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# Improvement in spontaneous emission rates for InGaN quantum wells on ternary InGaN substrate for light-emitting diodes

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The spontaneous emission characteristics of green- and red-emitting InGaN quantum wells (QWs) on ternary InGaN substrate are analyzed, and the radiative recombination rates for the QWs grown on ternary substrate were compared with those of InGaN QWs on GaN templates. For green- and red-emitting InGaN QWs on $In_{0.15}Ga_{0.85}N$ substrate, the spontaneous emission rates were found as ~2.5-3.2 times of the conventional approach. The enhancement in spontaneous emission rate can be achieved by employing higher In-content InGaN ternary substrate, which is also accompanied by a reduction in emission wavelength blue-shift from the carrier screening effect. The use of InGaN substrate is expected to result in the ability for growing InGaN QWs with enhanced spontaneous emission rates, as well as reduced compressive strain, applicable for green- and red-emitting light-emitting diodes. © *2011 American Institute of Physics*. [doi:10.1063/1.3668117]

## I. INTRODUCTION

III-Nitride semiconductors have applications for lasers[1–3] and energy-efficient technologies, including solid state lighting,[4–14] thermoelectric solid state cooling,[15,16] and photovoltaic[17] applications. Specifically, the use of InGaN alloy[4–14] is of great interest as light-emitting diodes (LEDs) active region. In the conventional approach, the growths of visible LEDs employ InGaN quantum wells (QWs) grown on GaN templates,[4–14] which lead to the existence of large QW strain arisen from the large lattice mismatch ($\Delta a/a$) between InGaN QW and GaN substrate/barrier materials. The compressive strain in InGaN QW, with respect to the GaN substrate or template, leads to large piezoelectric polarization in the QW. The large piezoelectric polarization, in addition to spontaneous polarization, leads to charge separation effect in QW, which reduces the optical matrix element in InGaN QW.[18–20] The large QW strain and charge separation issues lead to additional challenges in achieving high-efficiency green- and red-emitting InGaN QWs. Several approaches by using InGaN QWs with large overlap designs have also been pursued to address the charge separation issue.[21–28]

Previously, Shimizu and co-workers had reported the growths of InGaN ternary templates on sapphire substrates by metalorganic vapor phase epitaxy.[29] Recent works by hydride vapor phase epitaxy have also led to successful growths of high quality InGaN ternary substrates,[30,31] which are applicable for LED epitaxy.[30,31] The use of InGaN substrate has the potential for enabling the growth of InGaN QW with reduced QW strain. Recent work by Sharma and Towe[32] has pointed out the possibility of achieving emission wavelength in the green up to red spectral regimes by using InGaN QW on $In_{0.15}Ga_{0.85}N$ substrate. In addition, the use of strain-compensated InGaN/InGaN QW,[33] similar to staggered QW,[21–23] has also been proposed for green-emitting QWs on the ternary substrate. However, up to today, no comprehensive studies on the spontaneous emission characteristics of InGaN QW grown on the InGaN substrate have been reported, and these studies are important in order to clarify on the optical properties and optimized QWs grown on ternary substrates for nitride-based LEDs.

In this work, we present a study on the optical properties of InGaN QWs on ternary InGaN substrate. Specifically, the spontaneous emission rates of the InGaN QWs on $In_{0.15}Ga_{0.85}N$ substrate are compared with those of InGaN QWs on conventional GaN template for emission wavelength from green up to red spectral regimes. The spontaneous emission rate characteristics of the InGaN QW on different ternary substrates are also compared for the green-emitting active region. The band structure and wave function analysis are based on self-consistent 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism for wurtzite semiconductor taking into account the valence band mixing, strain effect, spontaneous and piezoelectric polarizations, and carrier screening effect.[34–37] The band parameters for the III-Nitride alloys used here were obtained from Refs. 37–39.

