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Growth of GaN on Si (111) using simultaneous AlN/α-Si_3N_4 buffer structure

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1. Introduction

Recently, silicon as a substrate has attracted much attention for the epitaxial growth of group-III-nitride semiconductors because of its low cost, large size in large diameters up to 12 inches and potential in the integration of microelectronic and optoelectronic devices. However, large difference in in-plane thermal expansion coefficient (56%) [1,2] between GaN and Si, which causes a large tensile stress in the GaN epilayers during cooling down process resulting in cracked layers especially in MOVPE system [3]. In MBE grown samples the critical thickness is higher than in MOVPE grown because of the lower growth temperature. The large difference in the lattice constant of the Si and GaN yields 16.9% mismatch resulting in a high dislocation density in the GaN layer. To overcome this problem, various types of buffer layers such as 3C-SiC [4], AlN [5], γ-Al_2O_3 [6] and β-Si_3N_4 [7] have been used to reduce the mismatch between GaN and Si. Shangjr Gwo et al. have [7] demonstrated the high temperature β-Si_3N_4 to suppress the auto-doping effect in GaN on Si. Unfortunately, the c-axial lattice constant of β-Si_3N_4 is 2.907 Å which indicates large tensile strain in the layer. The large tensile strain can induce the cracking problem [8]. In addition, the thickness of GaN layer only 240nm and it was not whether the layers exhibit cracks or not.

In this study, crack free GaN layers were demonstrated by using low temperature (LT) simultaneous AlN/α-Si_3N_4 buffer structure. Besides, it also reduces the mismatch, stress and improves the structural and optical properties.

2. Experiments

The growth of GaN/AlN/α-Si_3N_4 was carried out on Si (111) substrates by RF-MBE (ULVAC MBE system). Two-inch Si (111) wafers (p-type doping) were etched by 10% HF without DI water rinsed for suppressing oxide formation. Clear (7×7) surface reconstruction confirmed by high-energy electron diffraction (RHEED) at ~830℃ [Fig. 2(a)]. In this study, two different samples for GaN growth on Si (111) substrates were prepared for comparison. One sample consists of an LT simultaneous AlN/α-Si_3N_4 buffer structure. The other one is direct growth GaN layer on Si. Figure 1 schematically depicts the process of LT simultaneous AlN/α-Si_3N_4 structure. Al pre-seeding layer was deposited on Si surface at 400℃. 3nm thick AlN was grown at 500 to 600 ℃ by temperature grading method. The simultaneous α-Si_3N_4 layer was formed during AlN growth process. The ramping rate is 30℃/min in grading process. The simultaneous α-Si_3N_4 layer is around 1.5-2.0 nm. The 0.98 μm thick GaN epilayer were grown on LT simultaneous AlN/α-Si_3N_4 buffer structure at 740 ℃. The samples with LT simultaneous AlN/α-Si_3N_4 structure is crack free after 0.98 μm thick GaN epilayer growth.

3. Results and discussion

Si wafers were further thermally degassed to remove the fluorine and remaining oxide layer on surface at high temperature. Figure 2 shows the evolution of RHEED patterns, along the Si [110] azimuth during the growth process. Figure 2 (a) shows the clear (7×7) surface reconstruction at 830℃. Figure 2 (b) and (c) show streaky (1×1) RHEED pattern of AlN after 150 sec and 0.98μm thick GaN epilayer, respectively. Streaky (1×1) RHEED pattern indicates 2D growth and flat surface morphology for each layer. After the MBE growth, the grown GaN surface (cooled to 250-400℃) showed a (2×2) reconstruction pattern, indicating a Ga polar surface. But the direct growth samples showed a (3×3) reconstruction pattern, indicating an N polar surface.

The crystalline quality of the GaN growth on Si is investigated by XRD in the θ-2θ scan mode as shown in Fig. 3. The diffraction peak at 34.6^o and 73.06^o is intense and is identified as wurtzite GaN (0002) and (0004) diffraction. The full-width at half-maximum (FWHM) of X-ray rocking curve (XRC) in the ω mode shows the GaN (0002) reflection is 1200 arcsec. The weak diffraction peak near 32.98^o is attributed to the (100) diffraction of the AlN. The diffraction peak near 31.1^o and 64.85^o is attributed to the (002) and (303) diffraction of the α-Si_3N_4 layer which was formed during AlN growth process. The c-axial lattice constant of α-Si_3N_4 is 5.621 Å which indicates small tensile strain in the layer. Therefore, the crack free surface can be achieved by using α-Si_3N_4 layers.

