Effects of Spontaneous Polarization on Optical Properties of Ultraviolet BAlGaN/AlN Quantum Well Structures

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***Abstract*—Effects of spontaneous polarization on electronic and optical properties of ultraviolet (UV) $B_xAl_yGa_{1-x-y}N$/AlN quantum well (QW) structures were using the multiband effective-mass theory. The spontaneous emission peak begins to decrease when the boron composition exceeds a critical value. The critical value is found to increase rapidly with decreasing the absolute value of the spontaneous polarization constant. In addition, the light intensity is reduced with decreasing spontaneous polarization. However, the spontaneous emission peak of BAlGaN/AlN QW structures is found to be greatly improved with the inclusion of the boron, irrespective of the spontaneous polarization. Hence, we expect that BAlGaN/AlN QW structures can be used as a high-efficiency light source for optoelectronic applications in ultraviolet spectral region.**

***Index Terms*—BAlGaN, AlN, quantum well, light-emitting diode, polarization**

I. INTRODUCTION

THe group-III nitrides have attracted special attention with respect to their application in light-emitting devices operating in the visible and ultraviolet (UV) spectral regions [1]. Among them, AlGaN-based light-emitting diodes (LEDs) emitting in the UV spectral range has been highly attractive to researchers for its wide applications such as biomedicine, fluorescence spectroscopy, photolithography, optical data storage, and purification or sterilization of air and water [2], [3]. The performance of UV LEDs has markedly increased due to the improved quality of high-Al-composition AlGaN layers and also the optimization of LED designs. However, several obstacles still impede further improvement for higher performance UV LEDs [4]. One of the major challenges is the large internal fields induced by the lattice mismatch in the active region. This results in the reduction in the radiative recombination rate and serious electron leakage out of the active region.

Recenlty, the BAlGaN system has been proposed to reduce the lattice mismatch in the active region because the growth of the lattice-matched BAlGaN quaternary system to AlN is possible with the inclusion of the small boron ($<$ 12 %) [5]–[8]. The maximum boron contents up to 13 % and 9 % were demonstrated experimentally for BAlN and BGaN, respectively [5]. On the theoretical side, Dreyer *et al.* [9] repoted that the magnitude (-2.174 C/m^2) of the spontaneous polarization for wurtzite BN is significantly larger than that for the other III nitrides. This value is about thirty times larger than that of AlN. On the other hand, no experimental data to compare this prediction with are avaliable. Hence, an investigation of spontaneous polarization effects on electronic and optical properties of UV $B_xAl_yGa_{1-x-y}N$/AlN QW structures will be very useful for the design of the BAlGaN-based active region because their light emission characteristics are significantly affected by the internal field related to the spontaneous polarization.

In this research, we investigate light emission characteristics as a function of spontaneous polarization for UV $B_xAl_yGa_{1-x-y}N$/AlN QW structures using the multiband effective-mass theory and non-Markovian model. Here, we consider the free carrier model with the band-gap renormalization. We assume that a BAlGaN/AlN QW structure is grown on a thick AlN buffer layer and the well width of the active layer is fixed to 2.5 nm. The self-consistent (SC) solutions are obtained by solving the Schrödinger equation for electrons, the block-diagonalized 3×3 Hamiltonian for holes, and Poisson's equation iteratively [10], [11]. The expression for the non-Markovian spontaneous emission spectrum $g_{sp}(\omega)$ is given in Refs. [12] and [13]. The material parameters for GaN and AlN used in the calculation were taken from Refs. [14], [15] and references therein. The parameters for $B_xAl_yGa_{1-x-y}O$ are obtained from the linear combination between the parameters of BN, AlN, and GaN. However, several material parameters for BN are not well known and we assumed its parameters to be equal to those of AlGaN as a first approximation in the case of a lack of published data.

