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EFFECT OF GA CONCENTRATION VARIATION ON THE BAND GAP OF IN1-XGAXAS TERNARY COMPOUND

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ABSTRACT
Semiconductors are used in fabrication of electronic components and manufacturing of electronics equipment. Band-gaps play prominent role in determining some characteristic properties of electronics devices, such properties include conductivities and optical wavelength. In this project, band gaps of Indium Gallium Arsenide,(InGaAs) ternary semiconductor compounds were calculated using generalized gradient approximation within Density Functional Theory as embedded in Quantum espresso package. The optimized values of k-point and cut-off energies of Indium Arsenide and Gallium Arsenide were used to optimize their respective experimental lattice constants. Lattice constants of Indium Gallium Arsenide, at varying concentration of Gallium, were calculated using additivity equation and later optimized to obtain stable equilibrium values using convergence test. These equilibrium values were used to calculate energy gaps of the ternary compounds by varying concentration, x (0.00, 0.25, 0.50, 0.70, 0.80, 0.90 and 1.00) of gallium. The results show that lattice constants, calculated at each concentration are 11.055, 10.808, 10.562, 10.364, 10.266, 10.167, 10.068 Å, and energy gaps were zeros for $x \leq 0.5$*, 1.02, 1.2, 1.4, 1.6 eV respectively. And the results compare favorably well with experimental values. This results show that the ternary compound exhibited property at x=0.7, 0.8, 0.9 and 1.0.*

INTRODUCTION
Indium Gallium Arsenide (InGaAs) is a semiconductor that has conductivity between that of a conductor and an insulator. This attribute

enables semiconductors' applications in all facets of electronics. Semiconductors can be grouped into two; elemental semiconductor and compound semiconductors. Elemental semiconductors are carbon, silicon and germanium.

Compound semiconductors are formed from two or more elements in the periodic table typically from groups (iii-v) and (ii-vi).

Examples of compound semiconductors are binary semiconductors, GaAs and InAs; ternary semiconductors, InGaAs and quaternary semiconductors, AlInGaP

In this project InGaAs had been chosen because of its use in high power, high frequency electronics and its superior electron velocity over other compounds. Its band gap also makes it the detector material of choice in optical fiber communication (Pearsall et al., 1997). InGaAs can also be used in infrared detectors, lasers, photovoltaic and transistors.

The conductivity of any semiconductor may easily be modified by introducing impurities into their crystal lattices. In this project the concentration of Ga is varied in the InGaAs compound.

Statement of the Problem

Materials possessing good conductivity properties are essential for technological growth. Materials with varying energy gap are preferable due to their electronic and optical properties thus impact of variation of Ga concentration on $In_{1-x}Ga_xAs$ will be studied.

Significance of the Study

The significance of this project is to study the band gap of InGaAs by varying Ga concentrations making it possible to calculate/estimate range of properties of InGaAs such as the optical wavelength and conductivity.

Objectives of the Study

To calculate the range of band gaps obtainable from $In_{1-x}Ga_xAs$ by concentration variation of Ga using Density Functional Theory.

To calculate the range of optical wavelengths obtainable from the influence of concentration variation of Ga in InGaAs ternary compound.

Scope of the study

In this project bandstructures of $In_{1-x}Ga_xAs$ will be obtained using density functional theory as embedded in quantum espresso package. Energy gaps will be measured and wavelengths calculated.

LITERATURE REVIEW

Energy gaps of (Al, Ga, In)V binary compounds were undertaken using Density functional theory in the Local Density Approximation (LDA) by applying the correction for excited state proposed by Fritsch and his co-workers (Remediakis and Efthmos, 1999).

The structural, electronic and thermodynamic properties of $Pb_{1-x}Sr_xS$ had been studied by varying concentrations of Strontium (Sr) semiconductors using scalar relativistic Full Potential Linearized Augmented Plane Waves (FP-LAPW) approach as implemented in WIEN 2K code within the framework of density functional theory (Labidi, Meradji, Ghemidand Hassan, 2010).

