the relaxed atomic position was used by applying the conjugate gradients (CG) method in molecular dynamics. Maximum force tolerance in CG coordinates optimization set at 0.04 eV/Å. In these computations exchange-correlation energies were obtained using local density approximation (LDA). The results showed that the curvature has prominent effect on the band structure of SWGaNNTs, the energy bandgap decreases as the decrease the diameter. The calculated bandgap of (9,0) is 1.8126 eV are good experiment with the previous reported by theoretical studies. It is also observed that, there is a corresponding relation between the electronic transport properties and the valley of state density of GaNNT. In addition, the I-V graph of GaNNT is approximately linear for lower bias voltage and increases rapidly after that show ballistic transmission.

Keywords: GaN nanotube, electronic transport properties, DFT.

I. INTRODUCTION

Since the discovery of carbon nanotubes (CNT's) by Iijima in 1991 at the NEC fundamental research laboratory in Tsukuba, Japan [1] in the multiwall form and in 1993, Iijima's group [2] and Bethune *et al* [3] at IBM, Almaden research centre, San Jose, California synthesized single wall carbon nanotubes (SWCNT's), it has served as a model systems for theoretical calculations as well as critical experimental studies. CNT's can be either a metal or semiconductor depending on their diameters and helical arrangement. SWCNT's are basically graphite sheets rolled up into a cylinder with diameter of the order of few nanometer range, where as their length can even be much larger than its diameter [4], which are characterized by two integers (n-m) defining the rolling vector of graphite [5]

Theoretically, tight-binding method is a convenient tool for electronic structure. However, it contains empirical parameters to be determined in some other ways, so that one cannot use tight-binding method to predict the band gap. DFT based LDA calculation is parameter-free and powerful technique and it has been successfully applied to variety of materials to describe their electronic as well as other properties. As far as band gap is concerned, LDA tends to underestimate the gap of semiconductors; the LDA gap is typically half to two-third of the experimental gap. Therefore, the gap of carbon nanotube is still an open question in spite of its importance.

Gallium nitride (GaN) is one of the critical semiconductor materials, and has wide bandgap energy (3.4 eV). Currently, interest in gallium nitride based one-dimensional structures (nanowires, nanotube or nanorods), both on a commercial and scientific level, is high because of the potential to apply it in ultraviolet (UV) or blue emitters, detectors, laser diodes (LDs), high speed field-effect transistors, high temperature and radiation-resistant electronic devices. Though two dimensional (2D) structure GaN materials were synthesized successfully for several years, research on one-dimensional (1D) GaN materials is limited due to the difficulties associated with their synthesis. Since, pure boronnitride and boron-carbon-nitride nanotubes have been successfully produced by arc discharge [6, 7], therefore, it open the possibility of other nitride nanotube synthesis such as CN and GaN. In The study show that the strain energy costs necessary to wrap up graphitic GaN sheets into nanotubes are comparable with those of carbon nanotubes, ensuring again the possibility of GaN nanotube formation. Band structures reveal that GaN zigzag nanotubes are semiconductors with a direct band gap, whereas armchair nanotubes have an indirect band gap. The band gap of GaN zigzag nanotubes decreases with the decreasing tube diameter, whereas that of GaN armchair nanotubes is almost constant over a wide range of the diameter, which is contrary to the case of carbon nanotubes. Ultimate nanoscale optoelectronic devices for a wide range of wavelengths may be realized using GaN nanotubes.

In this paper, *ab initio* transport calculations were carried out within the framework of density-functional theory (DFT) combined with the nonequilibrium Green's function method (NEGF), as implemented in the TranSiesta module within SIESTA-3.1 code [8]. We have also analyzed the effect of curvature on their electronic structure and diameter dependence of band gap Band structure, density of states then Transmission Coefficients of (9,0) GaNNts will be discussed using NEGF techniques.

II. COMPUTATIONAL DETAIL

Many theoretical studies have been devoted into investigating the electronic transport properties of semiconducting and conducting materials such as tight-binding calculations, density functional theory (DFT) and many-electron Green's function approach within GW approximation. Among those methods, DFT calculations adopt parameter-free self consistent field calculations, and their reliability has been broadly proved in solid state field and nano-scale systems. Thus, most of the theoretical investigations have been carried out with DFT calculations.

The electronic transport properties were carried out using the first-principles self-consistent method implemented in the TranSiesta. The exchange–correlation energy and electron–ion interaction are described by the Perdew–Zunger (PZ) [9] local density approximation (LDA) and normconserving pseudopotentials [10] in the fully nonlocal form respectively.

The plane wave mesh cutoff energy finalized on the basis of convergence and we found that, in all the cases, total energy converges at plane-wave mesh cutoff of 250 Ry, which is used in the further calculations.

To fix the number of k points for k-point sampling, Monkhorst-Pack special k-point scheme has been used. The convergence of total energy with respect to number of k-points was investigated and we found that total energy converges at number of k-point equal to 13 which corresponds to 1 x 1 x 20 Monkhorst-Pack for GaNNTs. Owing to the very large lattice constants of the supercell along x and y direction, k-point sampling has done only along the tube axis i.e. along z-direction. The band energies were calculated along high-symmetry directions Γ (gamma) and X.

