



First principles calculation of the optical properties of zinc-blende $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{1-y}\text{I}_y$

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Informations	Abstract
Key-words : FP-LAPW quaternary alloys, lattice matched *Correspondance : Reçu le, Révisé le, Accepté le	We have presented The structural, electronic and optical properties of $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{1-y}\text{I}_y$ quaternary alloys in the zinc-blend phase have been calculated by using the full potential-linearized augmented planewave method within density functional theory. (DFT). We use both Wu—Cohen and Engel-Vosko generalized gradient approximations of the exchange-correlation energy that are based on the optimization of total energy and corresponding potential, respectively., We study the effect of composition on lattice constants, bulk modulus, band gap ,optical dielectric constant and refractive index shows a non-linear dependence and. reflectivity, absorption coefficient and energy-loss, The energy band gap $E_g(x,y)$ alloy deviates from a planar behavior displaying a two-dimensional gap bowing in the $x - y$ plane. . In addition, the energy band gap of zinc-blende $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{1-y}\text{I}_y$ quaternary alloys lattice matched to GaAs substrate is investigated. It should be noted that the present work is the first theoretical study of the quaternary alloys of interest.

1. Introduction

The I-VII copper halides CuCl, CuBr and CuI crystallize under ambient conditions in the zinc blende structure(space group F-43m) ,and known to be semiconductors with a large and direct gap falls between 1 and 3 eV.

The 3d level of Cu plays an important role in the electronic properties of the copper halides. Unlikely to III-V and II-VI compounds which have a localized 3d level (core states), in the copper halides this level is very close to those of the p levels of the halogen. This fact leads to a very heavy hybridization between the 3d and p electrons and increases noticeably the number of valence electrons per unit formula from 8 to 18. Accordingly, the electronic behaviors of copper halides were misused because of the presence of this 3d level of Cu. In particular, the spin-orbit splitting was found to be negative in these compounds [1], due to a strong admixture of the d copper electrons to the p electrons of the amon.

Copper halides attract much attention. Because of the possibility of producing microcrystals [2]. As promising candidates for photosensitive and semiconducting materials,

silver halides have attracted considerable interest of experimental and theoretical researchers due to their prime role in the valued technological applications

The silver halides also find application in different areas like photographic processes [31, as well as in photo- and electro-chemistry [41 They are also very good solid electrolytes [51, holography [6], catalysis [7,8] and as liquid semiconductors [9] , etc. . The promotion of electrons from the valence to the conduction bands in these halides by light capture plays a major role in the photographic process. Silver bromide (AgBr) (I—VII) under normal conditions in the rock-salt (space group Pm3m) structure ,whereas silver iodide (AgI) (I—VII) crystallizes in the zinc-blende structure as well as in wurtzite structure at ambient conditions but at high pressures it transforms first into NaCl structure and at further high pressure then into CsCl structure [10-11].

The silver atom possesses a completely filled 4d shell, followed by a lone 5s electron which can be transferred to the halide atom. However, there is also hybridization of the silver d states and the halide p states leading to a more

complicated electronic structure. In fact, on the Phillips [13]. ionicity scale, silver halides lie close to the borderline dividing ionic and covalent compounds; and AgBr is on the ionic side and AgI is on the covalent side.

The strong p—d hybridization separates the silver halides from the other compounds of the group II-VI, III-V and IV-IV.

In this work, we have examined the lattice constants, bulk modulus, band gap and refractive index, dielectric, constant reflectivity, a bsorption coefficient and energy-loss. Calculations are performed over the entire composition range of x and y . Second, the energy band gap, natural band offset, optical properties of alloys of interest lattice matched to Cul and Inp substrate have been investigated.

After introducing the problem, the remaining paper is organized as follows. In Section 2 a brief description of the ab initio theoretical method is given. In Section 3, we describe the computational details; results and discussions for structural, electronic properties of the investigated quaternary alloys and their related binary compounds and ternary alloys. Finally, our work is summarized in Section 4.

2. Theoretical aspects and

Table 1- Calculated lattice parameter (a), bulk modulus (B), and gap energy (Eg) for the binary compounds in the zinc -blende structure at equilibrium volume.

