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Structural, electronic and optical properties of the quinary $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$:First-principles study

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Abstract: *The structural, electronic and optical properties of $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$ have been investigated using a full potential linearized augmented plane wave (FP-LAPW) method within the local density approximation (LDA).The structural properties such as the lattice parameter, bulk modulus B, pressure derivative B' are determined and electronic properties such as band gap and density of states have been pursued. On the other hand, the dielectric function, refraction index, reflectivity, conductivity function, and energy-loss spectra were obtained and analyzed on the basis of electronic band structures and density of states.*
Keywords: *Full-Potential-LAPW; Local density approximation; Quinary alloys; Semiconductors III-V.*

I. Introduction

Researchers have been interested in III-V multi-element alloy semiconductors for several decades. Their band gaps extend widely from infrared to ultraviolet regions and the lattice constants can be tailored by controlling their composition. They also provide the material basis for a number of well-established commercial technologies. These multi-component alloys are promising candidates for many device applications such as high speed electronic and long wavelength photonic devices.

Continuing progress in III-V optoelectronics requires the synthesis of semiconductor alloys with specific structural, electronic and optical properties. The quaternary alloys lattice- matched to the given substrate provide new possibilities to realize the desired material properties and are very useful for reducing defects, dislocations and piezoelectric field. InGaAsP, GaInNAs, AlGaInN etc., quaternary alloys have been widely adopted for device applications [1–5].

The search for new semiconductor materials with structural and electronic properties for the advancement of optoelectronic applications, such as thin-film solar cells or laser diodes, constitutes one of the central challenges in materials science. II–VI and III–V compound semiconductors have long been viewed as promising materials for the device applications in electronic and optoelectronic technologies. Many of these binary semiconductors crystallize in a cubic zinc-blende structure.

The plan of the manuscript is as follows: The next Section 2 gives a brief description of the method used of the calculations; Section 3 presents the analyses of the calculated results and finally, the conclusion is given in Section 4.

II. Computational method

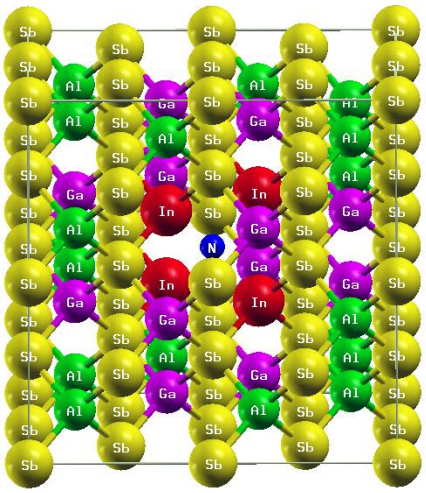
The calculations for the structural, electronic and optic properties of $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$have been performed using the FP-LAPW method based on the density functional theory implanted in the WIEN2K code [6, 7]. The maximum *l*-value for the wave function expansion inside the atomic spheres was confined to l_{max} =10. In order to achieve energy eigenvalues, the wave functions in the interstitial region are expanded into plane waves with a cutoff of $R_{MT}.K_{MAX}$=7 (where K_{MAX} is the maximum reciprocal lattice vector, and R_{MT} is the average radius of the MT spheres). The *k* integration over the Brillouin zone is performed using the Monkhorst-Pack mesh, yielding 73 k points in the irreducible wedge of the Brillouin zone, and the iteration process is repeated until the calculated total energy of the crystal converges to less than 0.1 mRy as used in this study [8]. Local density approximation is used for the exchange-correlation energy (Exc) in a Kohn-Sham functional using a 64 atom supercell. We chose to add 16 Al atoms (16/32 = 0.5 =50%), 12 Ga atoms (12/32=0.375≈ 38%), 4 In atoms (4/32=0.125≈ 12%), one N atom (1/32 = 0.03125 ≈3%) and 31 Sb atoms (31/32=0.96875≈ 97%).

III. Results and discussions

3.1. Structural properties

Fig. 1 Shows the unit cell of $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$who has a simple cubic structure, with space group 215_P-43m, and we have calculated the structural properties of this structure using LDA for the exchange-correlation functional [9],volume optimization was performed by minimizing the total energy with

respect to the unit cell volume, using Murnaghan's equation of state [10].



