Growth and Characterization of GaN Thin Films on SiC SOI Substrates

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SiC semiconductor-on-insulator (SOI) structures have been investigated as substrates for the growth of GaN films. The SiC SOI was obtained through the conversion of Si SOI wafers by reaction with propane and H_2. (111) SiC SOI have been produced by this carbonization process at temperatures ranging from 1200 to 1300°C. X-ray diffraction (XRD) and infrared spectroscopy (FTIR) are used to chart the conversion of the Si layer to SiC. Under our conditions, growth time of 3 min at 1250°C is sufficient to completely convert a 1000Å layer. XRD of the SiC SOI reveals a single SiC peak at $2\theta = 35.7°$ corresponding to the (111) reflection, with a corrected full width at half-maximum (FWHM) of ~590±90 arc-sec. Infrared spectroscopy of SiC SOI structures obtained under optimum carbonization conditions exhibited a sharp absorption peak produced by the Si-C bond at 795 cm^{-1}, with FWHM of ~ 20–25 cm^{-1}. Metalorganic CVD growth of GaN on the (111) SiC SOI was carried out with trimethylgallium and NH_3. The growth of a thin (≤200Å), low temperature (500°C) GaN buffer layer was followed by the growth of a thick (~2 μm) layer at 1050°C. Optimum surface morphology was obtained for zero buffer layer. XRD indicates highly oriented hexagonal GaN, with FWHM of the (0002) peak of ~360±90 arc-sec. Under high power excitation, the 300°K photoluminescence (PL) spectrum of GaN films exhibits a strong near band-edge peak (at λ_p~371 nm, with FWHM = 100–150 meV) and very weak yellow emission. Under low power excitation, the 370 nm PL emission from the GaN/SiC SOI structure increases rapidly with SiC carbonization temperature, while the yellow band (~550–620 nm) correspondingly decreases.

Key words: Carbonization, characterization, GaN, photoluminescence, SiC, SOI

INTRODUCTION

The rapid development of III-V nitride technology[1] is leading to major advances in related devices, including commercial blue and multi-color light-emitting diodes (LED). Recently, the feasibility of blue semiconductor diode lasers[2] has been reported. Due to the absence of commercial GaN bulk crystals, the investigation of alternate substrate materials is a very important task. The main requirements for an appropriate substrate for GaN epitaxial growth are:

- Dimensional lattice-matching;
- Thermal expansion coefficient matching; and
- Availability in large quantities, with large diameter and at low cost.

The substrate of choice to date has been sapphire (α-Al_2O_3) because of its commercial availability and excellent surface preparation. However, sapphire has a very large lattice mismatch with wurtzite GaN: ~33° for the aligned basal planes and >20% considering a 30° rotation of the GaN basal plane with respect to the sapphire basal plane. This inevitably leads to a large defect density of GaN epitaxial layers. Hexagonal (6H)-SiC offers a much smaller lattice mismatch (3.5%), which, although too large for perfect heteroepitaxy, is small enough to reduce the dislocation density significantly.[3] 6H-SiC, however, suffers from limited availability, small diameter (<5 cm) substrates, and very high cost. In this paper, we discuss an alternative substrate approach for epitaxial growth of GaN, which has the potential of providing large area, low cost 3C-SiC (111) substrates with fairly small lattice mismatch (3.5%). An additional consideration in heteroepitaxy is the mismatch

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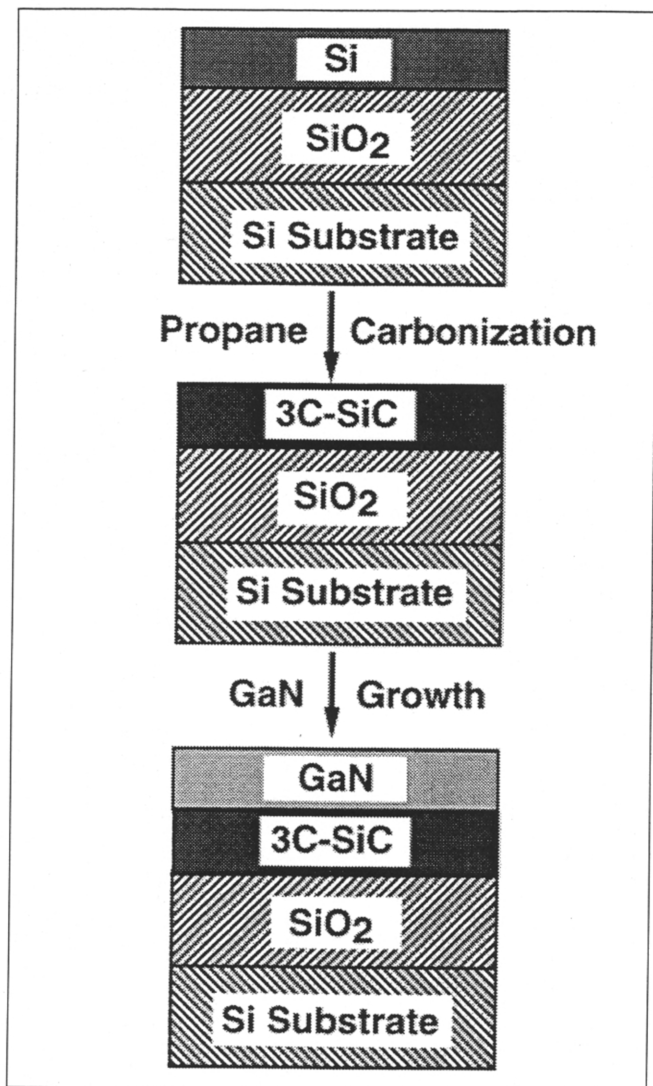

