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DFT INVESTIGATION OF ELECTRONIC STRUCTURE OF InGaAs/Ge FOR SOLAR CELL APPLICATION

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Abstract: Efficiency of solar cell depends on the energy states. GaAs and its derivatives have potential application as solar cell. First principle calculation for structural and electronic properties of GaAs, InGaAs and Ge are reported. We have used local density approximation (LDA) for this study. Calculations are executed on density functional theory (DFT) based Quantum espresso code. Calculated lattice constant is nearly equal to the experimental value. Energy band gap of GaAs, InGaAs and Ge calculated with Perdew-Barle-Emzerhof approximation. Energy band gap is close to the experimental value. Vacancy defects shows change in energy band gap and rise in extra energy states within energy band gap. It shows a good carrier concentration and hence good candidate for multijunction solar cell.
Keywords: Density Functional Theory; InGaAs; vacancy defects; solar cell.

1. INTRODUCTION

Gallium Arsenide (GaAs) is a III-V direct band gap semiconductor. It because of having unique characteristics like higher electron mobility and saturated electron velocity etc. is used to manufacture devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infrared light emitting diodes, laser diodes, solar cells and optical windows. It has certain advantages over other semiconductor materials owing to unique characteristics such as, better resistant to radiation, speed operation in conjunction with small power use, and moreover potential to transfer electrical signals to optical signals [1]. It is also considered one of the best photovoltaic materials for solar cell technology. Therefore researches are interested in GaAs both experimentally and theoretically [2-9]. GaAs is often used as a substrate material for the epitaxial growth of other III-V semiconductors including InGaAs, AlGaAs and others.

Most of the theoretical investigations of the material properties like electronic structure, structural properties, optical properties etc are done using DFT approach. It is because DFT provides a framework to simplify quantum many body problem and is contributing a significant role in designing new materials as well as tuning and investigating different physical properties.

In presented study, comparison between electronic structure of GaAs and InGaAs is done. Also electronic structure of Ge is investigated for multijunction InGaAs/Ge solar cell application. InGaAs is a ternary alloy of Indium Arsenide and Gallium Arsenide. As GaAs, InGaAs also have potential in many applications. InGaAs is used in multijunction solar cell where Ge used as substrate. Lattice parameter of Ge and InGaAs is nearly same therefore it helps in transport of electrons from one layer to other. Energy states of GaAs, $In_{0.5}Ga_{0.5}As$ and Ge are investigated. Because of synthesis environment, high energy radiation, heating treatment etc these solar cells could have vacancy defects. These vacancies act as either a hole or electron trap depending on their position. This affects the overall performance of the solar cell. To predict the metastable states induce in the energy band gap theoretical study of GaAs, $In_{0.5}Ga_{0.5}As$ and Ge with vacancies are carried out. Finally conclusions are drawn from the observations.

2. COMPUTAIONALDETAILS

Quantum mechanical calculations based on local density approximation exchange correlation function (LDA) and non relativistic projector augmented wave (PAW) method are executed in linux operating system based Quantum espresso (QE), an open-source DFT based package widely used to perform the first principle calculations [10]. The structure of the required materials was designed with consideration of necessary parameters. Perdew-Barle-Emzerhof approximation method is employed. Convergence threshold of 10^{-8} for better self-consistency and geometry relaxation was carried out with the ionic forces less than 0.002eV. DFT calculations were performed to obtain energy band structure and density of states (DOS) of GaAs, $In_{0.5}Ga_{0.5}As$ and Ge. A plane wave cutoff energy for the basis is set to 408eV for $In_{0.5}Ga_{0.5}As$ supercell. Monkhorst-Pack Brillouin zone describing the k mesh values are considered in the calculations. Initially the Zinc-Blende structure of GaAs was studied, from which other structures were derived based on their atomic replacement and relaxation as per requirement. The exact exchange fraction for electronic properties was taken to be 0.30. All the calculations were carried out in a sequential manner with proper lattice constant and geometrical optimization. The estimated errors in these calculations are seen to be around ±0.05eV.

3. RESULT AND DISCUSSION

Structural properties (the equilibrium lattice parameter) of GaAs, $In_{0.5}Ga_{0.5}As$ and Ge yield through the analysis of total energies versus volume. These parameter were calculated using LDA scheme. It was found that lattice parameters 10.6828bohr, 11.0908bohr, 10.63bohr respectively of GaAs, $In_{0.5}Ga_{0.5}As$ and Ge are proper for the further calculations. Obtained lattice parameters are closely associated with the experimental value. DFT approach allows a more detailed analysis of some aspects of the DOS and Fermi energy which are responsible for determining the various energy levels that are occupied by the electron in the transport phenomenon, considerable changes in the DOS and Fermi value will vary the electric characteristics of the semiconductor material [11]. Therefore electronic properties of pure GaAs, $In_{0.5}Ga_{0.5}As$ and Ge and with vacancy defects are analyzed.

