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Study of carrier dynamics and radiative efficiency in InGaN/GaN LEDs with Monte Carlo method

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In this paper, we have applied the Monte Carlo method to study carrier dynamics in InGaN quantum well. Vertical and lateral transport and its impact on device radiative efficiency is studied for different In compositions, dislocation densities, temperatures, and carrier densities. Our results show that the non-radiative recombination caused by the defect trapping plays a dominating role for higher indium composition and this limits the internal quantum efficiency (IQE). For lower indium composition cases, carrier leakage plays some role in the mid to high injection conditions and carrier leakage is strong in very high carrier density in all cases. Our results suggest that reducing the trap density and QCSE are still the key factors to improve the IQE. The paper examines the relative roles of leakage and non-radiative processes on IQE.

1 Introduction Nitride based light-emitting diodes are playing a dominant role in the solid state lighting [1, 2]. However, the efficiency of InGaN LED is still low especially in the longer wavelength range [3–6]. In c-axis growth devices the strong quantum confined Stark effects (QCSE) caused by the piezoelectric and spontaneous polarization causes the electron and hole to be spatially separated increasing the radiative lifetime. Several efforts have been made to decrease the electron hole separation. These include use of a staggered InGaN quantum well [7–10] with various compound materials or use of electron blocking layer [11] and polarization matched layer [5] to prevent leakage. However, there is still no clear answer for how to bring the device IQE to 100%. Most papers addressing the efficiency of LED use A (non-radiative), B(radiative), C (Auger) coefficients and drift-diffusion solver from the commercially available software to empirical fit the experimental results. These approaches provide a macroscopic view of the physical mechanism in the InGaN LED and sometimes may be too simplified. Work has been reported using non-quasi-equivalence model to improve the simulations [12]. In this paper we use a Monte Carlo approach to study a more statistical dynamic behavior of carriers in the quantum well which we believe can reveal more of the underlying physics in the InGaN quantum well.

Our approach allows us to examine lateral and vertical transport of free carriers once they are in the InGaN QWs. This transport occurs under very low electric field and is important as it determines how carriers laterally diffuse towards regions of dislocations before they recombine radiatively or non-radiatively. To study this phenomenon, we have developed a Monte Carlo program [13] which includes several 2D scattering mechanisms to study the lateral mobility of carriers in the InGaN quantum wells and the performance of the device. The impact of parameters such as dislocation density, interface roughness, indium composition and junction temperature on the internal quantum efficiency(IQE) is discussed in this paper.

2 Method To investigate the carrier transport in the QW, we use the one dimensional (1D) Poisson, Schrödinger and drift-diffusion equations solver [14] to obtain the carrier density, wavefunctions, and spontaneous emission rate ($R_{\rm sp}$), and then calculate the carrier dynamics by MC method [15]. The MC method includes several 2D scattering mechanisms, such as charged dislocation scattering [16], interface roughness scattering [17], alloy scattering, 2D polar optical and acoustic phonon scattering [18], and electron-electron scattering [19]. We recognize that the allowed transition states will become restricted when the carrier density is high and subband states are filled with carriers. Therefore, the Fermi-Dirac distribution function is used to determine if the final scattering state is occupied or not. Before adding the non-radiative term, we calculate the carrier mobility to know the diffusion coefficient of carriers in the quantum well.