Fig. 1. Overall concept diagram.

in linear thermal expansion coefficient between growth layer and substrate over the growth temperature range. The average expansion coefficient[4] from 25°C to 1000°C for GaN is 4.9×10^{-6}/K, which matches quite well with the value of 4.7×10^{-6}/K for 3C-SiC. On the other hand, the only expansion coefficient value over the same temperature range related to sapphire which we have found in the literature is that of alumina,[5] which is 9.25×10^{-6}/K. This value probably understates the expansion mismatch, as the expansion coefficient of alumina also changes much more with temperature than that of GaN. The combination of these two considerations clearly indicates that strain in the GaN overlayer should be significantly reduced by the use of a 3C-SiC substrate.

We have fabricated SiC SOI structures and utilized them as substrates for GaN growth. As shown in Fig. 1, the starting point for SiC SOI is a silicon SOI wafer consisting of a normal Si substrate, an oxide layer and a thin Si device layer. The Si SOI structure is produced[6] either by thermal bonding and etch back of two Si wafers or by oxygen ion implantation. The thin Si device layer (from several hundred to a few thousand Ås) can be rapidly and completely converted to cubic (3C) SiC by a chemical vapor deposition (CVD) process through exposure to propane or other carbon-containing gases at high temperature. This minimizes the formation of voids and other defects which accompany the carbonization of conventional Si substrates,[7,8] where Si atoms can diffuse out from the bulk along <111> planes until the surface is completely sealed. Next, a thick GaN layer of several μms can be grown by a variety of deposition techniques. The SOI substrate has several additional advantages over the use of conventional Si substrates. The presence of the oxide layer is beneficial in absorbing growth-generated stress and dislocations.[9] The oxide layer can also provide improved performance through electrical isolation between devices, as in Si SOI devices and circuits. Finally, if the GaN film is grown thick enough (>100 μm) to be self-supporting, the oxide can serve as a "quick-release" layer through selective etching.

Si SOI device technology is currently experiencing intense development for commercial low power and very large scale integration (VLSI) applications,[6] resulting in the rapid development of SOI substrates in terms of wafer diameter, quality, and cost. Therefore, the approach of using the SiC SOI structure as a substrate for GaN growth can directly benefit from the progress obtained by the much larger SOI community.

SIC SOI FORMATION AND CHARACTERIZATION

The use of insulating substrates for the CVD growth of cubic SiC has been reported by Pazik et al.[10,11] and Tang et al.[12] utilizing Si-on-sapphire (SOS) and by Steckl et al.[13,14] utilizing the SOI structure discussed above. A similar SiC SOI has been pursued by Yang et al.[15] where the use of MBE growth for the carbonization was investigated. In the work reported here, we have utilized (111) Si SOI structures with a thin Si (111) device layer (900–1000Å), a 1 μm SiO_2 layer and a Si (100) substrate. The crystal orientation of the Si (111) layer was tilted 2.4–4° off-axis. The starting SOI was produced[16] by thermal bonding and etch back. To provide the 0.1 μm Si device layer with high uniformity over the wafer area required a specialized plasma etching process.[17] SiC growth on the (111) Si was selected on the basis of superior results[18] with growth of thicker 3C-SiC films directly on (111) and (100) Si substrates. In addition, the (111) SiC surface, which closely resembles the c-plane of 6H-SiC, is a better match for subsequent growth of III-N films.

