Microphotoluminescence mapping of laterally overgrown GaN layers on patterned Si (111) substrates

L. Macht, a P. R. Hageman, S. Haffouz, and P. K. Larsen
Experimental Solid State Physics III, Institute for Molecules and Materials, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

(Received 20 January 2005; accepted 26 July 2005; published online 19 September 2005)

Spatial distribution of optical properties of GaN layers grown on patterned Si (111) substrates by maskless metalorganic chemical vapor deposition has been investigated. The Si substrates were prepared with a pattern of 1.5 μm diameter holes at a 3.5 μm distance from each other. The holes were overgrown by GaN until coalescence, creating GaN areas with no substrate underneath. Microphotoluminescence mapping measurements with 0.8 μm lateral resolution show a five-fold increase in luminescence intensity coming from the overhang areas as compared to the layer directly over the substrate. This is accompanied by a slight redshift of the luminescence peak wavelength. Photoelectrochemical etching shows that the dislocation density is much lower in those areas while the photoluminescence redshift is attributed to lesser strain relaxation resulting from a lower dislocation density. © 2005 American Institute of Physics. [DOI: 10.1063/1.2042546]

Despite extensive research into the growth of gallium nitride (GaN), there are still no industrially available free-standing GaN wafers. This fact enforces the use of foreign substrates and, therefore, results in layers exhibiting large numbers of dislocations. Among the possible substrates, silicon offers some potential advantages as a substrate for GaN; these include: Low cost, large-scale availability, and well-established processing technology. Additionally, growth of nonpolar r-plane GaN layers can be realized on Si (001) by careful control of the nucleation layer. However, silicons' large lattice mismatch with GaN (17%) and additionally their difference in thermal expansion coefficients makes it very challenging to grow GaN layers of high enough quality to ensure proper operation of devices. Apart from a high density of dislocations (in the order of 1010 cm⁻²) created at the substrate-layer interface, the thermal expansion coefficient mismatch leads to the generation of cracks for layers thicker than 1 μm. Several methods of growth optimization can be used to improve these unfavorable characteristics, for instance, various modifications to the the AlN nucleation layer. An additional SiNx layer, or AlGaN/GaN superlattice structure also serves to release strain and lower the overall dislocation density. A significant improvement can be obtained by using the epitaxial lateral overgrowth (ELO) technique. In fact, dislocation densities as low as 5 × 10⁷ cm⁻² have been obtained. However, these techniques require complicated and costly ex situ processing during an interruption of the GaN growth.

The present letter reports on the photoluminescence (PL) characteristics of ELO GaN epilayers on (111) Si substrates patterned with hole openings. The results are discussed in terms of strain distribution and dislocation density as shown by photoelectrochemical (PEC) etching. According to PL results, these layers exhibit characteristics favorable for the growth of low cost light-emitting diode structures and are therefore industrially feasible.

Prior to the growth of the GaN layers, the Si substrates were etched in a hole pattern creating 4 μm deep circular holes with a diameter of 1.5 μm and center to center distance of 3.5 μm, arranged in a hexagonal plan. The etching was done in a series of dry etching steps: Inductively coupled plasma (ICP) etching followed electron cyclotron resonance (ECR) plasma etching. First, an oxide mask was deposited in an ICP C4F8 plasma, and, subsequently reactive ion etching-oxygen plasma etching was used to remove the organic resi-

![Figure 1](image-url)

**FIG. 1.** (a) SEM micrograph at 45° inclination of the GaN layer overgrowing the pits in the substrate. Complete coalescence can be observed, however, the growth run was too short for complete smoothing of the surface. (b) Schematic drawing of the overgrowth process. The arrows indicate lateral and vertical growth directions and solid line indicates the sample surface at the end of the growth run. The dotted lines show growth surfaces during the growth and the dashed line shows projected surface if the growth run had been continued.
PEC etching was employed to visualize the threading dislocations and to give an estimate of the dislocation density. It was performed in a stirred aqueous KOH solution (0.004 M) at room temperature. The UV illumination was provided by a 450W UV-enhanced Xe lamp. The nature and physical background of PEC etching can be found elsewhere.