II. RESULTS AND DISCUSSION

Figure 1 shows (a) strain and (b) internal field in the well as a function of the boron composition for $B_xAl_yGa_{1-x-y}N$/AlN QW structures (L_w=2.5 nm, y=0.2) with several spontaneous polarization constants. The well is under the compressive strain for the conventional AlGan/AlN QW structure. The compressive strain is reduced gradually with increasing boron composition in the well because of the reduction in the lattice mismatch between the well and the substrate with the inclusion

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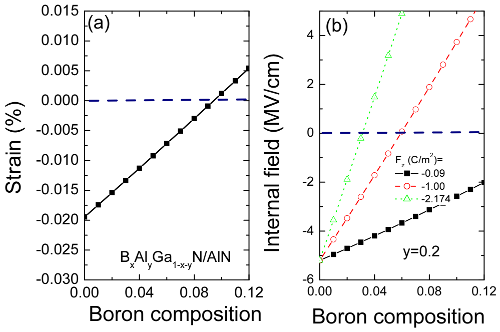

Fig. 1. (a) Strain and (b) internal field in the well as a function of the boron composition for $B_xAl_yGa_{1-x-y}N/AlN$ QW structures (L_w=2.5 nm, y=0.2) with several spontaneous polarization constants.

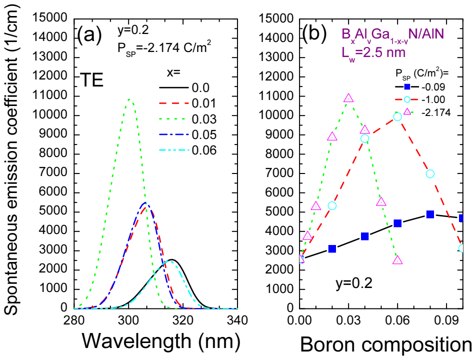

Fig. 2. (a) Spontaneous emission coefficients for $B_xAl_yGa_{1-x-y}N/AlN$ QW structures ($P_{SP} = -2.174C/m^2$, y=0.2) with several boron compositons and (b) peak intensities as a function of the boron composition for $B_xAl_yGa_{1-x-y}N/AlN$ QW structures (y=0.2) with several spontaneous polarization values.

of the boron. That is, the the lattice constant in the well is decreased with increasing boron composition. As a result, the well is lattice-matched to the barrier or the substrate for the QW structure with a particular boron composition. For y=0.2 (Al composition), the boron composition to give the lattice-matched condition is 0.094. The internal field is shown to depend on the spontaneous polarization significantly. With increasing boron composition, the internal field rapidly decrease, becomes zero, and begins to increase. The boron composition to give zero internal field greatly depends on the magnitude of the spontaneous polarization constant. That is, it rapidly decreases with increasing the magnitude of the spontaneous polarization constant.

Figure 2 shows (a) spontaneous emission coefficients for $B_xAl_yGa_{1-x-y}N/AlN$ QW structures ($P_{SP} = -2.174C/m^2$, y=0.2) with several boron compositons and (b) peak intensities as a function of the boron composition for $B_xAl_yGa_{1-x-y}N/AlN$ QW structures (y=0.2) with several spontaneous polarization values. Spontaneous emission spectra are obtained at a sheet carrier density of $N_{2D} = 20 \times 10^{12} cm^{-2}$. The peak wavelength of the conventional AlGaN/AlN QW structure with the Al composition of 0.2 is shown to be about 315 nm. It is shifted to the short wavelength with increasing boron composition because of the increase in the bandgap energy and the internal field. We know that the spontaneous emission peak of BAlGaN/AlN QW structures is found to be greatly improved with the inclusion of the boron. In particular, the light intensity of the QW structure with x=0.03 is about four times larger than the conventional QW structure. However, the spontaneous emission peak begins to decrease when the boron composition exceeds a critical value, for example, x=0.03 for y=0.2. On the other hand, the critical value significantly depends on the spontaneous polarization. That is, it rapidly increases with decreasing the absolute value of the spontaneous polarization constant. We know that the light intensity is also reduced simultanelusly with decreasing P_{sp}.

III. SUMMARY

In summary, effects of spontaneous polarization on electronic and optical properties of UV $B_xAl_yGa_{1-x-y}N/AlN$ QW structures were using the multiband effective-mass theory and non-Markovian model. The spontaneous emission peak of BAlGaN/AlN QW structures is found to be greatly improved with the inclusion of the boron, irrespective of the spontaneous polarization. However, the spontaneous emission peak begins to decrease when the boron composition exceeds a critical value. The critical value significantly depends on the spontaneous polarization.

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