Once the lateral transport is evaluated, we start to estimate the IQE of InGaN quantum well LED. We arrange the locations of dislocation defects randomly in the QW with different average spacing. In the simulation process, the electron will laterally diffuse randomly in the QW within a calculated radiative lifetime. During the diffusion process, if the electron enters into the center of the dislocation defect, it will be captured by the defect and will recombine non-radiatively. Otherwise, it will keep diffusing until it recombines radiatively. Furthermore, to study the influence of carrier leakage especially for electron, we have included the non-equivalent intervalley scattering mechanism to account for how the phonon adsorption or emission assists electrons to overcome the potential barrier ΔE_c and causes leakage. Note that electron effective mass (≈ 0.2 m_0) is much smaller than the hole effective mass (≈ 1.6 m_0). Therefore, for the same quantum well size, electrons have a smaller density of states in the quantum well making it much easier for the quantum well to be filled up and cause leakage. Electron leakage effects have been observed by many experimental groups. Therefore, we only consider the electron leakage in this paper. The potential barrier is decided by the maximum potential in the p-GaN layer to the first eigenvalue of the quantum well in the conduction band obtained by the Poisson, drift-diffusion and Schrödinger solver. So the potential barrier will be influenced by the bias condition. With a larger forward bias, the barrier becomes smaller and therefore as injection density increases, there is a higher carrier leakage.

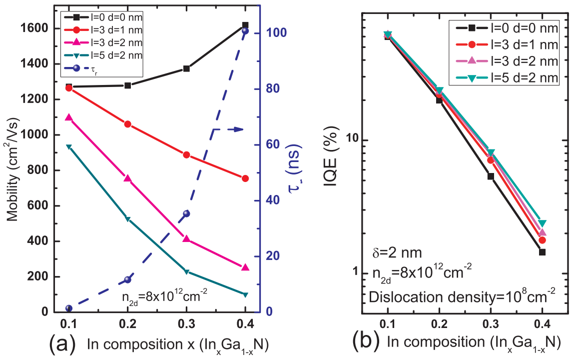

Figure 1 (a) The calculated mobility and radiative lifetime τ_r versus the indium composition with different interface roughness parameters. l and d are the interface roughness size horizontally and vertically, respectively.The quantum well width is 3 nm and n_{2d} is 8×10^{12} cm^{-2}. (b) The estimated maximum efficiency versus the indium composition. The capture cross section diameter,δ is 2 nm.

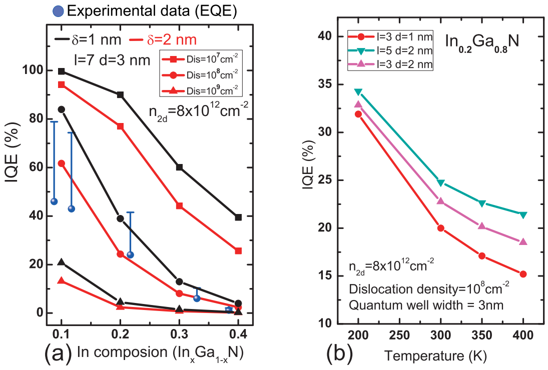

Figure 2 (a) The estimated maximum efficiency versus the indium composition with different dislocation densities when the n_{2d} is 8×10^{12} cm^{-2}. The circle points are the experimental results of EQE and range bar are the estimated possible IQE [20]. (b) The estimated maximum efficiency versus temperature with different roughness l and d for the 20% In QW.

3 Results and discussion We start by removing the defect traps so we can determine the carrier diffusion in the QW. Figure 1(a) shows the calculated mobility and radiative lifetime τ_r versus indium composition when n_{2d} is equal to 8×10^{12} cm^{-2}. Here l and d are the interface roughness size horizontally and vertically, respectively. Carrier mobility is inversely proportional to the effective mass so when the interface is perfect without surface roughness, the mobility of higher In composition is higher because of the smaller effective mass. Thus the carriers in the channel have a larger mobility. But the mobility does not increase too much since it becomes limited by the stronger alloy scattering. If the interface is not perfect, the mobility drops rapidly with larger interface roughness especially in higher indium cases where alloy scattering is stronger since the scattering potential ΔE_c is larger in higher indium composition alloys. In addition, the higher In composition has much longer τ_r due to the stronger QCSE. As a result, the efficiency becomes lower with higher In composition due to the higher capture rate as shown in Fig. 1(b). We find that for 10% In composition devices is (typical UV and blue LED range), devices have much better IQE because of the smaller QCSE and smaller τ_r. One can expect that a higher dislocation or defect density will lead to a higher capture rate. Figure 2(a) shows the relation of IQE, indium composition, and defect or dislocation density. If we can improve the fabrication process and make the dislocation or defect density drop to 10^7