Impact of varying Bi concentrations on the structural and electronic properties of $GaAs_xBi_{1-x}$ alloys had also been studied using Full Potential Linear Augmented Plane Waves (FP-LAPW) as implemented in WIEN 2K code (Reshak, Kamarudin, Auluck and Kityk, 2012).

The effect of increasing concentration of aluminuim on the structural properties of $Al_xIn_{1-X}P$ alloy using the Full Potential Linearized Muffin-Tin Orbital (FP-LMTO) method with both LDA and GGA (Ameri, Bentoual, Doui-Aice, Khenatic, Boufadi and Touric, 2011). Their result showed that LDA bulk modulus and lattice constant for AlP and InP correlated well with experimental than the GGA values while the calculated LDA and GGA bulk moduli decrease from AlP to InP which suggests that the compressibility of InP is higher than that of AlP. It was deduced that decrease in the lattice constant from InP to AlP with increasing Al concentrations was attributed to the smaller size of Al atom than that of In atom.

The structural and electronic properties of Zinc blende BN, AlN and their ternary $B_xIn_{1-x}N$ alloy for concentrations $x = 0.25$, 0.5 and 0.75 using the most recent version of Vienna package WIEN 2K code. The calculated LDA and GGA band gaps predicted metallic compounds for Zinc-blende InN and direct band gaps for $B_xIn_{1-x}N$ alloy which were underestimated due to the

fact that the simple form of GGA does not take into account the quasi-particle self –energy correctly which made it sufficiently flexible to accurately reproduce both exchange correlation energy and its charge derivative (Abdiche et al,. 2010).

The band gaps variety of ground state properties of the 3C, 2H and 4H polytypes of Silicon carbide and lattice dynamical properties of cubic SiC were investigated (Kare, et al., 1994) using plane-wave pseudo-potentials within local density approximation of the density functional theory

The effect of variation of composition factor on the electronic, structural, optical and thermodynamic properties of the Strontium compound and disorder effects in the ternary alloy using full potential linear augmented plane waves (FP-LAPW) method (Labidi, et al., 2010) had been investigated. The calculated band structure showed a transition from indirect to direct band gap at x= 0.82 which exhibits non-linear behavior or bowing effect with varying concentrations and increase of lattice parameters of the compounds with increasing Sr concentrations suggested small positive deviation from Vegard's behavior. In this research, impact of variation of Ga atom in InGaAs will be studied.

Basic Theory of Electronic Structure Calculation.

In the study of structural properties of material, energy of electrons in a periodic potential is calculated by solving the Schrödinger equation. For a one electron system and many electron systems,

$$\left(\frac{-h^{2}}{2m}p^{2}+V(r)\right)\varphi(r)=E\varphi(r)\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$\left(\frac{-h^{2}}{2m}\nabla^{2}+\left(V_{e-e}(r)+V_{e-n}(r)+V_{n-n}(r)\right)\right)\varphi(r)=E\varphi(r)\ldots\ldots\ldots(2)$$

can be used respectively. If either of the equation is solved for the system in question, energy band can be calculated from the band structure of the system enabling calculations of parameters useful for the electronic and optical technology with powerful computational technique.

Density Functional Theory

The derivation of the physical properties of interacting system is one of the most important goals of physics in this century but to derive these properties from the quantum mechanical law of nature is a problem.

This problem requires solution of a partial differential equation the (Schrodinger or Dirac equation) of 3N spatial variables and N-spin variables (for electrons) N is the number of particles in the system.

For atoms N ranges from one to 100 electrons and often more than 100 while in solid, $N \approx 10^{23}$ (Kohn W, 1999; Leenwen,1994). Therefore it is clear that the problem cannot be solved without approximation along the line, somewhere.

The main objective is to understand the properties of many-body particle systems and to calculate several measurable quantities like bonding energy, polarizability , conductivity, etc. rather than the wave function itself, (Harrison,1980).