The Si-to-SiC conversion was performed in a rapid thermal chemical vapor deposition (RTCVD) reactor which restricted exposure to high temperature to only the few minutes needed for in-situ cleaning and complete carbonization. Additional information on the operation of the RTCVD reactor for SiC growth can be found elsewhere.[7] Figure 2 contains a typical process diagram. After wet chemical cleaning, the samples

were introduced into the RTCVD reactor where they underwent in-situ cleaning in the presence of 3 lpm H_2 flow. The temperature was first ramped up to 400–500°C where it was held for 30 s to allow for moisture removal. Then the temperature was increased to 1000–1200°C where it was held for 1–2 min. Between cleaning and carbonization, the chamber was evacuated to its base pressure. The carbonization reaction was performed at atmospheric pressure and temperatures from 1100 to 1300°C with mixtures of propane (5 % in H_2) and H_2 at 760 Torr. The propane flow rate ranged between 10 and 12 sccm and the H_2 flow rate was 1 lpm. The temperature ramp-up rate for all process steps was always held to 50°C/s. The optimum carbonization temperatures were found to be in the 1200–1250°C range. The carbonization process is described in more detail elsewhere.[7,8] The carbonization produced a SiC layer with thickness approximately equal to that of the starting Si device layer.

The composition and structure of the SiC SOI samples have been characterized by Fourier transform infrared (FTIR) spectroscopy and by x-ray diffraction (XRD). FTIR spectroscopy can determine the formation of SiC during the carbonization reaction by monitoring the Si-C bond which produces a characteristic IR absorption peak at ~795 cm^{-1}. Absorbance spectra covering the 700–900 cm^{-1} range are shown in Fig. 3. The structures were carbonized at 1200°C for 3 and 6 min and at 1250°C for 3 min. The full widths at half maximum (FWHM) of the peaks are approximately 20–25 cm^{-1}, which is an excellent range for such thin films. Carbonization of (111) SOI at 1200°C for 3 min resulted in a very small FTIR peak indicating the formation of a very small SiC layer, while extending the time to 6 min or the temperature to 1250°C results in a well-defined large peaks.

In Fig. 4 are shown wide angular range XRD spectra for the same three (111) SiC SOI samples whose FTIR spectra were shown in Fig. 3. The sample which underwent carbonization at 1200°C for 3 min displays

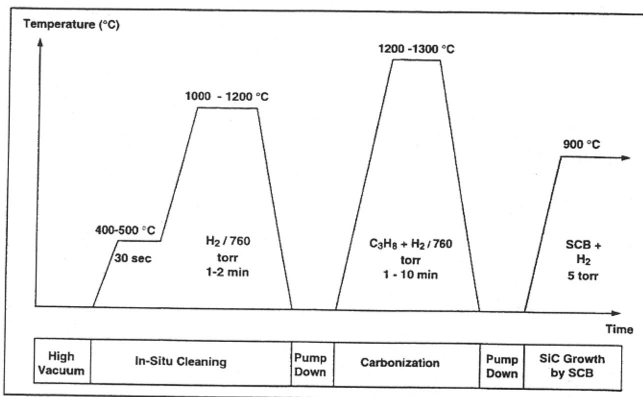

Fig. 2. SiC growth process time-temperature schematic.

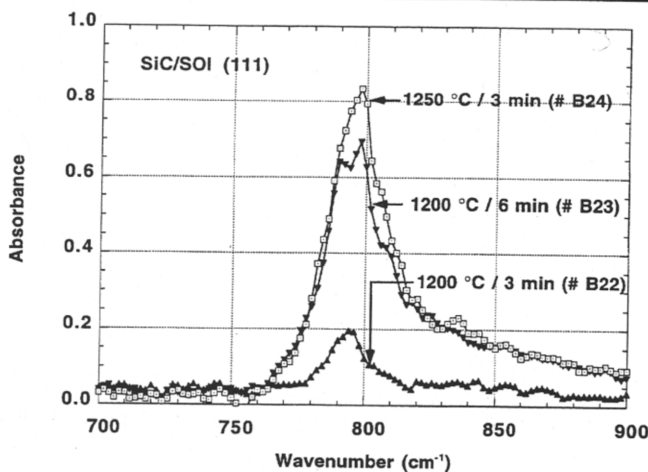

Fig. 3. Fourier transmission infrared spectra of (111) SiC SOI structures.

