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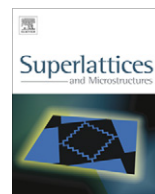
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First-principles calculations to investigate optical properties of $B_yAl_xIn_{1-x-y}N$ alloys for optoelectronic devices

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ABSTRACT

First-principles density-functional theory of Full-Potential Linear Augmented Plane Wave (FP-LAPW) within local density approximation (LDA) of the optical properties of $B_yAl_xIn_{1-x-y}N$ systems (with $x = 0.187$ and $y = 0.062, 0.125$ and 0.187) has been performed. Substitutional atoms of Boron induced in small amounts into the (Al_xIn_{1-x}) -cationic sublattice of $AlInN$ affects the energy gap of $BAlInN$. The higher band gap of $Al_{0.375}In_{0.625}N$ alloy can form a useful quantum well (QW) laser structure. A best choice of B-content, $B_yAl_xIn_{1-x-y}N$ could be an alternative to $Al_xIn_{1-x}N$. The results of accurate calculations of the band structures and optical properties show the better performance characteristics belong to the structure containing B-content (y) of 12.5%. The NaCl metallic $B_yAl_{0.1875}In_{0.8125-y}N$ has a direct character for $y = 12.5\%$. The imaginary part of dielectric function, reflectivity, refractive index, absorption coefficient and optical conductivity are investigated well and provide reasonable results for optoelectronic devices applications.

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1. Introduction

Being the most mysterious materials among the group-III nitrides, AlN , GaN , and InN and their alloys have attracted enormous interest for use in high-power microwave transistors, applications in light emitting diodes (LED's) and laser diodes (LD's) ranging from the visible spectrum [1–4] to the

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deep ultra-violet (UV) [5,6] and future chemical [7] sensors applications in quantum cryptography [8] or in photocatalysis [9]. Despite the intensive study of $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{Al}_x\text{Ga}_{1-x}\text{N}$, found to be useful as well layers and cladding layers in QW-LD structures, respectively [10–12], little attention has been paid to $\text{Al}_x\text{In}_{1-x}\text{N}$, due to difficulty in its growth mainly caused by thermal instability resulting from the spinodal phase separation phenomenon [13]. Although this phase separation makes the determination of AlInN structural properties difficult during its epitaxial growth, the possibility of lattice matching to GaN makes it an attractive alternative to InGaN and AlGaIn for applications in GaN-based devices, such as cladding layers, Bragg mirrors, insulating layers, or channel layers in field effect transistors [14–16] and active layer for LED's in the spectral region from UV to infrared (IR). $\text{Al}_{0.83}\text{In}_{0.17}\text{N}/\text{GaN}$ heterostructures are very useful and interesting when utilized as cladding layers with no strain leading to defects on LD's structures [17].

On the contrary, InGaIn layers grown on GaN template substrates have the disadvantage of lattice mismatch, leading (for high In-content) to high misfit dislocation densities limiting the range of In-composition [18]. To solve this problem, a Boron cause decreasing the lattice parameter of nitrides [19] is added to reduce the lattice mismatch between InGaIn epitaxial layers and GaN substrates [18]. The BInGaIn alloy offers the possibility to optimize the energy gap and lattice parameter independently of each other without inducing strain into layers, which is highly desirable for the band gap engineering of advanced optoelectronic heterostructures [20]. Another alloy belonging to the B-containing III-nitrides (B-III-N) group is BAlGaIn that grows on AlN substrates experimentally [21], has an energy gap ranging from 3.6 to 6.2 eV and corresponding to the 344–200 nm wavelength range, respectively with respect to its application in light-emitting devices operating in the UV spectral region.