## II. CONCEPT OF InGaN QUANTUM WELLS ON TERNARY SUBSTRATES

Figure 1(a) shows the energy band lineups of 3-nm $In_{0.325}Ga_{0.675}N$ QW surrounded by $In_{0.15}Ga_{0.85}N$ barriers on the $In_{0.15}Ga_{0.85}N$ substrate with the corresponding ground state conduction subband (C1) wavefunction and the ground state valence subband (HH1) wavefunction at zone center. The lattice constant of the $In_{0.325}Ga_{0.675}N$ QW is larger than that of the $In_{0.15}Ga_{0.85}N$ barrier, which induces the compressive strain in the QW. However, by employing the ternary $In_{0.15}Ga_{0.85}N$ substrate, the lattice-mismatch between the QW and the ternary substrate is reduced in comparison with that of conventional approach, which leads to reduction in internal electrostatic field in the QW.

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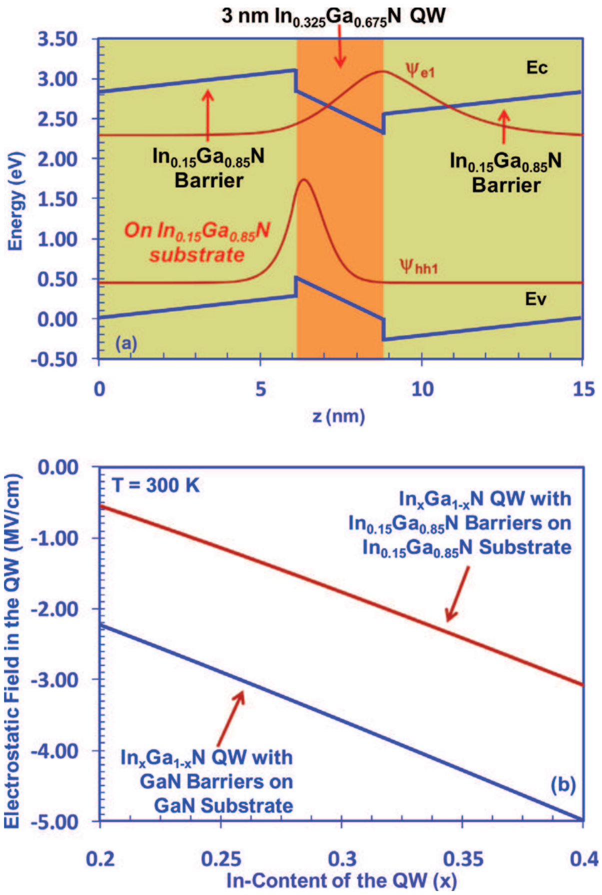


FIG. 1. (Color online) (a) The schematics of 3-nm $In_{0.325}Ga_{0.675}N$ QW with $In_{0.15}Ga_{0.85}N$ barriers on $In_{0.15}Ga_{0.85}N$ substrate with electron wavefunction EC1 and hole wave function HH1 and (b) electrostatic field in the $In_xGa_{1-x}N$ QW with $In_{0.15}Ga_{0.85}N$ barriers on $In_{0.15}Ga_{0.85}N$ substrate as a function of In-content of the QW.

Figure 1(b) shows the comparison of the internal electrostatic fields in the QWs for both $In_xGa_{1-x}N$ QW on $In_{0.15}Ga_{0.85}N$ barrier/substrate and conventional $In_xGa_{1-x}N$ QW on the GaN barrier/substrate, with the In-content ($x$) ranging from 20% up to 40%. The internal electrostatic field calculation was similar to the treatment in Ref. 36. The internal fields in the InGaN QWs grown on the ternary substrate can be reduced by ~40% up to ~75% [Fig. 1(b)], in comparison to those obtained in identical QWs grown on the conventional GaN substrate/barrier. Specifically, the internal fields in $In_{0.2}Ga_{0.8}N$ QW with GaN and $In_{0.15}Ga_{0.85}N$ substrates are −2.23 MV/cm and −0.55 MV/cm, respectively. In addition, the internal fields were calculated as −4.98 MV/cm and −3.08 MV/cm for $In_{0.4}Ga_{0.6}N$ QW/GaN substrate and $In_{0.4}Ga_{0.6}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate, respectively.

