# Delta InN-InGaN Quantum Wells With AlGaN Interlayers for Long Wavelength Emission

Ioannis E. Fragkos, Wei Sun, Damir Borovac, Renbo Song, Jonathan J. Wierer, Jr., *Senior Member, IEEE*, and Nelson Tansu, *Fellow, IEEE*

***Abstract*— An active region design based on InGaN / delta-InN quantum well (QW) with AlGaN interlayer (IL) and GaN barriers (delta-structure) is investigated for potential high-efficiency visible light emitters. Numerical simulations demonstrate a large wavelength redshift with a simultaneous increase of the electron-hole wavefunction overlap for the delta-structure as compared to the conventional InGaN QW with AlGaN IL and GaN barriers. Proof of concept experimental growths via the metalorganic chemical vapor deposition demonstrate the effect of the delta-InN insertion into the conventional InGaN-based QW.**

***Index Terms*— Light emitters, III-nitrides emitters, indium gallium nitride, III-nitride semiconductors, semiconductor physics, semiconductor optoelectronics, solid-state lighting, delta structure, delta indium nitride, indium nitride, pulsed MOCVD growth.**

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Ioannis E. Fragkos was with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA. He is now with Rockley Photonics Inc., Pasadena, CA 91101 USA (e-mail: i.e.fragkos@gmail.com).

Wei Sun was with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA. He is now with II–VI Incorporated, Sherman, TX 75090 USA.

Damir Borovac was with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA. He is now with OSRAM Opto Semiconductors GmbH, 93055 Regensburg, Germany.

Renbo Song is with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA.

Jonathan J. Wierer, Jr., was with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA. He is now with the Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27606 USA.

Nelson Tansu was with the Department of Electrical and Computer Engineering, Lehigh University, Bethlehem, PA 18015 USA, and also with the Center for Photonics and Nanoelectronics, Lehigh University, Bethlehem, PA 18015 USA. He is now with the School of Electrical and Electronic Engineering (EEE) and the Institute for Photonics and Advanced Sensing (IPAS), The University of Adelaide, Adelaide, SA 5005, Australia (e-mail: nelson.tansu@adelaide.edu.au).

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## I. Introduction

In RECENT years, the pursuit of high-efficiency InGaN-based quantum well (QW) light emitters towards the red spectral regime has proved challenging. The need for higher In-content in the InGaN active region to achieve longer wavelength emission results in phase separation of the InGaN alloy, defect formation due to lattice mismatch with the GaN substrates, and higher polarization fields which reduce the wavefunction overlap (Γe-h) between electrons and holes inside the QW. These factors are detrimental to the internal quantum efficiency (IQE) of the emitter and have resulted in the well-known "green-gap" problem [1]–[5]. The challenges for high In-content InGaN have hindered the development of relatively high-efficiency visible light emitters - without the need of phosphor down conversion - that could exploit a full-color gamut and enable LED devices for solid-state lighting and display applications [6].

Several theoretical and experimental approaches have been proposed to overcome these issues including, staggered InGaN QWs, strain compensated InGaN QWs, semipolar and non-polar InGaN QWs, ternary substrates and buffer layers, and high bandgap thin interlayers that cap the InGaN QW [7]–[23]. Recently, special research interest has been given for the latter, since the use of AlGaN and AInN inter-layers has resulted in the highest efficiencies in the red and green spectral regime [23]. In addition to the above solutions, a different approach that eliminates the need for high In-content has been proposed. In particular, theoretical studies have shown that inserting an ultra-thin layer [delta($\delta$)-like] of InN (~6 nm) in the middle of a conventional 3.0 nm $In_{0.25}Ga_{0.75}N$ QW with GaN barriers results in a significant wavelength shift towards the red spectral regime (~740 nm) with enhanced wavefunction overlap ($\Gamma_{e-h}$~50%) [24].

Experimental verification, via metalorganic chemical vapor deposition, of $\delta$-InN designs is challenging because of the evaporation and decomposition of In from the layer during the high-temperature GaN barrier growth. More specifically, the large discrepancy in growth temperatures between the InN (<600 °C), InGaN (~700 °C), and GaN (~850 °C) layers result in the decomposition and out-diffusion of In during the growth of the GaN barrier growth [25]–[29], thus creating a challenge to integrate $\delta$-InN layers.

