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Modeling of $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ light emitting diode structure on $ScAlMgO_4$ (0001) substrate for high intensity red emission

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Abstract. An $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ light emitting diode (LED) structure on $ScAlMgO_4$ (0001) substrate is modeled for high intensity red emission. The high indium composition (In > 15%) inside the *c*-plane polar quantum well (QW) for longer wavelength emission degrades the structural and optical properties of LEDs because of induced strain energy and quantum confinement Stark effect. To compensate these effects, it has been demonstrated by simulation that an $Al_yGa_{1-y}N$ cap layer of 2 nm thick and Al composition of 17% deposited onto QW of 3 nm thick and In composition of 35% will allow to have less defect density and higher intensity red emission at 663 nm than that of $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ LEDs grown on $ScAlMgO_4$ (0001) substrate. This LED structure has perfect in-plane equilibrium lattice parameter (a_{eq} = 3.249 Å) and higher logarithmic oscillator strength ($\Gamma = -0.93$) values.

Keywords: LED on $ScAlMgO_4$ (0001) substrate, red emission, equilibrium lattice parameter, oscillator strength, AlGaN cap layer.

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1. Introduction

Group III-Nitride materials paved the way for solid state lighting for its ability to emit within the visible spectral range [1]. It has very high external quantum efficiency (EQE) about 84% in the blue emission range [2]. However, the EQE drops drastically for longer wavelengths, since at yellow emission (576 nm) it is 13.3%, and at yellowish-red emission (629 nm) it is even lower only 2.9% [3-5]. The efficiency drop is caused by the high indium (In) composition within the $In_xGa_{1-x}N$ quantum well (QW) emitters [6]. Low growth temperature is required for this high In incorporation, which can degrade QW by unintentionally generated point defects, including In clustering, impurities incorporation, *etc*. Moreover, lattice mismatch between $In_xGa_{1-x}N$ and GaN as a host material induces strain within QW. This elastic deformation of the polar $In_xGa_{1-x}N$ crystal generates piezoelectric polarization, which lower the optical transition probability, because of the overlap between electron and hole wave-functions get reduced and also shifts the wavelength emission. This effect is known as Quantum Confinement Stark Effect (QCSE) [7, 8]. However, the excessive strain energy within QW can create defects like V-defects, misfit dislocations along with threading dislocations acting as non-radiative recombination centers [9]. Again, In-rich QWs affect the In fluctuation, carrier localization in the QWs, which influences on the structural and optical properties of devices [10-12].

To overcome the above mentioned limitations, several groups have tried to grow GaN on nonpolar [13] or semipolar substrates [14], thick InGaN templates on {0001} polar planes [15-17], even to use quantum dots [18], nanocolumns [19] and Eu-doped GaN [20] structure, which shows to be promising approaches. Some research groups tried to achieve improved green and yellow/amber light emission by using with or without AlGaN as capping layer on the top of InGaN QW grown on sapphire substrate [21-23]. However, recently, one research group showed that instead of sapphire substrate, $ScAlMgO_4$ (0001) or SCAM (0001) substrate can be used to achieve red emission with significantly higher PL intensity with $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ (where x > 0.2) structure [24].

LED with $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ on SCAM (0001) has been evaluated, but no further research has been conducted to see what impact of $Al_yGa_{1-y}N$ might be on $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ structure as a capping layer, yet. In this work, a comparative study has been performed to find out, what exactly the structure of an $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ grown on SCAM (0001) substrate should be to achieve a red emission LED with significantly high intensity.

2. Brief theoretical study

The $ScAlMgO_4$ (0001) substrate [25] has the in-plane lattice parameter $a = 0.3249$ nm, which leads to a lattice match with $In_{0.17}Ga_{0.83}N$ and a small mismatch with GaN of 1.8%. A thick $In_{0.17}Ga_{0.83}N$ buffer layer deposited on SCAM (0001) substrate has been demonstrated [26]. In this work, we considered the $In_{0.17}Ga_{0.83}N$ layer on SCAM (0001) substrate as our barrier layer for the structure.

We know pseudomorphicaly grown *c*-plane (0001) group III-Nitride material has intense piezoelectric polarization effect caused by its lattice mismatch as the coefficient of piezoelectric polarization is quite large [27, 28]. This effect plays a vital role in electric field generation within different epilayers of LED structure. For example, the internal electric field inside the well region (E_W) along with QW thickness (L_W) will deform the band structure of the LED and reduce the effective transition energy between different energy levels, *i.e.*, red-shift of targeted emission within the QWs. This will also reduce the overlap of electron-hole wave-function, which means reduction in overall emission intensity as the radiative lifetime is inversely proportional to the square of the overlap of the electron-hole wave-function integral [29]. Thus, the oscillator strength (F) of the system is a very significant parameter in this study, since it can be related with the square of the overlap of electron-hole wave-function $\left(F \propto \left|\langle \varphi_e | \varphi_{hh} \rangle\right|^2\right)$, where φ_e and φ_{hh} are wave-functions of electron and hole, respectively.

The internal electric field of any epilayer of a superlattice can be calculated using the following equation [30]:

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

where P_i and P_j are the total (both spontaneous and piezoelectric) polarization of the adjacent layer, ε_i and ε_j – permittivities of these two adjacent layers. For a three-layer system, where $In_{0.17}Ga_{0.83}N$ serves as a barrier, $In_xGa_{1-x}N$ as QW and $Al_yGa_{1-y}N$ as a capping layer, we may use i with the following correspondence: $i = 1 = In_{0.17}Ga_{0.83}N$, $i = 2 = In_xGa_{1-x}N$ and $i = 3 = Al_yGa_{1-y}N$, respectively. Under biaxial strain conditions, the equilibrium lattice parameter (a_{eq}) of a superlattice system can be calculated determining the minimum elastic strain energy of $E_{el}(a_{eq})$ of the system. The elastic strain energy per surface unit can be written as

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

where M_i is the biaxial modulus, L_i – layer thickness, Δ_i – strain in the growth plane. The strain can be expressed as $\Delta_i = (a_{eq} - a_i)/a_i$, where a_i is the relaxed lattice parameter of each i layer. By setting elastic strain energy (E_{el}) at the minimum, *i.e.*, $\frac{dE_{el}}{da_{eq}} = 0$, we can find the expression for equilibrium lattice parameter in the following form:

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

We can find the biaxial modulus M_i and relaxed lattice parameter a_i of an epilayer from the lattice parameters and stiffness constants of (Al, Ga)N and (Ga,In)N by using Vegard's law. In this work, the in-plane lattice parameters of GaN, InN and AlN are considered to be $a_{GaN} = 3.189$ Å, $a_{InN} = 3.538$ Å and $a_{AlN} = 3.113$ Å with the bowing parameter equal to zero ($b = 0$) [31, 32] and the stiffness constant values for c_{jk}(InN), c_{jk}(GaN), and c_{jk}(AlN) are considered similar to those by V.V. Nikolaev *et al.* [33].

3. Modeling the light emitting diode (LED) structure

First of all, we tried to find the relationship between In composition (0.20 up to 0.60%) inside QW and QW thickness (1 up to 6 nm) variation for red emission (630…670 nm), keeping the barrier layer thickness fixed at 12 nm. For each combination of In composition and QW thickness, we used the equation (1) to identify the internal electric field inside barrier and QW layers, then by solving the Schrödinger equation via envelop function formalism for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$, we obtained the output as shown in Fig. 1. We also calculated the equilibrium lattice parameter (a_{eq}) by using Eq. (3) and determined the logarithmic oscillator strength value (Γ) for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ LED structure. In Fig. 1, the red strip indicates the red emission (630 up to 670 nm) as the function of QW thickness (L_W) and percentage of In composition. We also incorporate the equilibrium lattice parameter (a_{eq}) in unit Å and the logarithmic oscillator strength value (Γ) as abscissa and ordinate, respectively, for different combinations of percentage of In composition and QW thickness for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ LED structure.