Recently, Bastek et al. [22] have investigated light matter coupling using a hybrid GaN based micro-cavity. They analyzed the emission of the structure without top Bragg mirror using photoluminescence spectroscopy, and found two emission peaks at nearly fixed energy but changing intensity ratio with respect to the position on the sample arise. Also, they investigated angle resolved photoluminescence at the full hybrid structure exhibit two emission peaks and stated predominantly excitonic behavior for the high and photonic-like behavior for the low energy peak. Also, Roqan et al. [23] have been obtained room temperature cathodoluminescence (RTCL) from Tm implanted $\text{Al}_x\text{Ga}_{1-x}\text{N}$ with different AlN contents and from implanted $\text{In}_x\text{Al}_{1-x}\text{N}$ with different InN contents close to the lattice match with GaN. They have been showed that the Tm^{3+} emission spectrum depends critically on the host material, how to enhance the emission up to a factor of 50 times with an increase of annealing temperature from 1000 to 1300 °C and the blue emission from $\text{In}_{0.13}\text{Al}_{0.87}\text{N}:\text{Tm}$, annealed at 1200 °C is more than 10 times stronger than that from $\text{Al}_x\text{Ga}_{1-x}\text{N}:\text{Tm}$. However, they have been stated that the intensity decreases significantly as the InN fraction increases from 0.13 to 0.19. While, Gautier et al. [24] have been grown BGaN materials with good structural quality and surface morphology on GaN template substrates by low pressure metal organic vapor phase epitaxy. They performed all the growths under 100% N_2 process gas and estimated boron concentration by HRXD measurements combined with SIMS analysis, where they have been obtained single-crystal layers of BGaN with B content as high as 3.6%.

To investigate the optical properties of BAlInN , our calculations have used a predictive single QW laser structure, similar to the $\text{InGaAsN}/\text{GaAs}$ experimental device fabricated by Peng et al. [25]. The aim of this work is performing first-principles calculations to investigate the optical properties of $\text{B}_y\text{Al}_x\text{In}_{1-x-y}\text{N}$ and give an important guideline on the material design of short-wavelength optical devices using these nitrides. The paper is organized as follows: An overview of theoretical approach in Section 2, results and their discussion are presented in Section 3. Finally, a conclusion is given in Section 4.

2. Computational method

All calculations of the optical properties, presented below are based on the self consistent first-principles calculations of Full Potential Linearized Augmented Plane Waves (FP-LAPW) method based on the density functional theory (DFT) [26] within the local density approximation (LDA) [27]. The

unit cell is divided into non-overlapping muffin-tin (MT) spheres around the atomic sites and an interstitial region. The MT radii (R_{MT}) for B, Al, In and N atoms were adopted to be 1.55, 2.05, 2.17 and 1.57 Bohr, respectively. In the MT spheres, the l -expansion of the non-spherical potential and charge density was carried out up to $l_{max} = 10$. The orbital of B ($1s^2 2s^2 2p^1$), Al ($3s^2 3p^1$), In ($4d^{10} 5s^2 5p^1$) and N ($1s^2 2s^2 2p^3$) are treated as valence electrons. In order to achieve energy eigenvalues convergence, the wave-functions in the interstitial region were expanded in plane waves with a cut-off of $k_{max} = 7/R_{MT}$. The k integration over the Brillouin zone (BZ) is preformed using the Monkhorst and Pack mesh [28]. A mesh of 20 special k -points was taken in the irreducible wedge of the BZ for the ternary and quaternary alloys. We adopted a supercell approach for the $Al_xIn_{1-x}N$ and $B_yAl_xIn_{1-x-y}N$ band structure calculations on which are based our optical properties. To investigate the B-incorporation effect on optical properties of $c-B_yAl_xIn_{1-x-y}N$, B substitutes on the In site in a 128-atom supercell, corresponding to $4 \times 4 \times 4$ supercell: the zinc-blende (ZB) crystal structure has the “ $F-43m$ ” space group. To model the $Al_xIn_{1-x}N$ and $B_yAl_xIn_{1-x-y}N$ random alloys with $x = 0.1875$ and $y = 0.0625, 0.125$ and 0.1875 , a 128-atom $B_mAl_nIn_{64-[n+m]}N$ supercell is used with $n = 12$ and $m = (0, 4, 8, 12)$. It is well-known that the use of the LDA to the density functional theory (DFT) usually leads to underestimate the energy band gap and lattice constant in semiconductors. This underestimation is mainly due to the fact that the LDA functional is based on simple model assumption which is not sufficiently flexible for accurate reproduction of the exchange correlation energy and its charge derivative. In order to overcome this shortcoming a scissors operation with a rigid upward shift of the conduction band has been used to correct the LDA energy band gap (E_0) error in both $Al_xIn_{1-x}N$ and $B_yAl_xIn_{1-x-y}N$ alloys. So, it is necessary to mention that the related energy shifts (ΔE_g) to correct these energy band gaps are:

$$\Delta E_{g(AlInN)} = x\Delta E_{g(AlN)} + (1 - x - y)\Delta E_{g(InN)} \quad (1a)$$

$$\Delta E_{g(BAlInN)} = \Delta E_{g(AlInN)} + y\Delta E_{g(BN)} \quad (1b)$$

Since no experimental data has been reported on the energy gap of $c-Al_xIn_{1-x}N$, a linearly interpolated result using $E_{0(AlN)} = 5.2$ eV and $E_{0(InN)} = 0.56$ eV is adopted [29]:

$$E_{0(AlInN)} = x5.2 + (1 - x - y)0.56 \text{ (eV)}. \quad (2a)$$

Assuming the Vegard's law: $E_{0(BAlInN)} = E_{0(AlInN)} + yE_{0(BN)} + (1 - x - y)E_{0(InN)}$ and using $E_{0(BN)} = 6.2$ eV [30], the following interpolated relationship to calculate E_0 of $B_yAl_xIn_{1-x-y}N$ has been deduced:

$$E_{0(BAlInN)} = x5.2 + y6.2 + (1 - x - y)1.12 \text{ (eV)}. \quad (2b)$$

Optical properties are of great importance in the design and analysis of optoelectronic devices such as light sources and detectors. At all photon energies $E = \hbar\omega$ have two parts, real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$, of the complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ describing these properties of a medium are connected by the well known Kramers–Kronig relations [29]. $\varepsilon_2(\omega)$ is strongly related to the joint density of states and optical matrix elements, and carried out by electronic structure calculation, where $\varepsilon_1(\omega)$ is derived from $\varepsilon_2(\omega)$.

3. Results and discussion

The optical properties of solids can be described in terms of the optical dielectric function. Previous results have been reported experimentally [31–35] and theoretically [36–38], they have been measured and calculated the absorption [31], imaginary part of the optical dielectric function [32,33,36,37], reflectivity [34–36] and the refractive index [39], respectively.

Since the imaginary part of the dielectric function $\varepsilon_2(\omega)$ can be strongly related to the joint band structure, we have seen that it is useful to calculate the two parts of ε for $B_yAl_xIn_{1-x-y}N$. The shift ΔE_g is to amend the energy band gap of $B_yAl_xIn_{1-x-y}N$ alloys, and used in calculations of the optical properties, are calculated from the experimental energy gap values for the binaries BN, AlN and InN that correspond to 6.0, 5.94 and 1.66 eV [39–41], respectively, and the available theoretical values of the same compounds are 5.74, 6.27 and 1.66 eV, respectively [39–41].

Acquaintance of electronic band structures of $B_yAl_xIn_{1-x-y}N$ is crucial to correct energy band gaps that underestimated by LDA [39,42] and improving characteristics of $B_yAl_xIn_{1-x-y}N$ light emitters.