This challenge can be addressed by growing an AlGaN interlayer at the same temperature as the $\delta$-InN layer (<600 °C) to cap and prevent decomposition at the higher

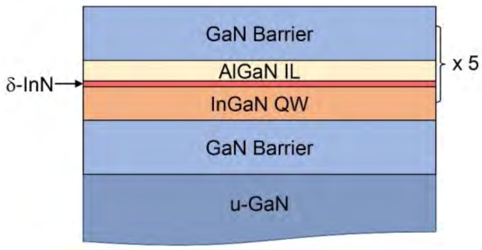


Fig. 1. Novel active region design consisted of an InGaN QW, $\delta$-InN and AlGaN interlayer between GaN barriers.

temperature growth of the GaN barrier [28], [29]. The capping and decomposition concept using an AlGaN IL has been demonstrated in conventional InGaN QWs. In addition, the AlGaN IL enables concurrent thermal annealing of the underlying layers during high-temperature GaN barrier growth, proving beneficial to the InGaN QW [19]. Moreover, despite the low-temperature growth of the AlGaN IL, it too experiences an improvement in crystal quality during the high-temperature GaN barrier growth [19].

The work presented in this letter exploits the concept of the $\delta$-InN layer in combination with a thin AlGaN interlayer (IL) integrated into a conventional InGaN QW with GaN barriers ($\delta$-structure) to achieve a high-efficiency long-wavelength emitter. The $\delta$ -structure depicted in Figure 1 is different from the one presented in reference [24], since it consists of a $\delta$-InN layer placed on top of the InGaN QW - rather than in the middle - followed by the AlGaN IL. Numerical simulations were carried out based on a six-band k.p formalism for wurtzite structure, considering crystal strain, valence band mixing, polarization fields, and carrier screening [9]. The energy band structure, wavefunction overlap, and spontaneous emission rates were calculated for the $\delta$-structure and compared to a reference structure. The reference structure consists of an InGaN QW, AlGaN IL, and GaN barriers with the same layer thicknesses and compositions as the $\delta$-structure.

## II. Numerical Simulations

Figure 2(a) and 2(b) depict the band structure of the reference and the $\delta$-structures, respectively. The reference structure consisted of a 2.6 nm thick $In_{0.2}Ga_{0.8}N$ QW with 1 nm thick $Al_{0.40}Ga_{0.60}N$ IL and 5 nm thick GaN barriers, while the $\delta$-structure has an additional 0.6 nm thick $\delta$-InN layer inserted between the $In_{0.20}Ga_{0.80}N$ QW and $Al_{0.40}Ga_{0.60}N$ IL. The reference structure is characterized by a transition (emitted) wavelength of $\lambda = 437$ nm, which is the blue spectral regime with an electron-hole (e-h) wavefunction overlap of $\Gamma_{e-h} = 43\%$. As presented in reference [24], the incorporation of a very thin $\delta$-InN layer with a much lower bandgap decreases the energy transition levels both in the condition band and valence band of the quantum well. It also redshifts the emitting wavelength. As shown in Figure 2(b), the insertion of the $\delta$-InN layer redshifts the transition wavelength from 437 nm to 634 nm (red) but at the expense of the e-h wavefunction overlap $\Gamma_{e-h}$, which is dramatically reduced to 3% as compared to the reference structure.

It is important to mention that the thickness of the inserted $\delta$-InN layer is close to its critical value of 0.6 nm, which

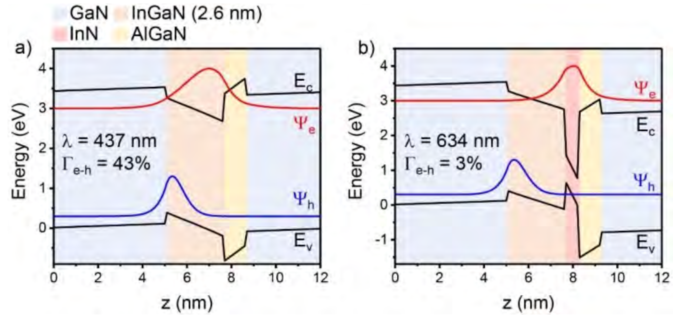


Fig. 2. Numerical simulations of band-structure and e/h wavefunction profile of (a) reference structure consisted of 2.6 nm $In_{0.20}Ga_{0.80}N$ QW + 5 monolayers $Al_{0.40}Ga_{0.60}N$ interlayer between 5 nm GaN barriers, and (b) $\delta$-structure consisted of 2.6 nm $In_{0.20}Ga_{0.80}N$ QW + 2 monolayers (0.6 nm) $\delta$-InN + 5 monolayers $Al_{0.40}Ga_{0.60}N$ inter-layer between 5 nm GaN barriers.