The figure clearly demonstrates that for red emission, we may consider either large QW thickness ($L_W = 6$ nm) with low indium composition (In comp. = 26%) or low QW thickness ($L_W = 1$ nm) with a much higher indium composition (In comp. = 65%). But in

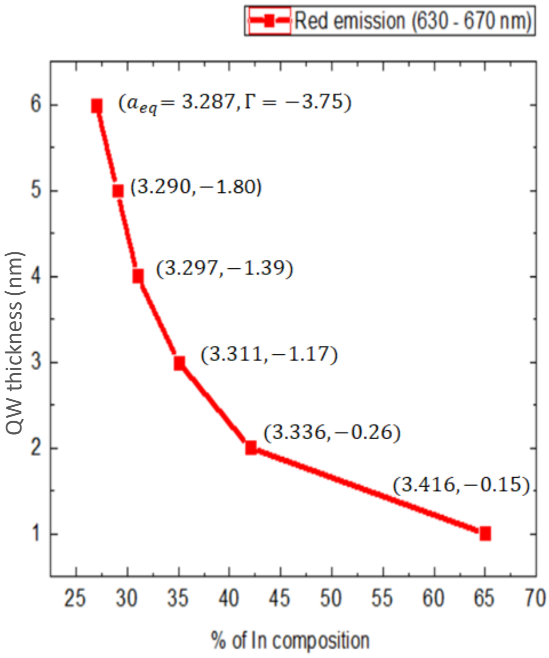

Fig. 1. Result of red emission as a function of QW thickness and In composition. The abscissa and ordinate indicate the equivalent lattice parameter (a_{eq}) in unit Å and logarithmic value of oscillator strength (Γ), respectively, for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ system.

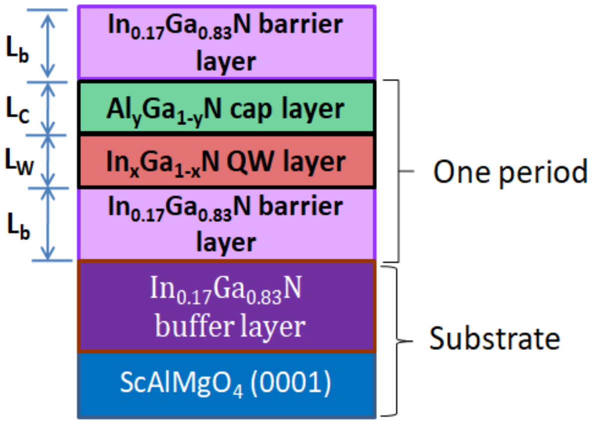

Fig. 2. Schematic diagram of $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ on $ScAlMgO_4$ (0001) LED structure.

either case, we have two extremes, *i.e.*, for the first case we may have low overall strain energy but low oscillator strength value, and for the second one, we may have much higher oscillator strength value but much higher overall strain energy inside the LED structures, as it is shown by the equilibrium lattice parameter (a_{eq}) and logarithmic oscillator strength value (Γ) given as abscissa and ordinate at different points of the graph, respectively. It is obvious that the higher strain energy will induce dislocations to get relaxed, and a lower oscillator strength value indicates the low intensity. Both cases are undesirable, since dislocations act as non-radiative recombination centers, and the oscillator strength indicates how bright the LED will be. Thus, to get red emission, it is better to compensate these two extremes and design a LED structure with QW thickness (L_W) within 3 to 4 nm range and In composition of 29 to 36%, since within these limits the equilibrium lattice parameter and oscillator strength are reasonable for the LED structure.

In this study, we incorporate $Al_yGa_{1-y}N$ as a capping layer on the top of $In_xGa_{1-x}N$ QW based on SCAM (0001) substrate. The overall LED structure of the proposed model is as shown in Fig. 2. We have made a comparative study, like to that we did for green emission from $GaN/In_xGa_{1-x}N/Al_yGa_{1-y}N$ on sapphire substrate [34] and tried to adjust the thickness of epilayers and composition of QW and cap layer to find out the best structural parameters with a much higher intensity of red emission.