3.1 ELECTRONIC STRUCTURE OF PURE GaAs

Gallium Arsenide is a material widely used in solar cell technology [12]. Electronic structure of pure GaAs is analyzed. FCC unit of GaAs spanned over infinite matrix is designed for the calculation. Monkhorst-Pack Brillouin zone with 4x4x4 k mesh is used for the calculation of Density of States. Energy state diagram was obtained with the high symmetry points for the FCC lattice. Figure 1 shows the structure of GaAs and figure 2a and 2b shows the DOS plot and energy state diagram of bulk pure GaAs.

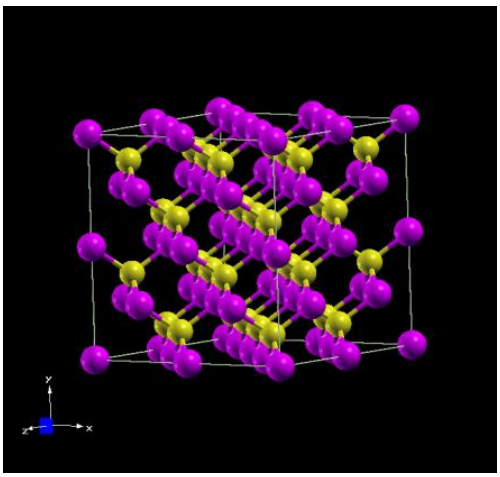

Fig.1 *structure of pure GaAs*

Simulation shows that Fermi energy is at 5.678eV. Energy states above Fermi energy are unoccupied molecular orbitals and bellow are the occupied molecular orbitals. Energy band gap was calculated as the difference between Lowest of Unoccupied Molecular Orbitals (LUMO)and Highest occupied Molecular Orbitals (HOMO) and it is observed to be 1.25eV. The value of obtained energy band gap is closely related to experimental value which is 1.43eV [13].

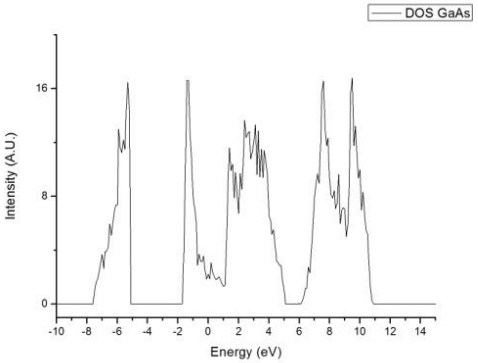

Fig.2a *DOS of pure GaAs*

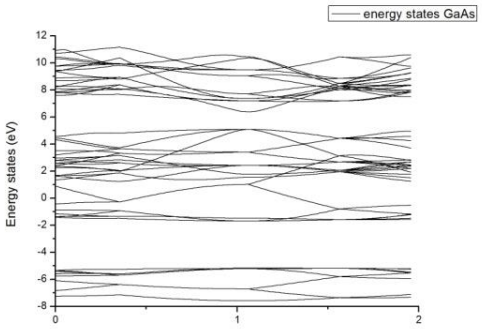

Fig.2b *Energy states of pure GaAs*

Energy states diagram shows that GaAs is a direct band gap semiconductor. Energy state diagram also shows the energy band gap of 1.25eV.The point of direct band gap measurement is at gamma point.

3.2 ELECTRONIC STRUCTURE OF $In_{0.5}Ga_{0.5}As$

$In_{0.5}Ga_{0.5}As$ can be derived from structure of GaAs. A pillar like structure was constructed as shown in figure where two unit cells are placed on one another. This pillar like geometry is further spanned over infinite matrix hence considered a bulk $In_{0.5}Ga_{0.5}As$. DOS were calculated for $In_{0.5}Ga_{0.5}As$ followed by DOS for Ga and In vacancy in one pillar like geometry. As is a heavy ion in the material and therefore chances of vacancy of As in very less. Because of this reason only Ga and In vacancy was studied. Monkhorst-Pack Brillouin zone with 12x12x12 k mesh is used for the for the calculation of DOS. Energy state diagram was obtained with the high symmetry points. Figure 3a, 3b and 3c shows the structure of pure $In_{0.5}Ga_{0.5}As$, $In_{0.5}Ga_{0.5}As$ with Ga vacancy and $In_{0.5}Ga_{0.5}As$ with In vacancy. DOS plots of pure $In_{0.5}Ga_{0.5}As$, $In_{0.5}Ga_{0.5}As$ with Ga vacancy and $In_{0.5}Ga_{0.5}As$ with In vacancy are shown in Figure 4a, 4b and 4c.