A double-z polarized basis set of numerical atomic orbitals is used and the energy cutoff for real space mesh is set after convergence. TranSIESTA provide the ability to the model open boundary conditions where the ballistic electron transport is taking place and compute electronic transport properties of GaN NTs at different potentials. The method is based on using non equilibrium Green's function (NEGF), that are constructed using the DFT Hamiltonian obtained from a given electron density.

The system setup for a (9, 0) zigzag GaN nanotube being constituted by three parts: the left (L) and right (R) semi-infinite GaN leads (electrodes), and scattering region which is described by 12 atoms in the unit cells of GaN nanotube. The size of scattering region is takes place enough to prevent the interaction between the left and right electrode. The fundamental theory of nonequilibrium Green's functions is used to obtain the transport properties of a scattering atomistic system coupled to electrodes. The Hamiltonian of the scattering region is approximated by the Kohn-Sham Hamiltonian from density-functional theory. The junction is constructed so that the periodic replicas of the GaNNT along the direction parallel to the electrode edge are separated by nanometer range.

The current through the contact region was calculated using Landauer-Buttiker Formula [11]

$$I(V_b) = G_0 \int_{\mu_R}^{\mu_L} T(E, V_b)\, dE$$

Where $G_0 = \frac{2e^2}{h}$ is the unit of quantum conductance and $T(E, V_b)$ is the transmission probability of electron incident at an energy E through the device under the bias potential V_b. The electrochemical difference between the left and right electrodes is $eV_b = \mu_L - \mu_R$

III. RESULTS AND DISCUSSION

The plane wave mesh cutoff energy finalized on the basis of convergence. The total energy converges at plane-wave mesh cutoff of 400 Ry for GaNNTs. Similarly values of k-points obtained using convergence criteria. Hence, these values are used in the further calculations. Electronic properties of an isolated (n, 0) zigzag GaN nanotube (for = 3-9) have been studied. We found that when *n* is increased by one, an extra state appears both in valance band and conduction band and is continuously shift towards the Fermi level as *n* was increased till a minimum distance from Fermi level was achieved. After achieving this minimum distance from Fermi level, these states starts shifting away from Fermi level as *n* was further increased and other newly appeared states starts shifting towards Fermi level to achieve a minimum distance. The results electronic band structures of zigzag GaNNTs are shown in Fig. 1 are direct-band-gap semiconductors, this result is consistent with other literatures. The band gap of GaNNTs is essentially unchanged. This is different from other articles. The reason is that the density functional theory is based on ground state theory in the calculations, but the energy gap is based on excited state, so the obtained results may have tolerance errors.

In Table 1, the theoretical as well as experimental results available in literature have also been included. In general there is no regular trend in the value of energy band gap with respect to increase the value of n. In case of CNT's the (3, 0) and (6,0) are metallic and in (9, 0) SWCNTs where newly appeared states in VB and CB attain minimum distance from Fermi level and make them small gap semiconducting in nature [12]. Whereas (3, 0) GaN nanotube is metallic in nature and (6, 0) & (9, 0) tubes are semiconducting in nature. The bandgap of these tubes are 1.0622 eV and 1.8126 eV respectively.

Table 1: Energy band gap SWGaNNTs at Γ-point.

Index (n,0)	Energy band gap (eV) of GaNNT		
	Present work (LDA)	Ref. 1 (Exp.)	Ref14 (Theo.)
(3,0)	Metallic		
(6,0)	1.0622		
(9,0)	1.8126		2.16

This shows that curvature of nanotubes has prominent effect on their electronic band structure. Unlike the alternating energy gap of zigzag carbon nanotubes, the band gaps of GaN nanotubes decrease monotonically with the decreasing diameter. The energy gap of (n, 0) GaN nanotubes decreases signifcantly with the decreasing diameter. The reason for decrement of energy bandgap simply reflects the ionic bonding character, i.e. *s* and *p* bands localized to Ga and N respectively are well separated. Wrapping of the graphitic sheet to tubes enhances the re-hybridization more seriously in zigzag nanotubes. More *p* states near the valence band edge and more *s* states near the conduction band edge are developed at smaller diameter of zigzag nanotubes.