## III. SPONTANEOUS EMISSION CHARACTERISTICS OF InGaN QWs ON InGaN SUBSTRATES

Figure 2 shows the spontaneous emission spectra for both (1) $In_xGa_{1-x}N$ QWs with $In_{0.15}Ga_{0.85}N$ barriers/substrate, and (2) conventional $In_yGa_{1-y}N$ QWs with GaN barriers/substrate for green and yellow emitting QWs at carrier density ($n$) of $1 \times 10^{19}$ cm$^{-3}$ at room temperature. In designing the respective QWs for comparison purposes, the

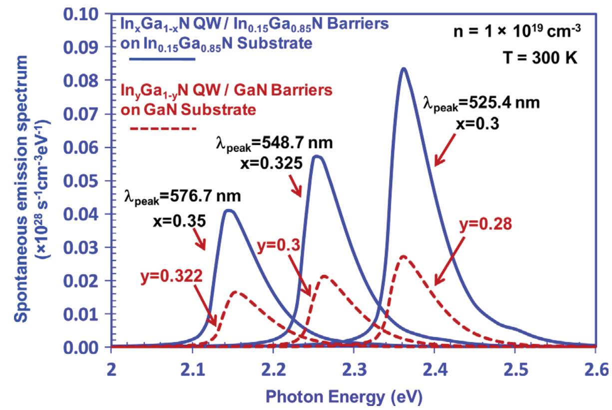


FIG. 2. (Color online) Spontaneous emission spectrum for both $In_xGa_{1-x}N$ QWs with $In_{0.15}Ga_{0.85}N$ barriers on the $In_{0.15}Ga_{0.85}N$ substrate and conventional $In_yGa_{1-y}N$ QWs with GaN barriers on the GaN substrate for green and yellow spectra regimes at $n = 1 \times 10^{19}$ cm$^{-3}$ at room temperature.

In-contents ($x$ and $y$) in the InGaN QWs were selected for similar emission wavelength at $n = 1 \times 10^{19}$ cm$^{-3}$. For green-emitting QWs at $\lambda_{peak} \sim 525.4$ nm ($\lambda_{peak} \sim 548.7$ nm), the spontaneous emission spectra peak of $In_{0.3}Ga_{0.7}N$ QW ($In_{0.325}Ga_{0.675}N$ QW)/$In_{0.15}Ga_{0.85}N$ substrate is ~3.1 times (~2.7 times) of that of $In_{0.28}Ga_{0.72}N$ QW ($In_{0.3}Ga_{0.7}N$ QW) on the conventional GaN substrate. For yellow-emitting QWs ($\lambda_{peak} \sim 576.7$ nm), the peak of the spontaneous emission spectra for $In_{0.35}Ga_{0.65}N$ QW on the $In_{0.15}Ga_{0.85}N$ substrate is ~2.5 times of that for $In_{0.322}Ga_{0.678}N$ QW on the GaN substrate. Note that the ternary substrate requires slightly higher In-content in the InGaN QW due to the less red-shift from the reduced built-in quantum confined Stark effect, however larger spontaneous emission spectra peaks are obtained for all the QWs on the ternary substrate.

Figures 3(a) and 3(b) show the spontaneous emission recombination rate per unit volume ($R_{sp}$) as a function of carrier density for both green- and yellow-emitting QWs at T = 300 K. For the green-emitting QWs ($\lambda_{peak} \sim 548.7$ nm) [Fig. 3(a)], the $R_{sp}$ of $In_{0.325}Ga_{0.675}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate was calculated as ~3.2 times of that of conventional $In_{0.3}Ga_{0.7}N$ QW/GaN substrate at $n = 2 \times 10^{19}$ cm$^{-3}$. For the yellow emitting QWs ($\lambda_{peak} \sim 576.7$ nm) [Fig. 3(b)], the $R_{sp}$ of $In_{0.35}Ga_{0.65}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate is ~2.9 times of that of $In_{0.322}Ga_{0.678}N$ QW/GaN substrate at $n = 2 \times 10^{19}$ cm$^{-3}$. The improved $R_{sp}$ of InGaN QWs on the ternary substrate can be attributed to the larger optical matrix elements arisen from the reduced strain and internal field in the QW.