	<u>Lattice constant a (Å)</u>			<u>Bulk modulus B (GPa)</u>			<u>Ep (eV)</u>			
	This work	Exp	Theo	This work	Exp	Theo	This work mbjGGA	Exp	Theo	EV
CuI	5,988	6,050	6.062	50,495	36.6	39.447h, 35.2i	2,345	1,091	1,97	2.95C1.764q
CuBrAgI	6.082i			55,411	36.6	44d, 34.8 ^k	1,731	0,383	1,346	2,911
AgBr	5,624	5.69 p	5.732 k	34,54	24e	40.4c , 26.66 7q	3,896	0,632	1,464	2.7s
	6,48	6,49a	6.61b , 6.36 ^c	53, 1466	410	60.3r , 38m	2,516	0,465	0,712	
	5,682	5.751i	5.6+							

computational method

The calculations were performed by the FPLAPW method [27] within the DFT to solve the Kohn Sham equations as implanted in the WIEN2K code [28]. In the FP-LAPW method the wave function, charge density and potential were expanded differently in two regions of the unit cell by spherical harmonic functions inside non-overlapping spheres surrounding the atomic sites (muffin-tin spheres(MT)) , and by plane waves basis set in the remaining space of the unit cell (interstitial region(I)). Our calculations for valence electrons were performed in a scalar-relativistic scheme. The calculated total energies using WCGGA scheme at many different volumes around

approximation, with neglecting spin-orbit coupling, while the core electrons were treated fully relativistic. In this program, the valence and core states origin energies have been separated, and the -6Ry energy bound separating between the valence electrons and the core states was chosen. The exchange correlation potential for structural properties was calculated by the Perdew-BurkeErnzerhof generalized gradient approximation (PBE-GGA) [29], while for electronic properties in addition to that, the Engel-Vosko (EV-GGA) formalism [30]

In the calculations reported here, we use the maximum l quantum number for the wave function expansion inside atomic spheres was confined to lmax = 10. The plane wave cutoff of Kmax = 8.0/RMT where RMT is this equation should be the smallest muffin-tin radius in the unit cell) is chosen for the expansion of the wave functions in the interstitial region while the charge density is Fourier expanded up to Gmax = 14(Ryd)^{1/2}. The muffin-tin radius RMT was assumed to be 2.4, 2.5, 2.5 and 2.2 a.u. for Cu, Ag, Br and I atoms, respectively.

A mesh of 72 special k points for binary compounds, 32 special k points for ternary alloys, and 32 special k points for quaternary

alloys were taken in the irreducible wedge of Brillouin zone. for the energy calculation,

3. Results and discussion

3.1 Binary compounds

The quaternary compounds CuI-x AgxBry11-y are bordered by the ternary alloys AgBr1-xIy, AgBr1 - xIy, CuI-x AgxI, Cu1-xAgxBry11-y which are bounded, in their turn, by four binary compounds CuI, CuBr and AgI in the zinc blend structure and AgBr, in the NaCl structure.

equilibrium were fitted by Murnaghan's equation-of-state [31]. The equilibrium lattice

parameter, bulk modulus and gap energy were presented and compared with the experimental data in Table 1. It is seen that the structural parameters are in good agreement with theoretical and experiment results.

The computed band structures of binary compounds using mbj and EV schemes indicate a direct band gap for CuI and CuBr and AgI, while AgBr are an indirect band gap with the X-L-r ordering of the conduction valley minima. In fact the results are presented in Table 1., these results within mbj are in very good agreement with the available experimental values. This is mainly due to the fact that the functionals within this

approximation have simple forms that are not sufficiently flexible to reproduce accurately both exchange-correlation energy and its charge derivative.

3.2 Ternary alloys
In this section, our simulations was to study the pseudobinary AgBr_{1-x}I_x, CuI_{1-x}Ag_xI, CuI_{1-x}Ag_xBr and CuBr_{1-x}I_x alloys which have been modeled at some selected compositions x=0.25, 0.5, 0.75 with ordered structures described in terms of periodically repeated supercells following the SQS approach. The second step of our calculations was to study the structural properties of AgBr_{1-x}I_x, CuI_{1-x}Ag_xI, CuI_{1-x}Ag_xBr and CuBr_{1-x}I_x alloys. Our calculated lattice constants at different compositions, as shown in Fig. 1(a), were found to vary almost linearly following Vegard's law with a marginal upward bowing parameters equal to -0,69956 +0,48696, -0,07716 and 6516A, respectively. However, violation of Vegard's law has been reported in semiconductor alloys both experimentally, and theoretically

