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# Intersubband energies in $\text{Al}_{1-y}\text{In}_y\text{N}/\text{Ga}_{1-x}\text{In}_x\text{N}$ heterostructures with lattice constant close to $a_{\text{GaN}}$

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## ABSTRACT

We have studied the conduction band profile and the intersubband transition energy,  $E_{12}$ , of  $\text{Al}_{1-y}\text{In}_y\text{N}/\text{Ga}_{1-x}\text{In}_x\text{N}$  quantum well structures. We have considered how material parameters such as non-parabolicity and the uncertainty in the bowing parameter affect  $E_{12}$  and the corresponding wavelength,  $\lambda_{12}$ . The calculations include strain and cover the transition range from telecommunication wavelengths (1.55  $\mu\text{m}$ ) to the mid-infrared ( $\sim 10 \mu\text{m}$ ).

Our results show that the transition energies of strain-free  $\text{Al}_{1-y}\text{In}_y\text{N}/\text{Ga}_{1-x}\text{In}_x\text{N}$  quantum well structures, which are lattice-matched to GaN ( $y = 17.7\%$ ,  $x = 0$ ), resulted in wavelengths above  $\sim 2 \mu\text{m}$ . To reach shorter wavelengths, we explored structures with other indium concentrations but maintaining a small mismatch to GaN. For  $\sim 1\%$  lattice mismatch the wavelength  $\lambda_{12}$  could be reduced to less than 1.55  $\mu\text{m}$ . The results serve as a starting point for designing and epitaxial growth of photonic intersubband structures.

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## 1. Introduction

III-Nitride based heterostructures have great potential for optoelectronic applications as they cover a huge wavelength range from the infra-red (IR) to the ultra-violet (UV). Linked to the interband transitions, a major achievement was the realization of light-emitting diodes (LEDs) covering red-yellow to near UV “colors”. Subsequently this gave way to the fabrication of the white LED [1–4] with good

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quantum efficiency and high light output. The most spectacular achievement for GaN-based heterostructures is the realization of blue laser diodes operating continuously with a long life-time at ambient temperatures [5]. Another type of application is associated with intersubband (ISB) transitions in this system. Specific devices are quantum well photodetectors and quantum-cascade lasers (QCL) [6–10]. The high conduction band (CB) discontinuities between compounds within the III-nitride family allow reaching shorter wavelengths than for arsenide or antimonide heterostructures [11]. The CB offset for AlN/GaN heterostructures is large, about 2 eV, and the lattice-mismatch, 2.5%, is large enough to generate structural defects. For AlN/InN the CB offset is 3.6 eV, while the mismatch is as much as 13%.

The design and engineering of AlN/GaN-based heterostructures for unipolar devices with intersubband transitions is a demanding task; a quantum cascade laser for telecommunication applications at 1.3 and 1.55  $\mu\text{m}$  has yet to be realized. However, intersubband transitions at wavelengths as short as  $\sim 1 \mu\text{m}$  [12–15] have been reported in the AlN/GaN system. To reach such short wavelengths, the well width is required to be only one or a few monolayers. At this scale the intersubband absorption unfortunately exhibits a large peak broadening ( $>100 \text{ meV}$ ) [13]. Another major issue for AlN/GaN heterostructures is the high dislocation density, which arises because of the 2.5% lattice mismatch. For AlN/GaN heterostructures grown on GaN, crack formation is likely to occur [16–18]. Therefore, III-nitride heterostructures must be designed to minimize the formation of structural defects during the epitaxial growth. For instance, we can make use of the fact that AlN with  $\sim 18\%$  indium is in-plane lattice matched to (0001) GaN [17]. For a growth temperature below  $550^\circ\text{C}$ , indium is reproducibly incorporated at fractions below  $\sim 20\%$ . Such layered structures have been studied with X-ray diffraction (XRD), transmission-electron microscopy (TEM), photoluminescence and photoabsorption [17,19–21]. The concept of strain-balance, that is matching the optimal lattice constant of a free-standing heterostructure to that of the cladding layers, is also discussed theoretically for wurtzite structures [22].

We are interested in  $\text{Al}_{1-y}\text{In}_y\text{N}/\text{Ga}_{1-x}\text{In}_x\text{N}$  structures deposited on a GaN substrate. This substrate could be bulk GaN or pseudosubstrates, thick layers of GaN grown on sapphire templates. In this work, we study QW structures with two confined levels. The aim is to identify structures that result in intersubband-transition wavelengths suitable for telecommunication applications for as small lattice mismatch as possible. The starting point is strain-free structures where both wells and barriers are lattice-matched to GaN. Next, we study strained heterostructures with large enough CB offset to reach the telecommunication wavelengths. The effects of non-parabolicity and the uncertainty in bowing parameter on the transition energy between ground state and first excited state,  $E_{12}$ , are also studied.

## 2. Theory

The electronic states depend strongly on the  $x$  and  $y$  values of the  $\text{Al}_{1-y}\text{In}_y\text{N}/\text{Ga}_{1-x}\text{In}_x\text{N}$  structures. Within the envelop function approximation, the wave-functions and energy levels are obtained by solving the following Schrödinger equation

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left( \frac{1}{m^*(z)} \frac{d}{dz} \psi_i(z) \right) + U(z) \psi_i(z) = E_i \psi_i(z) \quad (1)$$

$$U(z) = \begin{cases} eF_b(z - z_1) + eF_w(z_2 - z_1) + \Delta E_c & z < z_1 \\ -eF_w(z - z_2) & z_1 \leq z \leq z_2 \\ eF_b(z - z_2) + \Delta E_c & z > z_2 \end{cases} \quad (2)$$

The interface positions are given by  $z_1$  and  $z_2$  (see Fig. 1). The electric fields in the well and barrier materials are denoted  $F_w$  and  $F_b$ , respectively. These internal electrical fields arise from spontaneous and piezoelectric polarization [23,24], because the total polarization of the layers differ, as given by  $\Delta P$ , along the  $c$ -axis. Spontaneous polarization in wurtzite structures are linked to the lack of inversion symmetry. In superlattices of wells and barriers, the electric fields are given by

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