Energy gaps and Lattice constants

Energy gaps is the energy difference between the conduction band minimum and valence band maximum in a band structure of a given semi-conductor. In graded semiconductor structures, composition is varied by a change in band gap energy and this change can be accompanied by a variation of lattice constants. The dependence of forbidden- gap energy in terms of parabolic (linear plus quadratic) for graded alloy, dependence is;

$$E_g^{AB} = xE_g^A + (1-x)E_g^B + x(1-x)E_b \ldots\ldots\ldots\ldots (3)$$

The corresponding lattice constant is

$$a_o^{AB} = xa_o^A + (1-x)a_o^B + x(1-x)a_b \ldots\ldots\ldots\ldots . (4)$$

Parameters a_b and E_b are called bowing parameter. For heavy elements (In, Ga, Bi & As), bowing parameter is vanishingly small such that the composition is governed by

$$a_o^{AB} = xa_o^A + (1-x)a_o^B \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

$$E_g^{AB} = xE_g^A + (1-x)E_g^B \ldots\ldots\ldots\ldots\ldots (6)$$

These equations can be used to obtain wavelength of interest for the chosen alloy using

$$E_g = \frac{hc}{\lambda} \ldots\ldots\ldots\ldots\ldots\ldots\ldots . . (7)$$

MATERIALS AND METHOD

Materials used for this research are Acer Aspire Es11 Laptop which has 500GB hard disk capacities and 4Gb memory disk capacities. The system was partitioned into Windows 10 pro and Ubuntu operating software on which Quantum Espresso-6.0 software packages was downloaded and installed.

First principles total energy calculations were performed within the framework of Density Functional Theory, (Giannozzi et al., 2009).

The exchange correlations used was generalized gradient (GGA-PBE) approximation for the ternary compound. Atomic positions used for the ternary compound was designed in FCC super cell structure using VIESTA code.

Convergence tests was performed to obtain stable k-points sampling and self-consistent field total energy versus cut offs was plotted to obtain stable cut offs kinetic energy.

Experimental lattice constants were generated for varying concentrations of Ga using the formula:

$$a_0(In_{1-x}Ga_xAs) = a_0(GaAs)(x) + (1-x)a_0(InAs) \dots\dots\dots\dots\dots\dots (8)$$

Since convergence with respect to energy cut offs is a property of pseudo potentials it was carefully performed for each compound up to the energy difference of 10^{-3}Ry.

RESULTS AND DISCUSSION

Energy gaps of InGaAs varied with the increase in the concentration of Ga such that increase in the concentration of Ga causes an increase in the energy gap. This shows that the concentration of Ga is directly proportional to the energy gap and vice-versa.

Convergence

Literature revealed that the suitable required number of k-points for a given semiconductors and insulators which do not have Fermi surface is required. (Zbigniew, 2007). Thus, Monk-Horst Park(MP) 888 111 k-points were used throughout for the compound (InGaAs). Calculated parameters used were energy cutoffs and lattice constants. The calculated lattice constants for each concentration of Ga is shown in table1

Table1: Calculated Lattice constant, a_o (a.u) for varying concentrations of Ga.

CONCENTRATIONS OF Ga	Lattice constant a_o(a.u)
0.00	11.055
0.25	10.808
0.50	10.562
0.70	10.364
0.80	10.266
0.90	10.167
1.00	10.068

TABLE II: Calculated Energy gap (Eg) in eV for InGaAs

CONCENTRATION	ENERGY GAP(eV)
0.00	0.00
0.25	0.00
0.50	0.00
0.70	1.02
0.80	1.20
0.90	1.40
1.00	1.60

DISCUSSION

ENERGY GAP

There is a strong relation between the concentration variations and corresponding energy gaps in InGaAs ternary compound without spin orbit coupling. This results shows that from concentrations 0 - 0.5 no energy gap was observed but from concentrations of 0.7 - 1.0 the energy gap gradually increases with increasing concentration of Ga. This shows that only at concentrations ranging from 0.7 to 1.0 can the InGaAs compound have an energy gap.