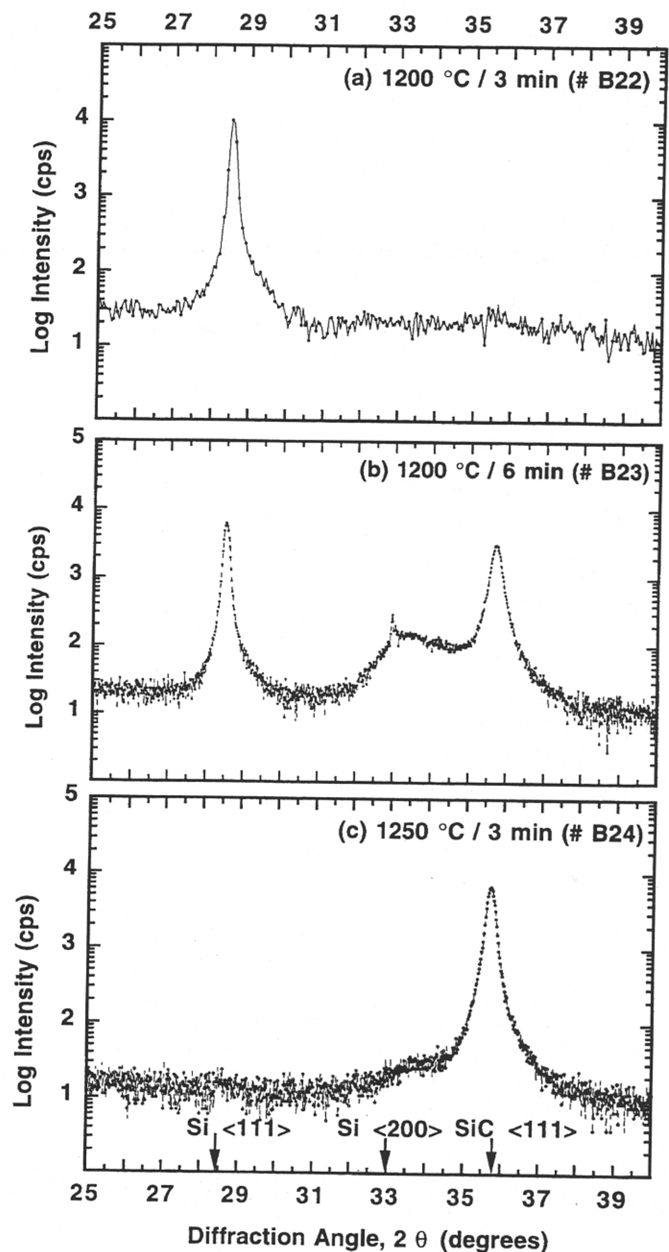

Fig. 4. Wide angular range x-ray diffraction spectra of (111) SiC SOI structures obtained by carbonization at 1200 and 1250°C.

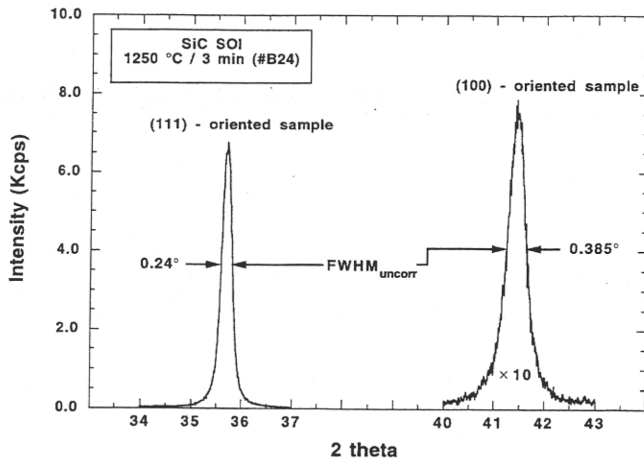

Fig. 5. High resolution XRD spectra of the main SiC peaks of <111> and <100> SiC SOI structures.

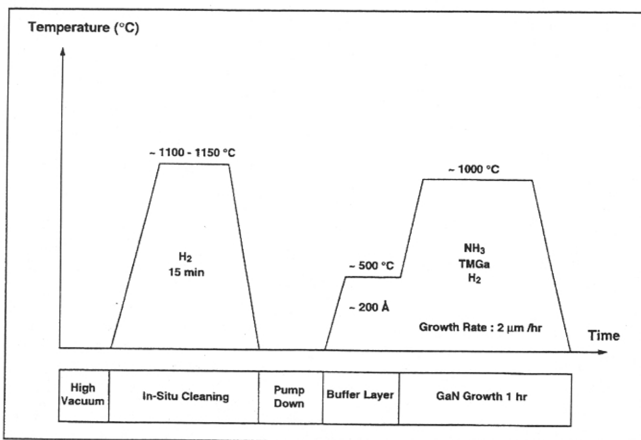

Fig. 6. GaN growth process time-temperature schematic.

only the Si <111> peak at $2\theta \approx 28.4°$ (as shown in Fig. 4a). No SiC XRD peak is observed for this sample, whereas a weak peak was observed by FTIR (Fig. 3b). The sample obtained by carbonization for 6 min at 1200°C (Fig. 4b) exhibits the Si <111> peak and two additional contributions at $2\theta \approx 33°$ and 35.7°. The latter two peaks are identified with Si <200> from the Si substrate and SiC <111> from the converted Si device layer, respectively. The structure carbonized at 1250°C reveals only a single sharp peak at 35.7° corresponding to the SiC (111) plane reflection.

Thermally bonded (100)-oriented Si SOI substrates (2.2 ± 0.5 µm Si layer and 1 µm SiO_2 thickness) were occasionally used for comparison purposes. The main SiC peaks of SOI (111) and (100) structures obtained by carbonization at 1250°C for 3 min are shown in Fig. 5 at higher angular resolution. The (111) sample exhibits a peak with an uncorrected FWHM of ~0.24°, while the (100) sample has an FWHM of ~0.39°. Correcting for XRD system broadening reduces the FWHM by about 0.05–0.1°, resulting in FWHM values of 590±90 arc-sec and 1134±90 arc-sec for the <111> and <100> peaks, respectively. In addition, the x-ray signal intensity from the (111)-oriented sample is approximately ten times larger that produced by

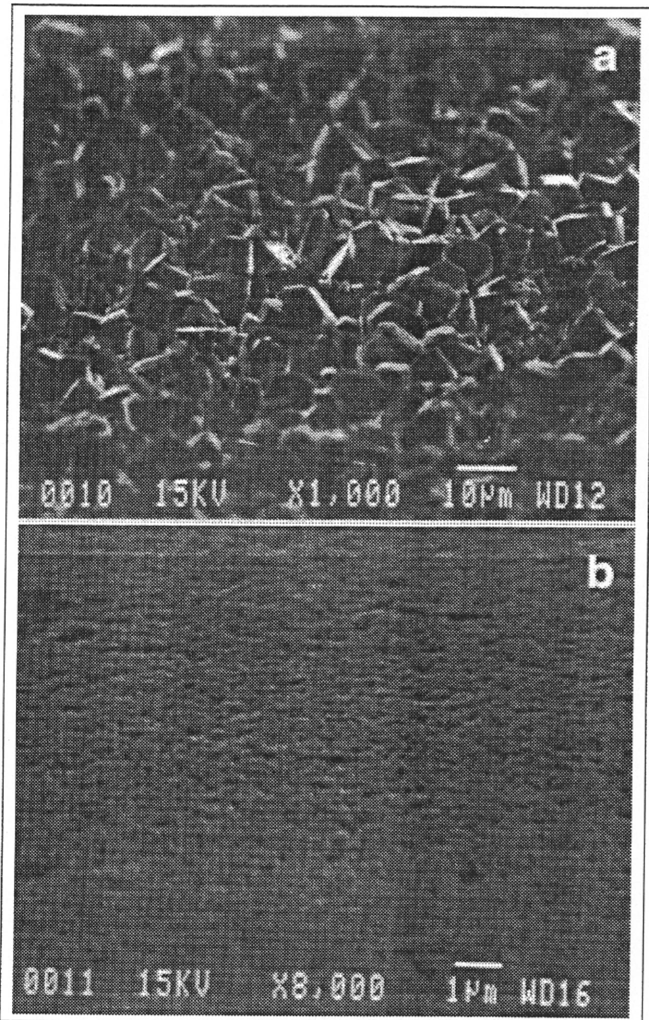

Fig. 7. SEM microphotographs of the GaN surface morphology obtained with: (a) with 200Å buffer layer - 1000× magnification, and (b) with zero buffer layer - 8,000× magnification.

the (100)-oriented sample. These XRD values indicate that the carbonization process produces a superior SiC layer when utilizing a (111) Si SOI starting substrate to that obtained from (100) Si SOI by the same process.

GaN THIN FILM GROWTH AND CHARACTERIZATION

Metalorganic CVD (MOCVD) growth of GaN layers on the (111) SiC SOI structures was carried out in a stainless steel, rotating disk reactor (EMCORE Discovery 180) using trimethylgallium (TMGa) and ammonia (NH_3) precursors. The substrate disk rotates in a horizontal plane while the reactants are introduced vertically through an array of nozzles. The high rotation speed of the substrate holder and the low pressure of the chamber produce a thin, uniform boundary layer which results in uniform, high growth rate epitaxy over a large area.[19] The overall growth process[20] is shown schematically in Fig. 6. The SiC SOI substrates were first ex-situ cleaned with acetone, etched in 10% HF and rinsed in deionized H_2O. This

was followed by in-situ cleaning through exposure to a high flow of H_2 at 1100°C for 15 min. A thin GaN layer was grown first, by reaction of TMGa and NH_3 at low temperature (~500°C). This produces an amorphous or polycrystalline layer which is crystallized as the temperature is ramped up to ~1000–1100°C for the final GaN growth step. At 1000°C, a GaN growth rate of ~2 μm/h is achieved with NH_3 flow rate of 16 slpm, TMGa flow rate of 180 μm/min, pressure of 55 Torr, and substrate rotation of 1000 rpm.

