High-efficiency BGaN/AlN quantum wells for optoelectronic applications in ultraviolet spectral region

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***Abstract*—Light emission characteristics of ultraviolet (UV) BGaN/AlN quantum well (QW) structures were investigated using the multiband effective-mass theory and non-Markovian model. The BGaN/AlN QW structures show a much larger light intensity than the conventional AlGaN/AlN QW structures. This is mainly due to the fact that the internal field is significantly reduced by increasing boron contents. The spontaneous emission peak shows a maximum at the critical value (x= 0.04) and begins to decrease when the boron content is further increased. Hence, we expect that BGaN/AlN QW structures with small boron contents can be used as a TE-polarized light source with a high efficiency in UV region.**

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

I. Introduction

AlGaN materials have attracted special attention with respect to their application in light-emitting devices operating in the visible and deep ultraviolet (UV) spectral regions because of many applications such as water purification, biochemical agent detection, medical research/health care, and high-density data storage [1]. However, it was found that there exists a large internal field 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 [2]–[6].

Recently, the BAlGaN or BInGaN system has been proposed as a promising candidate for UV and deep UV applications because the growth of the lattice-matched system to GaN or AlN is possible with the inclusion of the boron [7]–[12]. Similarly, the BGaN system was also proposed as novel class of materials lattice matched to AlN and SiC substrates [13]–[15]. Thus, it will be interesting to investigate electronic and optical properties of BGaN/AlN QW structures for application to novel light-emitting devices in the UV spectral region. In particular, on the theoretical side, many fundamental properties of these QW structures are not yet well understood because studies based on these structures are in an early developmental stage.

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In this research, we theoretically investigate light emission characteristics of BGaN/AlN QW structures using the multiband effective-mass theory. Here, we consider the free carrier model with the band-gap renormalization. We assume that a BGaN/AlN QW structure is grown on a thick AlN buffer layer. 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 [16], [17].

II. Theory

The non-Markovian spontaneous emission spectrum $g_{sp}(\omega)$ is given by [18], [19]

$$\begin{aligned} g_{sp}(\omega) &= \sqrt{\frac{\mu_o}{\epsilon}} \sum_{\sigma=U,L} \sum_{l,m} \left(\frac{e^2}{m_o^2\omega}\right) \int_0^\infty dk_{||} \frac{k_{||}}{\pi L_w} \\ &\cdot\ |\hat{\epsilon}\cdot\mathbf{M}_{lm}^{\sigma}(k_{\|})|^2 f_l^c(k_{||})[1-f_m^v(k_{||})] \\ &\cdot\ \mathrm{Re}L(E_{lm}(k_{\|},\hbar\omega)), \end{aligned} \quad (1)$$

where ω is the angular frequency, μ_o is the vacuum permeability, ϵ is the dielectric constant, $\sigma = U$ (or L) refers to the upper (lower) blocks for the effective-mass Hamiltonian, e is the charge on an electron, m_o is the electron mass, $k_{||}$ is the magnitude of the in-plane wave vector in the QW plane, L_w is the well thickness, $\hat{\epsilon}$ is a unit vector in the direction of the optical electric field, $|M_{lm}|^2$ is the momentum matrix element in the strained QW, f_l^c and f_m^v are the Fermi functions for the conduction band states and the valence band states, respectively, and $\hbar$ is the Planck constant. The indices l and m denote the electron states in conduction band and heavy hole (light hole) subband states in the valence band, respectively. Also, $E_{lm}(k_{\|},\hbar\omega)$ is the renormalized transition energy between electrons and holes. The line-shape function $L(E_{lm}(k_{\|},\hbar\omega))$ is Gaussian and given in Refs. [18], [19]. The material parameters used in the computations are taken from Refs. [20]–[22]

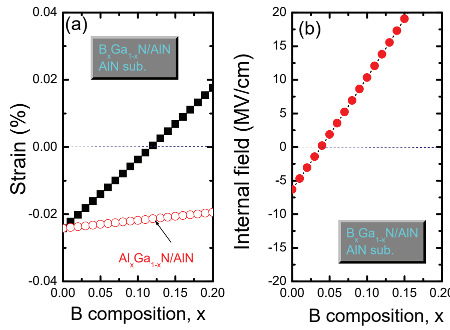

Fig. 1. (a) Strain and (b) internal field as a function of B content for B_xGa_{1-x}N/AlN QW structures (L_w=2.5 nm) gorown on AlN substrate.

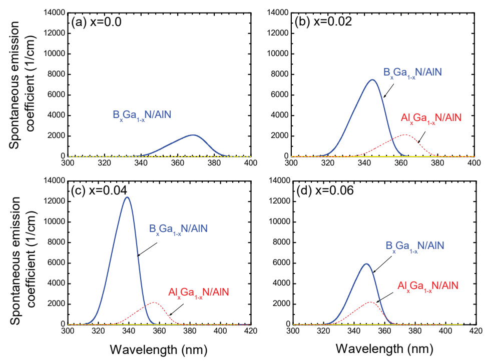

Fig. 2. Spontaneous emission coefficients for B_xGa_{1-x}N/AlN QW structures with (a) x=0, (b) 0.02, (c) 0.04, and (d) 0.06.

III. Results and discussion

Figure 1 shows (a) strain and (b) internal field as a function of B content for B_xGa_{1-x}N/AlN QW structures (L_w=2.5 nm) grown on AlN substrate. The dashed lines are guidelines for the zero strain ($\epsilon = 0$) and the zero internal field (F_z=0). The absolute value of strain rapidly decreases with increasing boron composition and becomes zero at a cirtical composition. Similar result is observed for the internal field. However, we observe that strain values of BGaN/AlNQW structures are smaller than those of AlGaN/AlN QW structures. The boron composition to give zero internal field is shown to be much smaller than that to give zero strain.

Figure 2 shows spontaneous emission coefficients for B_xGa_{1-x}N/AlN QW structures with (a) x=0, (b) 0.02, (c) 0.04, and (d) 0.06. Spontaneous emission spectra are obtained at a sheet carrier density of $N_{2D} = 20 \times 10^{12} cm^{-2}$. The peak wavelength of the conventionall AlGaN/AlN QW structure with x=0.0 is shown to be about 368 nm. It is shifted to the short wavelength with increasing boron composition because of the increase in the bandgap energy. The spontaneous emission peak of BGaN/AlN QW structures is found to be greatly improved with the inclusion of the boron. In particular, in the case of x=0.04, the light intensity of the QW structure is about six times larger than the conventional AlGaN/AlN QW structure. However, the spontaneous emission peak begins to decrease with the blueshift of the wavelength when the boron composition exceeds a critical value. The decrease in the spontaneous emission peak is related to the decrease in the optical matrix element due to the increase in the internal field.

IV. Summary

In summary, light emission characteristics of UV BGaN/AlN QW structures were studied using the multiband effective-mass theory and non-Markovian model. The QW BGaN/AlN structures show much larger light intensity than the conventional GaN/AlN QW structure. We expect that BGaN/AlN QW structures can be used as a TE-polarized light source with a high efficiency in UV region.

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