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Comprehensive study of group III-nitride light emitting diode structures based on sapphire and $ScAlMgO_4$ (0001) substrate for high intensity green emission

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Abstract. To mitigate the green gap problems existing in GaN/InGaN/AlGaN system on sapphire substrate, an $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ based LED structure on $ScAlMgO_4$ (0001) substrate has been introduced for green light (525…565 nm) emission. On $ScAlMgO_4$ (0001) substrate, 35% of In composition with 1.6 nm well thickness and only 15% of Al composition with 1.1 nm thick AlGaN as capping layer on top provide the best LED structure. It provides minimum equivalent lattice mismatch (0.01%) with reasonable overall elastic energy value (0.47 J/m^2). Most importantly, it provides at least 10% brighter green light emission than that of sapphire based LED structure.

Keywords: InGaN-green emission LED, sapphire substrate, $ScAlMgO_4$ (0001) substrate, AlGaN capping layer.

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1. Introduction

Group III-nitride materials are promising candidates for solid state lighting as they can emit light within visible spectrum range and beyond it [1]. However, the external quantum efficiency (EQE) of such device grown on sapphire substrate varies at different wavelengths [2]. It has been reported that the efficiency is about 80% at violet emission [3], whereas at yellow emission (570 nm) it is only 19.3% at 20 mA [4]. The drop of efficiency at higher wavelength is caused by the fact that the high indium (In) incorporation (> 20%) within InGaN quantum well (QW) is required [5]. The high In composition in InGaN alloys causes low thermal stability [6] and low growth temperature of deposition process, which results in unintentional point defects [7], including In clustering and QW thickness undulation [8]. It also creates strains within QWs, since the lattice parameter of the InGaN layer differs from that of GaN barrier, when been grown pseudomorphically on *c*-plane or polar direction, which can lead to formation of additional defects, namely: V-defects, misfit dislocations (MDs) along with threading dislocations (TDs), to release stress energy [9, 10]. In addition to that, the polar (*c*-plane) GaN/InGaN structure suffer from polarization effect that reduces the oscillation strength (*i.e.*, intensity) and also causes a red shift of emission wavelength due to internal piezo-electric field known as quantum confinement Stark effect [11, 12].

To compensate the above mentioned limitations, many research groups tried different approaches like to grow GaN on nonpolar [13] or semipolar [14] substrates, thick InGaN templates [15] on {0001} polar planes, use quantum dots [16], nanocolumns [17] and Eu-doped GaN structures [18]. Somebody tried to have more intensive light emission of green or even yellow/amber emission by using with or without few nm thick AlGaN as cap layer covering InGaN QWs grown on sapphire substrate [19–22]. However, instead of using sapphire, $ScAlMgO_4$ (0001) or SCAM (0001) substrates can be applied to achieve even higher wavelength (red) emission with $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ (where $x > 0.2$) structure [23]. Recently, our research group showed through simulation studies that by using AlGaN as a capping layer, one can reach even higher intensity red light emission with lower In composition within InGaN QWs [24].

Being motivated by our recent findings, in this work we tried to do a simulation based comparative study between $GaN/In_xGa_{1-x}N/Al_yGa_{1-y}N$ structure grown on sapphire substrate to that of $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ on SCAM (0001) substrate for green, yellowish green (525…565 nm) light emission. We tried to find the best structural parameters for both structures, and attempts were made to identify the significant features between these two structures, which will eventually allow us to have higher EQE and better intensity in green, yellowish green (525…565 nm) emission after fabrication.

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2. Theoretical analysis

The in-plane lattice parameter of ScAlMgO$_4$ (0001) substrate ($a = 0.3249$ nm) matches with that of In$_{0.17}$Ga$_{0.83}$N relaxed layer. Researchers were able to deposit a thick In$_{0.17}$Ga$_{0.83}$N layer as a buffer layer on SCAM (0001) substrate [25]. Since then SCAM (0001) becomes an alternative substrate for developing group III-nitride LED structure instead of using the sapphire substrate. Due to excessive cost of SCAM (0001) substrate, not intense experimental researches were reported till to date. That is why, a simulation based comparative studies between the LED structures developed on SCAM and sapphire substrate has research interest for further development.

