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Exploring electronic transport properties of AlN nanoribbon molecular device – A first-principles investigation

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ABSTRACT

The novel AlN nanoribbon molecular device is investigated using density functional theory for different voltage bias. The electronic transport properties of AlN nanoribbon are discussed in terms of device density of states, electron density, transmission spectrum and transmission pathways. It is evident that increasing the bias voltage leads to transition of electrons from the valence band to the conduction band across AlN nanoribbon. The electron density is found to be more along nitrogen sites. The transmission increases with the increase in bias voltage. The transmission can be fine-tuned at different energy intervals by varying the bias potential. The transmission pathways provide the insight for transmission of electrons along AlN nanoribbon. Mostly, the transmission is observed along the top and bottom regions of AlN nanoribbon. The results of the present work will give a clear picture to improve the electronic transport property along AlN nanoribbon.

1. Introduction

The technological progress in group III nitride optoelectronic devices attracted the scientific community to enhance the transport properties of these materials in the past decade. Among GaN, InN, AlN and their alloys, Aluminium nitride (AlN) attracted much attention due to its properties. AlN possesses high electrical resistivity, high thermal conductivity and high thermal expansion coefficient. The band gap of bulk AlN was reported to be 6.2 eV and this high band gap energy makes AlN suitable for optical devices emitting blue wavelength, excellent electrical insulation applications in microelectronic devices, heat sinks and power transistors [1–3]. The dielectric constant of AlN is found to be approximately 8.2–8.9. The other interesting features of AlN are its large piezoelectric coupling coefficient and high acoustic velocity [4]. These features make AlN suitable for surface acoustic wave (SAW) applications such as SAW resonators, sensors and filters [5]. The nanoscale quantum confinement geometries of AlN namely nanotubes, nanowires, nanoparticles are particularly important in underlying fundamental concepts in optical, electronic and mechanical properties. The future nanodevice includes nanoscale light emitting diodes and field effect transistors [6–10]. The different morphologies of AlN nanostructures such as nanotubes [11], nanocones [12,13] and nanobelts [14] exhibits excellent field emission properties. The transport phenomena of electrons in molecular electronic devices are one of the challenging tasks in applied science field. The molecular electronic device assembly with a single molecule or a layer of molecules between the source and drain electrodes is a favorable option for conventional electronics [15]. Recent reports show that rectification, switching and controlling the current flow across the molecular device with bias voltage or applied magnetic field are possible [16–19]. Nevertheless, the contact between the electrode and scattering region is a challenging task which gives rise to atomistic changes in metal-molecule contact due to quantum effects [20]. Moreover, if the scattering region is too small there is a possibility of tunneling of electrons across the scattering region. In spite of all these facts, the development of accurate theoretical model to describe the transport across the molecular device is required. The state-of-the-art of the present work is to design AlN nanoribbon molecular device and to study the transport property under different voltage bias. Motivated by these features of AlN, AlN nanoribbon based molecular device model is proposed in the present work. Based on the literature survey, most of the reported work is in the synthesis of AlN. AlN is synthesized by different methods, namely radio frequency magnetron sputtering [21], chemical vapor deposition [22], molecular beam epitaxy [23], self-templated synthesis [24] and reactive magnetron sputtering [25] methods. J.M. Vail et al. studied nitrogen vacancy in aluminium nitride [26]. Yan Jiao et al. reported

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adsorption of CO_2 and N_2 on aluminium nitride single walled nanotubes using density functional theory [27]. The density functional theory (DFT) is a better approach to study the electronic transport properties of AlN nanoribbon [28–30]. The novel aspect of the present work is to study the transport property of AlN nanoribbon molecular device under different voltage bias.

2. Computational details

The geometrical optimization of AlN nanoribbon device is carried out using DFT method which is expanded based on the basis set of atom. In the present work, optimization is performed with a DFT utilizing TranSIESTA module in the SIESTA package [31]. The generalized gradient approximation (GGA) through Perdew–Burke–Ernzerhof (PBE) exchange correlation functional for electron–electron interaction is used throughout the calculation [32–34]. The molecular geometry is optimized by reducing the atomic forces of atoms to be smaller than 0.05 eV/Å. In the present model, the Brillouin zones are sampled with $1 \times 1 \times 100$ k-points. The real-space grids for electrostatic potentials are determined by mesh cutoff energy of 10^{-5} eV is used to achieve the balance between the calculation efficiency and accuracy. The optimization of the molecular device and electronic transport properties of AlN nanoribbon is studied with single zeta polarization (SZP) basis set for aluminium and nitrogen in the present work [35].

