KMITL Sci. Tech. J. Vol. 9 No. 2 Jul. - Dec. 2009

Density of States Calculation for Indium-Arsenide Zincblende Based on Density Functional Theory

Mohd Faudzi Umar[1]*and Ahmad Puaad Othman[2]

[1]*Department of Physics, Faculty of Science and Mathematics, Universiti Pendidikan Sultan Idris, 35900 Tanjong Malim, Perak, Malaysia
[2] School of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

Abstract

Ab initio study of the density of states on InAs zincblende phase is calculated using the linearized augmented plane wave method based on density functional theory, implemented with WIEN2k codes. These calculations used the local density approximation for the exchange and correlation potential. The result shows that InAs is the n-type smiconductor (donor) which has direct band gap of 0.388eV which is in agreement with experimental result. There is an internal gap between upper valence band and lower valence band. The result indicates a strong hybridization between arsenide atom and 5p state of indium atom, which belongs to the InAs at upper valence band.

Keywords: Density of states, indium-arsenide, density functional theory

1. Introduction

Group III-V semiconductors are currently used in many established electronic devices such as photo-electrochemical cells, transistors, detectors, photodiodes, photoconductors and photovoltaic solar cells. InAs is one of the compounds in Group III-V semiconductors belongs to a family of anion III-V semiconductor and has the wavelength range between 1 to 4.0 μm which is suitable for the infrared detectors application. It has been used in higher-power applications at room temperature without any cooler for lower noise [1, 2]. Experimentally indium-arsenide (InAs) is direct bandgap with 0.36eV and used for diode lasers [3].

InAs has another applications such as semiconductor quantum dot which performs in a monolayer on gallium-arsenide (GaAs) substrate [4]. The electronic properties of nanosize give the numerous applications and improve the efficiency in electronics and photonics device. InAs based nanowires have been used to improve electronics in case of resonant tunneling diodes and single electron transistor [3]. Experimentally, InAs grown on GaAs substrate via Molecule Beam Epitaxy [5] and metal-organic chemical vapor deposition and the distribution InAs in subtrate was observed using Scanning Tunneling Microscope (STM) [6].

*Corresponding author: Tel: +605-4506416 Fax: +605-4583616
E-mail: faudzi@fst.upsi.edu.my

Density Functional Theory (DFT) developed by Hohenberg and Kohn [7] in 1963 following by Kohn and Sham [8] in 1964, was used throughout the fields including physics and chemistry [9]. It is started with the solution for many body problems, since we know it is quite complicated for their classical approximation even analytical solution, where Born and Oppenheimer [10] made a simple assumption to eliminate the kinetic energy for nuclei and Coulomb interaction nuclei-nuclei terms. The further medication of many body problems, namely Hartree-Fock (HF) method [11], perfomed accurate in solution for atoms and molecules but less accurate in solids. To treat HF, Hohenberg and Kohn found two theorems of early density functional theory. Later, Kohn and Sham provided the proper exchange-correlation potential into the theory.

Previously, Zanolli and Barth calculated the structural and electronic properties of InAs and GaAs in wurzite and zincblende [12]. Ahmed *et. al.* [13] observed the effect of various chosen exchange-correlation functional namely local density approximation or LDA. Generalized gradient approximation parameterized by Engel and Voskov [13] was called as EV-GGA and generalized gradient approximation (GGA) [14] upon band structure of InAs and EV-GGA and GGA gave a better accuracy than LDA. The objective of this work is to investigate the calculation of density of states performed by linearized augmented plane wave (LAPW) method and local density approximation as the exchange and correlation potential. Density of states is an important electronic properties for material especially semiconductor compounds, where the density of states (DOS) at certain system are defined as the number of states at each energy level that are available to be occupied. A high DOS at a specific energy level means that many states are available for occupation. A DOS of zero means that no states can be occupied at that energy level and moreover, it provides sufficient information for a through characterization of the electronic properties of a material, we can also determine whether the materials have conductor, semiconductor or insulator properties. The calculation in this work provided within WIEN2k [15] software package based on DFT and employed with the LAPW method [16].

2. Methods

The calculation of electronic properties performed by DFT provided by the linearized augmented plane wave (LAPW) [16] method using WIEN2k code [15]. LAPW is among the accurate method for performing electronic properties study. The exchange-correlation potential of calculation was treated by local density approximation (LDA) parameterized by Perdew and Wang [14] and the latest developed by Perdew *et al.* [17]. Many researchers calculated the exchange-correlation using LDA corrected with generalized gradient approximation, but in this article we only focused on LDA as our accurate calculation.