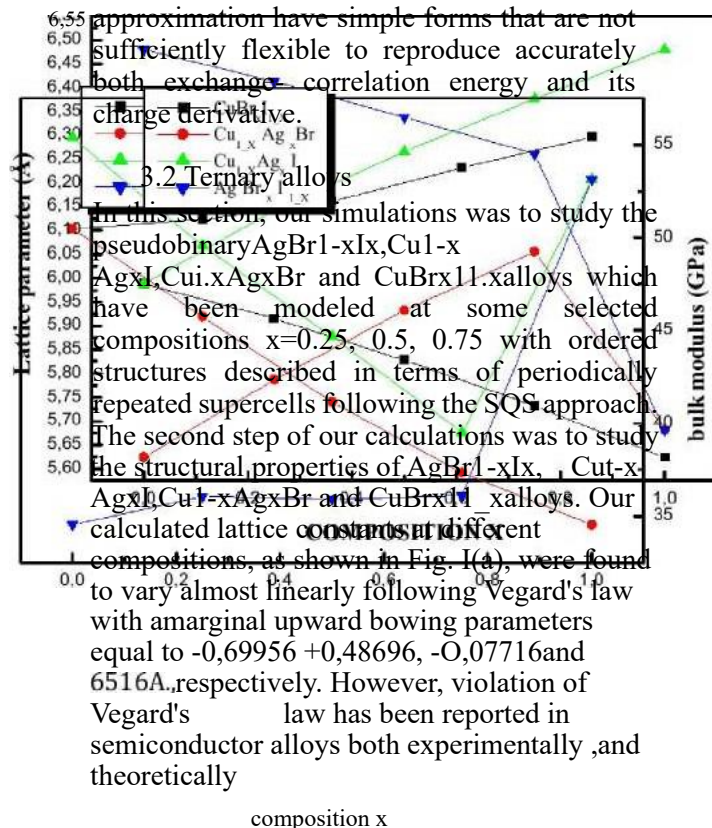


Fig. 1. Composition dependence of the calculated lattice constant (a) and bulk modulus (b) of the four pseudo-binary alloys using WC-GGA.

A comparison of the lattice constant and bulk modulus of these alloys shows that an increase of the earlier parameter is accompanied by a decrease of the later one, which is in agreement with the well-known relationship between B and the lattice constant: $B \propto V_0^{-1}$, where V_0 is the unit cell volume. It represents bond strengthening or weakening effects induced by changing the composition [50],

We observe an important deviation of the bulk modulus from the linear concentration

dependence in Fig. 1 (b) with downward bowing equal to -1,0712, 1,266, 1,0596 and -0,5892 GPa for AgBr_{1-x}I_x, CuI_{1-x}Ag_xI, CuI_{1-x}Ag_xBr and CuBr_{1-x}I_x alloys, respectively. It should be noted that the values of the bulk modulus bowing are closed each other which should be mainly due to the small mismatches of the bulk modulus of the binary compounds. A more precision comparison of the behaviors of the AgBr_{1-x}I_x, CuI_{1-x}Ag_xI, CuI_{1-x}Ag_xBr and CuBr_{1-x}I_x ternary alloys (Fig. 1) shows that the decrease of the lattice constant is accompanied by the increase of the bulk modulus. It represents bond strengthening or weakening effects induced by changing the composition. We turn our attention to study the electronic properties of the ternary alloys via calculating the energy gaps.

The results of the gap bowing parameter of AgBr_{1-x}I_x, CuI_{1-x}Ag_xI, CuI_{1-x}Ag_xBr and CuBr_{1-x}I_x alloys are, respectively, equal to 3,732, 2,466, 2,144 and 2,332 eV for (mbj), while for EV-GGA they are equal to 1,566, 1,511, 2,056, 1,24 and 1,973 eV.

The variation of the energy band gaps as a function of composition x for ternary alloys providing a positive gap bowing.

Hence it is usually expressed by

$$E_g = xE_{AC} + (1-x)E_{BC} - b_0x(1-x) \quad (1) \text{ and } E$$

Where E is the gap bowing and It is clearly seen that the direct band gap increases non-linearly with increasing concentration x, and seen that the band gap values given by MBJ are in good agreement with the experiments. Fig. 2 shows the composition dependence of the calculated band gaps for the material of interest.