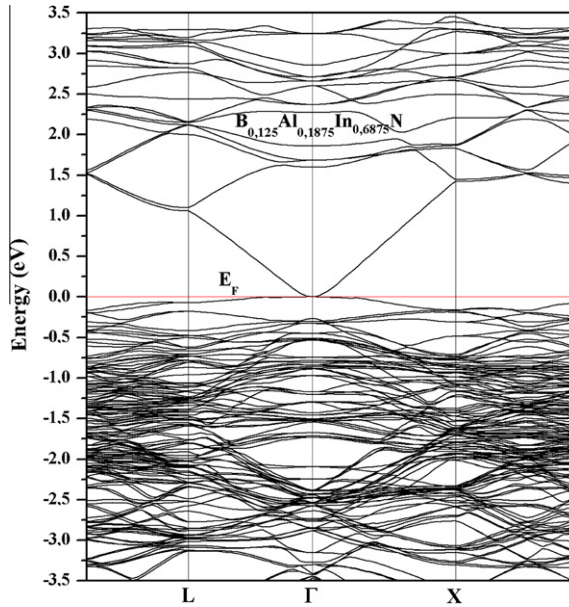


Fig. 1. Band structure of $B_{0.125}Al_{0.1875}In_{0.6875}N$ alloy.

Fig. 1 gives the schematic band structure of $B_yAl_xIn_{1-x-y}N$ for $x = 0.187$ and $y = 0.125$. One can easily remark the direct character of the NaCl metallic $B_{0.125}Al_{0.1875}In_{0.6875}N$, which is of great interest for optical transitions, as remarked previously for II–VI semiconductors alloys [43].

Different methods are established as a flexible and valuable tool for studying the physical properties [39,43–47] in a wide variety of materials [48], falls short of being a complete and general solution to many-electron problem.

Imaginary part ϵ_2 indicates two inter-band transitions as shown in Fig. 2; $B_yAl_xIn_{1-x-y}N$ is characterized by a strongest peak at 5.0 eV, might be strongly dependent on the ionic polarization of the

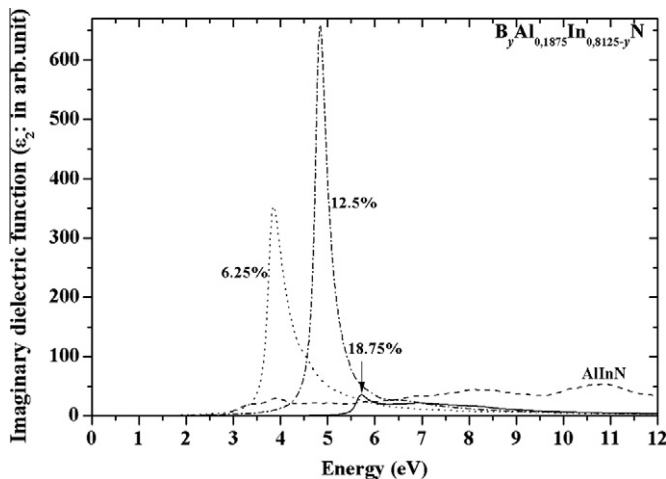


Fig. 2. Imaginary part of the dielectric function of $B_yAl_xIn_{1-x-y}N$ alloys.

$B_yAl_xIn_{1-x-y}N$ crystal due to the large electronegativity of N, and a weakest one for $B_yAl_xIn_{1-x-y}N$ at 5.71 eV.

Fig. 3(a) shows the reflectivity spectra along for $B_yAl_xIn_{1-x-y}N$ systems. It is interesting that there is an abrupt reduction in the reflectivity spectrum after 20 eV for the researched system confirming the occurrence of a collective plasmon resonance. The normal-incidence reflectivity $R(\omega)$ [29] is:

$$R(\omega) = \frac{[n_r(\omega) - 1]^2 + k(\omega)^2}{[n_r(\omega) + 1]^2 + k(\omega)^2} \quad (3)$$