The low temperature deposition of an intermediate ("buffer") layer is routinely used (see for example Morkoç et al.)[21] in the growth of GaN films on sapphire in order to achieve uniform nucleation on the substrate surface. As the temperature is subsequently ramped up, the grains of the buffer layer become oriented producing a more suitable substrate surface for growth of the final GaN film. While most often an AlN buffer layer is utilized, a low temperature GaN buffer layer has been shown by Nakamura[22] to produce GaN epitaxial films of equal or superior quality. Growth of GaN on sapphire by the process described above typically utilizes a 200Å buffer layer. For growth on SiC SOI substrates, we have experimented with GaN buffer layers with thickness ranging from zero to 200Å. We have found that the surface morphology improved significantly as the buffer layer thickness was reduced. Figure 7 contains photomicrographs of GaN films grown on SiC SOI at 1050°C for 1 h. The sample in Fig. 7a, which incorporated a 200Å buffer layer, reveals numerous individual crystallites and hence a very rough surface. On the other hand, the sample in Fig. 7b, which was grown with no buffer layer, reveals a much smoother (though still far from perfect) surface. XRD spectra of GaN/SiC SOI structures are shown in Fig. 8. For all films, we observe the largest peak to be that due to the <0002> reflection (with powder diffraction value of 2θ = 34.637°) and several smaller peaks corresponding to the <10$\bar{1}$0> and <10$\bar{1}$1> reflections (at powder diffraction values of 2θ = 32.443 and 36.998°, respectively). This indicates a highly oriented wurtzite GaN film with dominant growth orientation along the c-axis. The peak at ~31° (see Fig. 8b) which apears in the XRD of all the films investigated (including GaN/sapphire) was not identified. Changing the thickness of the buffer layer appears to have some effect on the XRD spectrum characteristics in terms of the precise angle, intensity, and width of the main peaks. However, to draw unambigous conclusions on this point requires further investigation.

For the film grown without a buffer layer, the uncorrected FWHM of the (0002) peak shown in Fig. 8a is approximately 0.16° or ~580 arc-sec. Correcting for system broadening results in an FWHM of ~360±90 arc-sec. This value is roughly comparable to that obtained[23] for GaN grown on 6H-SiC substrates (~310 arc-sec). Interestingly, the XRD spectrum (Fig. 8b) of the GaN film grown on (111) SiC SOI without a buffer layer displays a peak at 2θ ≈ 35.6°, which is attributed to <111> SiC from the underlying layer. The enlarged view of the SiC peak shown in Fig. 9 indicates an FWHM of ~0.25°, which is very close to the value obtained before GaN growth (see Fig. 5).

The optical properties of the GaN layers grown on SiC SOI were investigated by photoluminescence (PL) at 300°K using both relatively high (pulsed N_2 laser at λ_{exc}~337 nm with a peak incident power on the sample of 0.1 MW/cm²) and low (cw He-Cd laser at λ_{exc} ~325 nm with 0.1–1.0 W/cm²) power levels. High power PL spectra of several GaN films grown on <111> SiC SOI with buffer layers of different thick-

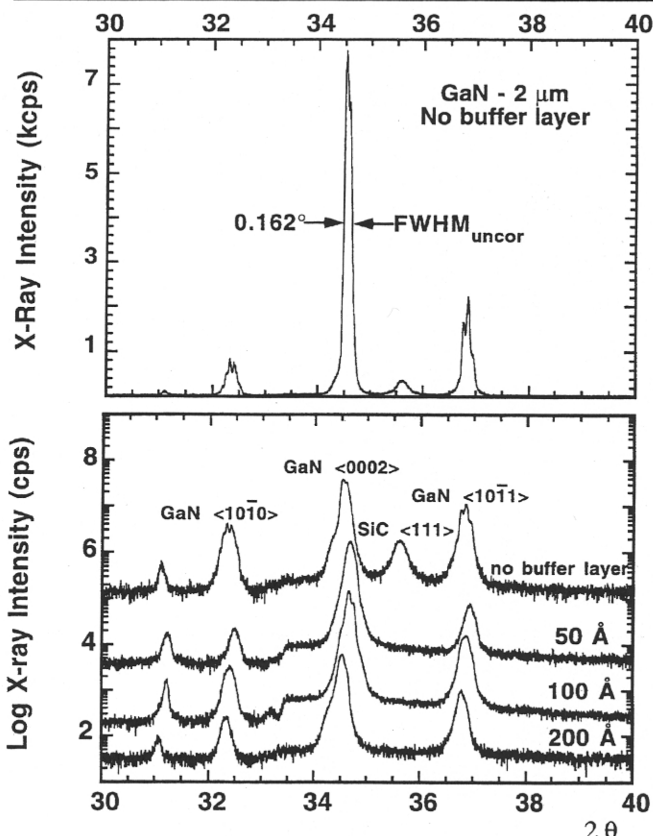

Fig. 8. X-ray diffraction spectrum of GaN/SiC SOI structure: (a) no buffer layer-linear scale, and (b) various buffer layer thicknesses-log scale.

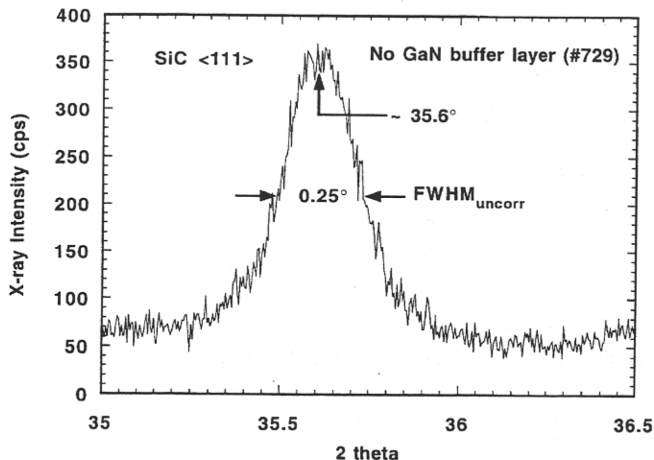

Fig. 9. SiC <111> XRD peak from GaN/SiC SOI structure.

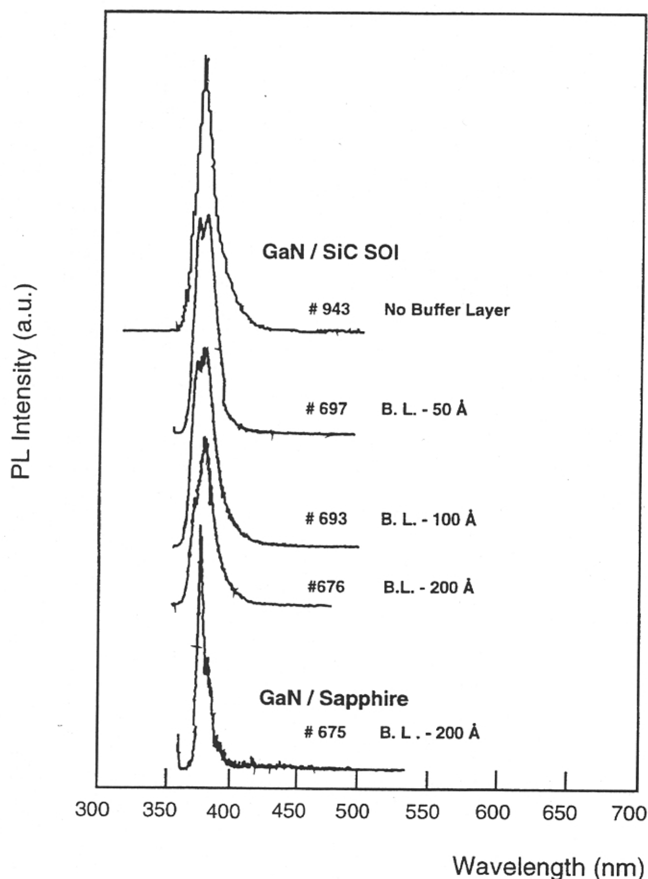

Fig. 10. Room temperature PL of GaN/SiC SOI structure obtained under high power excitation (pulsed N_2 laser): (a) various buffer layer thicknesses, and (b) no buffer layer.

ness are shown in Fig. 10. The carbonization in all cases was performed at 1200°C. For comparison, the PL spectrum of GaN film grown on sapphire is also included. Strong near band-edge emission (at λ_p~365–375 nm) and weak yellow band emission (not shown in Fig. 10) was obtained from all films under high power excitation. The film grown on sapphire with a 200Å buffer layer has a main emission peak at ~365 nm (with an FWHM corresponding to ~70–75 meV). The shoulder at 372–375 nm is probably due to emission related to the presence of native defects (i.e. N vacancies). By comparison, the GaN film grown on SiC SOI with the same buffer layer thickness exhibits the reverse situation: the main PL peak is shifted to 375 nm with only a shoulder appearing at 365–368 nm. As the buffer layer thickness is reduced, first to 100Å and then to 50Å, the component at 368 nm increases until it is comparable to the component at 375 nm. Finally, for the GaN film grown on SiC SOI without a buffer layer, a single PL peak is obtained at 371 nm, with an FWHM of 145–150 nm.