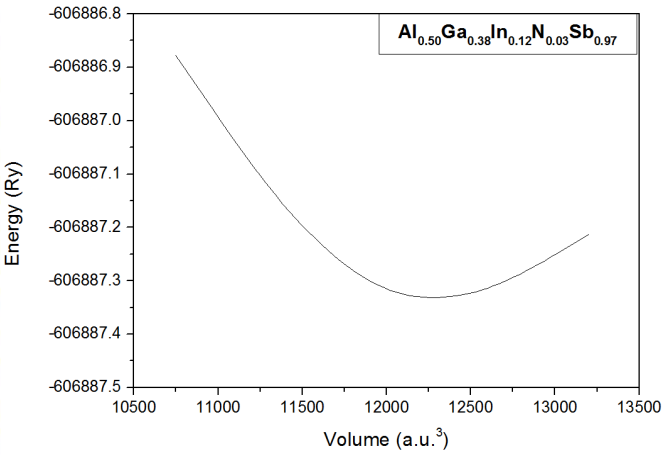


Fig. 1 crystal structure of quinary $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$Fig. 2Variation of total energy as a function of volume of $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$

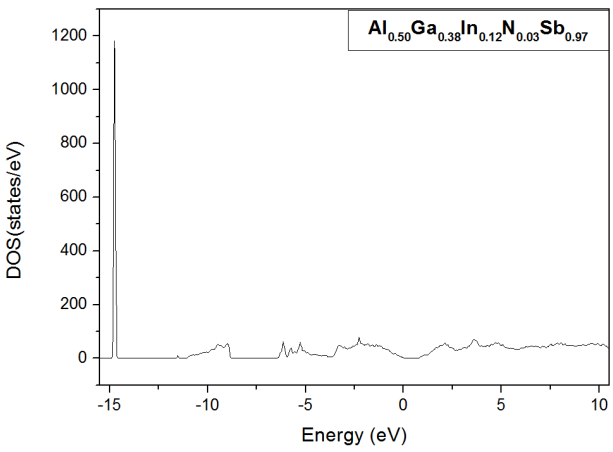
To this end, equilibrium structure parameters such as the lattice constant a and the bulk modulus B and its pressure derivative B' have been projected in Table 1and Fig.2.

Structure	**Space group**	**a(*Å*)**	**B(GPa)**	**B'**
$Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$	215_P-43m	6.10273[a], 6.11165[b]	55.7014[a]	2.6112[a]

Table 1.Lattice parameter, bulk modulus and B' for $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$.
[a] is purely of this work, where [b] is of our work using Vegard's law

3.2. Electronic properties

Analysis of electronic and optical properties of crystalline solids requires the knowledge of electronic density of states (DOS). The DOS for $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$ have been calculated using LDA scheme. As we know Al, Ga, In, N and Sb have the valence electron configuration $1s2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$,$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$,$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^1$,$1s^2\ 2s^2$ 2pand $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^3$, respectively, Fig. 3 Shows the total density of stats (TDOS).The band structure calculations give a direct band gap $E_g^{\Gamma-\Gamma}$ and have been shownin Fig. 4 and Table2.



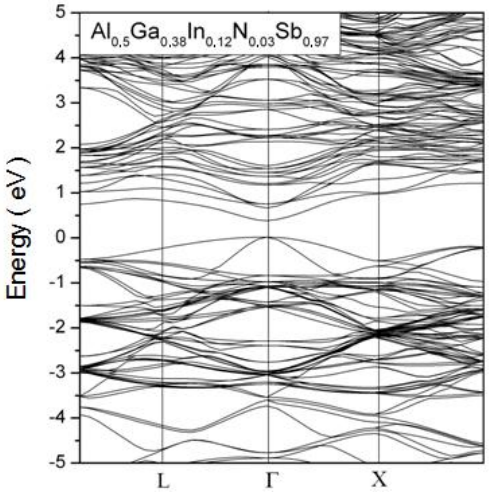


Fig. 3Calculated total densities of states (TDOS) $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$

Fig. 4 Calculated band structure for $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0}$.97 of

structure	E_g(eV)	Nature of Energy Gap Eg
$Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$	0.36105[a]	Direct

Table 2. Calculation of energy gap for $Al_{0.5}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$.[a] is from this work.