The electronic configuration of InAs within In: [Kr],$4d^{10},5s^{2},5p^{1}$ and As:[Ar],$3d^{10},4s^{2},4p^{3}$ was provided. Before we started our calculation, we had to differentiate between electronic configuration of inner shell and valence state. For inner shell, electronic configurations of In and As are $1s^{2},2s^{2},2p^{6},3s^{2},3p^{6},4s^{2},4p^{6}$ and $1s^{2},2s^{2},2p^{6},3s^{2},3p^{6}$ and for valence states for In and As are $4d^{10},5s^{2},5p^{1}$ and $3d^{10},4s^{2},4p^{3}$. The type of lattice for InAs was face centered cubic FCC (F-43m, no.216) with position In (0, 0, 0) and As (0.5, 0.5, 0.5) and the lattice parameter of FFC InAs, we chose the value that has already been studied, i.e a=6.0584**Å** [18].

In this calculation, we treated the unit cell divided by interstitial region and non-overlapping muffin tin spheres. We used the plane waves in the interstitial region and linear combination of radial functions multiplied by spherical harmonics in non-overlapping muffin-tin spheres. For InAS, we performed covergence studies and determine the optimum value for cut-off

parameter $R_{MT}K_{MAX}$ = 11; where K_{MAX} is the maximal value of the respirocal lattice vector and R_{MT} is the smallest atomic sphere radius in the unit cell.

We chose k-points at 1000 (10x10x10) and the separation energy of core and valence states equal to -9.0 Ry because we wanted to ensure that charge could leak to the atomic sphere. The R_{MT} values for In and As in InAs compound are 2.5 atomic units (a.u.) and 2.2 a.u., respectively. Our calculation included relativistic and neglecting spinor orbit coupling because it did not produce any significance effect to our result.

3. Results and Discussion

3.1 Partial density of states of indium (5s and 5p states)

From the result, it was found that the region for DOS is separated by three regions, where valence band is composed of two parts, namely lower valence band (core state) and upper valence band (start from -11.2eV until 2.42eV), but they separated by internal gap about 9.0eV. The Fermi energy level is located at 0.0eV. Conduction band starts from 2.5eV and above. Figure 1 showed the partial density of state for atom indium at *5s* and *5p* state, respectively, where the peaks in Figure 2 looks dominant at conduction band rather than Figure 1, this implies that In-p contributed more number of occupation available as conduction state. It indicates that the most outer electron consised at configuration *5p* state. The maximum peak in Figure 1 is located at -5.12eV, in the valence band. Moreover there are slightly hybridization between In-s and In-p at region 0.08eV until -3.78eV.