Figure 2 shows the GaN layer after PEC etching. Due to its nature, PEC etching reveals dislocations of edge, mixed, and screw type as well as narrow inversion domain boundaries. Because the sample exhibits Ga-polarity, formation of inversion domains does not seem probable. Therefore, all the whiskers visible on the figure are attributed to dislocations and the density is calculated to be ~8 X 10^9 cm^-2. No whiskers can be seen in the overgrown areas. There are two reasons for that. First, as shown in Ref. 8, the dislocations which nucleated at the edge of a hole in the Si substrate tend to bend toward the center and either annihilate or become basal plane dislocations. Second, no new dislocations are generated in the overhanging GaN layer. The dislocations are known to suppress band edge luminescence and this is clearly reflected in Fig. 3. Figure 3(a) shows a map of luminescence intensity at the spectral position of the peak for a theoretical diffraction limit for the lens used (numerical aperture 0.6) is 0.66 µm.
The bright circular areas represent over-the-void voids show even lower emission energy than those directly above the Si substrate and those directly over the void due to the lack of dislocations.

In summary, it has been shown that GaN layers can be grown on patterned Si substrates exhibiting locally much lower dislocation density and better structure quality. This enhancement is accompanied by a large increase in luminescence intensity and a slight shift of luminescence peak toward lower energies. This redshift indicates higher levels of tensile stress which is caused by a locally lower density of dislocations.

**Fig. 4.** Spectral scans of PL at the points designated as A and B on the PL maps.

15×15 μm area. This peak position is not constant and it varies from spot to spot, the intensity of luminescence is taken at the actual spectral position of the peak for each point and not at an arbitrary energy. Thus, the measured intensity of overgrown areas is, on average, five times higher than intensity measured in the areas directly over the substrate. In Fig. 3(a), the bright circular areas represent over-the-void layer.

A corresponding map of the same area shown in Fig. 3(b) shows peak emission energy. The luminescence from the overgrown areas of the GaN layer have markedly lower energy than those from areas above the Si substrate and the values are 3.400 eV and 3.405 eV, respectively. Figure 4 shows PL spectral data from two points designated as A and B in Fig. 3. The scans show the difference between luminescence intensity as well as the spectral position of the peaks. The latter value is consistent with value of 3.406 eV reported elsewhere for GaN/Si layers. For comparison, GaN/sapphire which is believed to be in small compressive strain at room temperature emits at 3.424 eV, while completely unstrained GaN emits light at 3.420 eV.

GaN layers grown on Si substrates are believed to be in tensile strain at room temperature resulting in the emission wavelength shifted toward lower energies. This is also the case for our samples as can be seen by lower emission energies than those for relaxed GaN. It is also believed that layers grown over a mask in the ELO process or, in this case, over a void should be relaxed and therefore have emission at comparably higher energy. Figure 3(b) shows exactly the opposite behavior, as spots corresponding to areas grown over the voids show even lower emission energy than those directly over the substrate.

The reason for such an effect can be explained by the dislocation formation mechanism and the strain relaxing properties of dislocations. There are two major reasons for the existence of dislocations. One is the fact that growth is usually started as three-dimensional growth and the layers coalesce at a later time which induces the creation of low angle grain boundaries at the spots of coalescence, creating rows of dislocations. The second reason is the differences in thermal expansion coefficients which induce stress upon cooling of the sample and dislocations appear postgrowth as a means of relaxing that stress. Differences between the density of GaN nucleation islands result in the general differences of statistical dislocation density between GaN layers grown on different substrates.

In the case of this sample, the PL results shown in Fig. 3(b) suggest that GaN areas grown over a void have higher tensile stress than the ones over Si substrate. This can be explained by the fact that the areas over Si have very high in-grown dislocation density. Those dislocations relax strain, whereas a much lower dislocation density in the areas over the voids does not present such an opportunity. The mismatch in the thermal expansion coefficients between Si and GaN induces tensile strain when the sample is cooled down to room temperature, which can be partially relaxed by the in-grown dislocations directly over substrate but will be much less relaxed over the void due to the lack of dislocations.

**μ-PL mapping** has been used to study local optical properties of the samples and it is proved to be a suitable tool for local strain mapping of GaN layers.

The authors are grateful to E. W. J. M. van der Drift for preparation of the silicon substrates. This work has been financially supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM).