3D structural construction of GaN-based light emitting diode by confocal micro-Raman spectroscopy
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ABSTRACT
The key issue for light emission strength of GaN-based LEDs is the high defect density and strain in MQWs causing the electric polarization fields. In this work, we construct 3D confocal microspectroscopy to clarify strain distribution and the relationship between photoluminescence (PL) intensity and pattern sapphire substrate (PSS). From 3D construction of E$_2^{\text{high}}$ Raman and PL mapping, the dislocation in MQW can be traced to the cone tip of PSS and the difference in E$_2^{\text{high}}$ Raman mapping between substrate and surface is also measured. The ability to measure strain change in 3D structure nondestructively can be applied to explore many structural problems of GaN-based optoelectronic devices.

Keywords: GaN, pattern sapphire substrate, confocal Raman microspectroscopy

1. INTRODUCTION
GaN and related compound semiconductors are attractive material for optoelectronic device applications such as light-emitting diodes (LEDs), and laser diodes, etc. The InGaN/GaN LEDs have become the most important optoelectronic devices in solid-state lighting application due to the wide tunable range of the emitting wavelength from ultraviolet (UV) to near infrared (NIR) and the high overall electric-optical conversion efficiency which has been improved rapidly.[1, 2]

Although there are many advantages, lack of native substrates is a big issue and limited the development of GaN-based devices. Without native substrates, the GaN-based devices are commonly grown on sapphire substrates by the heteroepitaxy approach, but the large lattice mismatch induces large defect and dislocations in the subsequent grown GaN films.[3, 4] In order to improve the crystal quality of GaN-based devices grown on sapphire substrate, patterned sapphire substrate (PSS) is widely applied and it can not only reduce the defect and dislocation density, but also enhance the light extraction efficiency.[5, 6] Although the PSS technique was introduced, large lattice mismatch between GaN films and PSS still causes a large built-in strain and an accompanied large internal electric field triggered by strain-related quantum-confined Stark effect (QCSE) in the commonly grown [0001] c-plane direction.[7, 8] The internal electric field leads to the band bending and mismatch of electrons and holes wavefunction in the quantum-well region which decreases the radiative recombination efficiency in the multiple quantum wells (MQWs). The suppression of efficiency of GaN MQWs now becomes more and more seriously with increasing of injection current which is so called efficiency droop phenomenon. [9, 10] The efficiency droop phenomenon is a great challenge for GaN-based LEDs to operate in higher injection current where nowadays chips are getting smaller but need to maintain the same output power or even achieve higher output power.

In the previous research, many groups try to change the structure of PSS, such as shape, height, or period of PSS, to release the compressive strain in GaN films and suppress dislocation density by bending the threading dislocation along the tilted surface of PSS.[11] In the research of Y.-L. Li’s group, the spatial strain distribution was measured by micro-Raman spectroscopy and they observed that the PSS caused the spatial strain variation in the GaN films between the plane area and cone area of PSS.[12] The strain variation not only caused the difference of QCSE spatially, but also made the In content fluctuation in MQWs. The different droop behavior on a single device due to the fluctuation of...
effective band gap was also obtained in the research of Y. Lin’s group. The well design of pattern of sapphire substrate may reconstruct the strain distribution in GaN films and raised the efficiency and suppressed efficiency droop effect.[13] In this work, we use a GaN-based LED structure without p-GaN layer as reference sample in order to directly observe the characteristics of MQWs. The correlation between PSS and strain distribution in GaN films and the correlation between PSS and spatial light emission intensity in MQWs have been measured by spatially resolved photoluminescence (PL) and spatially resolved confocal Raman spectroscopy. Combining the mapping results, we have confirmed that periodically compressive strain fluctuation in GaN films and spatial In content variation are both correlated to PSS.

2. DEVICE DESIGN

In this work, the GaN-based LED structure was grown on the c-plane PSS by using metal organic chemical vapor deposition system (MOCVD) and the sample layer structures are shown in Figure 1, consisting of a 3 μm-thick undoped GaN, and 2.5 μm-thick Si-doped n-GaN from the PSS, followed by 60 pairs of In_{0.05}Ga_{0.95}N/GaN superlattice layers and InGaN/GaN multi-quantum wells (MQWs) as the active layer. Two different In content quantum well were designed in the MQWs: the first group with 8% In content for 6 wells, while the second group with a 15% In content for 9 wells, and the thickness of InGaN wells were 2.5–3 nm and that of GaN barriers were 12 nm for both groups.