3. Results and discussion

3.1. Structure of AlN nanoribbon molecular device

The hexagonal structured AlN molecular device is constructed with reference to International Centre for Diffraction Data (ICDD) card number 88-2369. AlN nanoribbon consists of 28 aluminium atoms and 28 nitrogen atoms along the scattering region. The scattering region of AlN nanoribbon is held between left and right electrodes. The left and right electrodes have 7 aluminium atoms and 7 nitrogen atoms each. The width of left and right electrodes is 3.15 Å. The bond length between aluminium and nitrogen atom is 1.82 Å. The dimensions of nanoribbon being n and m, with $n = m = 3$, the nanoribbon is repeated four times along z axis. The AlN nanoribbon is designed along (200) plane. The potential difference is maintained between AlN nanoribbon across left and right electrodes. The voltage across left electrode is varied in the order of 0 V, 0.5 V, 1 V and 1.5 V and right electrode is held at constant ground potential. The density of states, electron density and transmission spectrum of AlN nanoribbon molecular device are studied and the results are reported in the present work. The schematic diagram of designed AlN nanoribbon based molecular device is shown in Fig. 1.

3.2. Density of states of AlN nanoribbon device

The density of states (DOS) spectrum provides the insight to the density of charges present within the energy interval in the valence band and the conduction band of AlN nanoribbon [36–38]. The Fermi energy (E_F) level is taken as 0 eV Fig. 2(a) represents the projected density of states (PDOS) of AlN nanoribbon at 0 V. In the valence band of AlN nanoribbon, peak amplitudes are noticed and beyond the Fermi level, there are not many peaks observed. These peak amplitudes arise due to the orbital overlapping of aluminium and nitrogen. The major contribution is seen along p orbital overlapping of AlN nanoribbon. Fig. S2 (a) in supplementary material shows PDOS spectrum of pure Al nanoribbon. Since the electronic configuration of aluminium is *[Ne]* $3s^2\ 3p^1$, peak maximums are observed in s, p and d orbitals due to orbital overlapping. However, in the case of AlN nanoribbon the major contribution in PDOS spectrum is from p orbitals. Fig. 2(b) depicts the PDOS spectrum at 0.5 V; clearly it is evident that some peaks are seen in the conduction band near the Fermi level and peaks get reduced in the valence band. It indicates that the applied bias voltage makes the electrons to transit from the valence band to the conduction band in AlN nanoribbon. Gao Ting-Ge et al. reported first-principles study of aluminium vacancy in wurtzite aluminium nitride [39]. The peak amplitudes are observed to be more near the Fermi level, which is in agreement with the present result. Fig. S2(b) in supplementary material indicates PDOS spectrum of pure Al nanoribbon at 0.5 V bias, peaks get smoothened in the valence band and the conduction band. Fig. 2(c) illustrates the PDOS spectrum at 1 V. In this case, peaks are seen along 0.5 eV and 1.75 eV. This clearly indicates that the more potential difference between the electrodes makes the electrons to move deep into the conduction band. Fig. S2(c) in supplementary material represents PDOS spectrum at

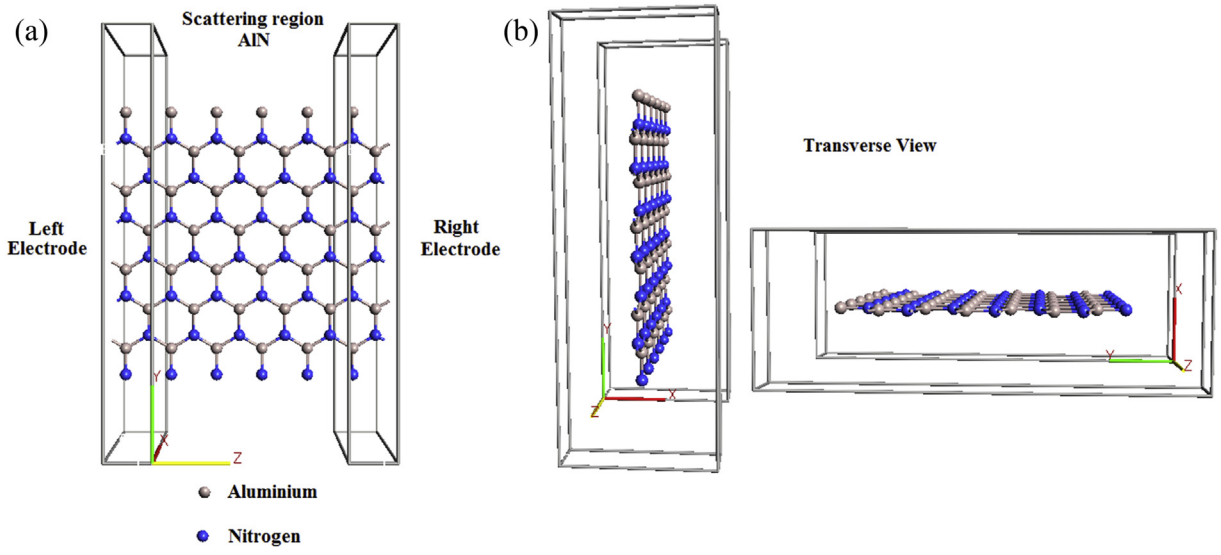

Fig. 1. (a) Schematic diagram of AlN nanoribbon molecular device. (b) Transverse view of AlN nanoribbon molecular device.