Optical properties of ultra-thin InN layer embedded in InGaN matrix for light emitters*

Yang Wei(杨 薇), Wu Yi-Yang(武翌阳), Liu Ning-Yang(刘宁炀), Liu Lei(刘 磊), Chen Zhao(陈 钊), and Hu Xiao-Dong(胡晓东)†

State Key Laboratory for Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking University, Beijing 100871, *China*

(Received 29 June 2012; revised manuscript received 21 August 2012)

We theoretically investigate the optical properties of an ultra-thin InN layer embedded in InGaN matrix for light emitters. The peak emission wavelength extends from ultraviolet (374 nm) to green (536 nm) with InN quantum well thickness increasing from 1 monolayer to 2 monolayers, while the overlap of electron–hole wave function remains at a high level (larger than 90%). Increase of In content in InGaN matrix provides a better approach to longer wavelength emission, which only reduces the spontaneous emission rate slightly compared with the case of increasing In content of the conventional InGaN quantum well. Also, the transparency carrier density derived from gain spectrum is of the same order as that in the conventional blue laser diode. Our study provides skillful design on the development of novel structure InN-based light emitting diodes as well as laser diodes.

Keywords: InN ultra-thin layer, spontaneous emission spectra, gain, laser diodes

PACS: 78.20.Bh, 78.55.Cr, 78.67.De **DOI:** 10.1088/1674-1056/22/4/047801

1. Introduction

After the correction of the energy band-gap of InN material at room temperature for 0.63 eV,[1] the group III–nitrides systems including InN, GaN, AlN, and their alloys were found to cover the whole spectrum range from deep ultraviolet (∼ 200 nm) to infrared (∼ 2000 nm). A conventional active layer for solid state lighting adopts the InGaN ternary alloy or AlInGaN quaternary alloy as quantum well (QW) structure, which would induce the undesirable effects of phase separation and atomic ordering. At the same time, the spontaneous and piezoelectric polarization induced electric fields in the conventional QW would lead to the quantum confined Stark effect (QCSE),[2] thus reducing the overlap of electron–hole wave function.

An ultra-thin InN layer (1∼2 monolayer ML) embedded in GaN (InGaN) matrix was considered as a novel structure of the active layer for high efficiency light emitting diodes (LEDs), due to remarkably reducing the QCSE and exempting from the problem caused by random alloy compositional fluctuation of the ternary InGaN material.[3] Due to the advance of InN growth on *c*-plane GaN template by molecular beam epitaxy (MBE) process, Yoshikawa *et al*.[3,4] first demonstrated the photoluminescences (PLs) of the above structure, respectively, with an emission wavelength of 398 nm (1-ML InN well) and 437 nm (2-ML InN well) and a preliminary LED sample with electroluminescence (EL) peak around 418 nm at room temperature. Then Dimakis *et al*.[5] fabricated similar ultraviolet LEDs by MBE with the peak emission wavelength at 384 nm, which was independent of injection current due to the absence of QCSE. Later, Yuki *et al*.[6] extended the PL wavelength to 480 nm at 15 K by using InGaN as barrier layer instead of GaN. This novel structure LED was also obtained through metal organic vapour phase epitaxy (MOVPE) in 2010 by Lin *et al*.,[7] which enabled the large mass production of fabrication compared with the MBE. However, there is little theoretical research about the optical properties for the novel structure, especially the spontaneous emission rate and the gain spectrum as a function of structure parameters.

In this work, we investigate the optical properties comprehensively with respect to structure parameters such as InN QW thickness (d) and In content (In%) of InGaN matrix. Interband transition wavelength and overlap of electron–hole wave function are first calculated to evaluate the emission range of the novel structure. Then, spontaneous emission rates for different values of d and In% are shown to determine the preference of a high efficiency structure. Finally, the gain spectrum and peak material gain are obtained to give the transparency carrier density and also applied to a typical laser diode structure.

2. Parameters and method

The calculation of the band structures and wave functions is based on a self-consistent gain module of APSYS program.[8] The conduction band structure is determined by solving the single band effective mass Hamiltonian using

*Project supported by the National Natural Science Foundation of China (Grant Nos. 61076013, 51272008, and 51102003), the National Basic Research Program of China (Grant No. 2012CB619304), the Beijing Municipal Science & Technology Commission (Grant No. D111100001711002), and the Specialized Research Fund for the Doctoral Program of Higher Education, China (Grant No. 20100001120014).

†Corresponding author. E-mail: huxd@pku.edu.cn

© 2013 Chinese Physical Society and IOP Publishing Ltd

parabolic approximation, while the valence band structure is obtained by self-consistent six-band $k \cdot p$ formalism.[9] The built-in polarization induced by spontaneous and piezoelectric polarizations is represented by interface charges through the method developed by Fiorentini and Fiorentini.[10] All the computation parameters (see Table 1) are obtained from the literature by Vergaftman and Meyer[11] and a recent review article by Wu.[12] The band-offset for InN/GaN is chosen to be 80:20.[13] The intra-band relaxing rate is determined to be 1×10^{-13} s.[14] By carefully choosing the specific material parameters, APSYS can be used to explore the internal physical process and in optimizing device performances.[15,16]

Table 1. Material parameters of the semiconductors GaN and InN, 1 Å = 0.1 nm.

Parameter	Symbol (unit)	GaN	InN
Lattice constant	a (Å) at $T = 300$ K	3.189	3.545
	c (Å) at $T = 300$ K	5.185	5.703
Energy band gap	E_g (eV)	3.510	0.78
Spin–orbit split energy	Δ_{so} (eV)	0.017	0.005
Crystal-field split energy	Δ_{cr} (eV)	0.019	0.041
Electron effective mass (c axis)	$m_e^{\parallel}(m_0)$	0.20	0.07
Electron effective mass (transverse)	$m_e^{\perp}(m_0)$	0.20	0.07
Hole effective mass parameter	A_1	–7.21	–8.21
	A_2	–0.44	–0.68
	A_3	6.68	7.57
	A_4	–3.46	–5.23
	A_5	–3.40	–5.11
	A_6	–4.90	–5.96
Hydrost. deform. potential (c axis)	a_1 (eV)	–4.08	–3.5
Hydrost. deform. potential (transverse)	a_2 (eV)	–8.16	–3.5
Shear deform. potential	D_1 (eV)	–3.7	–3.7
	D_2 (eV)	4.5	4.5
	D_3 (eV)	8.2	8.2
	D_4 (eV)	–4.1	–4.1
	D_5 (eV)	–4.0	–4.0
	D_6 (eV)	–5.5	–5.5
Elastic stiffness constant	C_{11} (Gpa)	390	223
	C_{12} (Gpa)	145	115
	C_{13} (Gpa)	106	92
	C_{33} (Gpa)	398	224
	C_{44} (Gpa)	105	48

3. Results and discussion

Figure 1 shows the inter-band transition wavelength (right) and the overlap of electron–hole wave function (Γ_{e_hh}) (left) each as a function of InN well thickness embedded in 12-nm GaN matrix. As InN well thickness (d) increases from 2.5 Å to 6 Å, the peak emission wavelength increases from 374 nm to 536 nm, covering the spectrum range from ultraviolet to green. It is worth noting that Γ_{e_hh} is insensitive to the value of d (about 5% change) and remains at a significant high value (larger than 90%), which is attributed to strong localization of electron and hole wave function in the ultra-thin InN well.[17,18] The emission wavelength also shows a red shift with In% of InGaN matrix increasing as shown in the inset of Fig. 1, with the InN well thickness fixed at 3 Å. If we combine the above two structure parameters (d and In%) with skillful design, this ultra-thin InN well novel structure can be further extended to longer wavelength such as yellow and red light (for example In% = 0.15, d = 6 Å, 592-nm yellow light).

