Structural and optical properties of GaAs and InAs for doping Sb under the effect of pressure and temperature: DFT and EPM investigations

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Abstract
We have developed first-principles calculations utilizing the empirical pseudopotential method and density functional theory to examine the basic behaviors of the GaAs and InAs semiconductor compounds for doped Sb. The electronic and optical responses of these compounds were calculated. We examined the impacts of the temperature and pressure with the energy band forbidden and parameters of optical parameters (static dielectric constant) of the considered compounds. The literature hasn’t fully analyzed the electronic and optical characteristics of the compounds with doping Sb under the impact of pressure and temperature for fixed composition (x = 0.5). So, we concentrated on the study of these properties.

Keywords Electronic properties · Optical properties · DFT · EPM · Pressure · Temperature

1 Introduction
The advancement of communications, computers, healthcare, military systems, transportation, renewable energy, and numerous more uses is made possible by semiconductors, which are a crucial part of electronic devices. The GaAsSb and InAsSb semiconductor alloys showed enormous application potential in optoelectronic devices and processed extraordinary development. Opto-electronic, mechanical, and structural properties of semiconductor alloys under the effect of temperature and pressure have been studied by several authors (Degheidy et al. 2017, 2018b; Degheidy and Elkenany 2013a, 2015a; Elkenany and Othman 2021; Othman 2020; Sharma et al. 2018). High-pressure investigations on GaAsSb and InAsSb compounds have been carried out extensively, resulting in a complete understanding of their structure-property relationships. The discovery of pressure and temperature-dependent features such as metallization and bandgap has had a significant impact.
on the further evolution of those materials. Through this viewpoint, we chiefly stress temperature and pressure dependence on the properties of these compounds as a function $x = 0.5$.

A decade ago, semiconductor materials gained significant consideration and concern from academic populations and industrialized zones all over the world, while they supplied marvelous perspectives in optoelectronic and photodetectors (Degheidy et al. 2018a; Degheidy and Elkenany 2015b; Dusabe et al. 2020; Sherzad Othman et al. 2021). They retain outstanding optical and electronic properties for their great absorption of coefficients, long carrier distribution lengths, and optical bandgaps, it was stated that these compounds were doped with a variety of metal ions including Al (Ritenour et al. 2015), In (Singh et al. 2019), and Sb (Ting et al. 2020).

It displayed that a rise in electric accessibility with a decline in band forbidden occurred due to the smaller ionic radius dopants (Dolia et al. 2017; Mikhailova et al. 2019). Also, it has been reported these compounds with temperatures using different methods. It has been about twenty years, and a great deal of research stressed the high pressure and temperature structural stability of these compounds, however, the stage figures of high-pressure of the GaAs and InAs compounds with Sb doping were not fully specified. Zunger et al. (Liu et al. 2007; Mäder and Zunger 1994; Wei et al. 1990; Wei and Zunger 1991) studied the physical properties for many of semiconductor materials and proposed the empirical pseudopotentials for the III–V compound semiconductors. Many modeling techniques were used to determine the physical properties of materials in material science (Abdelghany et al. 2015, 2021; Degheidy et al. 2018e; Elkenany 2021; Othman 2022). Besides that, some research theoretically and experimentally was implemented regarding some spectral parameters of GaAs-Sb alloys (Mochizuki and Nishinaga 1988), and studies were then kept publishing to indicate the electronic and optical behaviors of semiconductor compounds (Almi and Lakel 2020; Asadi and Nourbakhsh 2019; Aschenbrenner et al. 2010; Degheidy et al. 2018a, c, d; Degheidy and Elkenany 2015b, c, 2015d, e; Elkenany 2016, 2021).

In this work, doped Sb concentration ($x = 0.5$) with GaAs and InAs compounds afterward, under different temperatures and pressures were examined. The electronic properties as the electronic band structure, forbidden energy band, optical properties as optical absorption coefficient, and dielectric constants of the prepared compounds were studied theoretically with two different methods (DFT, and EPM).