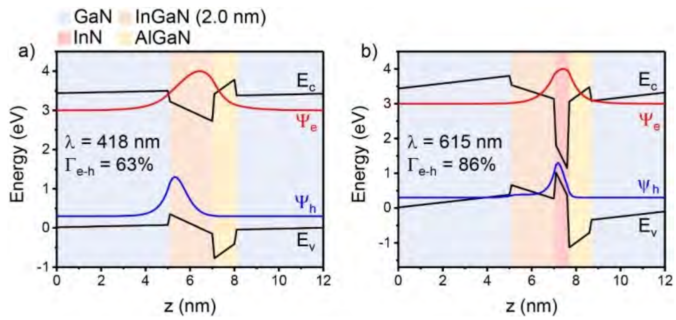


Fig. 3. Numerical simulations of band-structure and e/h wavefunction profile of (1) reference structure consisted of a 2.0 nm thick $In_{0.20}Ga_{0.80}N$ QW and 5 monolayers $Al_{0.40}Ga_{0.60}N$ interlayer between 5 nm GaN barriers, and b) $\delta$-structure consisted of a 2.0 nm thick $In_{0.20}Ga_{0.80}N$ QW, 2 monolayers (0.6 nm) of $\delta$-InN, and 5 monolayers of $Al_{0.40}Ga_{0.60}N$ inter-layer between 5 nm thick GaN barriers.

corresponds to a few monolayers ($\sim$ 2) of InN [30]. The main reason for the low e-h wavefunction overlap of the $\delta$-structure is the holes in the valence band. As shown in Figure 2(a), the peak of the hole wavefunction ($\Psi_h$) of the reference structure is located at the GaN/InGaN heterointerface, and its position does not change with the insertion of the $\delta$-InN layer. At the same time, the electrons move into the $\delta$-InN layer (Figure 2(b)).

To increase the e-h wavefunction overlap ($\Gamma_{e-h}$) in the $\delta$-structure, the peak of the $\Psi_{e-h}$ has to be shifted towards the $\delta$-InN layer. A simple way to accomplish this is to reduce the thickness of the InGaN layer. Figure 3(b) presents the case where the InGaN layer thickness is reduced to 2.0 nm. By doing so, the peak of the hole wavefunction is shifted into the $\delta$-InN layer, increasing the e-h wavefunction overlap Γe-h to 86% with an emitted wavelength $\lambda = 615$ nm. Figure 3(a) corresponds to a reference structure with a 2 nm thick $In_{0.20}Ga_{0.80}N$ layer. It is evident that the $\delta$-InN layer itself does not help achieve large e-h wavefunction overlap in this particular novel active region design. The thickness of the InGaN layer is very crucial. From the numerical calculations, it was observed for thin InGaN layers <2 nm with a few inserted monolayers of $\delta$-InN and an AlGaN IL, the $\delta$-structures will result in very high wavefunction overlap with a simultaneous wavelength shift towards red wavelengths compared to the reference structure without the $\delta$-InN layer.

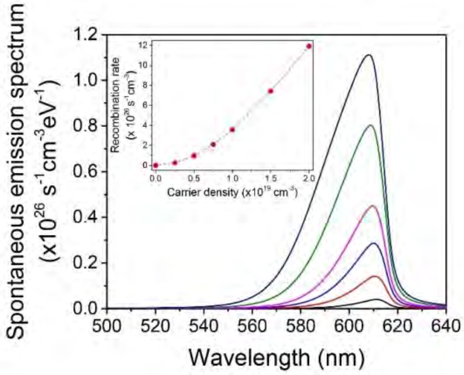


Fig. 4. Spontaneous emission spectra and radiative recombination rate of a $\delta$-structure consisted of a 2.0 nm thick $In_{0.20}Ga_{0.80}N$ QW, 2 monolayers (0.6 nm) of $\delta$-InN, and 5 monolayers of $Al_{0.40}Ga_{0.60}N$ between 5 nm thick GaN barriers.

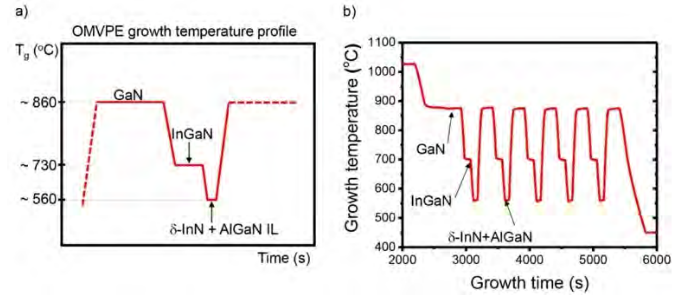


Fig. 5. (a) MOCVD growth temperature profile of 1 period of the $\delta$-structure. (b) Actual growth temperature profile of a 5 period $\delta$-structure. The reference structures exhibit similar growth temperature profile.

In addition to the wavelength shift and the high e-h wavefunction overlap, the $\delta$-InN structure should exhibit very high carrier injection efficiencies if the active region is implemented for LEDs. The high bandgap material of the AlGaN IL can act as an effective barrier for the injected electrons and holes into the active region by preventing them from thermionic escape from the quantum well [31]. It is ubiquitous in conventional InGaN QW-based LEDs to observe a blueshift of the emitted photon energy with increased injection current. This blueshift is attributed to 1) in the band-filling effect of localized energy states formed by potential profile fluctuations (due to In composition fluctuations) and 2) carrier screening of the strain-induced polarization fields (those fields are responsible for the quantum confined stark effect (QCSE). The carrier screening of the QCSE flattens the potential across the MQWs, increasing the quantum energy states into the QW.

For the case of the $\delta$-structure, the QCSE is expected to be strong enough (due to the significant lattice mismatch among the $\delta$-InN and AlGaN IL) so that the presence of the carries will not be able to screen it. This screening will result in a slight blueshift of the emitted wavelength of the spontaneous emission spectrum (assuming that there is not In-composition fluctuation into the active region of the $\delta$-structure). This peak stability can be seen in Figure 4 where the peak of the spontaneous emission spectrum of the $\delta$-structure increases from $0.04 \times 10^{26}$ to $1.12 \times 10^{26}$ $s^{-1}cm^{-3}eV^{-1}$ while the carrier density, n, increases from $2.5 \times 10^{18}$ to $2 \times 10^{19}$ $cm^{-3}$ respectively, with no observed blueshift on the transition wavelength.

## III. Proof-of-Concept Experiments

The numerical simulations indicate the $\delta$-structure with a relatively thin InGaN QW and an AlGaN IL can be used as a highly efficient light-emitting active layer. Proof-of-concept experiments are carried out to demonstrate the concept of the $\delta$-structure presented in this work. The proof-of-concept experiments were similar to the simulations and are divided into two parts. In the first part, the $\delta$-structure was studied for a $\sim$3 nm thick $In_{0.15}Ga_{0.85}N$ QW with $\sim$1 nm thick $Al_{0.40}Ga_{0.60}N$ IL, and for the second part, the $\delta$-structure was studied for a $\sim$2 nm thick $In_{0.15}Ga_{0.85}N$ with a QW $\sim$1 nm thick $Al_{0.40}Ga_{0.60}N$ IL. The composition of the InGaN layers among the two experimental parts are varied slightly, but this does not significantly alter the concept of the wavelength shift and e-h wavefunction overlap changes of the $\delta$-structures with respect to their reference structures.

As described in the introduction, the new design of the $\delta$-structure enables the experimental verification via the MOCVD. However, an issue that needs to be taken under consideration is the growth of the pure InN $\delta$-layer to prevent the presence of metallic-In. It is well known that the MOCVD growth of InN imposes very narrow optimized growth conditions, which are limited by the ammonia (NH3) dissociation and metallic-In formation. Nevertheless, this issue can be overcome by employing a pulsed MOCVD growth mode for the InN layer, which results in high quality, metallic-In-free InN films [25]–[29].