At the concentration of 0 – 0.5 no meaningful band gap was recorded this may be due to the low concentration of Ga in the compound.

Band Structures of $In_{1-x}Ga_xAs$ Using GGA

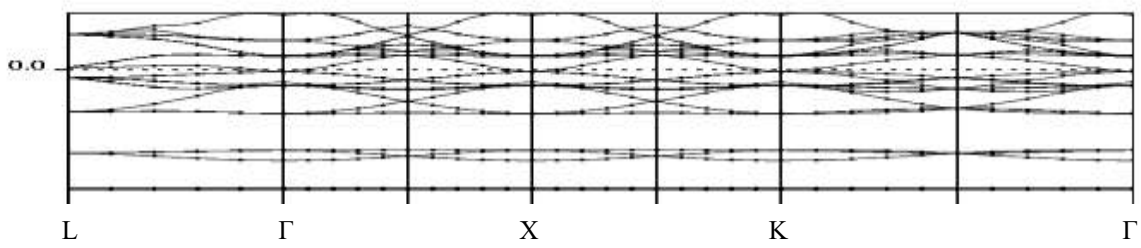

Fig.4.1 $In_{1.0}Ga_{0.0}As$

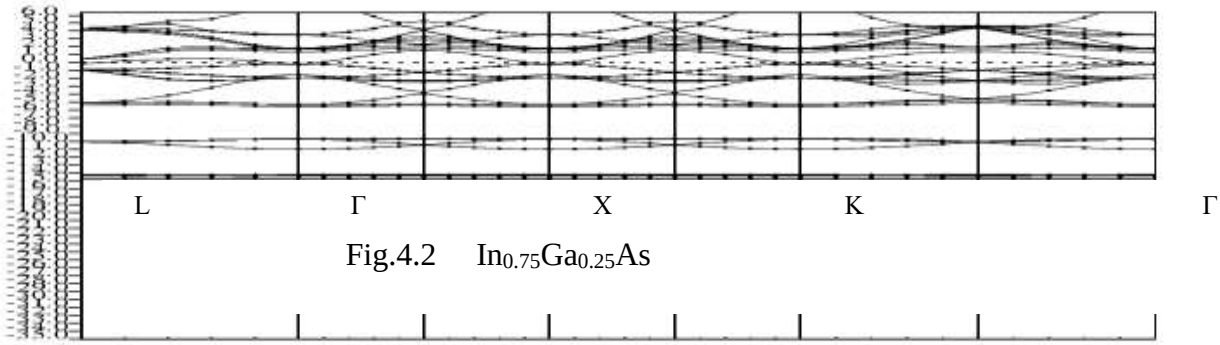

Fig.4.2 $In_{0.75}Ga_{0.25}As$

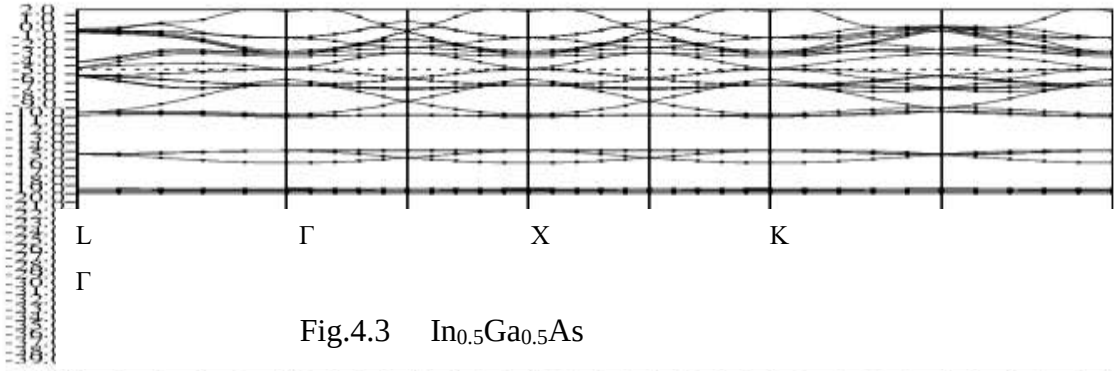

Fig.4.3 $In_{0.5}Ga_{0.5}As$

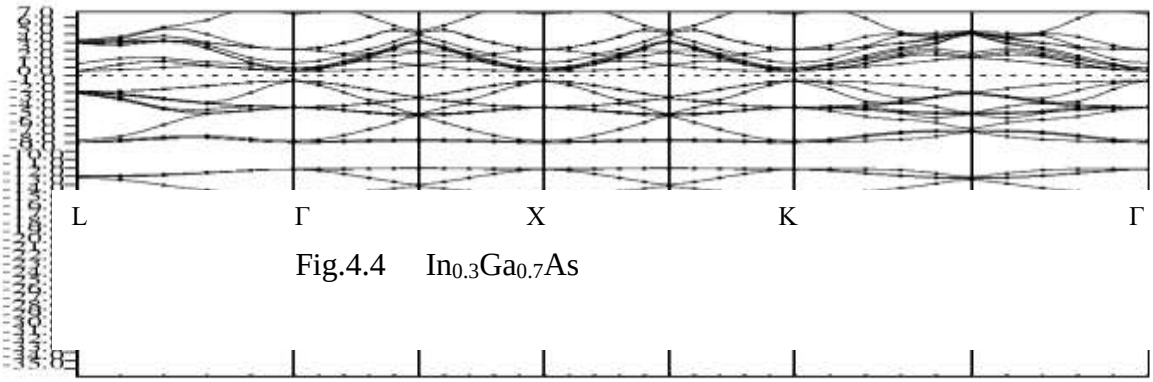

Fig.4.4 $In_{0.3}Ga_{0.7}As$