Using both the mBJ exchange potential approximation., EV-GGA ,we observed a direct band gap located at the point in the whole range of concentrations. The value of the bowing parameter at different concentrations is calculated by fitting the non-linear variation of the calculated direct band gap with polynomial function Results as shown in Fig. 2 are summarized as follows:

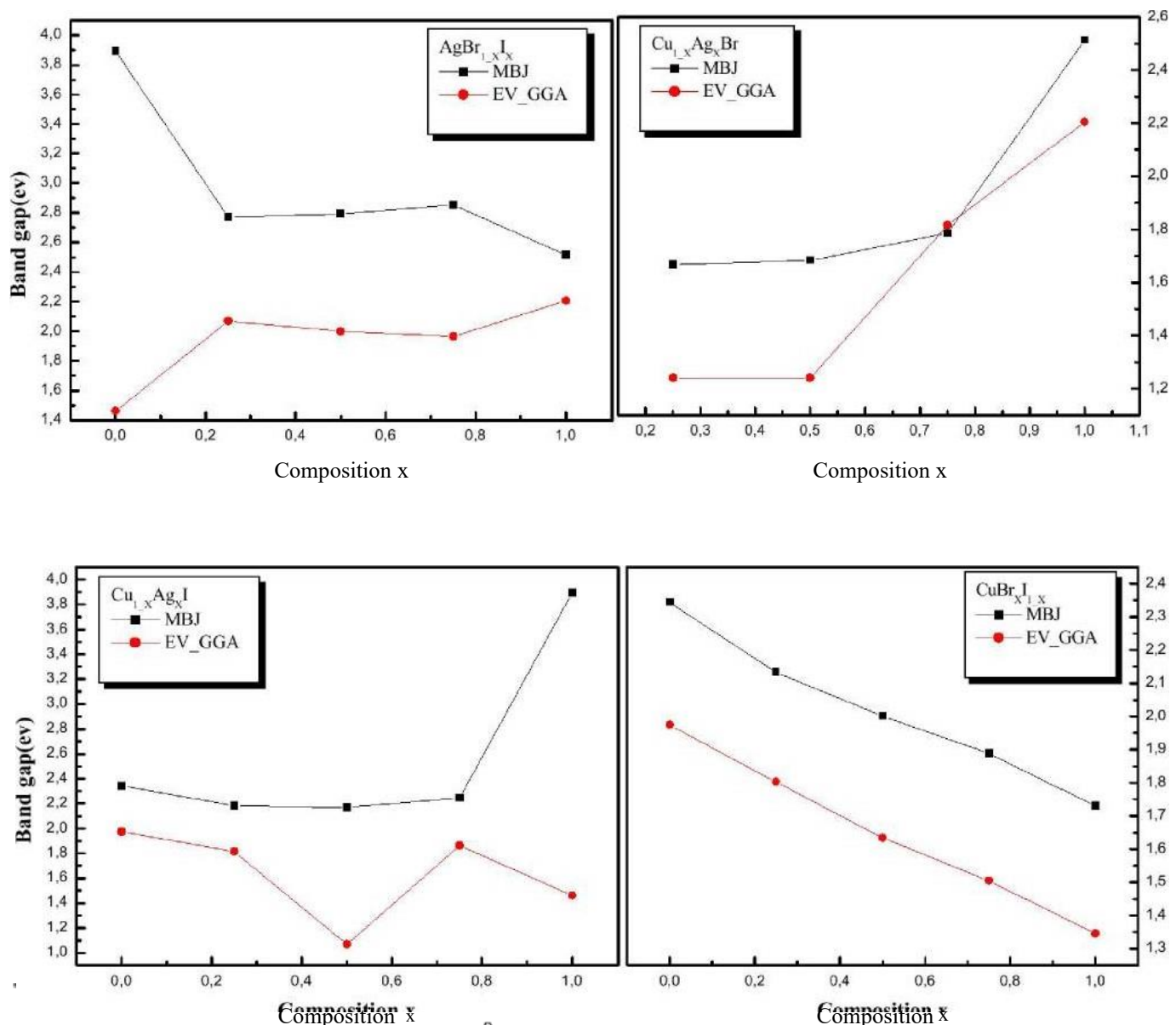


Fig. 2 - Energy band gap as functions of the composition x for the ternary alloys: (a) $\text{AgBr}_{1-x}\text{I}_x\text{Br}$, (b) $\text{Cu}_{1-x}\text{Ag}_x\text{Br}$, (c) $\text{Cu}_{1-x}\text{Ag}_x\text{I}$, (d) $\text{CuBr}_{1-x}\text{I}_x$ by MBJ and EV-GGA.