4. Results and discussion

From the equilibrium lattice parameter (a_{eq}) data for $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ system, we can conclude that the value is always larger than that of the in-plane lattice parameter of $In_{0.17}Ga_{0.83}N$ barrier layer ($a = 3.249$ Å) (Fig. 1). To bring the equilibrium lattice parameter (a_{eq}) near to 3.249 Å, we have considered two models for the proposed LED structure. In the model 1, we have taken the QW thickness close to 3 nm, In composition 35% (In comp., $x = 35\%$), and in the model 2 we have considered the QW thickness 4 nm, In composition 30% (In comp., $x = 30\%$) along with the $Al_yGa_{1-y}N$ cap layer thickness 2 nm and Al composition 17% (Al comp., $y = 17\%$) for both models. Using Eq. (3), we have found that

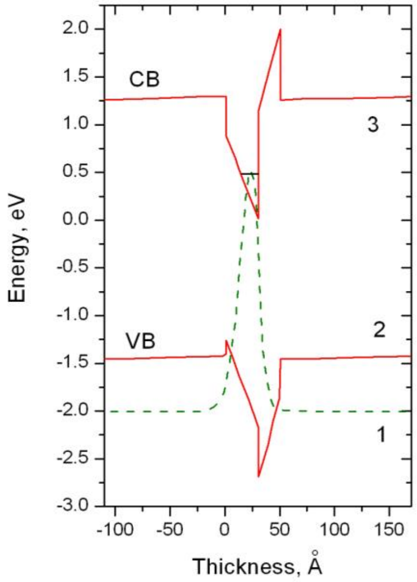

Fig. 3. Energy band diagram for the model 1, where the green line represents the electron wave-function and red lines are valence and conduction bands of the system.

Table 1. Variation of parameters while keeping QW thickness fixed at $L_W = 3$ nm.

Sl. No.	Indium composition (% of In)	Cap layer thickness, L_C (nm)	Aluminum composition (% of Al)	Emission wavelength, λ (nm)	Equilibrium lattice parameter, a_{eq} (Å)	Logarithmic value of the oscillator strength (Γ)
1	35	2	17	663	3.249	–0.93
2	35	2	18	663	3.249	–0.95
3	35	2	19	663	3.248	–1.28
4	37	2	17	698	3.252	–1.40
5	33	2	17	632	3.246	–3.84
6	35	1	17	644	3.271	–0.45

Table 2. Variation of parameters when keeping QW thickness fixed at $L_W = 4$ nm.

Sl. No.	Indium composition (% of In)	Cap layer thickness, L_C (nm)	Aluminum composition (% of Al)	Emission wavelength, λ (nm)	Equilibrium lattice parameter, a_{eq} (Å)	Logarithmic value of the oscillator strength (Γ)
1	30	2	17	647	3.249	–1.67
2	30	2	18	649	3.249	–1.50
3	30	2	19	650	3.248	–3.43
4	32	2	18	692	3.253	–1.70
5	28	2	18	632	3.245	–5.90
6	30	1	18	623	3.266	–1.84

the equilibrium lattice parameter for both models become exactly equal to the required value 3.249 Å. Then, to find the emission wavelength and oscillator strength values of the model structures, we used Eq. (1) to identify the internal electric field for each layer. For the model 1, the values are as follows: barrier electric field $E_b = 28.55$ kV/cm, QW electric field $E_W = 3174.3$ kV/cm and cap layer electric field $E_C = 4590.1$ kV/cm, as well as for the model 2 they are: barrier electric field $E_b = 3.11$ kV/cm, QW electric field $E_W = 2290.8$ kV/cm and cap layer electric field $E_C = 4562.8$ kV/cm, respectively. Using these values and solving the Schrödinger equation, we obtained that the emission wavelength of the system is within red emission (630…670 nm) and the logarithmic value of oscillator strength is much better than that of $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$ system. To adjust further, we tried to manipulate the composition and thickness of QW and cap layer and to identify their impacts on the wavelength and oscillator strength values. In each case, we kept the barrier layer thickness 12 nm thick. Tables 1 and 2 summarize the results for QW thickness 3 and 4 nm, respectively. From Table 1, we can find that with change in any parameter of the model 1, the overall performance changes. For example, if we change the Al composition of cap layer (% of Al), the oscillator strength values get reduced, but the equilibrium lattice parameter and emission wavelength remain almost the same (2nd and 3rd row entries of Table 1). Variation in In composition (% of In composition, x) and cap layer thickness (L_C) makes huge impacts on the emission wavelength, equilibrium lattice parameter and on oscillator strength values (4th to 6th row entries of Table 1). When increasing (decreasing) the In composition inside QW, red (blue) shifts of the emission are observed, since the bandgap of QW is inversely proportional to In composition. The oscillator strength values drop more drastically than those in the model 1, and chance of defect generation increases, because of the equilibrium lattice parameter changes from 3.249 Å. However, we get the largest oscillator strength value while keeping the cap layer thickness less than 2 nm ($L_C = 1$ nm as shown in Table 1). But in that case, emission gets blue shifted and chance of defect generation increases as the equilibrium lattice parameter ($a_{eq} = 3.271$ Å) becomes higher than 3.249 Å. The energy band diagram for the model 1 is shown in Fig. 3, where the green line shows the electron wave-function within the QW region.