3.3. Optic properties

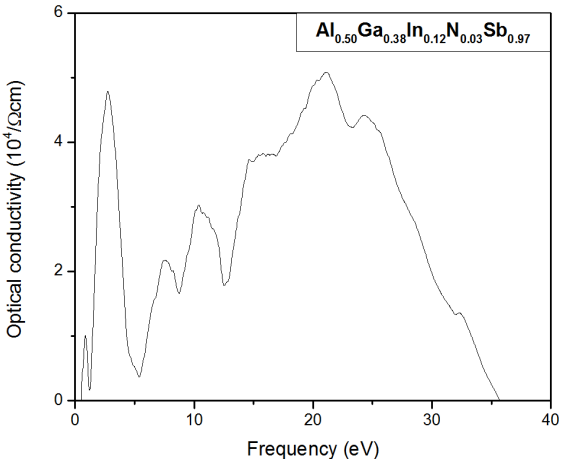


Fig. 5 Calculated conductivity σ(*ω*)

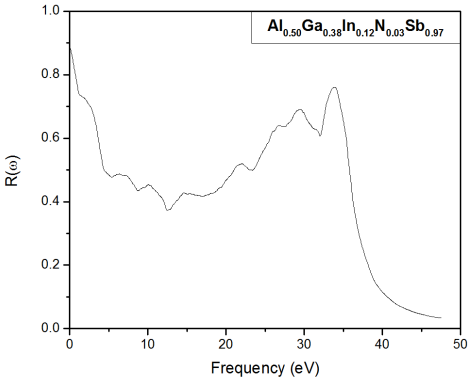


Fig. 6 Calculated reflectivity *R*(*ω*)

The optical properties of $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$are determined by the complex dielectric function $\mathcal{E}(\omega) = \mathcal{E}_1(\omega) + i\mathcal{E}_2(\omega)$[11], which describes, in fact, the features of linear response of the system to electromagnetic radiation, and governs the propagation behavior of radiation in a medium. The imaginary part $\mathcal{E}_2(\omega)$ of the dielectric function is calculated from the momentum matrix elements between the occupied and unoccupied states over the BZ and given as in [12].The real part $\mathcal{E}_1(\omega)$ can be derived from $\mathcal{E}_2(\omega)$ using the Kramers–Krönig relation [13] in the form equation (1) the knowledge of both the imaginary and real parts of the dielectric tensor allows the calculation of important optical functions such as the refractive index $n(\omega)$, reflectivity $R(\omega)$, conductivity function r(ω), and energy-loss spectrum $L(\omega)$ [14].

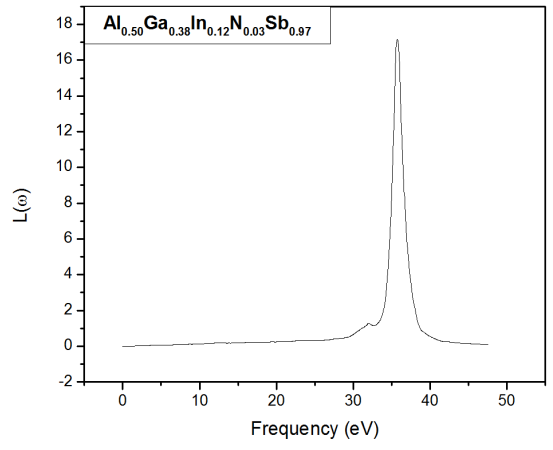


Fig. 7 Calculated energy loss function *L*(*ω*)

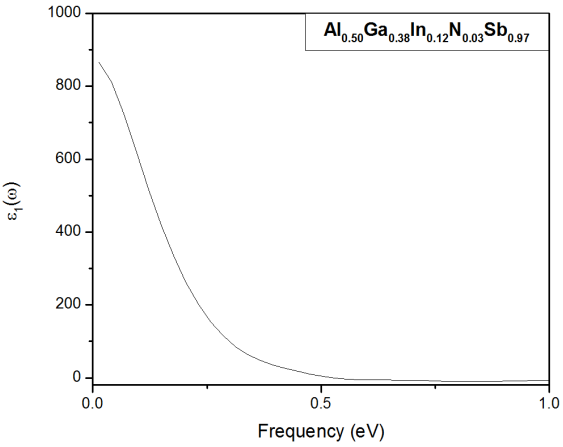


Fig. 8 Calculated real parts $\mathcal{E}_1(\omega)$

The frequency-dependent optical conductivity is also calculated and is shown in Fig. 5.Figure 6 shows the results of the reflectivity function *R*(*ω*).As can be seen from the graph Fig. 7, the peaks of *L*(*ω*) are located at about 35.74eV.