3.3 Quaternary $\text{Cu}_x\text{Ag}_y\text{Br}_{11-y}$ alloys

In this section, we present the structural, electronic and optical properties of the $\text{Cu}_x\text{Ag}_y\text{Br}_{11-y}$ quaternary alloys, which are crystallized in the zincblende structure, where the lattice parameter, bulk modulus, energy band gap and refractive index for different composition rates (x, y) have been adopted the

"Special Quasirandom Structures" (SQS) approach.

The supercell used in our calculations of $\text{Cu}_x\text{Ag}_y\text{Br}_{11-y}$ alloys was thus obtained by a simulated annealing procedure by among 64 atom simple-cubic structures including systems with random, high symmetry, and low symmetry atomic positions, the ones minimize the total

energy with respect to the cell parameters and the atomic positions were searched.

. We found out that the structure with the most symmetric atomic positions is the most stable system and has the least total energy. Our results concerning lattice constant and bulk modulus versus x and y concentration for Cu_{1-x}Ag_xBr_{1-y}I_y quaternary alloys is presented in Fig.3, respectively. have marginal deviation of the lattice constant from Vegard's law can be observed, and a large deviation of bulk modulus from linear concentration dependence (LCD) is visible.

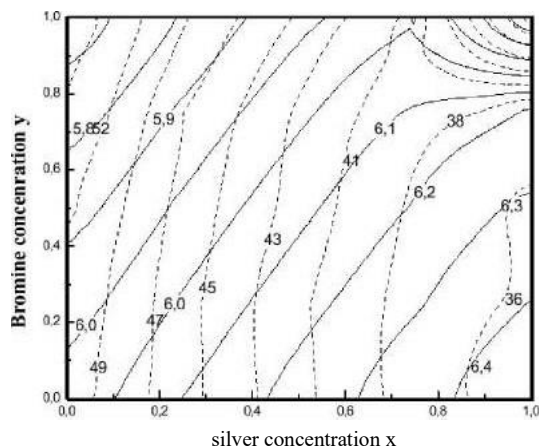


Fig.3 - Contour map of the calculated lattice constant in (Å) (solid lines) and bulk modulus in (GPa) (dashed lines) versus the compositions x and y for Cu_{1-x}Ag_xBr_{1-y}I_y quaternary alloys

The formation energies $E_{Form}(x, y)$ of quaternary alloys at different concentrations were calculated using the following formula:

$$E_{Form}(x, y) = E_{CuAgBrI} - xE_{AgBr} - (1-x)yE_{CuBr} - x(1-y)E_{AgI} - (1-x)(1-y)E_{CuI} \quad (2)$$

Where E_{Ag} , E_{CuBr} , E_{AgI} , E_{CuI} are the total energy of the binary compounds and $E_{CuAgBrI}$ is the total energy of quaternary alloys at the related concentration.

We note that the results of the formation energy do only to some extent provide insight onto stability and for a more complete study the entropy of the system should be included. Figure 4 shows the results in a contour plot form, the darker part of the graph the more stable the; corresponding alloy. It is clear the least stable alloys are around 25 and 75% concentrations of both Ag and Br atoms.

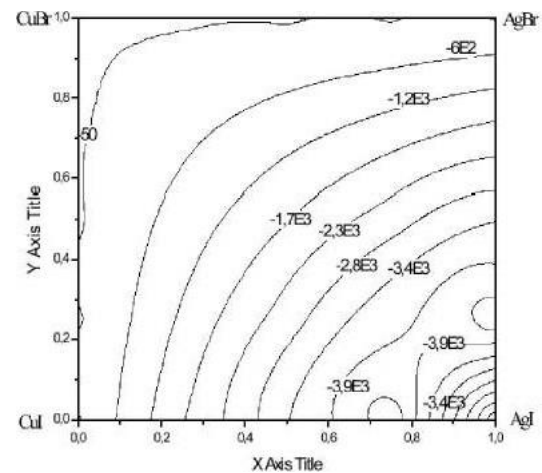


Fig.4 - Contour map of the calculated formation energy contour lines (Ryd/cell) versus the compositions x and y for Cu_{1-x}Ag_xBr_{1-y}I_y quaternary alloys.

