Influence of polar face on optical properties 
of staggered 440 nm InGaN/InGaN/GaN quantum-well light-emitting diodes

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Abstract – The influence of the polar plane on optical properties of staggered InGaN/InGaN/GaN quantum well (QW) light-emitting diodes was investigated using the multiband effective mass theory. The N-face staggered InGaN/InGaN/GaN QW structure has a greater spontaneous emission peak than the Ga-face staggered InGaN/InGaN/GaN QW structure because the former has a larger matrix element than the latter. On the other hand, the heavy-hole effective mass around the topmost valence band is not affected nearly by the polarity. We expect that the N-face staggered InGaN/InGaN/GaN QW structure has an improved characteristics compared to the Ga-face staggered InGaN/InGaN/GaN QW structure.

I. INTRODUCTION

III-Nitride diode lasers and light emitting diodes (LEDs) emitting in the 420-500nm region play important roles for medical, optical storage, and solid state lighting. One of major challenges preventing high performance conventional InGaN quantum well (QW) is a large internal field due to the strain-induced piezoelectric (PZ) and spontaneous (SP) polarizations.[1,2] As a result, the radiative recombination rate and the optical gain of these QW structures are reduced significantly due to the large spatial separation between the electron and hole wavefunctions. Several methods have been proposed in an effort to reduce the effect of the internal field due to polarizations.[3-5] In addition, an InGaN/InGaN/GaN QW structure with a staggered well has been recently proposed to reduce the internal field effect.[6] It was demonstrated that the QW structure with the staggered InGaN well shows significant improvement in output power. The staggered well offers an extra degree of freedom which may be employed to tune the emission wavelength. However, many fundamental properties of GaN-based QW structure with the staggered well are not yet well understood because studies based on these structures are in an early developmental stage. In particular, there has been very little work on the influence of the polar plane on optical properties of the staggered InGaN/InGaN/GaN QW structure. Both types of polarity (N- and Ga-faces) were found by ion channeling and convergent beam electron diffraction in GaN (0001) layers grown by MOCVD on c-plane sapphire.[7]

In this paper, we investigate the influence of the polar plane on optical properties of staggered InGaN/InGaN/GaN QW light-emitting diodes. The self-consistent (SC) band structures and wave functions are obtained by solving the Schrodinger equation for electrons, the 3x3 Hamiltonian for holes, and Poisson's equation iteratively.[8,9]

II. RESULT AND DISCUSSIONS

Figure 1 shows the potential profiles and the wave functions of the first conduction subband (C1) and the first valence subband (HH1) at zone center for the ground state of (a) Ga-face staggered and (b) N-face staggered InGaN/InGaN/GaN QW structures. The internal field F in layers can be obtained by using the periodic boundary condition \( \sum F = 0 \), where the sum runs over all the layers, including barrier layers, and \( t \) denotes the thickness of a layer.[10] The alignment of the piezoelectric and spontaneous polarizations is antiparallel in the case of compressively strain for Ga-face. If the polarity flips over from Ga-face to N-face material, the piezoelectric, as well as the spontaneous polarization changes its sign. The total thickness of the left side well \( (L_{w1}) \) and the right side well \( (L_{w2}) \) in a staggered QW structure is selected as the same as the well width \( (L_w) \) in the single QW structure. However, the
In compositions are selected to give a transition wavelength of 440 nm.

Both staggered InGaN/InGaN/GaN QW structures show that a spatial separation between electron and hole wavefunctions is reduced with the inclusion of staggered InGaN layer. Also, we observe that the potential profile and the spatial separation between wavefunctions for staggered QW structures depends on the polar face. On the other hand, we note that, in the case of the single QW structure, the spatial separation between electron and hole wavefunctions is independent of the polar face.

Figure 2 shows (a) optical matrix elements as a function of the in-plane wave vector and (b) spontaneous emission spectra for 440 nm (a) Ga-face staggered and (b) N-face staggered InGaN/InGaN/GaN QW structures. For comparison, we plotted the result for a conventional QW structure. The SC solutions are obtained at a sheet carrier density of $N_{2D} = 10 \times 10^{12} \text{ cm}^{-2}$. We know that a N-face staggered QW structure shows larger matrix element than a Ga-face staggered QW structure. Also, the optical matrix elements of staggered QW structures are shown to be larger than that of a conventional QW structure. This is mainly due to the fact that the internal field effect is reduced with the inclusion of staggered InGaN layer. The spontaneous emission spectra have only one peak which corresponds to C1-HH1 transition. In the case of a conventional QW structure, the peak position of spontaneous emission spectrum is blueshifted at a high carrier density of $N_{2D} = 10 \times 10^{12} \text{ cm}^{-2}$, compared to staggered QW structures. This means that the screening effect of the internal field is dominant in the conventional QW structure. Spontaneous emission peaks of both staggered QW structures are shown to be larger than that of a conventional QW structure. Also, the N-face staggered InGaN/InGaN/GaN QW structure shows a greater spontaneous emission peak than the Ga-face staggered InGaN/InGaN/GaN QW structure. This can be attributed to the fact that the before has a larger matrix element than the latter.

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