Enhancement of surface emission in deep ultraviolet AlGaN-based light emitting diodes with staggered quantum wells

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AlGaN-based light-emitting diodes (LEDs) with a high Al content can realize deep ultraviolet (DUV) light emission, which have potential applications in sterilization, medicine, and biochemistry. However, the external quantum efficiencies (EQEs) of reported Al-rich AlGaN-based LEDs are very low, about 1% or less, even though the high quality AlGaN epitaxial layers have been grown by improved growth technology [1,2]. Recently, it has been revealed that the intensity of light emission with TE polarized from c-oriented AlGaN-based alloys and related quantum wells (QWs) structure decreases dramatically with increasing Al content [3–5]. The suppression of the TE polarized component results in a significant reduction of surface emission from c-plane Al-rich AlGaN-based LEDs because the photons propagate perpendicularly to electrical polarization vectors [6]. So, it is considerably important to obtain DUV AlGaN-based LEDs with dominant TE polarized emission.

Several research results have shown that strong TE polarized emission for c-oriented AlGaN-based QWs can profit from in plane compressive strain and a small well width [7–10]. It has also been indicated that the use of semipolar and nonpolar substrates are beneficial to the improvement of surface emission from Al-rich AlGaN-based LEDs [11]. However, further decreasing well width or changing growth orientation will lead to crystal quality decline of AlGaN epitaxial layers. In addition, large TE polarized emission has been realized by the insertion of GaN delta-layer in Al-rich AlGaN-based QWs [12].

In this work, we present a practical method to enhance TE polarized emission from DUV AlGaN-based LEDs by using the particular staggered QW structure with step-function like Al content profile in the QW layer, which has been applied to improve output power from InGaN-based QWs [13–17]. The total well width and emission wavelength of the designed staggered AlGaN-AlGaN/AlN QW are equal to that of the conventional AlGaN/AlN QW. Numerical results show that the TE polarized emission from the AlGaN-based QWs can be remarkably enhanced by using staggered well structure. The changes of valence subband structure, including energy level order and subband coupling relation, are believed to be the reason for the increase of TE polarized emission and surface emission.

The subband structure and spontaneous emission properties of conventional and staggered AlGaN-based QWs are analyzed using the theoretical model based on the k · p method [18]. The strain effect, subband coupling, and polarization electrostatic fields are fully considered. However, the carrier screening effect, which should be included in the case of high carrier density, is ignored in this work for the low injection of 5 × 1017 cm−3 [19]. More details about the theoretical model can be found in other work [19–21]. The parameters for wurtzite GaN and AlN used in calculation are taken from [21–23].

For the heavy hole (HH) and light hole (LH) subbands, the wavefunctions have mainly |X⟩ and |Y⟩ components, and the |Z⟩ component is dominant in the wavefunction of crystal-field split off (CH) subband. Therefore, the transitions from conduction band to HH subband (C-HH) and LH subband (C-LH) contribute mainly to emission light with TE polarization, and the C-CH transition favors the TM polarized emission. As a result, the valence subband order becomes the primary origin of optical polarization properties of AlGaN-based QWs [7,24]. Also, the proportions of |X⟩, |Y⟩, and |Z⟩ components in wavefunctions of each valence subband can be influence by the subband coupling relation especially at k ≠ 0 [25]. That is, the optical polarization properties of AlGaN-based QWs can be determined by the valence subband structure including both energy level order and subband coupling relation. Then, it is a hopeful method for realizing dominant TE polarized emission by adjusting valence subband structure of the AlGaN-based QWs.

Figure 1(a) gives the calculated valence subband structure of conventional Al0.87 Ga0.13 N/AlN QW with 1.5 nm well width. It can be seen that the CH1 subband is the...
The spontaneous emission rates with TE and TM polarizations can be calculated using a momentum matrix element. Figure 3 gives the emission proportions contributed by the transitions from conduction band to CH1, HH1, and LH1 subbands for conventional Al0.87Ga0.13N/AlN QW and Al0.82Ga0.18N-Al0.92Ga0.08N/AlN QWs. As shown in Fig. 3(a), the C-CH1 transition contributes mainly to TM polarized emission and the TE polarized emission mostly comes from C-HH1 and C-LH1 transitions for conventional QW. It is also indicated that most light emissions in conventional QW come from the C-CH1 transition because the hole mostly populates in the CH1 subband as discussed in Fig. 1(a). As expected from the discussions of the momentum matrix element, there are both TE and TM polarized emissions that originated from the C-HH1, C-CH1, and C-LH1 transitions for staggered QW as shown in Fig. 3(d), and the TM emission from C-CH1 transition is greatly suppressed. It is noteworthy that the emission component with TE polarization from all the C-HH1, C-CH1, and C-LH1 transitions are greater than that of TM polarization due to valence

Fig. 2. (Color online) Momentum matrix elements contributed by transitions from the conduction band to the three topmost valence subbands in 1.5 nm (a) conventional Al0.87Ga0.13N/AlN QW and (b) staggered Al0.82Ga0.18N-Al0.92Ga0.08N/AlN QW.

Fig. 1. (Color online) Valence subband structure of (a) 1.5 nm conventional Al0.87Ga0.13N/AlN QW, (b) 1.0 nm Al0.87Ga0.13N/AlN QW, (c) 1.5 nm staggered Al0.82Ga0.18N-Al0.92Ga0.08N/AlN QW, and (d) 0.6 nm Al0.82Ga0.18N/AlN QW.
subband coupling. This leads to dominant TE polarized emission from the staggered QW.

Figure 4 further gives the total calculated spontaneous emission spectra of TE and TM polarized components for 1.5 nm conventional Al$_{0.87}$Ga$_{0.13}$N/AlN and staggered Al$_{0.82}$Ga$_{0.18}$N-Al$_{0.92}$Ga$_{0.08}$N/AlN QWs. The staggered QW is designed to have same peak wavelength emission at 216 nm with the conventional QW by modifying well width and Al content in the left and right side well layer. It is clear in Fig. 4 that the TE polarized emission is stronger than the TM component for the staggered QW structure, while the TM polarized emission is dominant in conventional QW. As a result, the surface emission of AlGaN-based LEDs with staggered QW structure can be enhanced significantly, and the EQEs of AlGaN-based LEDs with staggered QW structure can be improved as a result.

In summary, the optical polarization properties of staggered AlGaN-based QW structure were investigated using the theoretical model based on the $k \cdot p$ method. The particular emission wavelength equaling that of conventional AlGaN/AlN QW was realized by modifying the staggered AlGaN-based QW structure. Simulation results demonstrated that the valence subband structure including energy level order and subband coupling relation for staggered QW is beneficial to TE polarized emission. From the results of a staggered Al$_{0.82}$Ga$_{0.18}$N-Al$_{0.92}$Ga$_{0.08}$ N/AlN QW, dominant TE polarized emission with a 216 nm emission wavelength is realized. The polarization control for enhancing the surface emission using the staggered QW structure can be applied to high EQE DUV AlGaN-based LEDs.

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