Figure 4(a) shows the spontaneous emission spectrum for $In_xGa_{1-x}N$ QWs with $In_{0.15}Ga_{0.85}N$ barriers on $In_{0.15}Ga_{0.85}N$ substrate with various In-contents ($x$) calculated for $n = 1 \times 10^{19}$ cm$^{-3}$ at room temperature. By employing the $In_{0.15}Ga_{0.85}N$ substrate, large peaks of the spontaneous emission spectra can be obtained for InGaN QWs with peak emission wavelengths covering from blue ($3.98 \times 10^{27}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$, $\lambda_{peak} = 452.6$ nm) up to red ($2.23 \times 10^{26}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$, $\lambda_{peak} = 645.8$ nm) spectral regimes. The peaks of the spontaneous emission spectra decrease with longer emission wavelength, which is related to the increasing charge separation effect. In order to provide

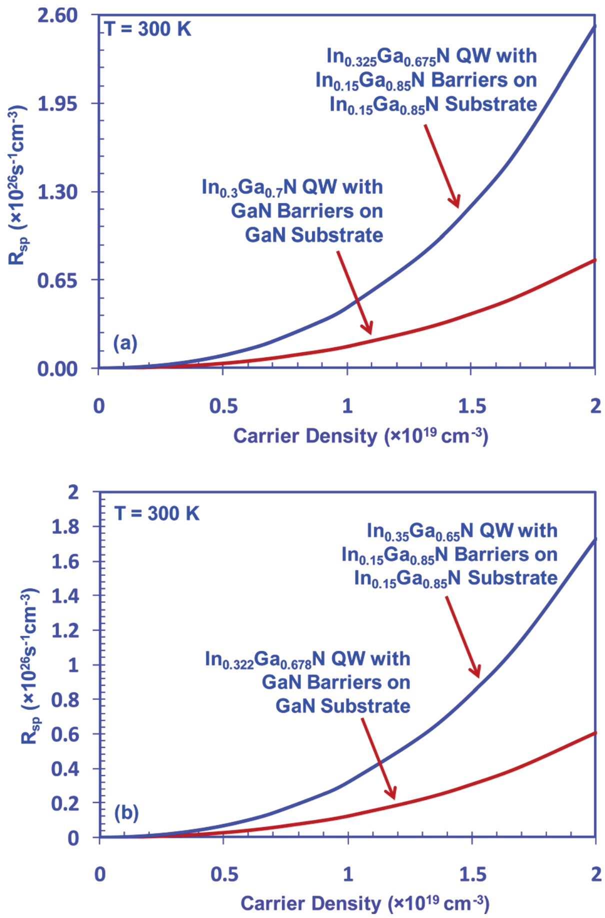


FIG. 3. (Color online) Comparison of $R_{sp}$ as a function of carrier density for (a) $In_{0.325}Ga_{0.675}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate and conventional $In_{0.3}Ga_{0.7}N$ QW/GaN substrate and (b) $In_{0.35}Ga_{0.65}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate and conventional $In_{0.322}Ga_{0.678}N$ QW/GaN substrate.

