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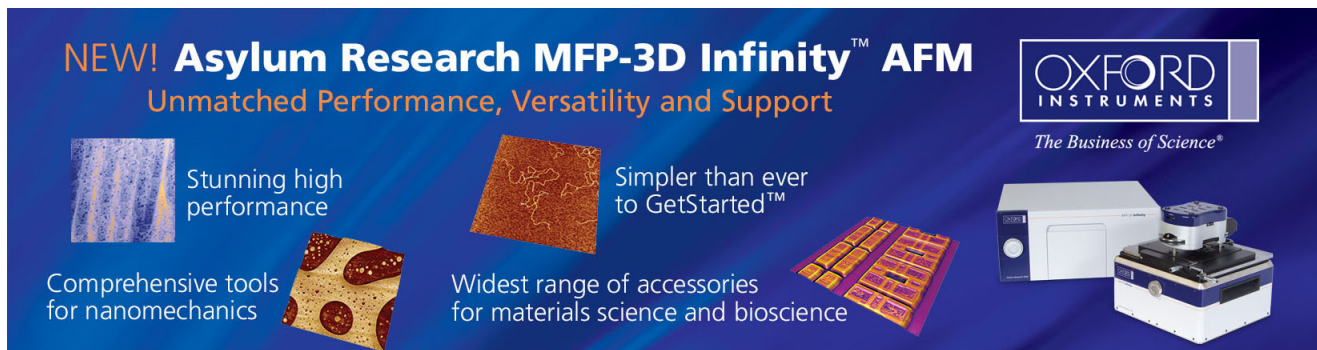
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Growth of GaN film on 150 mm Si (111) using multilayer AlN/AlGaN buffer by metal-organic vapor phase epitaxy method

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High quality GaN film was successfully grown on 150 mm Si (111) substrate by metal-organic vapor phase epitaxy method using AlN multilayer combined with graded AlGaN layer as buffer. The buffer layer structure, film quality, and film thickness are critical for the growth of the crack-free GaN film on Si (111) substrate. Using multilayer AlN films grown at different temperatures combined with graded $\text{Al}_{1-x}\text{Ga}_x\text{N}$ film as the buffer, the tensile stress on the buffer layer was reduced and the compressive stress on the GaN film was increased. As a result, high quality 0.5 μm crack-free GaN epitaxial layer was successfully grown on 6 in. Si substrate. © 2007 American Institute of Physics. [DOI: 10.1063/1.2818675]

GaN-based semiconductors have attracted much attention in the past decade as one of the most important semiconductor materials as they can be applied to high power and high frequency electronic devices as well as light emitting diodes (LEDs) and laser diodes. GaN growth on Si substrate has attracted considerable attentions due to its low cost, large size, good thermal conductivity, and the potential for integration with Si-based devices^{1,2} as compared with other substrates such as sapphire and SiC. The main issues for epitaxy of GaN on silicon substrates are large thermal expansion coefficient and lattice constant mismatches between GaN and Si substrates, which result in the occurrence of cracks and high defect densities on the films grown. In order to solve these problems, several approaches have been proposed to reduce the stress and minimize the cracks and defects for the film grown, such as creating a bridging interlayer of similar thermal expansion coefficients (CTE), adding compressively strained layers to the overall structure which reduces the tensile strain induced by the high temperature growth and cooling process, growing the high temperature (HT)-GaN film under compression to compensate for the tensile strain induced during cooling, and epitaxial lateral overgrowth using patterned Si substrates.³⁻⁹ To obtain high quality GaN films on Si, an important technology is the design of the interlayer structure between the GaN and the Si substrate. Using low temperature (LT)-AlN interlayer, the tensile stress in the GaN film can be further reduced upon heating to high temperature due to the CTE mismatch.⁸⁻¹⁰ However, the AlN film grown at low temperature shows a poor film quality as compared to that of the high temperature grown AlN, which influences the GaN film quality grown on top of it. Using high quality AlN buffer layer, the crack-free GaN film grown on large area Si substrates can be obtained.^{11,12} However, there is no systematical study of the effects of the buffer layer structure and growth parameters on the quality of the GaN film grown so far. In this letter, a series of GaN films

grown on Si (111) 6 in. substrates using different types of AlN multilayer buffers is investigated.

The AlN multilayer buffers and GaN films were grown on 6 in. Si (111) wafers by EMCORE D-180 metal-organic vapor phase epitaxy reactor. Trimethylgallium (TMGa), trimethylaluminum (TMAI), and ammonia (NH_3) were used as the reactant sources for Ga, Al, and N, respectively. High temperature baking at 1050 °C for 30 min in hydrogen between each GaN deposition run was used to remove Ga from the susceptor, chamber, and gas lines. The Si (111) substrates were chemically cleaned by $\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2:\text{H}_2\text{O}$ (3:1:1) and buffered-oxide-etch (BOE) HF (20:1) before loaded into the reactor, which resulted in oxide-free and hydrogen terminated Si surface. After being loaded into the chamber, the substrates were baked at 1050 °C for 30 min under a hydrogen atmosphere. After that, different types of buffers including HT-AlN/GaN, HT-AlN/LT-AlN/HT-AlN/GaN, and HT-AlN/LT-AlN/HT-AlN/graded AlGaN/GaN were used. The LT-AlN films were grown at 800 °C, and HT-AlN films, graded AlGaN films and GaN films were deposited at 1050 °C. The x-ray diffraction (XRD) and photoluminescence were performed to investigate the crystalline quality of the samples. Optical microscope was used for the investigation of the film surface morphologies and cracks. The buffer layer structures, AlN and GaN film thicknesses, the XRD diffraction full width at half maximum (FWHM) data, and the film qualities as well as the bow and radius of curvature of wafer are shown in Table I.

For the growth of GaN film on Si, due to the strong reaction between Si and nitrogen, a thin amorphous Si_xN_y layer can form on the Si substrate if nitrogen pressure is too high. Another well known problem is the meltback etching of Si by Ga during the deposition process. These reactions result in defects and formation of very poor quality GaN. Deposition of Al rich AlN film before GaN film deposition was used to avoid the diffusion of Ga into the substrate and the formation of Si_xN_y film. On the other hand, the value of

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TABLE I. Buffer layer structure and characterization results of GaN films grown on 6 in. Si (111) samples.

Sample	1	2	3	4	5	6
Buffer type	Single					
Buffer-layer thickness (nm)	HT-AlN	Multilayer-AlN ^a	Multilayer-AlN ^a	Multilayer-AlN ^a	Multilayer-AlN ^a	Multilayer-AlN/AlGaN ^a
GaN thickness (μm)	0	0	0.5	0.5	2	0.5
FWHM _{GaN} (004)	N/A	N/A	0.54°	0.315°	0.120°	0.223°
FWHM _{AlN} (004)	2.75°	1.02°	1.66°	0.865°	0.52°	0.343°
Wafer size(in)	6	6	6	6	6	6
Cracks	yes	no	yes	yes	yes	no
Radius of curvature(m)	80.45	32.17	25.24	48.65	72.91	238.96
Bow (μm)	-23.32	-54.36	-71.3	-52.3	-45.65	-8.63

^aMultilayer-AlN: HT-AlN/LT-AlN/HT-AlN.

the CTE of AlN is between GaN and Si, which can also be used to reduce the thermal mismatch between GaN and Si substrate. In order to grow high quality AlN on Si substrate, high growth temperature is required. However, AlN has 19% lattice mismatch and about 15% thermal mismatch with Si (111), which generates tensile stress of about 6.269 GPa on AlN. GaN grown with HT-AlN buffer showed the cracks near the edge of 6 in. wafer when the thickness was greater than 30 nm (sample 1 in Table I). In order to solve this problem, multilayer buffer of AlN (HT-AlN/LT-AlN/HT-AlN) structure was used for the growth of GaN on Si substrate. The first layer of HT-Al rich AlN film with thickness of about 10–50 nm grown at 1050 °C was used to prevent the reaction of Si with nitrogen. There were many defects and cracks formed on the first HT-AlN layer due to the relaxation of the stress in this layer. The second layer of LT-AlN film with thickness of about 10–50 nm was grown at 800 °C which was used as the nucleation layer for the growth of the top HT-AlN layer and was also used to stop the propagation of the cracks and defects from the first HT-AlN layer onto the top HT-AlN layer. LT-AlN can effectively block the defect propagation along the growth direction and reduce the dislocation density.¹¹ The third layer of HT-AlN film with thickness of about 50–200 nm was grown at 1050 °C to form a high quality AlN with lower defect density for further growth of the GaN film. Using the HT-AlN/LT-AlN/HT-AlN multilayer structure, over 100 nm crack-

free AlN films were grown on 6 in. Si (111) wafer (sample 2). The experimental results also exhibit that the AlN film quality improved with increasing film thickness. Figure 1 shows the XRD AlN (004) mosaic FWHM versus AlN film thickness, the FWHM of the XRD data decreases when the thickness increases. This means that to reach a high quality AlN film, enough AlN thickness is necessary. Due to the lattice mismatch between AlN and GaN, a compressive stress was generated on the GaN film during the epitaxial growth of GaN on the AlN buffer, the compressive stress can be used to compensate the tensile stress formed due to the CTE mismatch between AlN and GaN to make a crack-free GaN film on Si substrate. To study the buffer layer thickness effect on the quality of the the GaN films grown, AlN multilayer buffers with different thicknesses were used for the growth of GaN on Si substrates; the results are as shown in Table I. For samples 3 and 4, with 0.5 μm GaN film, only a few cracks were found near the wafer edge, the GaN quality improved with buffer layer thickness. Figure 2 shows the GaN XRD mosaic FWHM data correlation with the AlN film thickness. In this figure, AlN film quality has significant influence on the quality of the GaN film grown. This figure also confirms that in order to grow high quality GaN films, high quality AlN buffers are necessary. High quality GaN film (2 μm thick) was successfully grown on 6 in. Si (111) substrate with the mosaic FWHM of GaN (004) only 0.12° (sample 5),

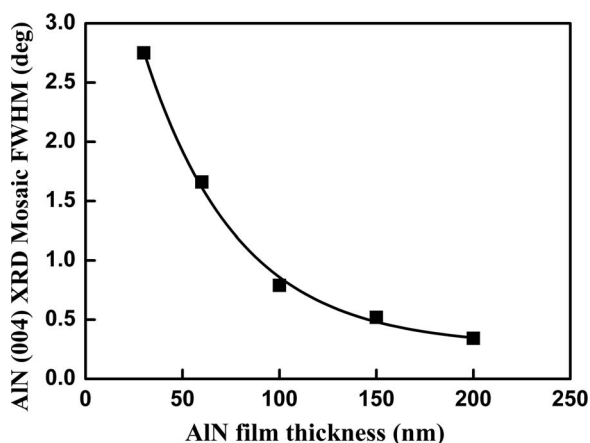
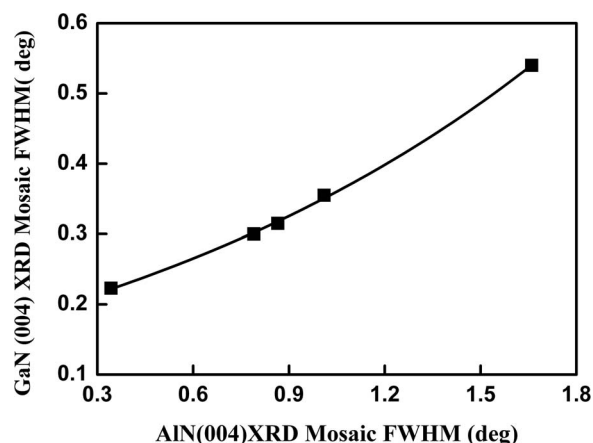


FIG. 1. AlN (004) mosaic FWHM (deg) vs AlN film thickness

FIG. 2. GaN (004) mosaic FWHM vs AlN (004) mosaic FWHM of 0.5 μm thick GaN with various AlN buffers on Si (111) wafers.

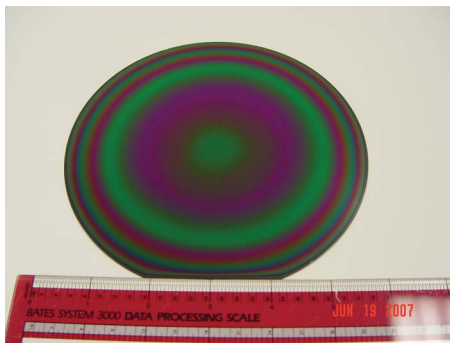


FIG. 3. (Color online) Optical photograph of GaN sample on 6 in. Si (111) substrate.

very few cracks formed between center and edge of this sample.

For the growth of perfect epitaxy GaN on AlN, the stress induced on GaN can be calculated from the theory. At room temperature, compressive stress on GaN is $\sigma_{\text{GaN}} = 11.8$ GPa, which is large enough to compensate the tensile stress induced by thermal mismatch during epitaxial growth. However, from *in situ* stress measurements, the maximum compressive stress generated from the lattice mismatch was only about 2 GPa. The reasons may be due to the poor AlN film quality or due to a mismatch of 2.4% in the in-plane lattice parameters between AlN and GaN; in these cases, the GaN lattice cannot exactly match the AlN lattice during the growth and many defects formed to release the compressive stresses induced. Therefore, obtaining maximum compressive stress on the top GaN film is very critical for the growth of thick crack-free GaN film on large size Si substrate. To further increase the compressive strain on the buffer, combining multilayer AlN films with graded $\text{Al}_{1-x}\text{Ga}_x\text{N}$ layers as the buffer were used for the growth of the crack-free GaN on Si substrate. Using the HT-AlN/LT-AlN/HT-AlN/graded $\text{Al}_{1-x}\text{Ga}_x\text{N}/\text{Al}_{0.42}\text{Ga}_{0.58}\text{N}$ buffer structure, $0.5 \mu\text{m}$ GaN film with a mirror surface without crack was obtained on 6 in. Si (111) substrate, as shown in Fig. 3 (sample 6 in Table I). Figure 4 shows the XRD reciprocal space mapping (RSM) of the same sample with the multilayer AlN/graded AlGaN buffer. In this figure, the AlN reciprocal-lattice points are distributed on the top of the solid line box region, which shows the AlN multilayer is under tensile strain (ϵ_a) of about 0.3%. The GaN reciprocal-lattice points distributed in the bottom of the solid line box region, which shows the GaN film is under small tensile strain (ϵ_a) of about 0.12%. The thin graded $\text{Al}_{0.66}\text{Ga}_{0.34}\text{N}$ and $\text{Al}_{0.42}\text{Ga}_{0.58}\text{N}$ reciprocal-lattice points distributed between AlN and GaN positions are under compressive strains of about -0.5% and -0.92% , respectively, which compensate the tensile stress on the AlN film and help in the growth of the crack-free GaN film on Si. The AlN film in sample 2 is thicker than the AlN film in sample

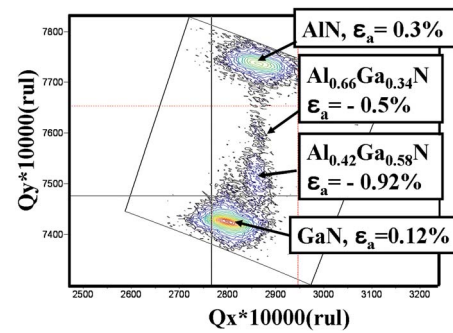


FIG. 4. (Color online) RSMs for GaN with AlN/AlGaN buffer on Si (111) substrate.

1, therefore, the bow in sample 2 is larger. Sample 5 has $2 \mu\text{m}$ thick GaN film but the strain was released due to the formation of cracks. Sample 6 has the smallest bow due to the incorporation of the compressive AlGaN buffer layer.

In summary, the effects of buffer layer structure and growth parameters on the quality of the GaN film grown on Si substrate were studied. The AlN buffer layer quality has a significant influence on the quality of the GaN film grown. A multilayer HT-AlN/LT-AlN/HT-AlN film structure combined with graded $\text{Al}_{1-x}\text{Ga}_x\text{N}$ film was proposed to reduce the tensile stress on the AlN film and increase the compressive stress of the GaN film grown, using the proposed buffer, high quality $0.5 \mu\text{m}$ crack-free GaN epitaxial layer was successful grown on 6 in. Si substrate.

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