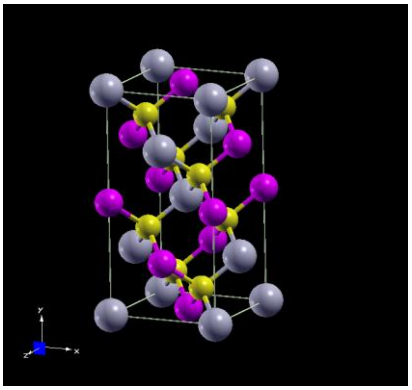

Fig. 3a *structure of pure $In_{0.5}Ga_{0.5}As$*

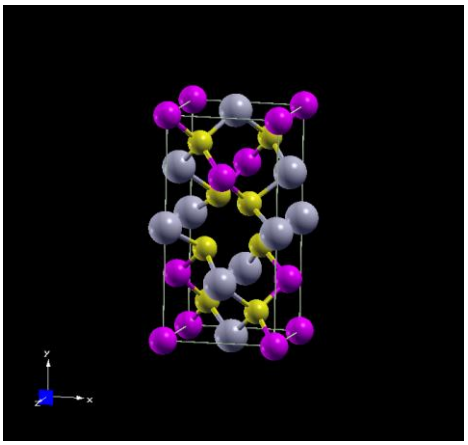

Fig. 3b *Ga vacancy in $In_{0.5}Ga_{0.5}As$*

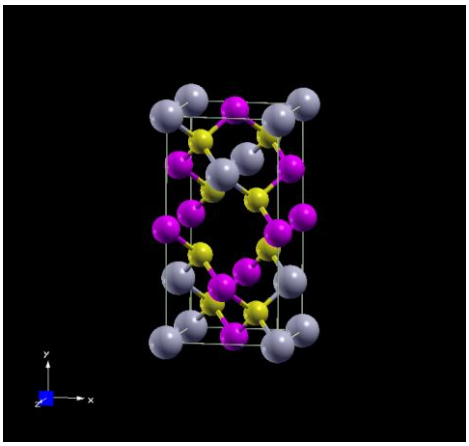

Fig. 3c *In vacancy in $In_{0.5}Ga_{0.5}As$*

DOS of pure $In_{0.5}Ga_{0.5}As$ and with Ga vacancy and In vacancy are shown in Figure 4a, 4b and 4c. Simulation shows the Fermi energies are at 4.566eV, 3.770eV and 3.574eV of pure $In_{0.5}Ga_{0.5}As$ and with Ga vacancy and In vacancy respectively. It is observed that Fermi energy is shifted towards valance band as vacancy defect is introduced. Fermi energy is in valance band in both the cases of vacancy defect. It shows that material shows charge carrier mobility due to holes. Energy band gap of $In_{0.5}Ga_{0.5}As$ and with Ga vacancy and In vacancy is 0.8eV, 0.7eV and 0.9eV respectively. Experimental value of energy band gap of $In_{0.5}Ga_{0.5}As$ is 0.74eV [14]. Obtained value of energy band gap is appreciable in comparison with the experimental value. It shows that energy band gap is reduced in comparison with the energy band gap of GaAs. It could be due to the extra energy states of In atom.