It is obvious that growing pseudomorphically any ternary alloy of (Al/In)$_x$Ga$_{1-x}$N material on *c*-plane (0001) buffer GaN layer on sapphire or In$_{0.17}$Ga$_{0.83}$N layer on SCAM substrate will have intense polarization effect as the coefficient of piezoelectric polarization is quite large [26]. The internal electric field of any epilayer of a superlattice can be calculated using the following equation [27]:

$$E_j = \frac{\sum_i \frac{(P_i - P_j)L_i}{\varepsilon_i}}{\varepsilon_j \sum_i \frac{L_i}{\varepsilon_i}}, \qquad (1)$$

where P_i and P_j are total polarization (sum of spontaneous and piezoelectric polarization) of the adjacent layers, ε_i and ε_j are permittivities of these two adjacent layers and L_i is the layer thickness of each i layer, respectively. Now for a three layer system, we can set the i value from 1 to 3 in the following manner: 1 – GaN layer or 1 – In$_{0.17}$Ga$_{0.83}$N, 2 – In$_x$Ga$_{1-x}$N and 3 – Al$_y$Ga$_{1-y}$N for LED structure grown on sapphire or SCAM (0001) substrate. The overall elastic strain energy per surface unit of a device with an equivalent lattice parameter a_{eq} can be written as follows:

$$E_{el}\left(a_{eq}\right) = \sum_{i=1}^{3} M_i L_i \Delta_i^2, \qquad (2)$$

where M_i is the biaxial modulus, Δ_i is the strain in the growth plane. For an equivalent lattice parameter a_{eq} of the device, the strain of individual layer Δ_i can be expressed as $\Delta_i = \frac{a_{eq} - a_i}{a_i}$, where a_i is the relaxed lattice parameter of each i layer. The equivalent lattice parameter a_{eq} of the structure can be found, after setting the elastic strain energy E_{el} of the system at the minimum, *i.e.* $\frac{dE_{el}}{da_{eq}} = 0$, as

$$a_{eq} = \frac{\sum_{i=1}^{3}\left(M_i L_i \prod_{j\neq i} a_j\right)}{\sum_{i=1}^{3}\left(M_i L_i \prod_{j\neq i} a_j^2\right)} \prod_{i=1}^{3} a_i\ . \qquad (3)$$

The biaxial modulus M_i and relaxed lattice parameter a_i of each epilayer of the system can be calculated using the Vegard law. In this work, the in-plane lattice parameter of AlN, GaN and InN are considered to be of 3.113, 3.189 and 3.538 Å, respectively, and the bowing parameter of zero ($b = 0$) has been considered [28]. Again, the stiffness constant values for $c_{jk}(\mathrm{InN})$, $c_{jk}(\mathrm{GaN})$ and $c_{jk}(\mathrm{AlN})$ have been taken from V.V. Nikolaev *et al.* [29].

The oscillation strength value is proportional to the overlap square of the electron and hole wave functions $F \propto \left|\langle \varphi_e | \varphi_{hh} \rangle\right|^2$, where φ_e and φ_{hh} are wave functions of electron and hole, respectively.

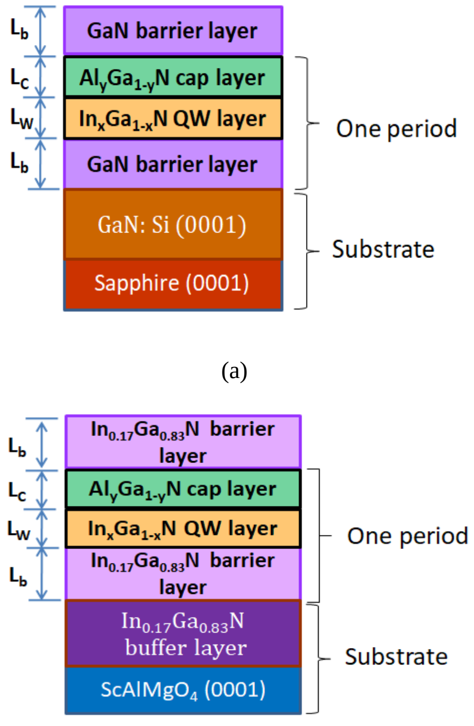
The radiative lifetime is inversely proportional to the square of the overlap of the electron and hole wave function integral as shown below [30]:

$$\tau_{rad}^{-1} = \frac{nd^2 E_0^3}{3\pi\varepsilon_0 h^4 c^3}\left|\int f_e \cdot f_h \cdot dz\right|^2 = \frac{E_0^3}{A}\left|\int f_e \cdot f_h \cdot dz\right|^2,$$

where d is the inter-band optical dipole of GaN, E_0 is the transition energy, f_e and f_h are wave functions of electron and hole, respectively. In this work, the logarithmic value of oscillation strength value is used to identify the light intensity and compare the light intensities for each change in device structure.

3. Model of the two structures

We have modeled two structures as first one considered to be grown on sapphire substrate with GaN as buffer and barrier layer, and the second one to be grown on ScAlMgO$_4$ or SCAM (0001) substrate with In$_{0.17}$Ga$_{0.83}$N as a buffer and barrier layer. To get a green or yellowish green emission (525…565 nm), we have set the barrier layer thickness of 12 nm, Al$_y$Ga$_{1-y}$N as capping layer with Al composition of $y = 17\%$ and thickness 1.2 nm on the top of In$_x$Ga$_{1-x}$N QW. The overall structures of LEDs are schematically shown in Fig. 1. Initially, we tried to compare the In composition within QW and its thickness for green emission between the two structure. The In composition and QW thickness have been varied from 20 up to 45%, whereas the thickness from 1 to 5 nm. In each step, the internal electric field of each layer, the equivalent in-plane lattice parameter and the overall elastic strain energy per surface unit have been calculated using the equations (1) to (3). For example, for the first model (on sapphire substrate) considering In composition within QW close to 27% with the QW thickness 2.0 nm, we have obtained internal electric field values in different layers, namely: in the barrier layer $E_b = 0.50$ MV/cm, in the QW layer $E_W = 4.28$ MV/cm and in the AlGaN cap layer $E_C = 2.12$ MV/cm. The equivalent lattice parameter a_{eq} is of 3.23 nm and the elastic energy is 0.67 J/m^2. Using these values, we have solved the Schrödinger equation *via* envelop formalism to determine the



(a)

(b)

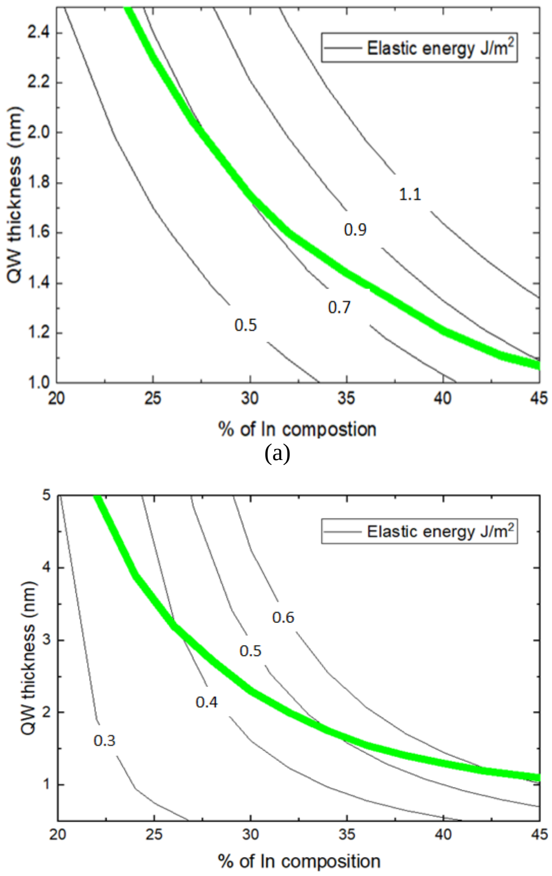
Fig. 1. (a) The first model with sapphire substrate and (b) the second model with $ScAlMgO_4$ substrate. The individual layers of the structures are indicated along with their thickness designations.

emission wavelength of the structure. In this case, the emission wavelength becomes 532 nm. Similar analysis has been done for the second model. The obtained results are summarized in Fig. 2.

4. Results and discussion

From Fig. 2, we can find that overall elastic energy lies between 0.65 to 0.9 J/m^2 for GaN/$In_xGa_{1-x}N/Al_{0.17}Ga_{0.83}N$ LED structure (Fig. 2a). Whereas the overall elastic energy lies between 0.35 to 0.65 J/m^2 for $In_{0.17}Ga_{0.83}$/$In_xGa_{1-x}N/Al_{0.17}Ga_{0.83}N$ LED structure (Fig. 2b), while changing the QW thickness and In composition to get the green light emission (green line in the plots indicates the emission in green/yellowish green light of 525 to 565 nm). Thus, it is obvious that the 2nd structure with $In_{0.17}Ga_{0.83}N$ barrier and buffer layer will generate less defects (threading dislocations (TDs), misfit dislocations (MDs), point defects (PDs) *etc*.) within the structure and will produce higher intensity green emission than that of the 1st model structure with GaN barrier and buffer layer.