## 2 Computational technique

### 2.1 Part a (DFT)

It is founded on DFT through a plane-wave basic for the protraction of the waves task (Sherzad Othman et al. 2021). Through the use of non-local ultrasoft pseudopotentials, the valence electrons were characterized. The Cambridge Serial Total Energy Package on the Board of Materials Studios was used to implement the calculations of the principal value that are shown at this point (Clark et al. 2005). Local-density approximations (LDA) were arranged with the PBE system to assess correlation energy. It is displayed that the results are properly related to this cutoff. The Ga ($3d^{10} 4s^2 p^1$), As ($3d^{10} 4s^2 4p^3$), In ($4d^{10} 5s^2 p^3$) and Sb ($4d^{10} 5s^2 5p^5$) were proceeded as valence band. The BFGS reduces internal matches to acquire the least amount of total energy (Broyden-fletcher Goldfarb-Shanno) system. The energy forbidden in materials is generally minimized by the local density approximation.
procedure. The first step of geometry optimization for the semiconductors GaAs\textsubscript{x}Sb\textsubscript{1−x} and InAs\textsubscript{x}Sb\textsubscript{1−x} with composition x = 0.5 was completed at various pressures (P = 0, 3, 6, 9, and 12 GPa) with symmetry \( P_1 \). After the structure parameters were calculated from symmetry directions. We calculated electronic band structures and determined the values of the energy band gaps with changing pressure. The optical behaviors were fixed for GaAsX and InAsX with doping Sb compounds with high pressure. Utilizing Kramer’s Kronig functions, the dielectric equations are used to characterize the optical linear response caused by the interaction of photons with electrons (Horsley et al. 2015; Tanner 2015).

2.2 Part b (EPM)

The empirical pseudopotential approach was created as a tool to solve the many-body problem of solving Schrodinger’s equation for bulk crystals without knowing the actual potential of an electron in a lattice. The pseudopotential approach is still in use today due to its efficacy and simplicity. The EPM has also been used in conjunction with CDE (compositional disorder effect) and VCA (virtual crystal approximation) (Bouarissa and Aourag 1995; Degheidy et al. 2018b, c; Degheidy and Elkenany 2017; Lee et al. 1990). Reference (Harrison 2016) offers further details about (EPM). Using our MATLAB-based technique, the current EPM calculations for the zinc-blende InAsSb and GaAsSb alloys were carried out (Higham and Higham 2016). With the aid of the references (Baranowski 1984; Bouarissa 2003), the electronic and optical properties of the substances under study were computed. The electronic energy spectra of these compounds were calculated using the local pseudopotential approach. The arrangements of the elements are attuned to provide an appropriate accord between the planned energy band forbidden and the matching of other simulation methods in this present value at high symmetry grades in the Brillouin area. As soon as the associated semiconductor form factors of Sb are marked, the calculations are going to be performed to resolve the band structure. For composition x = 0.5, by changing the adaptable parameter tile coordination was attained with the experimentations.

3 Results and discussion

The response of GaAsSb and InAsSb alloys at x = 0.5 with high temperature and pressure was calculated. Dielectric function (real section), optical band energy, and optical absorption have been discussed. Many physical properties such as cleavage, electronic band structure, and optical transparency are determined by crystal structure and symmetry. Crystal patterns determine the arrangement of atoms in a material. Additionally, it indicates a material’s bond lengths and lattice characteristics. Since the atomic configuration controls the material’s ductility and strength. Crystal structures for the InAsSb and GaAsSb compounds are specified in Fig. 1.

One of the most interesting topics in solid-state physics is band structure. The electronic levels in crystal formations are provided by it. The electronic band structure explains the energy ranges that an electron is permitted or forbidden to have. A material’s band structure determines various aspects, including its electrical and optical properties. As in the first step in calculations, the optically forbidden band energy corresponding to the \( \Gamma \) symmetry point is gained. Figure 2 displays the diagram band structure graph given for InAsSb and GaAsSb compounds under \( P = 9 \) GPa. The achieved electronic and band structures
outcome displayed that the structures get an immediate band zone. These values are found to be in submission with the different works (Elkenany and Othman 2021).

The electronic bandgap helps understand how light interacts with matter. The wavelength of light that will be absorbed by the material can be predicted using the electronic bandgap. It is the energy required for a valence electron that is bound to an atom to become a conduction electron that is free to move within the crystal lattice and also acts as a charge carrier in the passage of electric current. Figure 3 shows the optical band forbidden which is obtained by the two methods DFT and EPM for GaAsSb and InAsSb compounds under different pressure. The optical band forbidden of these compounds increases with increasing pressure factor. All values in the optical band forbidden are smaller than the experimental data (Adachi 2005) as a result of utilizing the LDA in the computations. Even so, it should be stated that the LDA emendation is not constant and does not alter precisely in response to the bandgap size. It has been noticed that the results of electronic band gaps produced by DFT are in good accord with those obtained by EPM.