The structures investigated in this study are depicted in Figure 1. The epitaxy of the structures was done in a vertical-flow shower-head type Veeco-P75 reactor under a growth pressure of 200 Torr. Ammonia was used as the group-V precursor, while triethylgallium (TEGa), trimethylindium (TMIn), and trimethylaluminum (TMAl) were used as group-III precursors for the III-nitride layers. Five periods of InGaN/ $\delta$-InN / AlGaN / GaN were grown on top of a 3 um thick n-doped GaN ($3 \times 10^{16}$ $cm^{-3}$) templates on a patterned c-plane sapphire substrate. The growth temperature profile of the structure is depicted in Figure 5. The InGaN layers were grown at $\sim$730 °C, while the GaN barriers were at $\sim$860 °C. To accommodate the growth of the InN at $\sim$560 °C, pulsed-the pulsed MOCVD growth was employed. During the growth of the InN $\delta$ -layer, the NH3 was constantly running into the reactor while the TMIn precursor was pulsed. Following the growth of the $\delta$-InN layer, the AlGaN layer was grown via the normal-MOCVD growth mode (constant metalorganic flow) at the same temperature of $\sim$560 °C.

To study the effect of the $\delta$-InN, a second structure without the $\delta$-InN layer was grown under the same growth temperature profile. Both MQW structures consisted of a $\sim$3 nm thick $In_{0.15}Ga_{0.85}N$ QW, $\sim$5 monolayers ($\sim$1 nm) thick $Al_{0.40}Ga_{0.60}N$ IL, and a $\sim$10 nm thick GaN barrier, all repeated 5 times. For the structure with the $\delta$-InN layer, the growth conditions of the pulsed growth mode were optimized

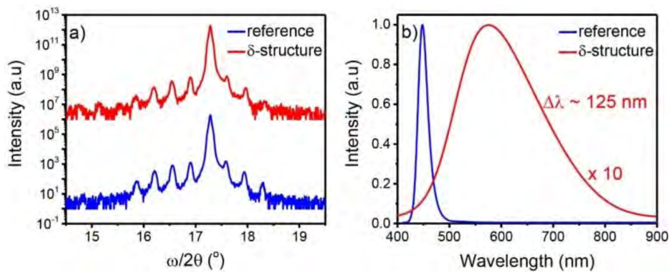


Fig. 6. (a) (002) plane X-ray $\omega/2\theta$ XRD scans, and (b) photoluminescence spectra of the reference and $\delta$-structure with a 3 nm thick InGaN layer.

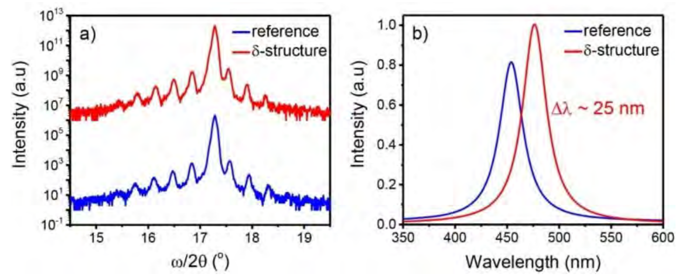


Fig. 7. (a) (002) plane X-ray $\omega/2\theta$ XRD scans, and (b) photoluminescence spectra of the reference and $\delta$-structure with a 2 nm thick InGaN layer.

to achieve metallic-In-free $\delta$-InN layer with nominal thickness of ~0.6 nm [28], [29]. This thickness of the $\delta$-InN layer corresponds to ~2 monolayers (~0.6 nm) which is the optimum thickness for the fully strained InN layer [30]. The two structures were characterized using a coupled $\omega/2\theta$ scan in the (002) - growth direction - via an X-ray diffractometer. As it can be seen in Figure 6(a), both structures exhibit sharp diffraction peaks, which is an indication that the crystallinity of the MQWs is maintained, despite the low growth temperature of AlGaN IL and the introduction of the $\delta$-InN layer. We believe that the high growth temperature of the GaN barriers assists in the re-crystallization of the $\delta$-InN and AlGaN IL, which in turn improves the overall crystal quality of the structure. It is also important to notice that despite the introduction of the $\delta$-InN layer, the picture of the X-ray $\omega/2\theta$ scan for the $\delta$-structure does not significantly change. One would expect smaller fringes between the satellite peaks for the MQW $\delta$-structure. However, the very thin layer of the $\delta$-InN in combination with the low resolution of the XRD diffractometer cannot detect its presence. Any detected signal would be buried into the noise between the adjacent picks of the MQW $\delta$-structure.