For the model 2, we observe that by slightly increasing the Al composition (from $y = 17\%$ to $y = 18\%$) of the cap layer, the logarithmic oscillator strength value (Γ) increases from –1.67 to –1.50 (see 1st and 2nd row entries of Table 2). Other than that similar type of impacts have been found due to change in In composition and cap layer thickness, which we have found for the model 1 (see 4th to 6th row entries of Table 2).

Finally, comparing these two models (see Tables 1 and 2), we can say that it is better to have LED structure of the model 1, since it allows us to have the highest logarithmic oscillator strength value (Γ = –0.93), red emission at 663 nm and perfect equilibrium lattice parameter close to 3.249 Å.

5. Conclusions

We have tried to determine a suitable LED structure with high intensity red emission on SCAM (0001) substrate. We have made the comparative study of In$_{0.17}$Ga$_{0.83}$N/In$_x$Ga$_{1-x}$N/Al$_y$Ga$_{1-y}$N system, where Al$_y$Ga$_{1-y}$N acting as a cap layer to that of In$_{0.17}$Ga$_{0.83}$N/In$_x$Ga$_{1-x}$N LEDs. Al$_y$Ga$_{1-y}$N cap layer of thickness (L_C) 2 nm and Al composition (y) of 17% deposited on In$_x$Ga$_{1-x}$N QW thickness of 3 nm with In composition (x) of 35%, allow us to have peak emission at 663 nm with the highest logarithmic oscillator strength value ($\Gamma = -0.93$) and also perfect equilibrium lattice parameter of 3.249 Å. This structure should have a higher intensity with the less defect density than that of In$_{0.17}$Ga$_{0.83}$N/In$_x$Ga$_{1-x}$N system, since either the overall equilibrium lattice parameter (a_{eq}) is much higher and/or the logarithmic oscillator strength value (Γ) is much lower in every combination of QW thickness *vs* percentage of In composition case for red emission (see Fig. 1). This LED structure can be used as a light converter on SCAM (0001) substrate, like to that we have seen the same with GaN/In$_x$Ga$_{1-x}$N on sapphire substrate [35]. The main challenge will be the accurate growth of the LED structure in near future.

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Моделювання структури світлодіодів $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ на підкладці $ScAlMgO_4$ (0001) для випромінювання червоного кольору високої інтенсивності

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Анотація. Створена модель структури світлодіода $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N/Al_yGa_{1-y}N$ на підкладці $ScAlMgO_4$ (0001) для випромінювання червоного кольору високої інтенсивності. Великий вміст індію (In > 15%) у полярній квантовій ямі *c*-площини (КЯ) для випромінювання з більшою довжиною хвиль погіршує структурні та оптичні властивості світлодіодів через індуковану енергію деформації та квантовий ефект Штарка. Щоб компенсувати ці ефекти, на КЯ шар товщиною 3 нм із вмістом In 35% нанесено шар $Al_yGa_{1-y}N$ товщиною 2 нм із вмістом Al 17%, що дозволило зменшити щільність дефектів і підвищити інтенсивність червоного випромінювання при 663 нм, ніж у світлодіодів $In_{0.17}Ga_{0.83}N/In_xGa_{1-x}N$, вирощених на підкладці $ScAlMgO_4$ (0001). Це було продемонстровано шляхом моделювання. Ця структура світлодіода має досконалу рівноважну сталу решітки (a_{eq} = 3,249 Å) і вищі значення логарифмічної сили осцилятора ($\Gamma = -0{,}93$).

Ключові слова: світлодіод на $ScAlMgO_4$ (0001) підкладці, випромінювання червоного кольору, рівноважна стала решітки, сила осцилятора, AlGaN шар.