Materials Science in Semiconductor Processing 35 (2015) 109–114

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

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

A first-principles study of transport properties of a gallium arsenide nanoribbon-based molecular device

R. Chandiramouli *

School of Electrical & Electronics Engineering, SASTRA University, Tirumalaisamudram, Thanjavur 613401, India

ARTICLE INFO

Available online 20 March 2015

Keywords:
Gallium arsenide
Molecular device
Nanoribbon
Transport property
Transmission pathways

ABSTRACT

GaAs nanoribbon based molecular device is investigated using density functional theory. The electronic transport properties of GaAs nanoribbon are discussed in terms of density of states, electron density, transmission spectrum and transmission pathways. The applied bias voltage increases the peak maximum in the valence band and the conduction band. The electron density is found to be more on the arsenic sites than in gallium sites across GaAs nanoribbon. The transmission spectrum provides the insight to the transmission of electrons at different energy intervals across GaAs nanoribbon. The transmission pathways give the visualization of possible path for the electrons, when the bias voltage is varied between the electrodes. The transmission pathways get modified with the applied bias voltage. The result of the present study gives clearer vision of enhancing the electronic transport properties of GaAs nanoribbon which is used in optoelectronic devices.

1. Introduction

The recent developments in new generation electronic devices using semiconducting nanostructures are in focus among the scientific community. Miniaturization and fabrication of electronic devices with single atomic chain, graphene like structures and nanowire are possible using nanotechnology [1,2]. The manipulation of quantum states in molecular level leads to improvement in the performance of functional nanomaterials. The building block of nanoelectronics starts from the molecular level, which gives rise to the fabrication of lasers, organic light emitting diodes, organic thin film transistors, solar cells and chemical sensors [3–8]. Usually in molecular devices, the conductance varies in a non-linear fashion with the applied voltages; it may also have spike-like and step-like features depending upon the molecular eigen states [9,10]. The key mechanism in transport properties through a molecular device arises due to the linkages across the molecules and lead terminals. Gallium arsenide (GaAs) is one of the important materials used in nanoelectronic and optoelectronic devices. Due to its high carrier mobility, small dielectric constant, high temperature resistance and direct band gap GaAs is widely used in optoelectronic devices [11,12]. Different nanostructures of GaAs can be synthesized by metal organic vapor phase epitaxy (MOVPE) [13,14] and molecular beam epitaxy [15,16].

The objective of the present work is to design GaAs nanoribbon and to study the transport properties of GaAs nanoribbon based molecular device. Besides, the motivation of the GaAs nanoribbon, the literature survey was conducted; to date, most of the reported work is in the synthesis and characterization of GaAs. The alloying properties, electronic and magnetic properties of doped GaAs nanowires are reported by other workers [17–22]. The novel aspect of the present work is to design and study the electronic transport property of GaAs nanoribbon, which is similar to zigzag type graphene nanoribbon under different voltage bias condition. Density functional method (DFT) is an efficient method to

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

http://dx.doi.org/10.1016/j.mssp.2015.02.076
1369-8001/

investigate the electronic properties of low dimensional materials [23,24]. Furthermore, the DFT approach in measuring the transport property is relatively rare as this is usually the realm of molecular dynamics simulation especially in device related issues. In the present work, GaAs nanoribbon based molecular device is modeled and successfully optimized using a DFT method for different bias voltages and the results are reported.