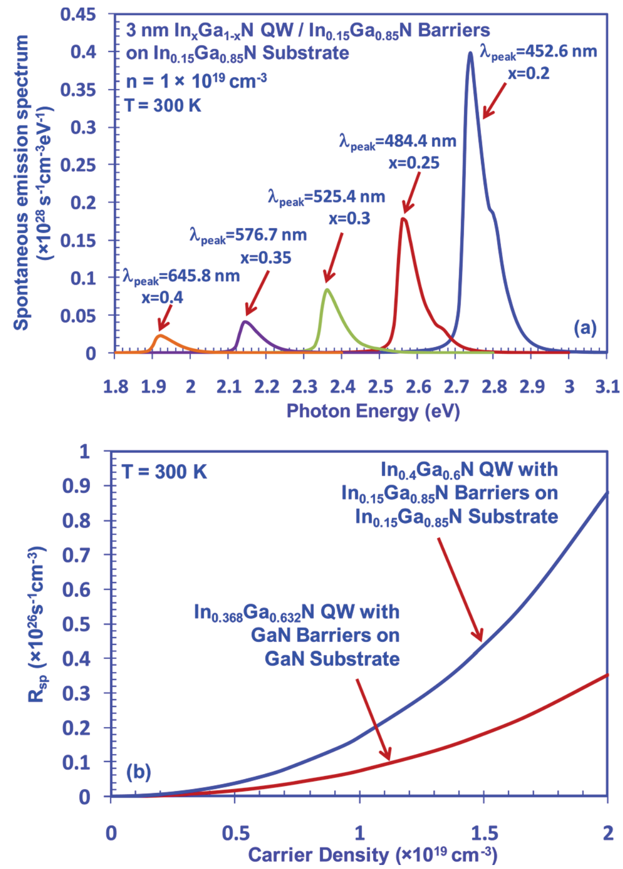


FIG. 4. (Color online) (a) Spontaneous emission spectrum for both $In_xGa_{1-x}N$ QWs/$In_{0.15}Ga_{0.85}N$ substrate from blue up to red spectral regimes at $n = 1 \times 10^{19}$ cm$^{-3}$ at room temperature and (b) comparison of $R_{sp}$ as a function of carrier density for $In_{0.4}Ga_{0.6}N$ QWs/$In_{0.15}Ga_{0.85}N$ substrate and conventional $In_{0.368}Ga_{0.632}N$ QWs/GaN substrate.

comparison for red-emitting QWs, Fig. 4(b) shows the comparison of the $R_{sp}$ as a function of carrier density up to $n = 2 \times 10^{19}$ cm$^{-3}$ for $\lambda_{peak} \sim 645$ nm. The $R_{sp}$ of the $In_{0.4}Ga_{0.6}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate was obtained as ~2.5 times of that of $In_{0.368}Ga_{0.632}N$ QW/GaN substrate at $n = 2 \times 10^{19}$ cm$^{-3}$. The significantly-improved $R_{sp}$ for InGaN QWs on the ternary substrate for emission wavelength across green and red spectral regimes confirm the strong potential for the use of ternary substrate to achieve high efficiency green- and red-emitting LEDs.

## IV. EFFECT OF TERNARY SUBSTRATE COMPOSITION ON SPONTANEOUS EMISSION OF InGaN QW

Figure 5 shows the comparison of the spontaneous emission spectrum for the $In_{0.3}Ga_{0.7}N$ QW on ternary InGaN substrates with In-contents from 5% to 20% calculated for $n = 1 \times 10^{19}$ cm$^{-3}$ at room temperature, as the In-contents of the commercially-available InGaN substrates range from 5% up to 20%.[30,31] The emission wavelengths of the $In_{0.3}Ga_{0.7}N$ QW show red-shift with lower In-content InGaN substrates. The peaks of the spontaneous emission spectra are larger for $In_{0.3}Ga_{0.7}N$ QW on higher In-content InGaN substrates ($1.5 \times 10^{27}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$ with $\lambda_{peak} = 521$ nm for $In_{0.2}Ga_{0.8}N$ substrate), which can be attributed to the reduced lattice-mismatch strain and internal electrostatic fields in the QW.