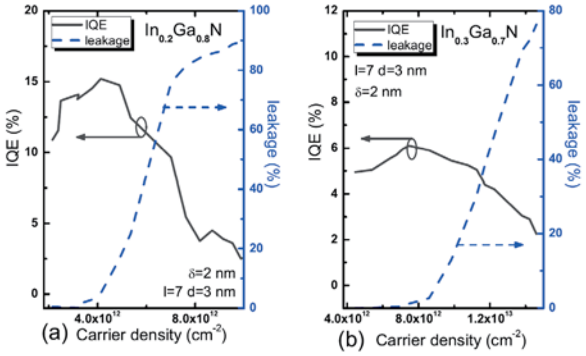

Figure 3 The estimated maximum efficiency and carrier leakage rate versus carrier density; (a) is for the 20% indium QW; (b) is for the 30 % indium QW.

cm^{-2}, the IQE can be improved significantly. For example, the IQE can increase to 30-40% for 40 percent In composition if the dislocation or defect density is 10^7 cm^{-2}. Also, reducing the radiative lifetime by non-polar or use of polarization matched material will be helpful in the high indium case. The circle points in Fig. 2(a) are experimental results of EQE and range bar are the possible IQE ranges by assuming a 50% light extraction efficiency [20]. For a typical dislocation density 10^8 cm^{-2}, our results show a good agreement if δ = 1 to 2 nm is assumed. For the higher In composition, the lattice mismatch is larger and it is harder to get a good crystal film even if the substrate is dislocation free. Therefore, it has been suggested that one use a thick InGaN buffer layer [21] to reduce the lattice mismatch in the system. This could be a possible solution to enhance the device performance.

The non-radiative recombination process will generate heat so we examine the role of temperature on IQE. Figure 2(b) shows the estimated maximum efficiency versus the temperature for 20 % In quantum well. We see that when the device temperature reaches 400 K, the diffusion length increases by 30% $\sim$ 60% depending on In composition because of the increase of τ_r. Therefore, the heating effect will make the non-radiative process even more dominated and may lead to the droop effect at higher current density. It is believed that the pulse measurement can completely remove the heating effect. However, the local heating effect at the active layer may not be avoided. In our previous work [22], the heat up time of the device in the active layer is only a few nanoseconds so that a very short pulse is needed.

Our studies show that the IQE will increase as the carrier density increases because of the reduction of QCSE and radiative lifetime. To understand the influence of carrier overflow versus carrier density, we need to include the overflow mechanism. Figures 3 (a) and 3(b) show the IQE and leakage versus carrier density for 20% and 30% indium compositions, respectively. We find that for carrier density larger than $4 - 8 \times 10^{12}$ cm^{-2}, the leakage becomes very important. For the higher indium case, the leakage starts to become strong at higher injection carrier density because of larger ΔE_c. However, since it has very large radiative lifetime caused by QCSE, the efficiency is quite low due to the non-radiative traps. For lower indium cases, due to high possibility of phonon assisted leakage, devices with higher quantum well numbers may be helpful to improve the performance. For the higher indium case, reducing the dislocation or trap density are still key issues to improve the IQE.

4 Conclusion We have analyzed the lateral and vertical transport behavior of free carriers in the InGaN/GaN QW and examined the role of lateral transport on IQE. Our calculation shows that peak IQE is strongly influenced by the dislocation density and radiative lifetime. By reducing the defect density or through the use of non-polar structures, the IQE can be improved considerably. When the phonon assisted leakage mechanism is included, it shows a strong leakage in the high carrier density condition. However, in green or yellow light emission, the peak IQE is still influenced by the defect trapping and reducing the defect density is more critical. In our future work, we will add the effect of multiple quantum wells and Auger effect to make this study more complete.

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