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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.

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 $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$, found to be useful as well layers and cladding layers in QW-LD structures, respectively [10–12], little attention has been paid to $Al_xIn_{1-x}N$, 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 AlGaN 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). $Al_{0.83}In_{0.17}N$/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, InGaN 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 InGaN epitaxial layers and GaN substrates [18]. The BInGaN 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 BAlGaN 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 microcavity. 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 cathodeluminescence (RTCL) from Tm implanted $Al_xGa_{1-x}N$ with different AlN contents and from implanted $In_xAl_{1-x}N$ 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 $In_{0.13}Al_{0.87}N$:Tm, annealed at 1200 °C is more than 10 times stronger than that from $Al_xGa_{1-x}N$: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% N2 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 InGaAsN/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 $B_yAl_xIn_{1-x-y}N$ 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