Figure 4 shows the optical band forbidden calculated by the EPM for GaAsSb and InAsSb alloys under different temperatures. It is noted that the band forbidden for GaAsSb and InAsSb is diminished with enhancing temperature from (0–500 K) from 1.515 to 1.324 eV and 0.1908–0.087 eV, respectively. The optical bandgap regulates how much of the solar spectrum is absorbed by a photovoltaic cell. Photons with energies smaller than the bandgap are not absorbed by semiconductor alloys, and the energy of the electron-hole pair created by a photon is equal to the bandgap energy.

To determine a material’s dielectric properties, a frequency-dependent complex dielectric function with real and imaginary components is utilized. The dielectric function describes how sensitive a semiconductor is to electromagnetic radiation carried by photons and electrons (Tripathy and Pattanaik 2016). The imaginary component of the dielectric
Fig. 2  Electronic band structure of InAsSb and GaAsSb alloys for composition 0.5 at $p = 9$ GPa

Fig. 3  Optical energy bandgap for GaAsSb and InAsSb compounds as a function of pressure
constant determines the absorption coefficient, while the real part of the dielectric constant determines the refractive index of a material. Figure 5 shows the variation of the real part of the dielectric function of the GaAsSb compound with energy under different pressures.

Fig. 4 Optical energy bandgap GaAsSb and InAsSb compounds as a function of temperature

Fig. 5 Dielectric function (real part) of the InAsSb and GaAsSb as a function of pressure
It rises with the increment of 1.73–5.02 eV and it is an average distinctive distribution. Raise in reflection and absorption are ready in the 1.73–502 eV energy interval of the GaAs and InAs compounds. Static dielectric constant $\varepsilon_1(0)$ with high-frequency dielectric constant $\varepsilon(\infty)$ of alloys system are investigated under different pressure, using DFT and EPM methods and given in Table 1. All semiconductor compounds have a substantial absorption limit in infrared spectrum zones.

Figures 6 and 7 give the variation of absorption of the GaAsSb alloy versus pressure. It is uneasy to achieve the precise optical energy bandgap. To fit the absorption edge to the experimental value, we applied the energy scissor approximation (Wang et al. 2019) with 0.93 eV in our calculations. This approach works for a wide range of systems. The relationship between the optical band gap and the data of absorption is provided (Costa et al. 2016; Makula et al. 2018). All data of these compounds relatively

| Pressure (GPa) | InAsSb ($\varepsilon_0$) | GaAsSb ($\varepsilon_0$) | GaAsSb ($\varepsilon(\infty)$) | InAsSb ($\varepsilon(\infty)$) |
|---------------|---------------------------|--------------------------|-------------------------------|-------------------------------|
|               | DFT | EPM | DFT | EPM | EMP | EMP | EMP |
| 0             | 15.68 | 17.09 | 8.93 | 7.82 | 7.20 | 7.82 |
| 3             | 14.99 | 14.84 | 9.06 | 8.14 | 7.18 | 8.14 |
| 6             | 13.31 | 12.63 | 9.48 | 8.47 | 7.01 | 8.47 |
| 9             | 12.72 | 10.99 | 8.67 | 9.06 | 7.09 | 9.06 |
| 12            | 11.91 | 9.73  | 7.92 | 9.73 | 7.33 | 9.14 |
increase with pressure. Also, decrease these values with temperature. It demonstrates that the variations with the pressure of InAsSb were rapprochement than GaAsSb compounds using different methods calculation.

4 Conclusion

We have performed first-principles calculations utilizing the DFT and empirical EPM to investigate the basic behaviors of the InAs and GaAs compounds doped with Sb elements at various pressures. These alloys’ electronic and optical properties were identified. Additionally, EPM was used to study the behaviors of the compounds under consideration at various temperatures. The electronic band structure, energy band gaps, static dielectric constant, high-frequency dielectric constant, and the absorption of the alloys under investigation have been determined. The pressure and temperature-dependent electronic energy bandgap and optical properties of the studied materials have been calculated. The influence of pressure and temperature on these compounds’ electronic and optical properties has not been completely explored in the literature. Subsequently, we concentrated on these behaviors’ impacts on pressure and temperature. The investigated materials could be applied in optoelectronic systems.

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Author's contributions Mazin SH. Othman and Elkenany B. Elkenany designed research, performed research, and wrote the paper. All authors have read and approved the final manuscript.
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Data availability  This manuscript has no associated data or the data will not be deposited.

Declarations

Conflict of interest  The authors have not disclosed any competing interests.

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