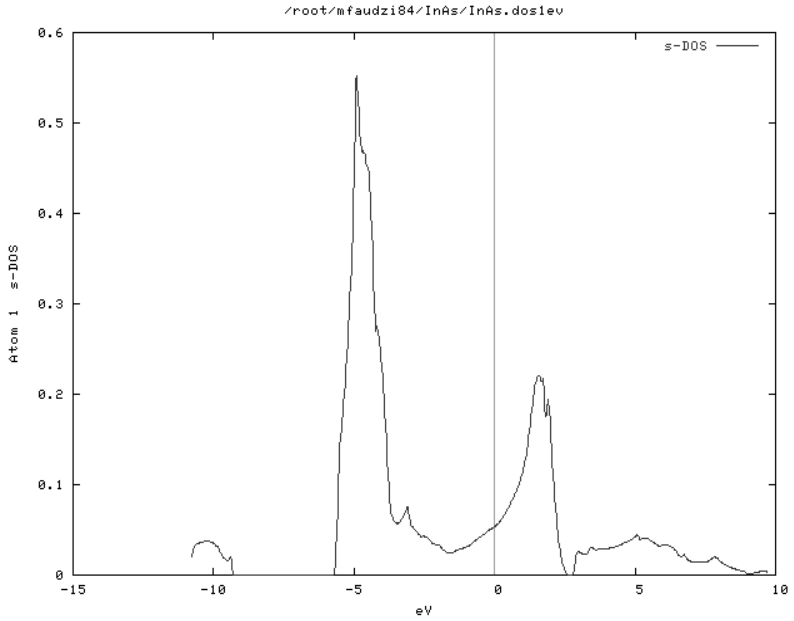

Figure 1 Partial DOS In-s

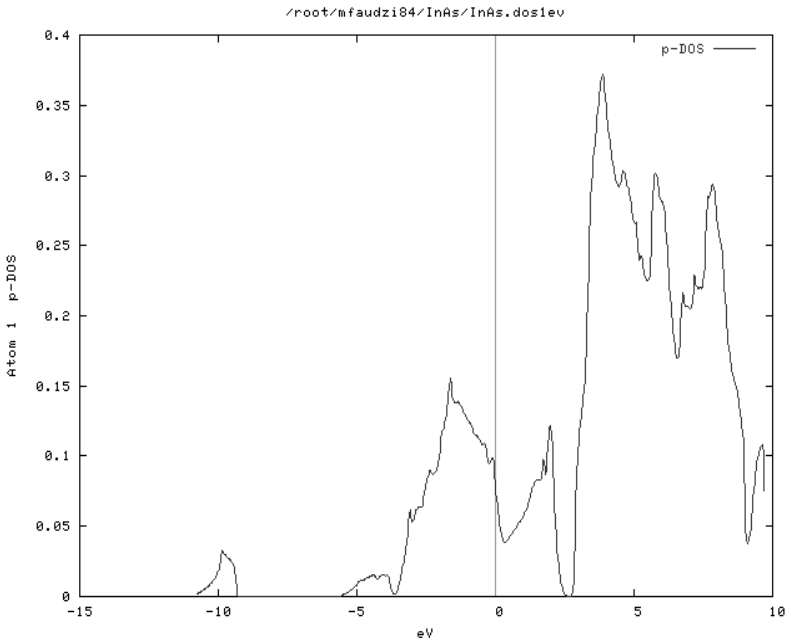

Figure 2 Partial DOS In-p

3.2 Total density of states of indium and arsenide

Figure 3 is the combination between partial DOS In-s and In-p. Peaks at the conduction band in the total DOS atom indium is dominated by peaks from partial DOS In-p and the maximum peak contributed by partial DOS In-s, indicates that In-s has tendency to be the lower valence state. Atom indium is relatively dominant contributed to the conduction band and the upper valence band.

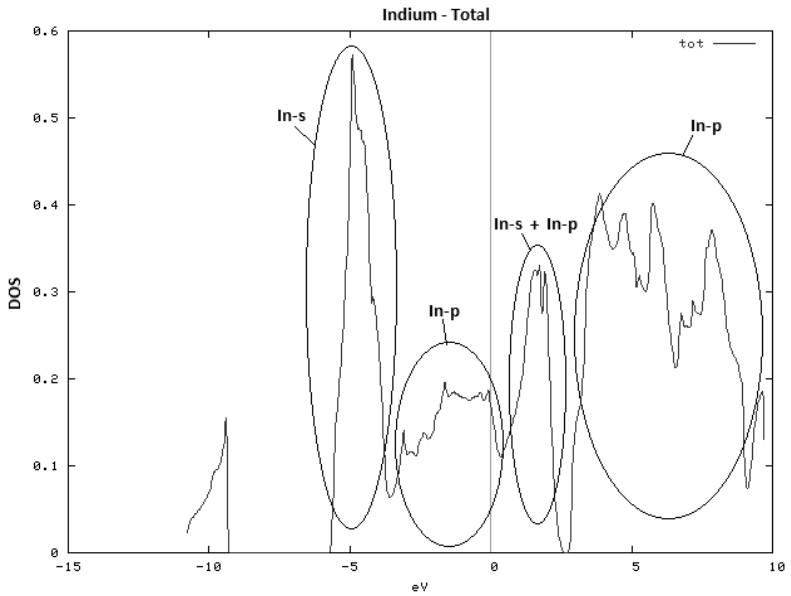

Figure 3 Total DOS Indium

Compared with atom arsenide (Figure 4), atom arsenide is relatively more dominant at lower valence band, especially at energy -9.38 eV (core), where it has maximum density of states at that point, which is about 1.68 eV^{-1} and the total DOS arsenide dominated at upper valence band as well. At conduction band, the total density of states of arsenide seem overlapping with the partial density of states of indium, It was observed that strong hybridization occurs between atom arsenide and indium at *5p* state.