The depth of the plasmon minimum is determined by the imaginary part of the dielectric function at the plasma resonance and is a representative of the overlap degree between the inter-band absorption regions. From the dielectric function used to describe the optical properties, the refractive index [42,49–53] is sensitive to study optoelectronics and can be given by [29]

$$n(\omega) = n_r(\omega) + i \cdot k(\omega) = \varepsilon(\omega)^{1/2} = [\varepsilon_1(\omega) + i\varepsilon_2(\omega)]^{1/2} \quad (4)$$

with $n_r(\omega)$ is the ordinary (real) refractive index and $k(\omega)$ is the extinction coefficient given differently as

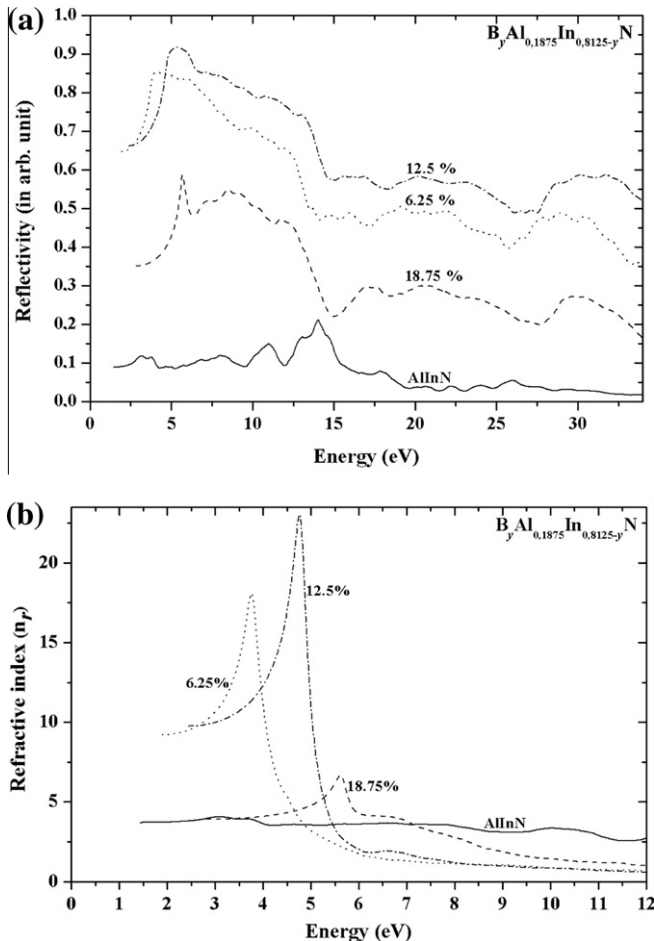


Fig. 3. (a) Reflectivity and (b) refractive index of $B_yAl_xIn_{1-x-y}N$ alloys.