2. Computational details

The calculations for GaAs nanoribbon are performed by the DFT method utilizing TranSIESTA module in SIESTA package [25]. The GaAs nanoribbon is optimized by reducing the atomic forces on the atoms in the nanostructure to be smaller than 0.05 eV/Å. The generalized gradient approximation (GGA) through Perdew–Burke–Ernzerhof (PBE) exchange correlation functional is used to study the electron–electron interaction throughout the study [26,27]. The Brillouin zones are sampled with $1 \times 1 \times 100$ k points. The present work is carried out using SEISTA package, in which the core electrons are substituted by Troullier–Martins pseudopotentials in their separable form for gallium and arsenic atoms. While applying Troullier–Martins type, pseudoatomic orbital basis set are used for the expansion of wave function for the valence electrons of gallium and arsenic atoms. Furthermore, the electronic wave functions of gallium and arsenic atoms are expanded in terms of basis set. The electronic wave functions can be expanded with the basis set of the atom that depends on the numerical orbitals. Using localized basis sets have advantages such as, the number of basis function required for the calculation is very few, computation can be done in less time, direct interpretation of the physical quantities like population analysis, projected density of states are possible. Moreover, vacuum padding is almost free and very high accuracy can be obtained using this kind of localized basis sets. The optimization of atoms along with their electronic properties of GaAs nanoribbon are carried out using double zeta polarization (DZP) basis set for GaAs scattering region and the same basis set is used in electrode regions in the present study [28]. To calculate the electronic properties of GaAs nanoribbon and to avoid the interaction of GaAs nanoribbon with its periodic images, a vacuum padding of 10 Å is modeled along x and y axes. In order to avoid the overlapping of the field interaction in the nanoribbon, a suitable amount of vacuum padding (10 Å) is made in GaAS nanoribbon. This will reduce the computational complexity while finding the density matrix Hamiltonian. The atoms along the nanoribbon are free to displace through their positions until the convergence with a force smaller than 0.05 eV/Å on every atom is achieved.

3. Results of discussion

3.1. Structure of GaAs nanoribbon

The GaAs nanoribbon molecular device is designed with reference to International Centre for Diffraction Data (ICDD) Card number: 80-0003, which exhibit hexagonal structure. The GaAs nanoribbon is constructed along (200) plane. The scattering region of the molecular device comprises of GaAs attached between two electrodes. The width of the scattering region is 12.6 Å and the width of left electrode and right electrode is 3.15 Å. The whole length of GaAs nanoribbon is 22.05 Å. The GaAs nanoribbon is repeated six times along c-axis. In GaAs nanoribbon, a potential difference is maintained between left and right electrodes. The designed GaAs nanoribbon consists of three regions, namely left electrode region, right electrode region and scattering region. The scattering region of GaAs nanoribbon, comprises of 28 gallium atoms and 28 arsenic atoms. The region on the left and right electrodes includes 7 gallium atoms and 7 arsenic atoms each. In total there are 42 gallium atoms and 42 arsenic atoms in the GaAs nanoribbon molecular device. In the present work, the potential at left electrode is varied as 0 V, 0.5 V, 1 V, and 1.5 V and right electrode is kept at ground potential. The variation of bias voltage leads to the change in density of states and transmission along GaAs molecular device. Fig. 1 shows the schematic diagram of GaAs nanoribbon molecular device.

3.2. Density of states of GaAs nanoribbon

The density of states (DOS) spectrum provides the visualization of charges along different energy intervals in GaAs nanoribbon [29–31]. The charges present along the valence band and the conduction band at different energy intervals in GaAs nanoribbon can be interpreted with DOS spectrum. The bias voltage is varied along the scattering region from 0 V to 1.5 V at intervals of 0.5 V. The Fermi level (E_F) is considered as zero, since the bias window between left and right electrodes are set to $[-V/2, V/2]$. The projected density of states (PDOS) spectrum arises with the overlapping of s, p, d orbitals of gallium and arsenic atoms along GaAs nanoribbon. The major contribution in PDOS spectrum in GaAs nanoribbon arises from orbital overlapping of p and d orbitals. Ding et al. reported the PDOS spectrum of bismuth alloying properties in GaAs nanowires [17]. A similar trend in PDOS spectrum is observed as that of the present work.

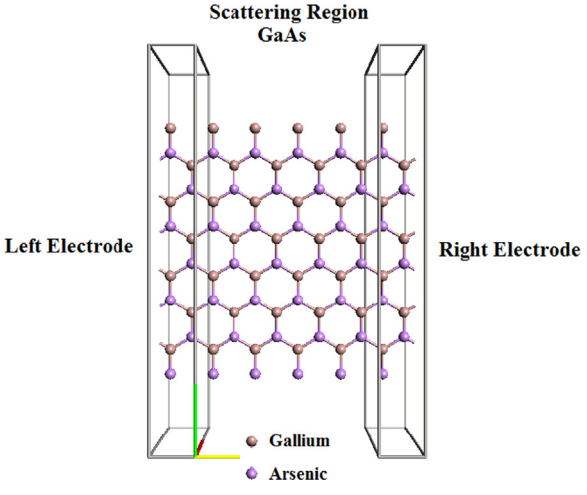

Fig. 1. Schematic diagram of GaAs nanoribbon molecular device.