Study on the Electronic Transport Properties of Zigzag GaN Nanotubes

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Abstract: The electronic transport properties of zigzag GaN nanotubes (n, 0) (4 ≤ n ≤ 9) have been calculated using the density functional theory and non-equilibrium Green’s functions method. Firstly, the density functional theory (DFT) is used to optimize and calculate the electronic structure of GaNNTs (n, 0) (4 ≤ n ≤ 9). Secondly, DFT and non-equilibrium Green function (NEGF) method are also used to predict the electronic transport properties of GaNNTs two-probe system. The results showed: there is a corresponding relation between the electronic transport properties and the valley of state density of each GaNNT. In addition, the volt-ampere curve of GaNNT is approximately linear.

1. Introduction

GaN has attracted much attention as a wide band gap semiconductor material[1]. Up to now, GaN bulk structures and GaN films have been studied extensively. In theoretical calculation, the main work of these research are calculations about some properties of one-dimensional GaN nanomaterials such as mechanics, electronic structure, light absorption, lattice vibration, electronic transportation characteristic and so on. However, in experiment, the prime task is only related to the preparation of one-dimensional GaN nanomaterials [2-3].

2. Calculation model and method

The structural optimization and the electronic structure calculation of the GaNNTs have been studied using first-principles method which is based on density function theory (DFT). During structural relaxation and electronic structure calculation, the generalized gradient approximation (GGA-PW91) is used to deal with the exchange of relevant potential energy. K-point sampling of Brillouin is 1 × 1 × 100 corresponded to simple Brillouin zone.

In this paper, the electronic transport properties of zigzag GaN nanotubes (n, 0) (4 ≤ n ≤ 9) have been calculated using ATK software based on DFT and NEGF. In this work, GGA is used as the exchange correlation function, with a 1 × 1 × 100 K-point sampling corresponding to simple Brillouin zone. ATK software can fully complete self-consistent process of the atomic-scale system and the semi-infinite electrodes coupling systems, the voltage across the conductor directly get involved in self-consistent calculation. System can be divided into three parts: central scattering region, left electrode and right electrode areas. The model is shown in Fig.1 and the current through this system can be obtained from Landauer-Biittiker formula according to the corresponding Green function [4].
\[ I = \frac{2e}{\hbar} \int T(E,V) \left[ f(E - \mu_r) - f(E - \mu_l) \right] dE \quad (1) \]

Here, \( \mu_l \) and \( \mu_r \) are Chemical potential of Left and right electrode respectively. \( (\mu_r - \mu_l)/e = V \) is the electrical potential difference between left and right ends, \( \mu_r = E_r - \frac{V}{2}, \quad \mu_l = E_r + \frac{V}{2}, \) \( [\mu_l, \mu_r] \) is energy integral interval, \( f(E - \mu_r) \) and \( f(E - \mu_l) \) are electronic fermi distribution function of the left and right electrodes respectively, \( T(E,V) \) is transmission coefficient when energy is E and biasing is V. The transmission coefficient of Fig.1 system has been obtained using ATK.

\[ \text{Fig.1 the electron transport model} \]

**3. Simulation results and analysis**

**3.1. Optimization analysis**

The optimized structures of zigzag GaNNTs \((4 \leq n \leq 9)\) are shown in Fig.2, dark indicate N atoms, light indicate Ga atoms. The positions of atoms in the model are the results of optimization. The result shows that the Ga–N bonds display a buckling with the N atoms moving slightly outwards and the Ga atoms moving slightly inwards, zigzag GaNNTs are a buckling of the Ga–N bond. The reason for buckling is that surface layer atom has dangling bonds, in order to reduce surface energy, chemistry bonding needs to readjust structure adjustment, this result is consistent with Lee’s \(^5\) results.

\( (4,0) \quad (5,0) \quad (6,0) \)

\( (7,0) \quad (8,0) \quad (9,0) \)

\[ \text{Fig.2 zigzag GaNNTs (n, 0) (4 \leq n \leq 9)} \]
The results electronic band structures of zigzag GaNNTs (n, 0) (4 \leq n \leq 9) are shown in Fig.3. (3, 0) GaNNT has a direct-band-gap semiconductors \(^5\), whereas the (4, 0) GaNNT has an indirect-band-gap. We think that the (4, 0) GaNNT has an indirect-band-gap because of a strong \(\pi - \pi\) hybrid. When n>4, like (5, 0), (6, 0), (7, 0), (8, 0), (9, 0), zigzag GaNNTs are direct-band-gap semiconductors, this result is consistent with other literatures. The band-gap of GaNNTs are 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.

**Fig.3** the band diagram of the zigzag GaNNTs (n, 0) (4 \leq n \leq 9)

### 3.2. Transport analysis

The transport properties of the two-probe system be using Au (001) as electrodes, which is exactly same with zigzag GaNNTs crystal face, we calculated the electronic transport properties of optimized zigzag GaNNTs \(^1\). In Fig.4, the density of states of zigzag GaNNTs under equilibrium conditions and the transmission spectrum are obtained when the electrons pass through nanotubes. 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 \( \pi \) orbital of the atomic \(^{12}\).

In this paper, the voltage was 0V to 2V, unit of changes is 0.2V. 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.4, the computation has obtained the transmission spectrum and the density of states. The transmission spectrum has a series of peaks and valleys, and the peaks and valleys of transmission spectrum and the density state curves have a similar trend.

![Graphs of transmission spectra for different zigzag GaNNTs configurations](image)

**Fig.4** the density of states and transmission spectra of the zigzag GaNNTs \((n, 0)\) \((4 \leq n \leq 9)\)

Zigzag GaNNTs \((4 \leq n \leq 9)\) I-V is characteristic as the curve in Fig.5 (dark behalf odd light behalf even). When voltage was 0V to 2V, performance of current and voltage has certain linear characteristics. In Fig.4, when the voltage was 0V to 2V zigzag GaNNTs\((4 \leq n \leq 9)\) I-V curve is approximately linear, the reason is that the zigzag GaNNTs density of state and the transmission
spectrum and electronic density of states have the linear variation region in the small energy range (-1eV to 1eV). It is also observed that, when n is an odd number, under the same voltage, the electric current increased with the increasing of n value, when n is an even number the case is just opposite to the previous one. But, in the odd number tube (5, 0) the GaNNT does not follow the rule above, we thought that π-π track's hybridization is advantageous with compared to the electronic transportation. The rehybridization of the π-π orbits of (5, 0) GaNNT is prominent compared to that of (7, 0) GaNNT

![Image](image.png)

**Fig.5** the current and voltage graph of the zigzag GaNNTs (n, 0) (4 ≤ n ≤ 9)

4. Conclusion

In this paper, we calculated the electronic structures of zigzag GaNNTs (4, 0) - (9, 0) using GGA method of the density functional theory, and then obtained their electronic energy structures. In the calculation results, we find that (4, 0) GaNNT is indirect band gap while the band gaps of (5, 0), (6, 0), (7, 0), (8, 0), (9, 0) GaNNTs are direct. By using the density functional theory and the non-equilibrium green's function method, the electronic transportation characteristic of zigzag GaNNTs (4,0) - (9,0) are predicted, it can be seen that there are certain corresponding relationships between electricity transportation characteristic and the valleys of density states; within small energy range, the I –V curves of Zigzag GaNNTs show linear features

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