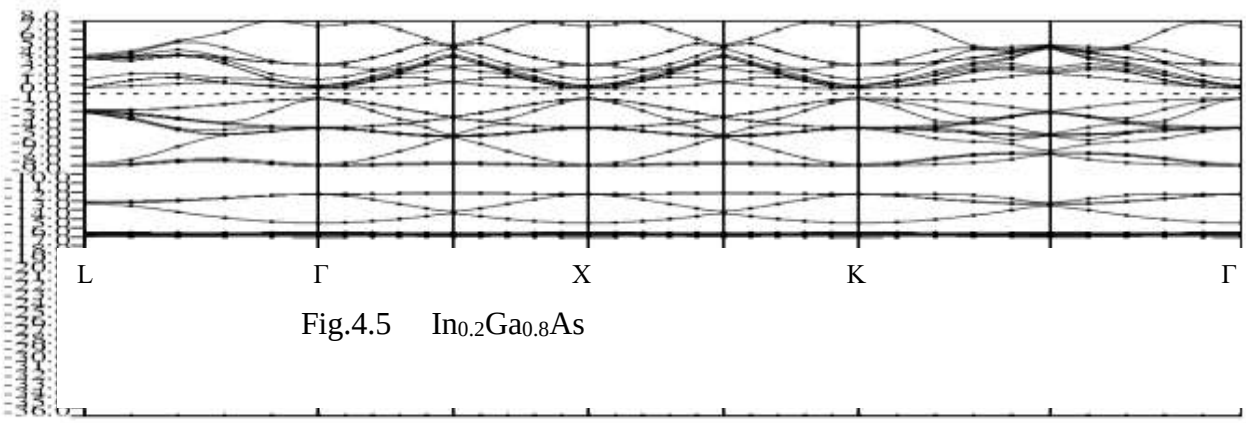

Fig.4.5 $In_{0.2}Ga_{0.8}As$

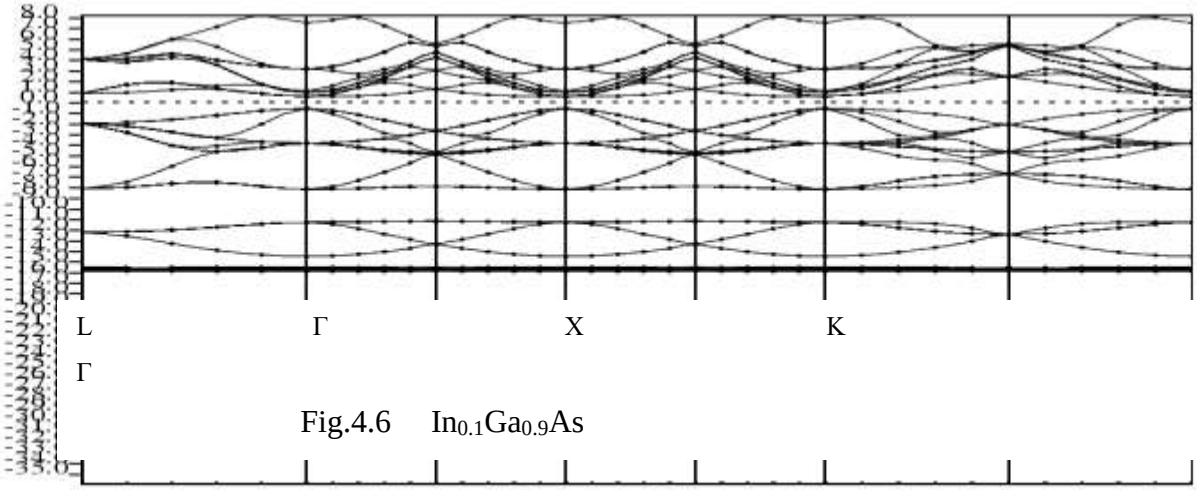

Fig.4.6 $In_{0.1}Ga_{0.9}As$

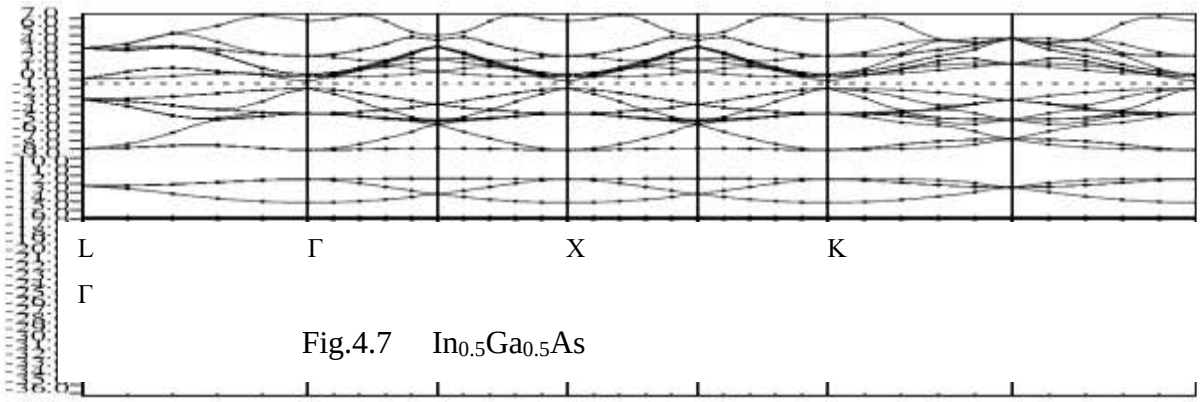

Fig.4.7 $In_{0.5}Ga_{0.5}As$

CONCLUSION AND RECOMMENDATIONS

In conclusion, it can be seen that the energy gaps increases with increasing concentrations of Ga with the exceptions of 0.25, 0.5.

The generalized gradient approximation has significant roles on energy gaps of ternary compounds in view of the different values calculated for the InGaAs compound. The facts that the results obtained correlate with experiments and published results show that the modern electronic structure techniques such as quantum espresso used in this research can produce fine details, thus giving further confidence in the predictive power of this technique,(Jeffrey Welser et al.,2010) and (Alguno, et al.,2009).

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