To find more suitable device parameters to get high intensity, less defect prone green emission structure, we have systematically changed the device parameters one by one, while keeping other parameters fixed, as we did the same type of analysis for $In_{0.17}Ga_{0.83}N$ /InGaN/AlGaN structure of red emission earlier [24].



(a)

(b)

Fig. 2. Plot of the quantum well (QW) thickness *versus* % of indium composition for green emission (525…565 nm) (as green strip line shows) along with total elastic energy (J/m^2) plot: (a) GaN/$In_xGa_{1-x}N/Al_yGa_{1-y}N$ on the sapphire substrate and (b) $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ on the SCAM substrate. (Color online)

The obtained device parameters for GaN/$In_xGa_{1-x}N$/ $Al_yGa_{1-y}N$ system along with logarithmic value of oscillation strength (Γ), percentage of equivalent lattice mismatch with respect to relaxed GaN barrier layer and elastic energy (J/m^2) are summarized in Table 1. We can also find the best device parameters for green emission with $ScAlMgO_4$ or SCAM (0001) substrate, where the QW thickness and In composition within QW may vary along with other parameters. The summary of the device parameters of LED structure with SCAM (0001) substrate is presented in Table 2.

From Tables 1 and 2, we can find that for both LED structures grown on sapphire and/or $ScAlMgO_4$ or SCAM (0001) substrates, QW with the low In composition (x = 16% and 24%) and high QW thickness (L_W = 4.2 nm and 4.3 nm) along with reasonable Al composition (y = 18% and 16%) and AlGaN capping layer thickness (L_C = 1.2 nm and 1.0 nm) has least elastic energy values (0.54 and 0.33 J/m^2, respectively). However, the logarithmic oscillation strength values are quite low of Γ = –3.66 and –1.77, respectively.

Table 1. Summary of device parameters for GaN/$In_xGa_{1-x}N/Al_yGa_{1-y}N$ system along with other obtained results.

QW In composition, *x*, %	Cap layer Al composition, *y*, %	Well thickness, L_W, nm	Cap layer thickness, L_C, nm	Logarithmic oscillation strength value, Γ	Percentage of equivalent lattice mismatch	Elastic energy, J/m^2
16	18	4.2	1.2	–3.66	1.22	0.54
21	24	2.9	1	–1.34	1.48	0.62
25	70	2.3	1.3	–0.93	0.91	0.83
30	66	1.8	1.2	–0.63	1.05	0.87
32	66	1.6	1.1	–0.50	1.11	0.86
35	70	1.5	1.1	–0.46	1.12	0.94
40	31	1.2	1.1	–0.32	1.58	0.83
44	37	1.1	1.1	–0.28	1.53	0.91

Table 2. Summary of device parameters for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ system along with other obtained results.

QW In composition, *x*, %	Cap layer Al composition, *y*, %	Well thickness, L_W, nm	Cap layer thickness, L_C, nm	Logarithmic oscillation strength value, Γ	Percentage of equivalent lattice mismatch	Elastic energy, J/m^2
24	16	4.3	1.0	–1.77	0.10	0.33
27	21	3.0	1.0	–1.21	0.08	0.39
30	17	2.2	1.0	–0.72	0.08	0.40
33	16	1.9	1.1	–0.62	0.06	0.46
35	15	1.6	1.1	–0.49	0.01	0.47
37	18	1.4	1.0	–0.40	0.03	0.48
40	10	1.2	1.1	–0.29	0.03	0.49
44	12	1.1	1.1	–0.28	0.03	0.55

Table 3. Results of comparative study between LED structures based on sapphire and $ScAlMgO_4$ (0001) substrates.

Substrate	In composition, *x*, %	Al composition, *y*, %	QW thickness, nm	Cap layer thickness, nm	Emission wavelength, nm	Logarithmic oscillation strength value, Γ	Percent of equivalent lattice mismatch	Elastic energy, J/m^2
Sapphire	25	70	2.3	1.3	540.0	–0.93	0.91	0.83
SCAM	35	15	1.6	1.1	536.4	–0.49	0.01	0.47