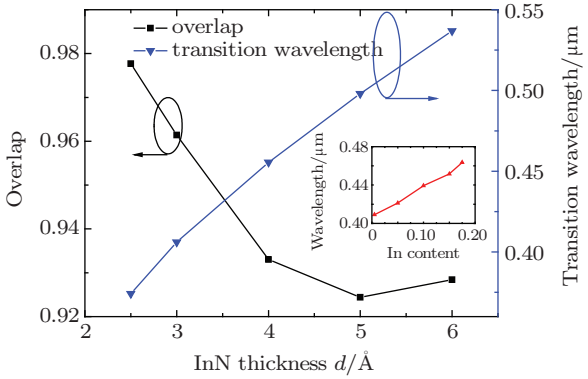


Fig. 1. (color online) Inter-band transition wavelength (right) and the overlap of electron–hole wave function (Γ_{e_hh}) (left) each as a function of InN well thickness embedded in 12-nm GaN matrix, the inter-band transition wavelength varies as a function of In% of InGaN matrix, with the InN well thickness fixed at 3 Å.

Figures 2(a) and 2(b) show the room temperature spontaneous emission spectra under different carrier injection levels (n) from 5×10^{18} cm^{-3} to 10×10^{18} cm^{-3} for different thickness values of InN well embedded in 12-nm GaN matrix (see Fig. 2(a)) and different values of In% of 12-nm InGaN matrix,

with InN well thickness fixed at 3 Å (see Fig. 2(b)). As shown in Fig. 2(a), the peak spontaneous emission rate increases from high energy (3.05 eV) to low energy side (2.49 eV) as InN well thickness increases from 3 Å to 6 Å. From Fig. 2(b), when the value of In% of InGaN matrix increases from 0 to 0.18, the spontaneous emission rate decreases slightly from 6.60×10^{27} cm^{-3}·s^{-1}·eV^{-1} to 5.35×10^{27} cm^{-3}·s^{-1}·eV^{-1} at $n = 10\times10^{18}$ cm^{-3}, which is attributed to the weaker carrier confinement in shallower QW with the value of In% of InGaN matrix increasing. Therefore, in order to achieve high efficiency light emitters in longer wavelength, larger InN well thickness is preferred rather than larger value of In% of InGaN matrix because the former exhibits larger spontaneous emission rate. As the critical thickness of InN grown on GaN is approximately 1 ML–2 ML (3 Å–6 Å) and the ability to grow InN with an accuracy of ML has been achieved according to the recent experimental studies,[19] high efficiency green LEDs with emission wavelength as long as 536 nm (as demonstrated in Fig. 1) may be available in the future.

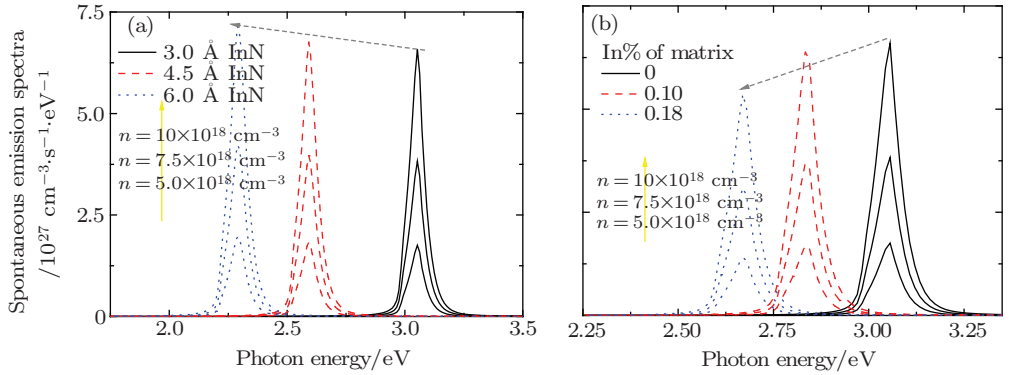


Fig. 2. (color online) The spontaneous emission spectra under different carrier injection levels each as a function of (a) InN well thickness embedded in 12-nm GaN matrix and (b) In% of InGaN matrix, with the InN well thickness fixed at 3 Å.

Note that the change of spontaneous emission rate in Fig. 2(b) is quite different from the situation in conventional InGaN/GaN QW structure, although for both cases the increases of In% shift the emission spectra toward longer wavelength. In the case of conventional QW, the increase of In% in the InGaN well will enhance the internal polarization field due to larger lattice mismatch inducing stronger piezoelectric polarization, thereby driving the electron and hole toward opposite directions in the QW and reducing $\Gamma_{\text{e_hh}}$ significantly. However, in the case of novel structure, the increase of In% in the InGaN matrix will reduce the internal polarization field due to smaller lattice mismatch, and spontaneous emission rate changes only a little. That is to say, the increase of In% in the InGaN matrix is a different and also a better approach to obtaining a longer wavelength emission than the increase of In% in the conventional InGaN well.

