Superlattices and Microstructures 83 (2015) 193–209

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Band structure and transport studies on InP nanotube – A first-principles investigation

R. Chandiramouli *

School of Electrical & Electronics Engineering, SASTRA University, Tirumalaisamudram, Thanjavur 613 401, India

ARTICLE INFO

Article history:
Received 17 March 2015
Accepted 19 March 2015
Available online 26 March 2015

Keywords:
Indium phosphide
Nanotube
Molecular device
Density of states
Electron density

ABSTRACT

The band structure and electronic transport property of InP nanotube molecular device are studied using density functional theory with GGA/PBE exchange correlation functional. The substitution of nitrogen in InP nanotube slightly widens the band gap. The substitution of nitrogen and aluminium in InP nanostructure modifies the density of states across InP nanotube. The electron density is found to be more on phosphorus sites than indium sites. The substitution of aluminium increases the electron density, whereas nitrogen substitution decreases the electron density across phosphorus site. The transmission spectrum provides the insight to transmission along InP nanotube molecular device. The transmission pathways get modified with the substitution impurity along InP nanotube molecular device. The results of the present work will give information on tuning the band structure and transport properties of InP nanotube molecular device.

1. Introduction

The development of nanoscale technology in semiconductor materials plays a vital role in the development of nanoelectronic devices. The low dimensionality and modified properties of nanostructures such as nanoribbon, nanowire and nanotube is in focus among the scientific community. Indium phosphide (InP) is an important group III–V semiconductor with direct band gap of 1.35 eV. This band gap of InP gives rise to significant applications in high-speed electronic devices, optoelectronic

* Tel.: +91 9489566466; fax: +91 4362 264120.
E-mail address: rcmoulii@gmail.com

http://dx.doi.org/10.1016/j.spmi.2015.03.042
0749-6036/

devices, high-speed logic circuits, fibre optic communication, microwave devices [1–6]. Moreover, high electron mobility, band gap around 1.34 eV and good heat conducting properties of InP find its potential application in microwave and optoelectronic devices. Owing to its significant photoluminescence and optical properties, InP is also used as light emitting diodes, light detectors and solar cells. InP can be synthesized in many methods such as hydrothermal route, co-evaporation technique, chemical vapour deposition, flash evaporation technique [7–11]. The presence of substitution impurity in InP nanostructure will enhance the transport property and the band structure can also be tailored with proper substitution impurity. With this as objective, literature survey was conducted by CrossRef metadata search and most of the reported works are in the synthesis and characterization of InP nanostructures. Tang et al. synthesized InP nanowires and nanotubes [12]. Khanna et al. synthesized InP nanoparticles [13]. Greenberg et al. reported InP nanowires grown by selective area vapour liquid solid epitaxy [14]. Tian et al. studied surface state and optical property of sulphur passivated InP [15]. Yamashita et al. reported growth of side facets in InP nanowires [16]. There are less work reported based on density functional theory (DFT) to study the transport property. The novel aspect of the present work is to study the band structure and transport properties of InP nanotube molecular device with substitution impurity in InP.

2. Computational details

Computations for present InP nanotube were performed using DFT methods employing SIESTA package [17]. DFT method is an efficient method to investigate the band structure, density of states and transmission coefficient of nanostructures [18–20]. The calculations are performed with generalized gradient approximation (GGA) with Perdew–Burke–Ernzerhof (PBE) exchange correlation functional throughout the study [21,22]. The Brillouin zones are sampled by $1 \times 1 \times 1$ k points. The electronic transport properties of InP nanotube are studied using vacuum padding of 10 Å modelled along x and y axes to overcome the interaction of InP nanotube with the periodic images. The real space grid for InP nanotube is calculated with mesh cut off energy of 10^{-5} eV. The geometry of molecules in InP nanotube is optimized by reducing the atomic forces between the atoms to be smaller than 0.05 eV/Å. InP nanotube is optimized with double zeta polarization (DZP) basis set [23]. The atoms in InP nanotube are free to move along with their positions till the convergence criteria rule with forces less than 0.05 eV/Å on each atom.

3. Results and discussion

3.1. Structure of InP nanotube

The InP nanotube was designed from InP nanosheet. At first, InP nanosheet was designed from International Centre for Diffraction Data (ICDD) card number 73-1983. The InP nanosheet is then rolled to form InP nanotube. The dimension of InP nanotube is $n = 5$ and $m = 2$ with the repetition along c-axis as one. In the present work, InP nanotube resembles chiral type which has different values of n and m. The pure InP nanotube comprises of twenty-six indium atoms and twenty-six phosphorus atoms to form InP nanotube. The nitrogen substituted InP nanotube consists of twenty-six indium atoms with twenty-three phosphorus atoms and three nitrogen atoms. Similarly arsenic substituted InP nanotube consists of twenty-six indium atoms with twenty-three phosphorus atoms and three arsenic atoms, three phosphorus atoms being replaced with three arsenic atoms which form part of a group-V semiconductors. The case of aluminium substituted InP nanotube comprises of twenty-two indium atoms with twenty-six phosphorus atoms and four aluminium atoms, four indium atoms being substituted with four aluminium atoms which form part of group-III semiconductors. The transport properties of the InP nanotube molecular device are studied with two probe method. The two ends of InP nanotube are attached to the left and right electrode and the bias voltage is varied along the left electrode and right electrode is kept at the ground potential. The transmission and transmission pathways are studied using two probe method. The schematic structures of pure, nitrogen substituted InP nanotube, arsenic substituted InP nanotube and aluminium substituted InP nanotube are illustrated in Figs. 1a–1d respectively.