

# Effects of strain distribution on the optical gain of InGaN/AlInGaN

D. Ahn<sup>1</sup>, S.-H. Park<sup>2</sup> and B. H. Koo<sup>3</sup>

<sup>1</sup>Department of Electrical and Computer Engineering, University of Seoul, Seoul 130-743, Korea

<sup>2</sup>Department of Electronics Engineering, Catholic University of Daegu, Hayang, Kyeongsbuk 712-702, Korea

<sup>3</sup>Wooree LST Corporation, Ansan-shi, Kyungki-do 425-833, Korea

Author e-mail address: [dahn@uos.ac.kr](mailto:dahn@uos.ac.kr)

**Abstract** -- Effects of the strain distribution on the optical gain of InGaN-AlInGaN QW light-emitting diodes (LEDs) is investigated. The amount of stress and strain in the multilayer quantum well structures are calculated taking into account the difference between crystalline parameters. Significant enhancement of optical gain is expected with the introduction of strain distribution layers.

## I. INTRODUCTION

It is well known that for III-V nitride quantum well based optoelectronic devices, strong built-in polarization fields caused by the strain exist in the active layers, which degrade the performance of the device significantly. Especially, the wurtzite GaN-based quantum wells grown along (0001) direction possess the piezoelectric (PZ) and spontaneous polarization (SP) fields of an order of MV/m [1,2]. These built-in internal fields reduce the optical gain and the luminescence by an order of magnitude as compared with other III-V semiconductors.

Here, we present an investigation of the strain distribution effect on the optical gain of InGaN-AlInGaN QW light-emitting diodes (LEDs) using the 6x6 Pikus-Bir Hamiltonian for wurtzite semiconductors [3] and the non-Markovian gain model with many-body effects [4]. The amount of stress and strain in the multilayer quantum well structures are calculated taking into account the difference between crystalline parameters such as lattice constant and thermal expansion coefficient of the composed multilayer structures [5]. In this strained multilayered structure where the  $i$ -th layer is characterized by the thickness  $d_i$  and the lattice constant  $a_i$ . Effective strain in the  $i$  th layer is then given by  $\epsilon_{xxi} = \frac{F_i}{E_i d_i} + \frac{d_i}{2R}$ , where  $F_i$  is the force per unit length of

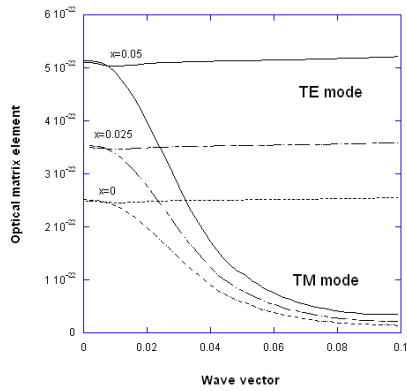
the  $i$ -th layer,  $R$  is the curvature radius and  $E_i$  is Young's modulus. The band structure of wurtzite quantum well is calculated within the 6x6 multiband effective mass theory<sup>8</sup> which takes into account the biaxial strain, spontaneous

polarization, and the piezoelectric effects. Non-Markovian model of the optical gain and the luminescence for the strained-layer wurtzite quantum well is employed taking into account of many-body effects within the time-dependent Hartree-Fock approximation. Plasma screening, bandgap renormalization, and Coulomb enhancement of optical transitions are included in the model. Non-Markovian lineshape is related to the memory effects in the system-reservoir interaction. Self-consistent band structure and wave functions are obtained by solving the Schrodinger equation for electrons, block diagonalized Hamiltonian for holes, and Poisson equation iteratively until the solution converges [5].

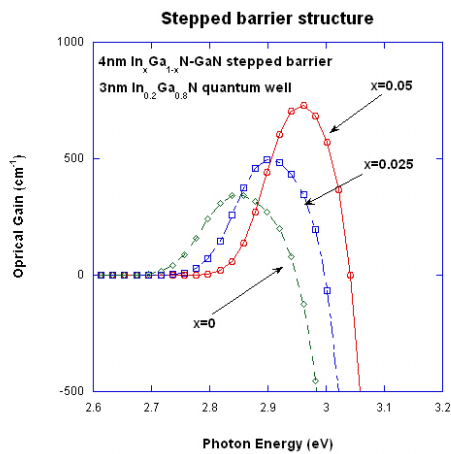
## II. RESULT AND DISCUSSIONS

As a numerical example, we first consider the symmetric In<sub>0.2</sub>Ga<sub>0.8</sub>N/In<sub>x</sub>Ga<sub>1-x</sub>N/GaN stepped quantum well, in which the In<sub>x</sub>Ga<sub>1-x</sub>N layers act as a strain relaxing region sandwiched between an In<sub>0.2</sub>Ga<sub>0.8</sub>N active region and GaN barriers. We assume the widths of the active layer and strain-relaxing layer as 3nm and 4nm, respectively and we denote the layer A for the active layer and the layer B for the In<sub>x</sub>Ga<sub>1-x</sub>N strain relaxing stepped barrier. Figure 1 shows the optical matrix elements of stepped structures for the indium fractions of  $x=0$ , 0.025, and  $x=0.05$ . When  $x=0$ , the amount of strain in layers A and B are -2.087% and 0.14%. On the other hand, those for  $x=0.5$  are -1.984% and -0.321%. From this result, one can see that the layer B absorbs part of the strain in the active region and as a result the piezoelectric field in the active region is reduced which in turn increases the optical dipole matrix element. In this figure TE mode and TM mode correspond to C1-HH1 transition and C1-LH1 transitions, respectively. The change of sign for the strain in the layer B when In is introduced to the layer composition increases the wave function overlapping between the electron and the hole.

layer. We assume that the 2.5 nm  $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$  quantum well as an active region and 15nm GaN buffer layer separate the active region and the strain distribution layer.



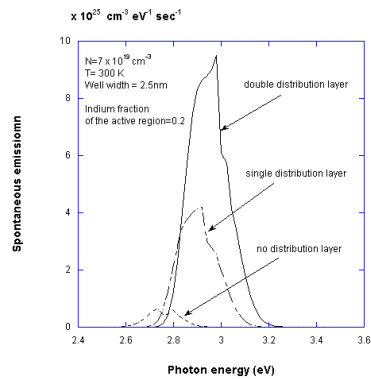
**FIG. 1** The optical dipole matrix elements of the stepped structure for various In mole fractions of  $\text{In}_x\text{Ga}_{1-x}\text{N}$  strain relaxing layer.



**FIG. 2** The optical gain of the stepped structure for various In mole fractions of  $\text{In}_x\text{Ga}_{1-x}\text{N}$  strain relaxing layer.

Figure 2 shows the optical gain of stepped structures for the indium fractions of  $x=0, 0.025,$  and  $x=0.05$ . It is expected that the optical gain is improved significantly when the In mole fraction in the strain relaxing layer B is changed from  $x=0$  to  $x=0.05$ . The improvement of the gain is mainly due to the enhancement of optical dipole matrix element which is related to the overlap of the electron and the hole wave functions.

As a second example, we consider the multilayer structure with separate 25nm thick  $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$  strain relaxing



**FIG. 3** The spontaneous emission spectra of the multilayer structure with separate strain distribution layers.

Figure 3 shows the spontaneous emission spectra for the multilayer structure employing separate strain distribution layers for the cases of (i) no distribution layer, (ii) single distribution layer, and (iii) double distribution layers. The amount of strain in the active region is changed from  $-2.19\%$  (no distribution layer) to  $-1.924\%$  in double distribution layer and the peak emission is expected to improve significantly.

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