The PL spectra of both structures are depicted in Figure 6(b). A 405 nm laser with a 95 mW power was used as the excitation source. The reference structure has a sharp luminescence with a peak wavelength of $\lambda = 448$ nm. With the insertion of the $\delta$-InN layer, the structure exhibits a lower intensity and a redshifted peak wavelength of $\lambda = 571$ nm. (Note, to measure the signal, the integration time of the digital spectrophotometer had to be increased by 10 times to that of the reference structure.) Although the measured emitted wavelength is in the yellow region of the spectrum, it cannot be discounted that this PL signal is yellow band luminescence of the GaN substrate and the active layer luminescence is weaker. In addition, considering the fact that the $\delta$-structure maintains relatively good crystal quality, according to the XRD spectrum, the very low luminescence could not be due to bad crystal quality. The reason for the low luminescence is most probably associated with poor e-h wavefunction overlap, as predicted from the numerical simulations.

The second part of the proof-of-concept experiments consists of a reference and $\delta$-structure. The reference structure consisting of a ~2 nm thick $In_{0.15}Ga_{0.85}N$ QW, ~1 nm thick $Al_{0.40}Ga_{0.60}N$ IL, and ~10 nm thick GaN barrier repeated 5 times. The $\delta$-structure is the same with the addition of

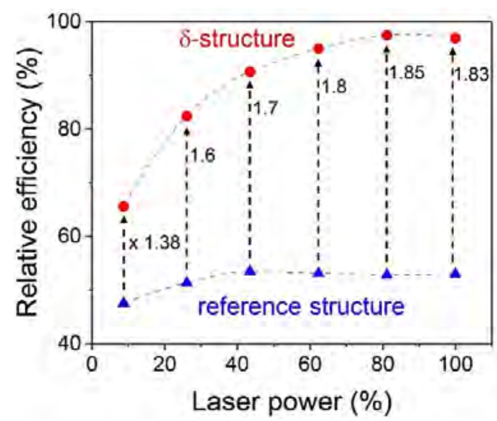


Fig. 8. Relative efficiencies versus excitation powers with a 405 nm laser for the reference and $\delta$-structure with 2 nm thick InGaN layer.

the $\delta$ -InN layer at ~0.6 nm thickness after the InGaN QW. Figure 7(a) shows the X-ray $\omega/2\theta$ scans of both structures. Sharp satellite peaks are observed, which is an indication of the excellent crystal quality of the structures.

Both structures were excited with a 405 nm laser at 95 mW power. The PL signal is depicted in Figure 7(b), both samples measured on the same scale. The reduction in the thickness of the InGaN layer to ~2 nm results in an increased luminescence for the $\delta$-structure from approximately 40000 to 49000 (1.22 times). The peak wavelength is slightly increased from 450 nm to 475 nm for the reference structure. This result is consistent with the overlap found in the numerical calculations for a 2 nm InGaN layer, where the reference structure exhibits an e-h wavefunction overlap $\Gamma e{-}h$ ~63% while the $\delta$-structure has $\Gamma e{-}h$ ~83% (1.36 times). However, the shift of the emitted wavelength is very small at ~25 nm.

These results indicate that the reduction of the thickness of the InGaN layer and the insertion of the $\delta$-InN layer improves the emitter's radiative efficiency and shifts the emitted wavelength as opposed to the structure with a thicker InGaN layer where the insertion of the $\delta$-InN layer completely eliminated the photoluminescence. However, it is important to mention that the experimental structures are not ideal, i.e., they most likely do not exhibit abrupt heterointerfaces and neither coherently strained and uniform layers as it is assumed for the numerical calculations. The above factors will certainly introduce unwanted crystal defects during the growth of the structures and shift the layers' energy states, which will impact their properties. This is the reason for the observed discrepancy in the absolute values of the wavelength shift between the simulation and the experiment. Further, improving the MOCVD process or even switching to molecular beam epitaxy (MBE), where the uniformity of the layers and strain are better controlled, may improve the properties of the $\delta$-structures. Nevertheless, the numerical calculations and the simulations should serve as a guide for the experimental design. The experimental trends are consistent with the trends of the numerical calculations presented in this work.

Figure 8 depicts a relative efficiency of the $\delta$-structure with respect to the reference structure with a 2 nm thick InGaN layer. The relative efficiency is defined as the integral of the PL spectra in the range of 350 nm - 550 nm over the relative output power of the laser (maximum output power of 350 mW at 100%). The $\delta$-structure exhibits almost 1.85 times higher efficiency than the reference structure. This is an indication that the insertion of the $\delta$-InN layer enhanced to some degree the wavefunction overlap, improving the internal quantum efficiency of the active layers.