3.4 Electronic properties

We discuss the band structure of Cu_{1-x}Ag_xBr_{1-y}I_y alloys for the transitions from the high-symmetry points Γ in the Brillouin zone. It should be noted that our direct band-gap value for composition $x=y=0.85$ (2.85 eV), using by mBJn view of Fig 5. The variation of the band gaps depends nonlinearly on the compositions especially at high concentration of Cu and Br.

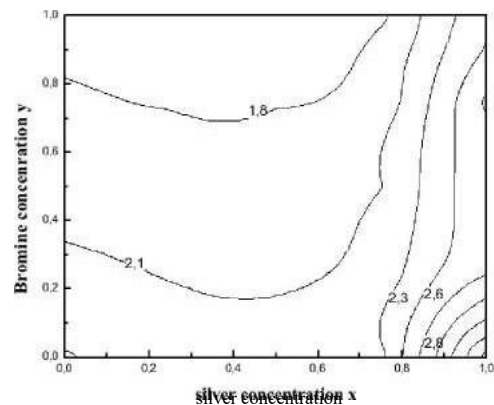


Fig.5 - Contour map of the calculated energy band gap in (eV) versus the compositions x and y for Cu_{1-x}Ag_xBr_{1-y}I_y quaternary alloys.

The optical properties of the Cu_{1-x}Ag_xBr_{1-y}I_y system are usually described in terms of the complex dielectric function $E(O)$, which represents the linear response of a system due to an external electromagnetic

field with a small wavevector. It can be expressed as [51,52]

$$\text{EGD} = \text{El}(\hbar) + \quad (3)$$

Where El and E2 are the real and imaginary components of the dielectric function, respectively.

$\text{E2}(\text{Q})$ The imaginary part of the frequency dependent dielectric function has been calculated directly from the electronic structure calculation using the joint density of states and the momentum matrix elements (the optical matrix elements) we use the corresponding eigen functions of each of the occupied and unoccupied states.

- ✓ The real part $\text{E1}(\omega)$ of the dielectric function can be extracted from the imaginary part E1 by the Kramers—Kronig relation.

The knowledge of both the real and the imaginary parts of the dielectric function allows the calculation of important optical functions. The optical constants such as refractive index $n = (x)$ and the extinction coefficient $k = (x)$ are calculated in terms of the real and imaginary part of the complex dielectric function given by: [53–55]

$$n(\omega) = \frac{\text{E}(\omega) + \sqrt{\text{E}(\omega)^2 - 4\text{E}_1(\omega)^2}}{2} \quad (4)$$

$$K(\omega) = \frac{\sqrt{\text{E}_1(\omega)^2 - \text{E}(\omega)^2}}{2} \quad (5)$$

At low frequency ($\omega=0$), we get the following relation

$$n(0) = c^2(0) \quad (6)$$

The refractive index and dielectric constants are very important to determine the optical and electric properties of the crystal.

Fig 6 displays the contour map of the calculated dielectric function versus the compositions x and y for $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ quaternary alloys. One can note that dielectric function index decreases with the increasing of x and y and depend nonlinearly on the

compositions. dielectric function of alloys are found to be, 2.2, 2.3, 2.4, 4.8 and 6.2 respectively.

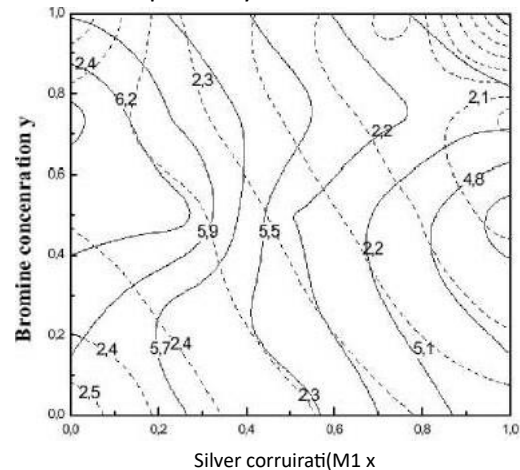


Fig. 6 - Contour map of the calculated dielectric function in (eV) (solid lines) and refractive index $n(\text{eV})$ (dashed lines) versus the compositions x and y for $\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ quaternary alloys.