Furthermore, we investigate the TE mode optical gain spectrum calculated from the spontaneous emission spectrum.[20] Figure 3 shows the material gain spectrum with injected carrier densities from 1×10^{19} cm^{-3} to 3.0×10^{20} cm^{-3} for 3-Å InN well layer embedded in 12-nm GaN matrix at room temperature, and the inset shows the peak gain coefficient as a function of carrier density. The differential gain coefficients and transparency carrier densities are determined to be 8.4×10^{-17} cm^2 and 8.2×10^{19} cm^{-3} respectively, similar to those of a conventional blue laser diode.[21] To demonstrate the application of this novel structure as an active layer for a laser diode emitting around 405 nm, we employ a typical three-QW laser structure with internal loss α_{i} of 43 cm^{-1} and optical confinement factor Γ_{opt} of 0.004 (considering the refractive index and ultra-thin thickness of InN well, the value of Γ_{opt} is scaled to 1/10 of that of LDs in conventional InGaN QW active region for a rough estimation).[22] The reflectivities of the coated facet front and end mirror are set to be $R_{\text{front}} = R_{\text{end}} = 0.5$ and the cavity length L is 550 μm. The threshold gain G_{th} for this structure is given by

$$\Gamma_{\text{opt}} \times G_{\text{th}} = \alpha_{\text{i}} + \frac{1}{2L} \ln\left(\frac{1}{R_{\text{front}} \times R_{\text{back}}}\right). \tag{1}$$

G_{th} is calculated to be 18534 cm^{-1} per QW, which corresponds to 3.0×10^{20} cm^{-3} for threshold carrier density from the inset of Fig. 3, on the same order as those reported n_{th}=1.8×10^{20} cm^{-3}.[21] The steady state rate equation for carrier injection gives

$$\frac{\eta_{\text{inj}} J_{\text{th}}}{q_{\text{e}} d} = \frac{n_{\text{th}}}{\tau}. \tag{2}$$

In the above equation, η_{inj} is the injection efficiency, J_{th} the threshold current density, q_{e} the elementary charge, d the thickness of active layer, and τ the carrier lifetime. As the thickness of QW for this novel structure (1–2 monolayers) is much smaller than that of conventional structure (2 nm∼3 nm), much smaller threshold current density can be

expected to have a threshold carrier density of the same order, both of which are of the same order. On the other hand, the coherent growth of ultra-thin InN QW less than the critical thickness can avoid/reduce the misfit dislocations,[3] resulting in a high-quality active layer very beneficial for laser performance, especially for high speed modulating.[23]

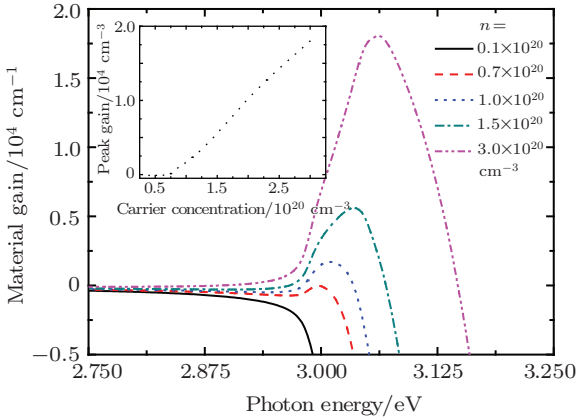


Fig. 3. (color online) The TE mode optical gain spectra for 3-Å InN well embedded in 12-nm GaN matrix emitting at $\sim$ 405 nm for the cases of some different carrier densities ($n = 0.1 \times 10^{20}$ cm^{-3}–3.0×10^{20} cm^{-3}), with the inset showing the peak gain coefficient as a function of carrier density.