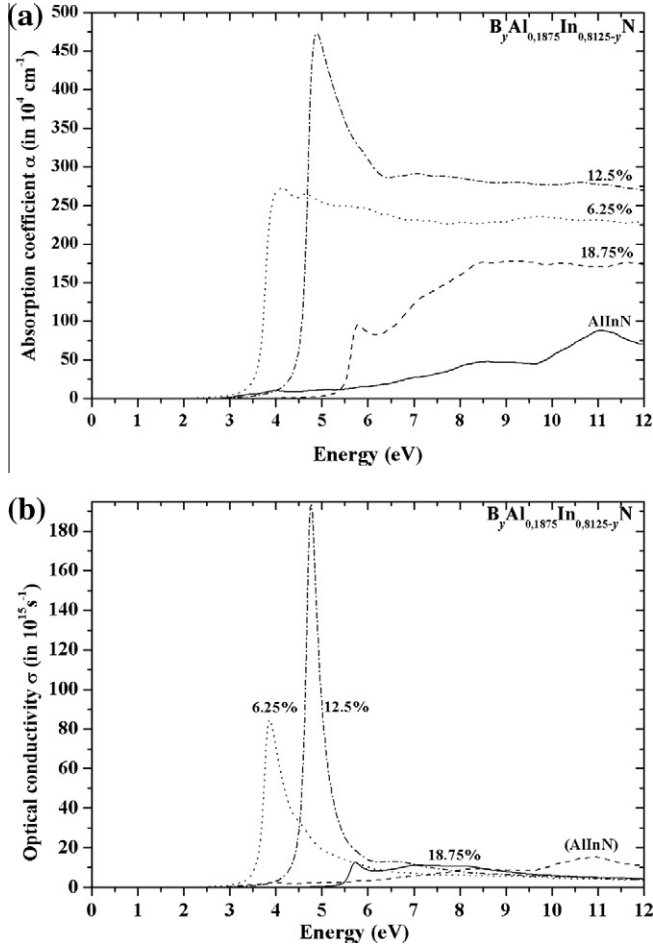


Fig. 4. (a) Absorption and (b) conductivity of $B_yAl_xIn_{1-x-y}N$ alloys.

$$n_r(\omega) = \left[\frac{[\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2]^{1/2} + \varepsilon_1(\omega)}{2} \right]^{1/2} \quad (5a)$$

and

$$k_r(\omega) = \left[\frac{[\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2]^{1/2} - \varepsilon_1(\omega)}{2} \right]^{1/2} \quad (5b)$$

The calculated refractive index is shown in Fig. 3(b). We note that at low energy these systems show high refractive indices, which decrease at higher energies.

The potential advantage of optoelectronic devices includes low sensitivity to temperature variations, low threshold current and high quantum efficiency (η) [54]. One of the key factors that determine η is the absorption coefficient $\alpha(\omega)$, which is a strong function of the wavelength [55] given by

$$\alpha(\omega) = \frac{4\pi}{\lambda} k(\omega) \quad (6)$$

where λ is the wavelength of light in vacuum.

The calculated absorption coefficient dispersion $I(\omega)$ is shown in Fig. 4(a). At low energies between 3.0 and 5.0 eV and at higher energies (at around 11.0 eV), this crystal shows a fast increasing absorption. A strong increase in optical conductivity with increasing the photon energy has been observed for $B_yAl_xIn_{1-x-y}N$ alloys. Beyond the photon energy of 5.07 eV, the conductivity of $B_{0.125}Al_{0.1875}In_{0.6875}N$ alloy dominates than of $B_{0.065}Al_{0.1875}In_{0.75}N$ alloy. The calculated optical conductivity dispersion $\sigma(\omega)$ for the investigated systems is shown in Fig. 4(b). The optical conductivity (OC) is related to the frequency-dependent dielectric function $\varepsilon(\omega)$ as $\varepsilon(\omega) = 1 + \frac{4\pi i \sigma(\omega)}{\omega}$. The peaks in the optical conductivity spectra are determined by the electric-dipole transitions between the occupied states to the unoccupied states [56–60].

4. Conclusion

Efficient first principles calculations using the FP-LAPW method within LDA scheme have been presented to investigate the optical properties of $B_yAl_xIn_{1-x-y}N$ alloys. The fact of choosing varying B-contents may allow to electronic and optical properties of B-III-Ns to be controlled. All of band structures of $Al_xIn_{1-x}N$ (with $x = 18.75\%$) and $B_yAl_xIn_{1-x-y}N$ (with x and y up $\leq 18.75\%$) alloys show a direct character, which is of great interest for optical transitions. The $B_{0.125}Al_{0.1875}In_{0.6875}N$ QW laser structure shows powerfully better performances, such as the strongest peak in refractive index at 4.75 eV and the main peak in reflectivity is at 5.43 eV, mainly related to the E_1 energy transition. The main peak in the absorption coefficient observed at 4.12 eV beyond the energy band gap and near to E_1 transition, is expected to show a significant interest in the design of QW solar cell structures over a wide range of wavelengths. $BAlInN$ alloys with energy band gap ranging from 0.56 to 6.2 eV (reaching the far UV wavelength range) may be not only an attractive alternative to $AlInN$ alloys for making devices operating in the UV spectral region but also a prototype to the B-III-N group.

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