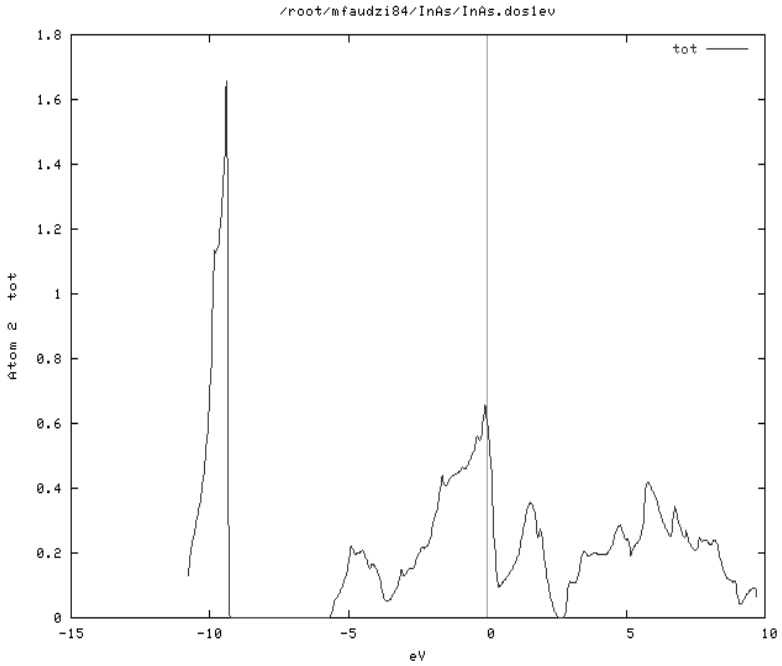

Figure 4 : Total DOS Arsenide

Figure **5** shows the combination of density of states from the total DOS arsenide and partial DOS indium (p and s). At the region 0.08eV until -3.78eV, there is slightly mixing density of states between arsenide and partial indium-5p, resulted in hybridization. The result showed that region between upper valence band and conduction band had no states of occupation around energy 2.421eV to 2.801eV and indicates that InAs is a semiconductor and has a bandgap about 0.38eV. It is in a good agreement to the experimental result about 0.36eV [19-21]. In addition, the shifted band gap to the upper Fermi energy level [19] indicated that InAs is the n-type semiconductor or donor. This property has been proven by Farah [22] with her undergraduate project to investigate the band structure of InAs, the result was similarly to the density of state calculation, and moreover Farah proves that InAs has a direct bandgap, which is agreed to the fact about InAs.

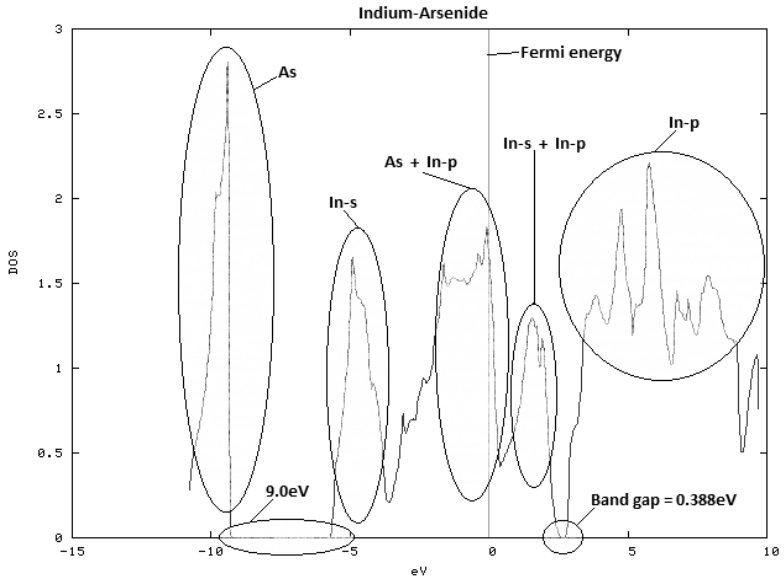

Figure 5 Total DOS Arsenide

References

[1] Korte, S., Farrer, I., Beere, H. E. and Clegg, W. J. **2008**. Discontinuous yield in InGaAs thin. *Surface & Coatings Technology* 203, 713-716.