4. Conclusion

In this paper, the optical properties of an ultra-thin InN well embedded in InGaN matrix are investigated theoretically. A self-consistent six-band $k \cdot p$ formalism is employed to calculate the band structures, wave functions, spontaneous emission rate, and gain spectrum with respect to InN well thickness and In% of InGaN matrix. The peak emission wavelength extends from ultraviolet to green with InN well thickness increasing from 1 ML to 2 MLs, while $\Gamma_{\text{e_hh}}$ remains at a high level (larger than 90%). The increase of In% in InGaN matrix provides another approach to long wavelength emission, which only reduces the spontaneous emission rate slightly compared with the case of increasing In% in conventional InGaN QW. Also, the transparency carrier density determined from the gain spectrum is of the same order of magnitude as that in conventional blue laser diodes. This novel structure is found to possess a high-efficiency light emitter in a rather broad regime.

References

[1] Wu J, Walukiewicz W, Yu K M, Ager Iii J W, Haller E E, Lu H, Schaff W J, Saito Y and Nanishi Y 2002 *Appl. Phys. Lett.* **80** 3967
[2] Takeuchi T, Wetzel C, Yamaguchi S, Sakai H, Amano H, Akasaki I, Kaneko Y, Nakagawa S, Yamaoka Y and Yamada N 1998 *Appl. Phys. Lett.* **73** 1691
[3] Yoshikawa A, Che S B, Yamaguchi W, Saito H, Wang X Q, Ishitani Y and Hwang E S 2007 *Appl. Phys. Lett.* **90** 073101
[4] Yoshikawa A, Che S, Ishitani Y and Wang X 2009 *J. Cryst. Growth* **311** 2073
[5] Dimakis E, Nikiforov A Y, Thomidis C, Zhou L, Smith D J, Abell J, Kao C K and Moustakas T D 2008 *Phys. Status Solidi (a)* **205** 1070
[6] Yuki A, Watanabe H, Che S B, Ishitani Y and Yoshikawa A 2009 *Phys. Status Solidi (c)* **6** S417
[7] Lin W, Li S and Kang J 2010 *Appl. Phys. Lett.* **96** 101115
[8] APSYS Version 2008.06.01, Crosslight Software, Inc., 1995–2005
[9] Chuang S L and Chang C S 1997 *Semicond. Sci. Technol.* **12** 252
[10] Bernardini F and Fiorentini V 2001 *Phys. Rev. B* **64** 085207
[11] Vurgaftman I and Meyer J R 2003 *J. Appl. Phys.* **94** 3675
[12] Wu J 2009 *J. Appl. Phys.* **106** 011101
[13] Wu G G, Li W C, Shen C S, Gao F B, Liang H W, Wang H, Song L J and Du G T 2012 *Appl. Phys. Lett.* **100** 103504
[14] Yeo Y, Chong T and Li M 1998 *IEEE J. Quantum Electron.* **34** 1270
[15] Lu T P, Li S T, Zhang K, Liu C, Xiao G W, Zhou Y G, Zheng S W, Yin Y A, Wu L J, Wang H L and Yang X D 2011 *Chin. Phys. B* **20** 108504
[16] Lu T P, Li S T, Zhang K, Liu C, Xiao G W, Zhou Y G, Zheng S W, Yin Y A, Wu L J, Wang H L and Yang X D 2011 *Chin. Phys. B* **20** 098503
[17] Che S, Yuki A, Watanabe H, Ishitani Y and Yoshikawa A 2009 *Appl. Phys. Express* **2** 021001
[18] Zhao H, Liu G and Tansu N 2010 *Appl. Phys. Lett.* **97** 131114
[19] Yoshikawa A, Hashimoto N, Kikukawa N, Che S B and Ishitani Y 2005 *Appl. Phys. Lett.* **86** 153115
[20] Ahn D, Chuang S L and Chang Y C 1988 *J. Appl. Phys.* **64** 4056
[21] Nakamura S 1997 *IEEE J. Sel. Top. Quantum Electron.* **3** 435
[22] Zhao H, Arif R, Ee Y K and Tansu N 2008 *Opt. Quantum Electron.* **40** 301
[23] Yoshikawa A and Che S B 2008 *Int. J. High Speed Electron. Syst.* **18** 993