## IV. Conclusion

In summary, an active region design of InGaN / delta-InN quantum well with AlGaN interlayer has been proposed to achieve high-efficiency visible light emitters at longer wavelengths. This design enables experimental demonstration via MOCVD because it helps to overcome the evaporation and decomposition of the $\delta$-InN layer during the growth of the structure. In particular, the growth of the thin AlGaN interlayer following the growth of the $\delta$-InN layer at the same temperature prevents the evaporation and decomposition of the InN during the high-temperature GaN barrier growth. In addition, the high-temperature GaN barrier growth anneals the underlying layers and improves the overall quality of the structure. The experimental trends are consistent with the numerical calculations which show (1) a $\delta$-structure with relatively thick InGaN layer reduces the e-h wavefunction overlap and reduces the efficiency of the emitter as compared to the reference structure, and b) a $\delta$-structure with a relatively thin InGaN layer provides a wavelength shift towards the and exhibits higher efficiencies compared to the reference structure.

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**Ioannis E. Fragkos** received the B.S. degree in physics and the M.S. degree in opto-microelectronics from the Department of Physics, University of Crete, Greece, in 2010 and 2012, respectively, and the Ph.D. degree in electrical engineering from Lehigh University, Bethlehem, PA, USA, in 2019. He was previously a Research Fellow with UNINOVA–Institute for the Development of New Technologies, Lisbon, Portugal, from 2012 to 2013. He is currently a Senior Laser Design Engineer at Rockley Photonics Inc., Pasadena, CA, USA. His research interests include the design, growth, and characterization of active and passive devices for photonic applications.

**Wei Sun** received the B.S. degree from the Department of Electrical and Information Engineering, Beijing Institute of Technology, in 2009, and the M.B.A. and Ph.D. degrees in electrical engineering from Lehigh University in 2014 and 2019, respectively. Currently, he is a Lead Design Engineer at II–VI Incorporated, Sherman, TX, USA. His research interests include the design, epitaxy, and characterization of high-speed and wide bandgap photonic devices.

**Damir Borovac** received the B.S. and Ph.D. degrees in electrical engineering from Lehigh University in 2015 and 2020, respectively. He is now working as a Hardware Development Engineer at OSRAM Opto Semiconductors GmbH, Regensburg, Germany. His research interests include III-nitride material science and device physics. He has (co)authored over 60 publications and conference publications.

**Renbo Song** received the B.S. and M.S. degrees in optics and condensed matter physics from Shandong University, China, 1998 and 2001, respectively, and the Ph.D. degree in electrical engineering from Lehigh University, Bethlehem, PA, USA, in 2009. He worked as an MOCVD Scientist at Valence Process Equipment from 2011 to 2015, and since then as a Scientific Manager at Lehigh University. His areas of interests include MOCVD and new epitaxy technologies for wide bandgap semiconductors.

**Jonathan J. Wierer, Jr.** (Senior Member, IEEE) received the B.S., M.S., and Ph.D. degrees in electrical engineering from the University of Illinois at Urbana–Champaign, Champaign, IL, USA, in 1994, 1995, and 1999, respectively. He was previously with Philips-Lumileds, San Jose, CA, USA; Sandia National Laboratories, Albuquerque, NM, USA; and Lehigh University, Bethlehem, PA, USA. He is currently a Professor with North Carolina State University, Raleigh, NC. He has authored or coauthored over 180 publications and conference publications and holds 42 patents.

**Nelson Tansu** (Fellow, IEEE) has been the Head of the School of Electrical and Electronics Engineering and a Professor of quantum electronics at The University of Adelaide, Adelaide, SA, Australia, since January 2021. Previously, he was the Daniel E. '39 and Patricia M. Smith Endowed Chair Professor with the Department of Electrical and Computer Engineering (ECE) and the Director of the Center for Photonics and Nanoelectronics (CPN), Lehigh University. He had made advances to the invention and innovation, fundamental sciences, and device technologies of III–V and III-Nitride semiconductors. He has more than 18 U.S. patents, and his work is integrated into today's state-of-the-art solid-state lighting technology. He has authored more than 160 refereed journals and 325 conference publications. He is the Editor-in-Chief of the open-access journal *Photonics*, and he serves as a member of the editorial boards for eight other leading journals in applied physics and nanotechnology. He is a fellow of the U.S. National Academy of Inventors (NAI Fellow; elected in 2016), an IEEE Fellow (Class of 2021), and Clarivate Analytics Highly Cited Researcher in 2018.