Superlattices and Microstructures 50 (2011) 277–288

Contents lists available at SciVerse ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

A theoretical study of band structure properties for III–V nitrides quantum wells

S. Ben Rejeb [a,*], A. Bhouri [a], M. Debbichi [a], J.-L. Lazzari [b], M. Said [a]

[a] Unité de Recherche de Physique des Solides, Département de Physique, Faculté des Sciences de Monastir, 5019 Monastir, Tunisia
[b] Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), UPR – CNRS 3118, Aix-Marseille Université, Case 913, Campus de Luminy, 13288 Marseille cedex 9, France

ARTICLE INFO

Article history:
Received 24 March 2011
Received in revised form 22 May 2011
Accepted 6 July 2011
Available online 9 August 2011

Keywords:
Cubic GaN
InGaN
AlInGaN
Band offsets
Strain
Quantum well

ABSTRACT

Reliable and precise knowledge about the strain and composition effects on the band structure properties is crucial for the optimization of InGaN based heterostructures for electronic and optoelectronic device applications. AlInGaN as quaternary barrier material permits to control the band gap and the lattice constant independently. Using the model solid theory and the multi-band k.p interaction model, we investigate the composition effects on band offsets and band structure for pseudomorphic $Ga_{1-x}In_xN/Al_zIn_yGa_{1-y-z}N$ (0 0 1) heterointerfaces having zinc-blende structure. The results show that both conduction and valence band states are strongly modified while varying In and Al contents in the well and barrier materials. Furthermore, it is found that using AlInGaN as the barrier material allows the design of heterostructures including InGaN wells with tensile, zero or compressive strain. Such results give new insights for III-nitride compounds based applications and especially may guide the design of white-light emission diodes.

1. Introduction

The vast potential of GaN, AlN, InN and their alloys for ultraviolet to far-red optoelectronic devices such as light emitting diodes (LEDs) or laser diodes, and electronic transistors for high frequency or power applications has been established [1–8]. Yet, issues involving numerous essential

* Corresponding author. Tel.: +216 73500274; fax: +216 73500278.
E-mail address: benrejeb.sana@yahoo.fr (S.B. Rejeb).

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doi:10.1016/j.spmi.2011.07.004

semiconductor properties remain unresolved. The large lattice mismatch between III-nitride compounds can result in device active layers experiencing significant biaxial strain especially for InGaN/AlGaN or InGaN/GaN hexagonal heterostructures. Furthermore, the piezoelectric polarization induced by the large lattice mismatch between the quantum well and the barrier, added to the spontaneous polarization, produces large internal field which can separate the wave functions of the electrons and holes. The later phenomenon dramatically changes the quantum well (QW) dispersion spectrum and thus reduces the radiative efficiency of the heterostructures [9–12].

Previous studies have been performed for devices based on InGaN/AlGaN or InGaN/GaN QWs. In this case, the InGaN well layer is subject to compressive stress. However, it is extremely wanted to understand and study InGaN QWs in which the well is under tensile or zero stress. To achieve this goal, it is proposed to use AlInGaN quaternary alloy as a barrier material for an InGaN QW. In fact, by adjusting the constituent compositions, it is possible to have an extra degree of freedom in controlling simultaneously the energy gap and the lattice constant. Also, it allows the lattice strain to be varied between compressive, zero and tensile strain [13–17]. Thus, for certain Al and In compositions, the AlInGaN/InGaN quantum heterostructures exhibits interesting features, such as emission intensities which are higher than those revealed by InGaN/AlGaN heterostructures based on ternary alloys [18].

Most of the progresses achieved so far are mainly based on the hexagonal (wurtzite) structures. The cubic metastable-phase layers are believed to possess potential advantages arising as promising alternatives for similar applications [18–24]. Since spontaneous polarization fields and piezoelectric fields are negligible in the cubic nitrides, their investigation would help understanding the relative roles of In-segregation and phase-separation on the radiative recombination processes in light emitting- and laser-diodes built-on $In_xGa_{1-x}N$. So far the effect of In-segregation on the luminescence properties of cubic $In_xGa_{1-x}N$ based heterostructures can be studied without influence of internal electrical field [25]. Indium clustering leads to potential fluctuations that limit non-radiative recombination of carriers by inhibiting their diffusion from regions of locally reduced band gap to non-radiative recombination centers such as dislocations [26]. Nonetheless, one has to be careful in considering the influence of Indium clustering on the band structure of cubic nitride alloys. All this makes the nitride alloys with In and Al particularly interesting also from a basic material research point of view.

Research efforts towards a more complete understanding of the cubic nitride based heterostructures have increased recently [18–26]. Despite the recent success of cubic AlInGaN based devices applications [13–17], many fundamental physical parameters are until now a controversial subject and not fully understood. Clearly, the application of cubic nitride structures in optoelectronic devices is difficult to realize correctly without detail knowledge of the band alignments of the corresponding QW interfaces. This has prompted us to perform such calculations using the Model Solid Theory [27] as we have previously done for nitride related alloys [28–30]. In addition, it is known that the most common method by which to achieve a white LED is to combine a phosphor wavelength converter with a GaN blue LED [9,31]. Thus, it is of great interest to design an integrated one-chip white LED by mixing red, blue and green emissions in different wavelengths with adequate intensities [9,31]. In such case, strain is very important in controlling the QW optical properties depending on whether the lattice is under tensile or compressive deformation, as it decreases or increases the energy band gap and the band offsets. With this in mind, we have calculated the strain dependent energy band gap in $In_xGa_{1-x}N/Al_zIn_yGa_{1-y-z}N$ heterostructures.

In this work, and after a brief introduction, we present and discussed in Section 2 the theoretical results concerning the band offsets and band structure in InGaN/AlInGaN interfaces. Conclusions are summarized in Section 3.

2. Results and discussion

2.1. Calculated band offsets for (0 0 1)-oriented $In_xGa_{1-x}N/Al_zIn_yGa_{1-y-z}N$ interfaces

For a relaxed-$In_xGa_{1-x}N$/strained-$Al_zIn_yGa_{1-y-z}N$ heterostructure along the $\langle 0\,0\,1\rangle$ growth direction, the lattice mismatch gives rise to a biaxial strain in the (0 0 1) plane. The effect of this strain on the energy band edges can be decomposed into hydrostatic and uniaxial contributions. The