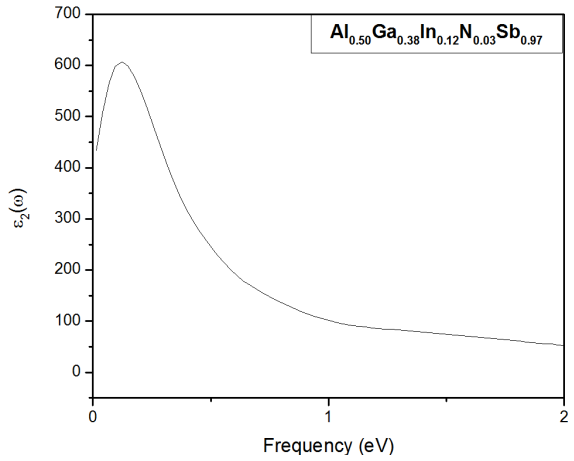


Fig. 9 Calculated imaginary $\varepsilon_2(\omega)$ of dielectric function

Fig.8 and Fig.9 shows the Calculated real parts $\varepsilon_1(\omega)$, and imaginary $\varepsilon_2(\omega)$ of dielectric function respectively. Absorption coefficient and refractive index n(ω) are calculated and is shown in figure 10 and figure 11 respectively**.**

$$\varepsilon_2(\omega) = \left(\frac{4\pi^2 e^2}{m^2\omega^2}\right)\sum\int \langle i|M|j\rangle^2 f_i(1-f_j)\delta(E_f - E_i - \omega)\mathrm{d}^3k \qquad (1)$$

$$\varepsilon_1 = 1 + \frac{2}{\pi}P\int_0^\infty \frac{\varepsilon_2(\omega')\omega'\mathrm{d}\omega'}{\omega'^2 - \omega^2} \qquad (2)$$

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2}\right]^{1/2} \qquad (3)$$

$$R(\omega) = \left|\frac{\sqrt{\varepsilon(\omega)} - 1}{\sqrt{\varepsilon(\omega)} + 1}\right|^2 \qquad (4)$$

$$\sigma(\omega) = \frac{\omega}{4\pi}\varepsilon_2(\omega) + i\left(\frac{\omega}{4\pi} - \frac{\omega}{4\pi}\varepsilon_1(\omega)\right) \qquad (5)$$

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} \qquad (6)$$

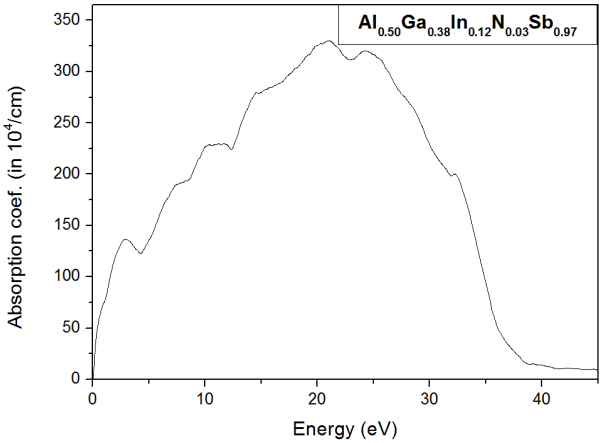


Fig.10 Calculated absorption coefficient

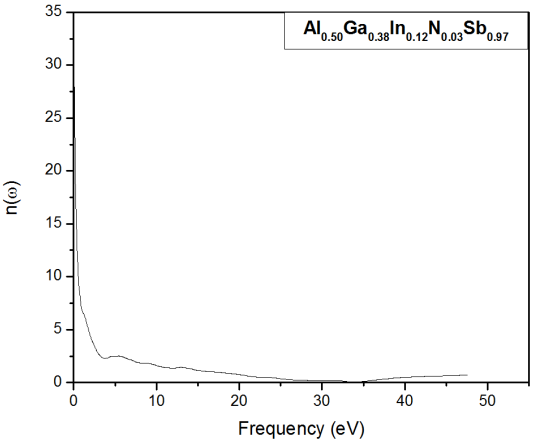


Fig. 11 Calculated refractive index n(ω)

IV. Conclusion

We have used the FP-LAPW method with the LDA form of exchange and correlation to determine the lattice constant, the bulk modulus, the electronic band structure and optical properties such as the imaginary and real parts of the dielectric function, the refractive index, reflectivity, and electron energy-loss of quinary compound semiconductors III-V $Al_{0.50}Ga_{0.38}In_{0.12}N_{0.03}Sb_{0.97}$.i- This structure crystallizes in cubic structure;the results show that the lattice parameter has very small deviations from Vegard's rule predictions. ii-Concerning the electronic properties, the calculation results show that the material studied is of direct gap type and have, thus, significant impact on the field of optoelectronic technology. iii- The imaginary and real parts of the dielectric function, the refractive index, reflectivity, and electron energy-loss spectra are calculated. The static dielectric constants $\mathcal{E}$ and refractive index *n* have been given for the first time.

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