On the overhand, the structure of the high In content ($x = 44\%$) and low QW thickness (L_W = 1.1 nm) and reasonable AlGaN capping layer thickness (L_C = 1.1 nm) with the different Al content ($y = 37\%$ and 12%) has the lowest logarithmic oscillation strength value Γ = –0.28 and the highest elastic energy value of 0.91 and 0.55 J/m^2, respectively. We know that the change in the oscillation strength value is due to QCSE, since it reduces the overall electron-hole wave-function overlapping in the case of QW with AlGaN interlayer thickness variation [31]. The overall elastic energy depends on both QW thickness and it's In composition value (as shown in Fig. 2). Both these cases are extreme as we need to have low logarithmic oscillation strength value for higher intensity light emission and less elastic energy within the system. The high elastic energy may create more defects that act as a non-radiative defect centres within the structure. After analyzing the obtained results (from Tables 1 and 2), we may state that it is better to have green emission from sapphire substrate (GaN barrier) with In composition of 25% and QW thickness of 2.3 nm along with Al composition of $y = 70\%$ and AlGaN capping layer thickness of 1.3 nm. In that case, the percentage of in-plane equilibrium lattice parameter mismatch of the structure is minimum of only 0.91% with logarithmic oscillation strength value of Γ = –0.93 and elastic energy of 0.83 J/m^2. Whereas, for LED structure with $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ grown on $ScAlMgO_4$ or SCAM (0001) substrates, we may have the highest intensity green emission from QW with the In composition close to 35% and well thickness 1.6 nm along with Al composition of only $y = 15\%$ and

AlGaN capping layer thickness of 1.1 nm as the percentage of in-plane equilibrium lattice parameter mismatch of the structure is minimum of only 0.01% with the logarithmic oscillation strength value Γ= –0.49 and elastic energy close to 0.47 J/m^2. The obtained result of comparison is summarized in Table 3.

It is clear that LED structure based on SCAM (0001) substrate will allow us to have much brighter emission than that of sapphire substrate as oscillation strength value is at least 10% higher (~11%). Moreover, it will have less defect density as the equivalent lattice mismatch and the overall elastic energy is quite low (0.01 and 0.47 J/m^2, respectively) as compared to that of LED structure on the sapphire substrate.

It should be also noted that the Al composition within AlGaN capping layer is only 15% in SCAM (0001) substrate based LED structure, whereas for the sapphire substrate based LED structure it is 70%. Again, the In composition (35%) within QW layer is less abrupt in SCAM based LED structure as the barrier layer ($In_{0.17}Ga_{0.83}N$) already has 17% of In incorporation in it. These two facts indicate that the growth process of LED structure on SCAM (0001) substrate will be easier than that in the structure based on the sapphire substrate. However, the production cost of SCAM (0001) substrate is much higher than that of sapphire substrate till today. The main challenge will be to reduce the cost per substrate to implement our proposed LED structure for brighter and less defect prone green emission in the nearest future.

5. Conclusions

A comparative analysis between $ScAlMgO_4$ or SCAM (0001) and sapphire substrate based group III-nitride LED structures has shown that after optimizing the device parameters, we can have brighter, less defective, prone and stable green light emitting diodes. An $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ system grown on SCAM (0001) substrate with 35% of In composition and thickness of 1.6 nm QW, 15% Al composition with 1.1 nm AlGaN as capping layer and 12-nm $In_{0.17}Ga_{0.83}N$ barrier layer will allow us to have the best device performance, since it has the lowest in-plane equivalent lattice mismatch (0.01%) and reasonably low elastic energy (0.47 J/m^2) than any other combination of device parameters. It will certainly reduce the chance of non-radiative defect generation possibilities and give brighter (at least 10% higher) green (~536 nm) emission as compared to that of a $GaN/In_xGa_{1-x}N/Al_yGa_{1-y}N$ system grown on sapphire substrate.

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Комплексне дослідження світлодіодних структур нітридів III групи на основі сапфірової та $ScAlMgO_4$ (0001) підкладок для отримання високоінтенсивного зеленого випромінювання

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Анотація. Щоб пом’якшити проблеми із зеленою ділянкою спектра, які існують у системі GaN/InGaN/AlGaN на сапфіровій підкладці, запропоновано світлодіодну структуру на основі $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ на підкладці $ScAlMgO_4$ (0001) для зеленого (525…565 нм) випромінювання. На підкладці $ScAlMgO_4$ (0001), 35% складу In із шириною квантової ями 1,6 нм і лише 15% вмісту Al з AlGaN товщиною 1,1 нм у ролі верхнього шару забезпечують найкращу світлодіодну структуру. Вона забезпечує мінімальну еквівалентну невідповідність решітки (0,01%) із прийнятним загальним значенням пружної енергії (0,47 Дж/м^2). Найважливіше те, що це забезпечує принаймні на 10% яскравіше випромінювання зеленого світла, ніж світлодіодна структура на основі сапфіра.

Ключові слова: зелений InGaN емісійний світлодіод, сапфірова підкладка, підкладка $ScAlMgO_4$ (0001), шар покриття AlGaN.