The comparison of the wavelength shifts for $In_{0.3}Ga_{0.7}N$ QW on different ternary $In_yGa_{1-y}N$ substrates ($y = 5\%$ – 20%) are shown in Table I. The peak spontaneous emission wavelengths show blue-shift at higher carrier density ($n = 2 \times 10^{19}$ cm$^{-3}$) for the $In_{0.3}Ga_{0.7}N$ QW with ternary substrates. The blueshift is suppressed by employing higher

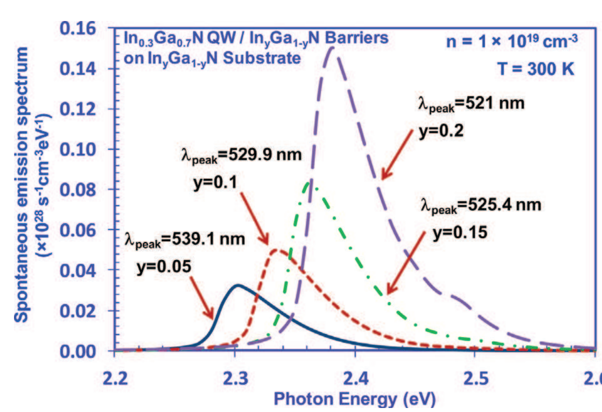


FIG. 5. (Color online) Spontaneous emission spectrum for $In_{0.3}Ga_{0.7}N$ QW on $In_yGa_{1-y}N$ substrates ($y = 5\%$ - 20%) at $n = 1 \times 10^{19}$ cm$^{-3}$ at room temperature.

TABLE I. The transition energy blue-shifts for $In_{0.3}Ga_{0.7}N$ QW on different ternary $In_yGa_{1-y}N$ substrates (y = 5% – 20%).

| Substrate composition | $In_{0.05}Ga_{0.95}N$ | $In_{0.1}Ga_{0.9}N$ | $In_{0.15}Ga_{0.85}N$ | $In_{0.2}Ga_{0.8}N$ |
|---|---|---|---|---|
| E21 at $n = 1 \times 10^{18}$ cm$^{-3}$ | 2.24 eV | 2.28 eV | 2.30 eV | 2.33 eV |
| E21 at $n = 2 \times 10^{19}$ cm$^{-3}$ | 2.37 eV | 2.39 eV | 2.42 eV | 2.42 eV |
| Blue-shift | 130 meV | 110 meV | 120 meV | 90 meV |

In-content InGaN substrate, as the lower lattice-mismatch strain leads to the reduction of the internal field. Specifically, the blue-shift of 90 meV is obtained for the $In_{0.3}Ga_{0.7}N$ QW/$In_{0.2}Ga_{0.8}N$ substrate (Table I), which is 40 meV less than that for $In_{0.3}Ga_{0.7}N$ QW/$In_{0.05}Ga_{0.95}N$ substrate.

Figure 6 shows the comparison of $R_{sp}$ as a function of carrier density up to $n = 2 \times 10^{19}$ cm$^{-3}$ for $In_{0.3}Ga_{0.7}N$ QW with $In_yGa_{1-y}N$ substrates (y = 5% – 20%) targeting at green spectral emission. The $R_{sp}$ of $In_{0.3}Ga_{0.7}N$ QW/$In_{0.2}Ga_{0.8}N$ substrate was obtained as ~6 times of that of $In_{0.3}Ga_{0.7}N$ QW/$In_{0.05}Ga_{0.95}N$ substrate at $n = 2 \times 10^{19}$ cm$^{-3}$. Therefore, by employing the ternary substrate with less lattice-mismatch to the InGaN QW, this approach leads to increase in spontaneous emission rate attributed to the reduced charge separation issue in the QW.

The comparison of the peak emission wavelengths as a function of $R_{sp}$ for $In_{0.3}Ga_{0.7}N$ QWs with various $In_yGa_{1-y}N$ substrates (y = 5% – 20%) at room temperature is shown in Fig. 7. As the carrier injection in the $In_{0.3}Ga_{0.7}N$ QWs with various ternary substrates increases, the spontaneous emission rate of the QWs increases. As the spontaneous emission rates for all QW structures increase, the peak emission wavelengths also reduce due to the carrier screening effect. The use of lower In-content $In_yGa_{1-y}N$ substrates (y = 5%, and 10%) leads to relatively low spontaneous emission rate, which is also accompanied by large emission wavelength blueshift. In contrast, the use of higher In-content InGaN substrates (y = 15%, and 20%) leads to large spontaneous emission rate, as well as the significantly reduction in wavelength blueshift. Specifically, the use of $In_{0.2}Ga_{0.8}N$ ternary substrate exhibits relatively low blue-shift (~10 nm) for achieving spontaneous emission rate ($R_{sp}$) of $R_{sp}$ ~$3.76 \times 10^{26}$ s$^{-1}$ cm$^{-3}$, while the use of the $In_{0.15}Ga_{0.85}N$ ternary substrate will lead to blue-shift up to ~20 nm for achieving a similar spontaneous emission rate.