[2] Anantathanasarn, S., Barbarin, Y., Cade, N. I., van Veldhoven, P. J., Bente, E. A. J. M., Oei, Y. S., Kamada, H., Smit, M. K. and Nötzel, R. **2008**. Wavelength tunable InAs/InP (100) quantum dots in 1.55-μm telecom devices. *Materials Science and Engineering: B*, Volume 147, Issues 2-3, 124 -130.

[3] Rashid Ahmed, Javad Hashemifar, Hadi Akbarzadeh, Maqsood Ahmed and Fazal-e-Aleem. **2007**. Ab initio study of structural and electronic properties of III-arsenide binary compounds. *Computational Materials Science* 39, 580 -586.

[4] Bugge, F., Zorn, M., Zeimer, U., Pietrzak, A., Erbert, G. and Weyers, M. **2008**. MOVPE-growth of InGaAs/GaAsP-MQWs for high-power laser diodes studied by reflectance anisotropy spectroscopy. *Journal of Crystal Growth,* In Press, Accepted Manuscript,

[5] Kamil Kosiel. **2008**. MBE—Technology for nanoelectronics. *Vacuum*, Volume 82, Issue 10, 951-955.

[6] Suzuki, T., Temko, Y., Xu, M. C. and Jacobi, K. **2005**. The atomic structure of InAs quantum dots on GaAs (112). *Surface Science* 595, 194-202.

[7] Hohenberg, P. and Kohn, W. **1964**. Inhomogenous electron gas. *Physical Review B136*, 864-871.

[8] Kohn, W. and Sham, L. **1963**. Self-consistent equations including exchange and correlation effects. *Physical Rev*iew *140*, A1133-1138.

[9] Mahan, G. G. and Subbaswamy, K. R. **1990**. Local density theory of polarizability. New York, Plenum Press.

[10] Born, M. and Oppenheimer, R. **1927**. On the quantum theory of molecules. *Annalen Physik* 84, 457-484.

[11] Hatree, D. R. **1928**. The wave mechanics of an atom with a non-Coulomb central field. Part I. Theory and methods. *Mathematical Proceeding of the Cambridge Philosophical Society*, 24, 89-110.

[12] Zanolli, Z. and Barth, U. V. All-electron study of InAs and GaAs wurzite: Structural and electronic properties. arXix: con-mat/0610066v2.

[13] Engel, E. and Vosko, S. H. **1993**. Exact exchange-only potentials and the virial relation as microscopic criteria for generalized gradient approximations. *Physical Review B* 47, 13164-13174.

[14] Perdew, J. P. and Wang, Y. **1992**. Accurate and simple analytic representation of the electron-gas correlation energy. *Physical Review B* 45, 13244-13249.

[15] Blaha, P., Schwarz, K., Madsen, G. K. H., Kvasnicka, D. and Luitz, J. **2001**. WIEN2K, An Augmented Plane Wave+Local Orbitals Program for Calculating Crystal Properties. Vienna University of Technology, Vienna, Austria.

[16] Madsen, G. K. H., Blaha, P., Schwarz, K., Sjőstedt, E. and Nordstrőm, L. **2001**. Efficiency linearization of the augemented plane-wave method. *Phyical Review B 64*, 195134-195142.

[17] Perdew, J. P., Burke, K. and Emzerhof, M. **1996**. Generalized gradient approximation made simple. *Physical Review Letter* 77, 3865-3868.

[18] Jeong, J., Schlesinger, T. E. and MilnesX-ray, A. G. **1988**. Characterization of $In_xGa_{1-x}As$/GaAs quantum wells. *Journal of Crystal Growth* 87(2-3), 265-275.

[19] Elliot, S. R. **1997**. The Physics and Chemistry of Solids. London, John Wiley & Sons Ltd.

[20] Bouarissa N., **2001**. Optoelectronic properties of $InAs_{1-x}P_x$ semiconducting alloys *Materials Science and Engineering B* 86 (1), 53-59.

[21] Bhat, R., Dutta, P. S. and Guha, S. **2008**. Crystal growth and below-bandgap optical absorption studies in InAs for non-linear optic applications. *Journal of Crystal Growth* 310 (7-9), 1910-1916.

[22] Farah, H. Z. **2007**. Simulasi profil struktur jalur bahan semikonduktor InAs berdasarkan Teori Fungsian Ketumpatan. Undergraduate project. University Kebangsaan Malaysia.