The results of the index refractive are given in Fig 6., the compositional dependence of the index refractive of the alloy has the same trend as that of the dielectric function in the region between 2.1 and 2.5 eV.

The reflection coefficient (R) is among the most important optical constants related to the dielectric function. It characterizes the reflective light energy part at the cleaved facets of the resonant cavity. For normal-incidence the reflectivity is [56, 57]

$$R = \frac{(n_r - 1)^2 + k^2}{(n_r + 1)^2 + k^2} \quad (7)$$

Fig 7 displays the contour map of the calculated reflectivity versus the compositions x and y for $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ quaternary alloys. One can note that the reflectivity coefficients decrease with the increasing of Ag and Br and depend nonlinearly on the compositions. The reflectivity coefficients decrease in the region between 0.13 and 0.18 eV.

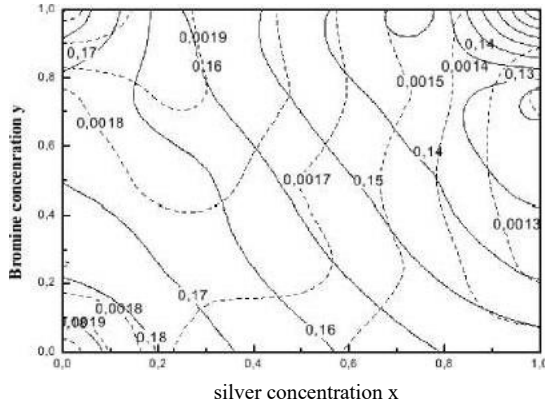


Fig. 7 - Contour map of the calculated reflection coefficient in (eV) (solid lines) and absorption coefficient in (eV) (dashed lines) versus the compositions x and y for $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ quaternary alloys.

The light incident on the $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y/\text{ZnB}$ structure may cause excitation of the ground state electrons from the VB to the CB or from one sub band to a higher sub band, where the required energy is supplied by the photons and the light is absorbed [58]. The absorption coefficient $\alpha(\omega)$ characterizing such a phenomenon, defined as the light energy absorbed in unit length per unit incident energy, depends on both parts of it is given by [56, 67].

$$\alpha(\omega) = \frac{4\pi}{\lambda} k(\omega) \quad (8)$$

λ is the wave length of light in the vacuum. It is well known that the optical absorption coefficient $\alpha(\omega)$ is one of the most crucial evaluation criterions in application of the photoelectric materials.

The results of the absorption are given in Figure 7., the compositional dependence of the absorption of the alloy has the same trend as that of the dielectric function. We observe lower absorption coefficient under the scissor operation in the range of 0.0013 and 0.0019 eV. These semiconductors have fundamental absorption limit at Infrared spectrum regions.

The electron energy loss function $L(\omega)$ for the quaternary alloy is displayed in Fig. 8. It can be determined by using the dielectric function:

$$\text{LGD} = \frac{\epsilon_2(\omega)}{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} \quad (9)$$

The energy-loss function is usually used to describe the energy loss of a fast electron traversing in the material [59]. Energy loss function defines the energy loss of the electrons passing between bands.. Energy loss functions

of alloys according to x and y values. The maximum of the energy loss function is related to plasma frequency. The material shows the dielectric or metallic characteristics when the photo frequency is above or below the plasma frequency [60]. The energy loss function maximum at 25% and 50% concentrations of both Ag and Br atoms.

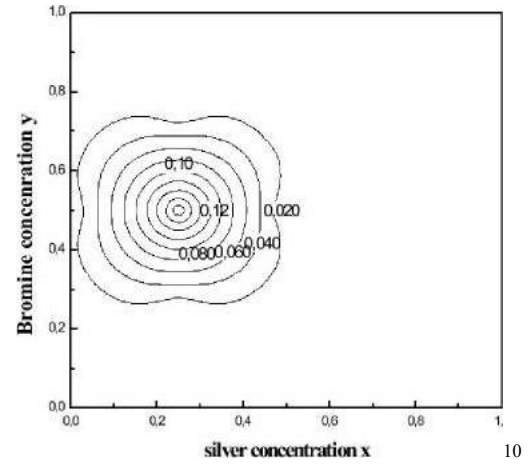


Fig.8- Contour map of the calculated energy loss versus the composition x and y for $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ quaternary alloys.

