Numerical Simulation on Electroluminescent property of GaN Nanorod LED array

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Abstract. The quantum well thickness and In concentration of the multi-section nanorod array structure increase with the sidewall height. At present, a two-section nanorod structure with a 466 nm spectrum at the bottom of the nanorod and a 488 nm spectrum at the top has been prepared. In this paper, according to the theory of yellow-blue light mixing to achieve white light, we have proposed a structure of the two-section nanorod, with a white LED model emitting a blue light spectrum at the bottom of the nanorod and a yellow light spectrum at the top. By varying the In concentration in the structure, the spectra of different In concentrations in different positions of the sidewall quantum wells were simulated to obtain the blue light in the sidewall quantum wells. We observed that the blue light of In cooperation range are 0.15~0.22, the yellow light of In cooperation are 0.27~0.34, and the corresponding wavelengths varied from 443nm to 498nm and 542nm to 610 nm. Therefore, the proposed structure will be a potential candidate in phosphor-free white-color emission LED.

1. Introduction

The fabrication of InGaN/GaN quantum well (QW) nanorod (NR) light-emitting diode (LED) arrays has attracted much attention, due to the advantages of dislocation-free crystal quality, larger emission area and non-polar quantum wells growth for efficient emission [1,2]. The self-organized GaN NRs have been widely grown on sapphire and silicon substrates with molecular beam epitaxy (MBE) [3,4] and metalorganic chemical vapor deposition (MOCVD) in randomly-distributed manner [5-7]. Selected area epitaxy (SAE) growths of GaN NRs have also been implemented with MBE and MOCVD. In regularly SAE growth, vertically oriented NRs of uniform size and height distributions can be obtained. With MOCVD growth, the pulsed growth technique is a common method for growing NR in vapor-liquid-solid (VLS) growth mode [8,9]. In this growth method, the Ga and N sources are switched on and off alternatively. When the supply durations of both Ga and N are kept constant, a single-section NR of a uniform cross-section could be obtained. However, if we decrease the Ga supply duration, while maintaining a constant N supply duration, a tapering section of decreasing cross-sectional size can be formed. Based on such a tapering process, two-section NRs of changing cross-sectional size can be grown [10].

For the growth of InGaN/GaN QW LED structure, n-type GaN NRs can be first grown along the c-axis based on the aforementioned pulsed growth method. Then, the QW structures can be deposited onto the hexagonal sidewalls (m-plane) to form nonpolar QWs in two-dimensional (2-D) growth mode. The broad emission spectrum from such an NR-LED array is observed, which can be attributed to the non-uniform distributions of QW thickness and indium composition on a sidewall. Normally, both QW
thickness and indium composition increase with height on a sidewall, leading to the increasing trend of emission wavelength along height on a sidewall of a single-section NR. However, the range of spectral variations for single-section NR is too narrow to meet the requirement broad wavelength emission application. To solve this problem, a two-section NR is fabricated through tapering process [11-13]. After depositing sidewall QWs, a broader QW emission spectrum compared to a single section NR is obtained, due to the larger variations of QW thickness and indium composition among different NR sections. Although the fabricated device can hardly meet the white-color emission requirement, this technique offers us a useful way to design and experimentally fabricate white-color emission LED based on two-section NR arrays.

In particular, the issue of white-color emission from such an NR structure without using phosphor is attractive for practical application. Without using phosphor, the Stokes loss in photon down-conversion can be removed for increasing the device overall efficiency. Also, the modulation bandwidth of a white-color LED can be significantly increased for visible communications. Motivated by the above advantages and fabrication method, a white-color LED model based on a two-section NR is proposed and simulated with COMSOL software. The influence of QW thickness and the indium concentration on the emission spectrum is demonstrated. Thanks to the tapering section, the LED model with light emission in the wavelengths of blue and yellow spectral peak are realized at the top and bottom parts of NR respectively.

2. LED device modeling
The growth model of single and two-section NR have been established in our previous work to explain the growth mechanism of QW structure on NR sidewalls. Especially, the height-dependent variation of QW thickness and indium composition are demonstrated, which properties are important for us to design the phosphor-free white-color LED arrays. In that model, the growth of QWs on single-section NR are contributed by downward diffusion of adatoms collected on the slant facets at the NR top, the upward diffusion of adatoms collected on the substrate, and the direct adsorption of atoms on the sidewall from the vapor phase. For a two-section NR, the upward and downward diffusions of adatoms collected on the slant facets of the tapering section between the two uniform sections and downward diffusions of adatoms from the top pyramid facets serve as extra adatom supply sources. Hence, by carefully control the growth time of tapering section and top facets, their geometric size can be adjusted accordingly. That means through the introduction of tapering section and top facets, the QW thickness and indium composition between upper and bottom parts of NR can be designed separately. Then, the specified intensity and spectral peak of emission will be satisfied at the designated parameters.

In this section, the performance of single-quantum well InGaN/GaN NR LED device of our design is investigated. This structure consists of n-type GaN core, InGaN/GaN active region and surrounded by p-type GaN layers. The parameters used in our simulation are listed in Table 1. The COMSOL software is implemented for device modeling. Here, we set three steps that considered to analyze the effect of current driving on LED spectrum in our modeling. First, the doping and transition from the continuous quasi-Fermi heterojunction model to the thermal emission model are studied. Second, the applied voltage from 0 to the appointed value is evaluated for current-voltage (I-V) relation. Third, the solution of the second step is utilized for current bias study. The applied current from 10 to 100 mA is swept for device analysis. Finally, the emission spectrum and the internal quantum efficiency (IQE) of LED device are characterized with respect to the current bias. In Table 1, the band gap of InGaN is changed with various In compositions, the other parameters for GaN and InGaN is the same in our simulation model.
Table 1. Parameters used in the model

| Material                  | GaN        | InGaN     |
|---------------------------|------------|-----------|
| Relative permittivity     | 9.7        | 9.7       |
| Band gap                  | 3.4[eV]    | InGaN_bg  |
| Electron affinity         | 4.1[eV]    | 4.1[eV]   |
| Electron mobility         | 1000 [cm^2/(V*s)] | 1000 [cm^2/(V*s)] |
| Hole mobility             | 350 [cm^2/(V*s)] | 350 [cm^2/(V*s)] |
| Auger recombination factor of electrons | 1.7e-30 [cm^6/s] | 1.7e-30 [cm^6/s] |
| Auger recombination factor of Hole | 1.7e-30 [cm^6/s] | 1.7e-30 [cm^6/s] |
| Electron lifetime, SRH    | 1e-8s      | 1e-8s     |
| Hole lifetime, SRH        | 1e-8s      | 1e-8s     |

3. Simulation results and Discussion

The model we studied is schematic illustrated in Fig.1. It consists of one quantum well structure of InGaN with thickness of 1nm on NR sidewalls, two quantum barrier layers of GaN of 5nm, p-type of 150nm and n-type layers of 145nm. The In concentrations in the upper and bottom parts of NR are set as 17% and 28% calculated from Fig.1(a), so as to obtain white-color emission spectrum. For effective current spreading over the sidewall QWs, conformal growth of transparent conductor, GaZnO, is undertaken on each NR. Here, one can see that on top of GaZnO, p-contact metals of Ni/Au (150∕50 nm) and n-contact metals of Ti/Au (150/50 nm) are deposited. As shown in Fig. 1, the injected current can flow along the conformal GaZnO layer and pass through the sidewall QWs for excitation. In Fig. 1(b), the detailed demonstration of device structure in one dimension is given. The combined illuminated effects from upper and bottom parts of NR will be given in the following.

![Schematic illustration of the model](image)

Fig. 1(a) Schematic illustration of the model (b) detailed demonstration of one-dimensional structure along horizontal direction of NR.

Figure.2 shows the relationship between injection current and applied voltage (I-V curves). The applied voltage varies from 0 to 3.3V with the turn-on voltage of 2.9V, which is consistent with experimental result obtained by Prof. C. C. Yang’s group. [8,9]. The inset shows the excitation spectrum at 2.8V and 2.9V respectively. As we can see from the figure, the relative intensity at 2.8V is much smaller than that of 2.9V, confirming the value of turn-on voltage of 2.9V.
Fig. 2 Relations between injection current and applied voltage with the turn-on voltage of 2.9V. The insets show the excitation spectrum at 2.8V and 2.9V respectively.

The simulation result of two-section NR LED device with applied current from 10mA to 100mA is shown in Fig.3. Due to different In concentrations in the upper and bottom parts of NR array, the emission of blue- and yellow-color light at the NR sidewall QWs can be obtained simultaneously. The wavelengths of light corresponding to different In concentrations are shown in Table 2. The combined effect of blue and yellow light with intensity ratio around 0.6 results in white-color emission from the whole output. From the figure, we can see that the blue-shift of the blue and yellow spectrum with the increased current are 11nm and 15nm respectively. The output spectral peak is expected to be fixed in an LED with m-plane QWs when injection current increases. The blue-shift trend of output spectral peak shown in Fig.3 is due to the non-uniform distribution of QW emission wavelength on a sidewall. Because the potential of a higher-indium QW is lower, when injection current level is low, it mainly flows through the QW portion of higher indium content and excite long-wavelength emission. As injection current becomes higher, the injected carriers can spread into the QW portions of higher potentials (lower indium contents) and excite shorter-wavelength emission. The two peaks of spectral wavelengths are centered at 466nm and 558 nm at 100mA, corresponding to blue and yellow wave band.

Fig.3 The spectrum of InGaN/GaN NR array at injection current from 10mA to 100mA. The two peak wavelengths are centered at 466nm and 558 nm at 100mA. The spectral blueshift with increasing current from 10mA to 100 mA is observed.
Table 2. Comparison of wavelengths of different In concentrations in the blue light yellow band

| Indium concentration | 0.15 | 0.16 | 0.17 | 0.18 | 0.19 | 0.2 | 0.21 | 0.22 |
|----------------------|------|------|------|------|------|-----|------|------|
| Wavelength (nm)      | 447  | 455  | 462  | 470  | 479  | 486 | 495  | 504  |

| Indium concentration | 0.27 | 0.28 | 0.29 | 0.3  | 0.31 | 0.32 | 0.33 | 0.34 |
|----------------------|------|------|------|------|------|------|------|------|
| Wavelength (nm)      | 549  | 558  | 462  | 579  | 588  | 599  | 609  | 621  |

4. Conclusions
In summary, due to the unique properties of indium distribution on NR QWs from experimental observation, the LED device based on two-section NR is designed and simulated. The geometric parameters of NR such as height, radius and size of tapering section are analyzed in order to achieve white-color emission, as In diffusion length and its incorporation rate is highly dependent on the chosen parameters. We conclude that the blue light In cooperation range of 0.15~0.22 and the yellow light of 0.27~0.34, the corresponding wavelengths varied from 443 to 498nm and 542 to 610 nm. Therefore, our proposed structures shows a potential and alternative solution in white-color LED design and fabrication.

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