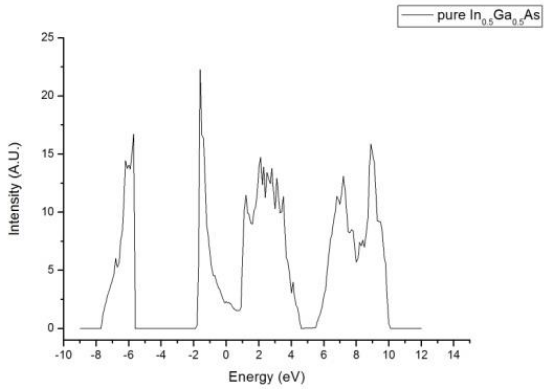

Fig. 4a *DOS of pure $In_{0.5}Ga_{0.5}As$*

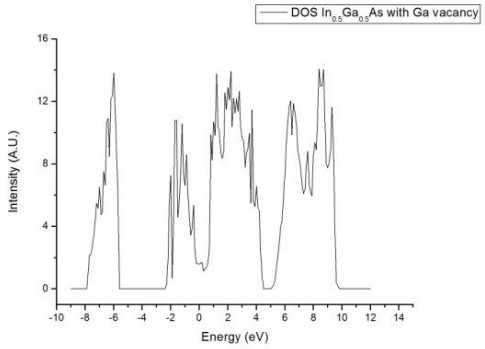

Fig. 4b *DOS of Ga vacancy in $In_{0.5}Ga_{0.5}As$*

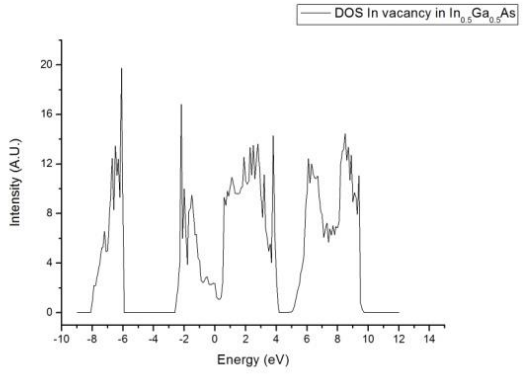

Fig. 4c *DOS of In vacancy in $In_{0.5}Ga_{0.5}As$*

3.3 Electronic structure of Ge

Ge is used as the substrate in double junction or multijunction solar cell. FCC unit cell designed for the calculation is shown in Figure 5. Monkhorst-Pack Brillouin zone with 12x12x12 k mesh is used for the for the calculation of DOS. Lattice parameter is closely related with the lattice parameter of $In_{0.5}Ga_{0.5}As$. It shows the lattice matching and hence $In_{0.5}Ga_{0.5}As$ could be pasted over Ge substrate. Because of good lattice match charge carriers could travel easily within the layers.

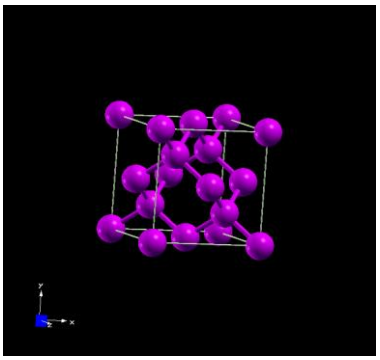

Fig. 5 *structure of Ge*

DOS plot is shown in Figure 6. Fermi energy is at 5.755eV. Calculated energy band gap of germanium is 0.6eV and it is very close to that of experimental value i.e. 0.67eV.

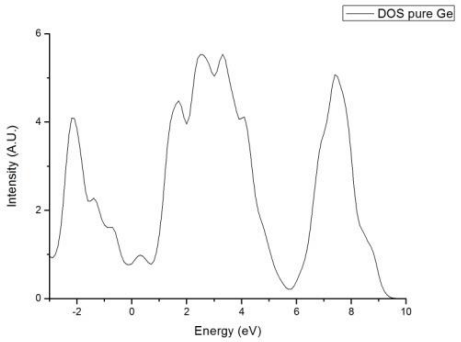

Fig. 6 DOS of pure *Ge*

Effect of vacancy of one Ge atom was studied. DOS of Ge with vacancy of one atom of Ge is shown in figure 7. Observed Fermi energy is at 4.315eV. In the case of vacancy of one Ge atom ions in FCC unit cell does not balance and therefore charge remains on the overall structure. Due to this band gap observed in pure Ge vanished and it act as conductor. DOS plot shows that extra energy states are arise within the band gap of pure Ge, results in metal like behavior.

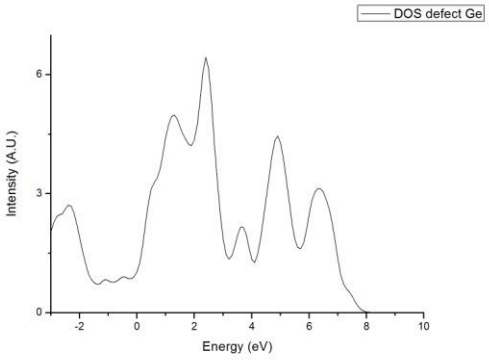

Fig. 7 *DOS Ge with vacancy of one Ge atom*

4. CONCLUSIONS

Electronic structure of GaAs, pure $In_{0.5}Ga_{0.5}As$, $In_{0.5}Ga_{0.5}As$ with Ga and In vacancy and Ge were studied. GaAs is a semiconductor material popularly used in solar cell. Its derivative i.e. $In_{0.5}Ga_{0.5}As$ is also potential candidate for the solar cell applications. Study of $In_{0.5}Ga_{0.5}As$ and Ge shows lattice match. Density of states shows good concentration of energy states. Therefore, good candidate for the solar cell applications. Because of their compatibility they can be used for the multijunction solar cell.

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