## V. SUMMARY

Despite the potential advantages of the ternary InGaN substrate for LED applications, it is important to note that the development of InGaN substrates is still at a relatively early stage.[29–31] Further advances in the development of high quality InGaN substrate are of great importance for realizing high-efficiency LEDs based on this technology.

Note that our current studies are primarily focused on the investigation of the spontaneous emission characteristics of the InGaN QWs on various ternary InGaN substrates as active regions for green- and red-emitting LEDs. However, future studies to investigate the optimized structures and compositions of the InGaN QW and barrier combinations on ternary substrates are of interest for achieving further improvement in the spontaneous emission rate of the LEDs active regions in particular for emission in the green up to red spectral regimes.

In summary, the spontaneous emission characteristics of InGaN QWs on the ternary $In_{0.15}Ga_{0.85}N$ substrate emitting in green and red spectral regimes are analyzed. The $R_{sp}$ of the green- and yellow-emitting InGaN QWs grown on $In_{0.15}Ga_{0.85}N$ substrate were found as ~2.9–3.2 times of those of QWs grown on the conventional GaN substrate. For red-emitting $In_{0.4}Ga_{0.6}N$ QW/$In_{0.15}Ga_{0.85}N$ substrate, the $R_{sp}$ was ~2.5 times of that of the conventional approach. By using higher In-content InGaN substrates, a significant increase in spontaneous emission rate and reduction in blue-shift from carrier-screening effect are observed. The use of the ternary InGaN substrate leads to reduction in QW strain and increase in optical matrix element, which in turn results in large spontaneous emission rates for InGaN QWs applicable for green- and red-emitting LEDs.

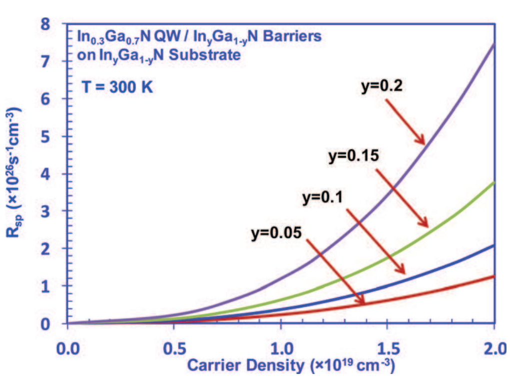


FIG. 6. (Color online) Comparison of $R_{sp}$ as a function of carrier density for $In_{0.3}Ga_{0.7}N$ QW with $In_yGa_{1-y}N$ substrates (y = 5% – 20%).

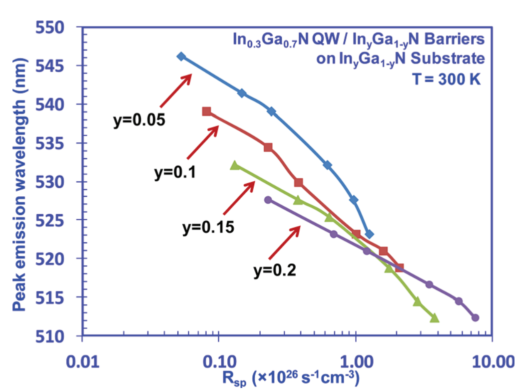


FIG. 7. (Color online) Peak emission wavelength as a function of $R_{sp}$ for $In_{0.3}Ga_{0.7}N$ QW with $In_yGa_{1-y}N$ substrates (y = 5% – 20%) at room temperature.

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