The room temperature PL obtained under low power excitation exhibits significantly different characteristics. PL spectra are shown in Fig. 11 from GaN films grown under the same conditions on SiC SOI substrates carbonized at different temperatures. At these low excitation levels, a much stronger "yellow" band

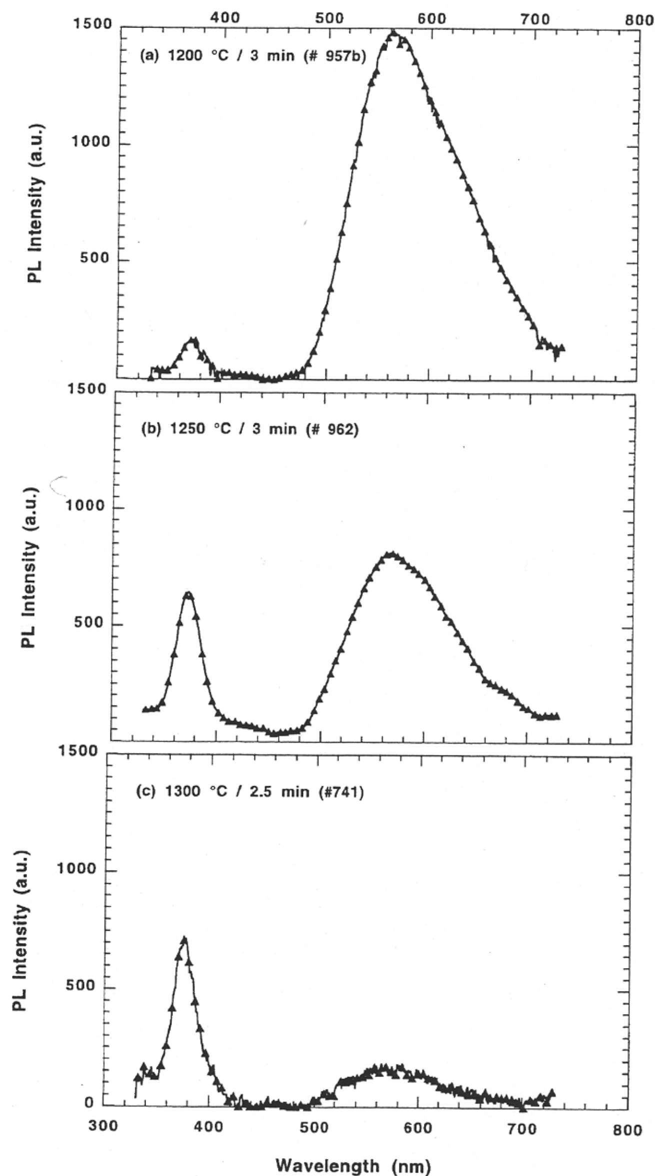

Fig. 11. Room temperature PL obtained under low power excitation (cw He-Cd laser) from GaN films grown on (111) SiC SOI substrates carbonized at different temperatures.

emission (with a peak at ~560–575 nm) is observed and the UV emission (with a single peak at ~370–373 nm) is significantly broadened. Furthermore, the relative strength of the UV-to-yellow (UV/Y) emission intensity appears to be a strong function of the extent of the carbonization. Carbonization at 1200°C, which does not completely convert the Si layer, produces a UV/Y ratio of 0.11. Increasing the carbonization temperature to 1300°C, which produces essentially complete conversion, produces a much stronger UV emission and supresses the yellow emission. The resulting UV/Y ratio is 4.27, or nearly 40× higher that of the GaN film grown on SOI carbonized at 1200°C. It is also interesting to observe that under these excitation conditions the GaN film grown on SiC SOI carbonized at 1300°C exhibited a much stronger UV emission than equivalent GaN films grown on either carbonized Si or sapphire substrates.

SUMMARY AND CONCLUSIONS

In summary, we have presented structural and optical properties of GaN/SiC SOI structures formed by propane carbonization and subsequent GaN growth by MOCVD. We have determined that under our growth conditions, the conversion rate of a 1000Å Si (111) layer to SiC at 1200°C is low enough to prevent complete conversion in 6 min; whereas at 1250°C, the carbonization process is complete in ~3 min. Excellent materials properties are achieved for such thin SiC films: XRD FWHM of ~600 arc-sec and FTIR FWHM of ~25 cm^{-1}. Subsequent GaN growth at ~1050°C indicated that significantly smoother films are obtained without the insertion of a low temperature (500°C) buffer layer. The highly oriented hexagonal GaN films have an XRD FWHM of ~350 arc-sec and a near band-edge PL FWHM of ~100 meV. The SiC carbonization conditions were seen to strongly influence the GaN PL characteristics, with the fully converted SiC layers resulting in a quenching of the yellow band emission and an enhancement of the UV emission. In conclusion, we have shown that SiC SOI structures obtained by carbonization have the potential to serve as useful substrates for GaN growth.

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