![Figure 1](attachment:figure1.png)

Figure 1. Schematic diagram of a (a) three-dimension and (b) a two-dimension of GaN films grown on PSS

3. RESULTS AND DISCUSSION

The spatial strain variation was measured by the powerful tool, spatially resolved confocal Raman spectroscopy which is able to obtain Raman spectrum mapping in the specific layer. The Raman intensity of E$_{2}^{\text{high}}$ at the MQW layer and substrate interface are shown in Figure 2(a) and the position of PSS and dislocation are determined. Fig. 2(d) shown the E$_{2}^{\text{high}}$ phonon peak position variation along the white line. Combining the result of Raman intensity mapping, we can see that there is a large strain fluctuation in the substrate interface and lower E$_{2}^{\text{high}}$ phonon peak position measured at the cone area. Although the strain fluctuation in the MQWs is not as large as that in the substrate interface, the correlation to the PSS is still be observed and the compressive strain in the MQWs above the cone area is relatively smaller than that above the flat area of PSS.
In order to clarify the impact of strain variation induced by PSS on the PL spectrum, the spatial PL measurement was done and shown in the Figure 3. In the Fig. 3(a), we demonstrate the PL intensity mapping in larger area and the Fourier transformed image of PL intensity mapping. The results show that there is periodical hexagonal distribution in PL intensity and the period of PL distribution is consistent with the PSS, shown in the Fig. 3(b). The higher PL intensity area is observed at the cone area and there are many small dark spots, which is nonradiative center caused by dislocation, on the top of cone tips. In the three-dimension mapping of $E_2^{\text{high}}$ phonon peak intensity, shown in the Figure 4, the relation between dislocation distribution and PSS are confirmed that most of dislocations are triggered from the cone tips of PSS.

Figure 3. Spatially PL intensity mapping image for (a) large scale about 60 $\mu$m2 (b) scale of one period of hexagonal PSS. The inset of (a) shows the fourier transform of image (a).
In addition, the PL peak position is also analyzed, shown in the Fig. 5, and there are two group of spectra with different main emission peaks observed. In the green area, the integrated PL intensity is higher and main emission peak is 450 nm which is the wavelength we designed. The PL emission at 440 nm rises and the integrated PL intensity decreases. The result shows that the strain distribution in the MQW causes the effective bandgap variation (or corresponding to In variation) in the MQWs. At the cone area, there is lower compressive strain and lower effective bandgap in comparison to those at the plane area so that the high compressive strain causes blueshift of PL emission from MQWs. The fluctuation of effective bandgap can enhance the localization effect in the MQWs and the carriers are preferred to accumulate at lower effective bandgap area. The local bandgap minimums provide carrier localization center and help to prevent the carrier diffusion to the defects and enhance the efficiency.

Figure 5. (a) The mapping of PL peak intensity of 440 nm (red region) and 450 nm(green region). (b), (c) PL spectrum of green region and red region.
In order to detailed study of carrier dynamics, the effective In content and the corresponding strain distribution based on the Raman peak and PL peak position mapping were both considered in calculation the rate equations to reveal the mapping of the radiative recombination rate shown in Figure 6. Since the radiative recombination rate distribution associated with the carrier density, the carriers accumulate at the area with higher In content and enhanced the recombination rate. The results are consistent with the experiment result of PL and Raman measurement. Combining the results in the previous research, by carefully designing the effective bandgap fluctuation to enhance localization effect can not only suppress the nonradiative recombination rate but also suppress efficiency droop effect.

Figure 6. (a)Simulation of In content fluctuation of MQWs (b)Simulation of radiative recombination rate of MQWs

4. CONCLUSION

In conclusion, we systematically measured the spatial strain distribution in GaN films by spatially resolved confocal Raman spectroscopy and PL mapping to confirm that the strain distribution is correlated to the PSS. We also confirmed that the strain fluctuation induced by PSS causes In fluctuation and strengthen localization effect. The experimental results are in good agreement with the simulation realization. Our demonstration is promising for the spatially resolved confocal Raman spectroscopy for nondestructive analysis and helpful contribution to design pattern of sapphire substrate in the future.

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