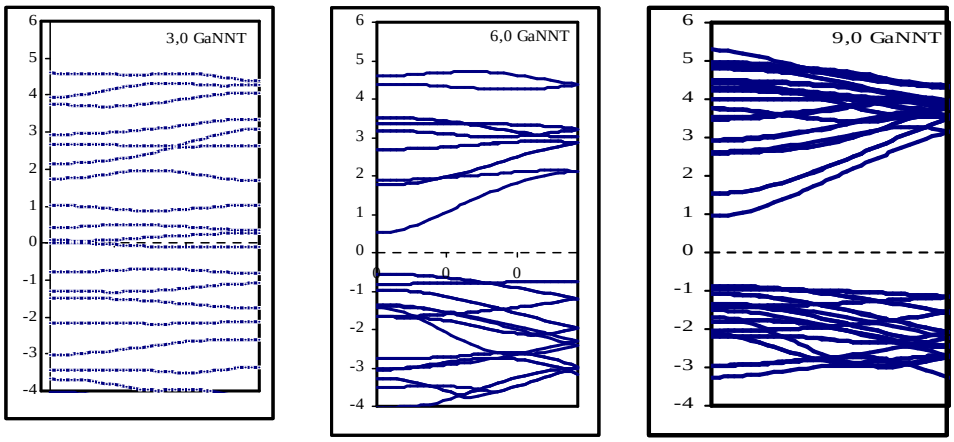

Fig. 1. Band structure of (3,0), (6,0) and (9,0) of GaNNTs.

The electronic transport properties of (9,0) GaNNTs are determined under equilibrium conditions and the transmission spectrum are obtained when the electrons pass through nanotubes shown in Fig. 2. The transmission spectrum T(E) measures the accumulated probability that the electrons will be transferred from incoming states on the left electrode to outgoing states on the right electrode. The results clearly show that the probability that the electronics pass through zigzag GaNNTs are closely related to the electron energy. With the change in the absolute value of the energy, the probability that the electronics pass through zigzag GaNNTs presents the shake trend; it is completely different from the condition when the electrons go through a conductor. The transmission probability reaches high, the main reason is that when the electronics resonate with the covalent π orbital of the atomic [13].

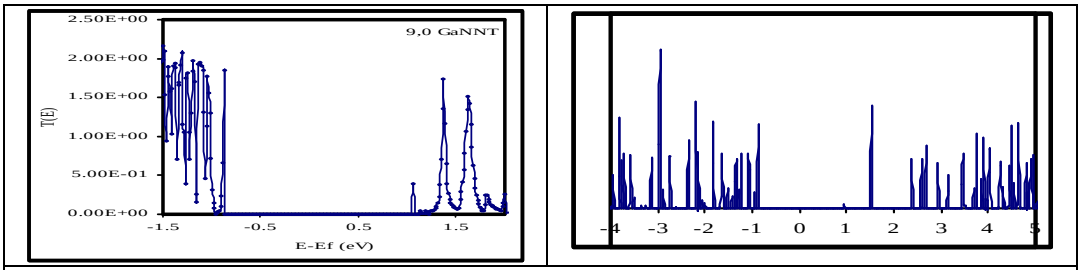

Fig. 3. Transmission spectrum and density of state of (9,0) GaNNT.

In this paper, the voltage was 0V to 1.2V, unit of changes is 0.4V. We found that in this voltage range, the transmission spectrum of the system is almost unchanged, the transmission spectrum in the equilibrium state could be used to analyze qualitatively. As the molecular orbital density of states (DOS) peaks has a significant contribution to the system eigen state and the interaction between molecules and electrodes can cause peak broadening and level shift.

The transmission coefficient peak is corresponding to the resonance passage when the electronics passed through the molecular state. From Fig. 2, the computation has obtained the transmission spectrum and the density of states.

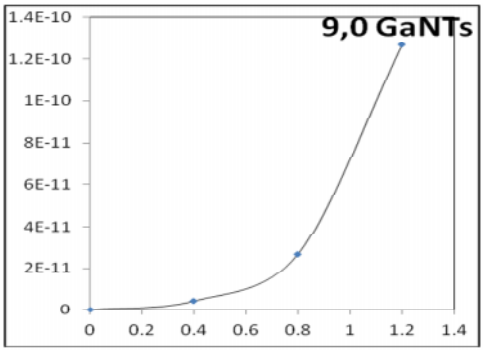

Fig. 3. I-V plot for 9,0 GaNNT.

The transmission spectrum has a series of peaks and valleys. It is clear that the peaks and valleys of transmission spectrum and the density state curves have a similar trend. In Fig. 3, the current as a function of the applied bias voltage for 0.0 to 1.2 V is shown the electronic structure is determined self-consistently under nonequilibrium conditions. The current is calculated by the Landauer-Buttiker Formula [11], which is determined by the transmission probability *T*(*E)* and the energy region (or integral window) of the current integral. For region 0-0.4V the current is almost zero, which means that the transmission probability T(E) in the integral windows is zero while the bias voltage in the range 0.4 V to 1.2 V the current is increases with valtage.

CONCLUSION

In the study of (9,0) GaN nanotubes, we found that, the GaNNTs are metallic for (3,0) and semiconducting for (6,0) and (9,0). There is no regular trend in increase or decrease of the value of energy band gap with the decrease in curvature in semi conducting zigzag GaN nanotubes. The curvature effect is responsible for their small energy band gap. The range of bandgap approximated upto 3.94 eV for the very large diameter of GaNTs. Study suggests that GaNNTs may be used for full color displays in the nanoscale optoelectronic devices which can be realized with sophisticated modern synthesis technique

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