The second goal of this work is to study the gap energy of $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ alloys lattice matched to CuI and InP semiconductors substrate. Similar to the ternary alloys. For this purpose we have used the relationships between the compositions x and y for lattice matched to quaternary alloys, is determined using Vegard's rule as

$$a(x, y) = x a_{\text{Ag}} + (1 - x) a_{\text{CuBr}} + y a_{\text{I}} + (1 - y) a_{\text{AgI}} \quad (10)$$

Where a_{Ag} , a_{CuBr} , a_{I} , a_{AgI} are the lattice constants of the binary compounds. By putting equal to the lattice constant of CuI and InP,

The lattice matching conditions for the quaternary alloy $\text{Cu}_{1-x}\text{Ag}_x\text{Br}_{11-y}\text{I}_y$ on CuI or InP substrate are as follows:

For CuI substrate

$$Y = \frac{-0.4912X}{-0.364804332} \quad (0 \leq x \leq 1) \quad (11)$$

Whereas, for InP substrate

$$Y = \frac{-0,338 - 0,4912x}{-0,364 - 0,4332x} (0 \leq x < 1) \quad (12)$$

The above expression specifies a line on the field of (x, y) silver and bromine concentration in which the corresponding alloy is lattice matched to the CuI and InP substrates. as obtained from calculations performed by WC_GGA scheme We have considered four different concentrations along the line of lattice matching to both CuI: (x, y) = (1/4, 8/32); (1/2, 13/32); (3/4, 17/32); and InP. (x, y) = (0/32, 11/32); (1/4, 16/32); (1/2, 20/32); (3/32, 23/32).

We observe nonlinear deviation of band gap versus concentration x leads to the gap bowing parameters of 1,077eV and 0,854eV respectively. (Figure 9). The results of the quaternary CuI-xAgxBr_{11-y} alloys should be useful for the design of optical devices with a continuous broad band gap in the Infrared spectrum regions when it is lattice matched to the CuI and InP substrates. The WCGGA calculated band gap of CuIAgxBr_{11-y} compound matched to CuI range from 0,865 to 0,771 eV, while in the case of the InP substrate, the corresponding range is from 0,859 to 0,679 eV.

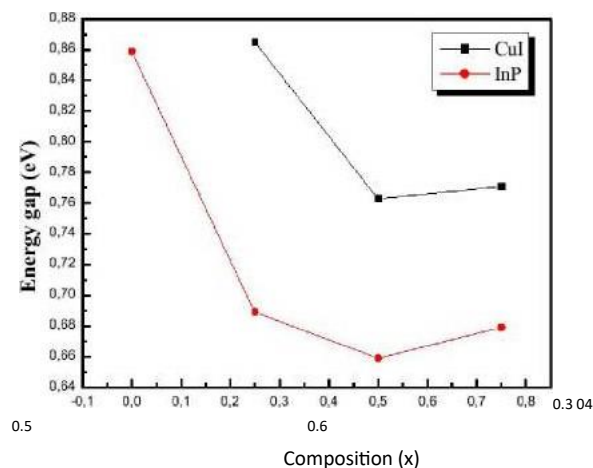


Fig.9 - Energy band gap of CuI-x AgxBr_{11-y} quaternary alloys lattice matched to CuI and InP as function of the x composition using WC_GGA scheme.

4. Conclusion

In summary, Employing the FP-LAPW method within DFT, we have investigated the structural and electronic and optical properties of the zinc blend CuI-x AgxBr_{11-y} quaternary and their four pseudobinary alloys as a function of the compositions x and y. A non-linear behavior of

the lattice constant, bulk modulus, band-gap and dielectric function, refractive index, reflection coefficient and absorption coefficient $\alpha(x)$ dependence on x and y has been observed.

- The calculations of formation energies showed that the least stable alloys are around 25% concentration of Ag atom and 75% concentration of Br atom
- The direct gap nature of the pure materials is conserved also in the alloys. The gap bowing of quaternary alloys was found strong at high compositions x and y
- Finally, the energy band gap of the quaternary alloys CuI-x AgxBr_{11-y} lattice matched to GaAs substrate, whose optical gaps range in the entire blue-green window, has been investigated. The results indicate that the band gap increases with the x composition.

Our results are predictions and may serve as reference for future experimental work.

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