The PL measurement is performed at 13K to investigate the optical properties of the GaN/AlN/α-Si_3N_4/Si structure as shown in Fig. 4. The 13K-PL spectrum shows a dominant emission peak at 3.49eV, which is attributed to the neutral-donor-bound exciton (D^oX) of the wurtzite GaN epilayer. The FWHM of the D^oX peak of the GaN is measured to be 20 meV. The defect-related yellow-band emission centered at 2.2eV is very weak.

Figure 5 shows the surface SEM morphology of the GaN/AlN/α-Si_3N_4/Si sample. The crack free surface is found in this sample even at the optical microscope analysis. The surface roughness is only 4 Å by AFM analysis.

4. Conclusions

High quality GaN epilayer on Si (111) substrate is obtained by introducing an LT simultaneous AlN/α-Si_3N_4 buffer structure by MBE. The GaN epilayer shows a wurtzite structure and exhibits excellent structural and optical properties as evidenced by XRD and PL measurements. The crack free surface of GaN epilayer was obtained by using LT simultaneous AlN/α-Si_3N_4 buffer structure. These results indicate that the crystalline quality and optical properties of the samples are comparable to those of GaN on sapphire samples.

Acknowledgements

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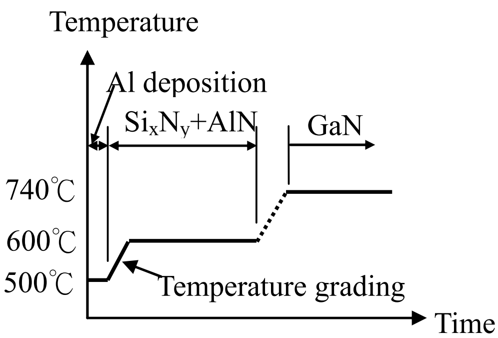

Fig. 1. Schematically depicts the process of LT simultaneous AlN/Si_3N_4 structure.

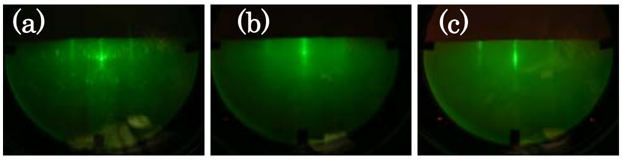

Fig. 2. The evolution of RHEED patterns, along the Si [110] azimuth during the growth process. (a) shows clear (7×7) surface reconstruction at high temperature. (b) and (c) show streaky (1×1) RHEED pattern of AlN after 150 sec and 0.98μm thick GaN epilayer, respectively.

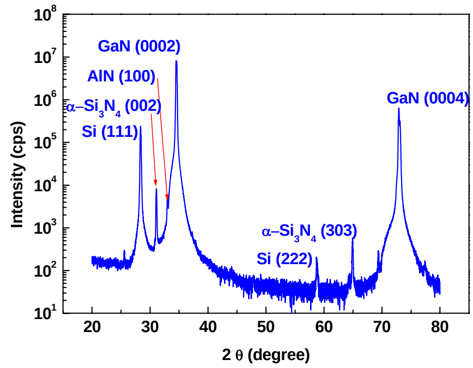

Fig. 3. A XRD pattern obtained from a 0.98 μm thick GaN epilayer on Si (111) substrate.

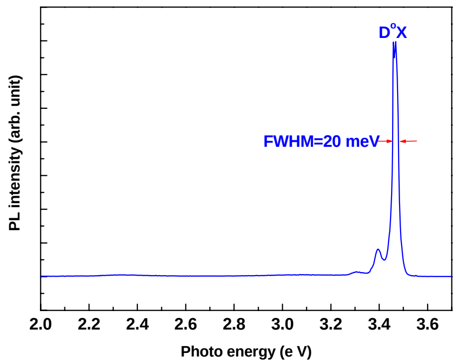

Fig. 4. PL of a GaN epilayer grown on Si (111) substrate measured at 13K

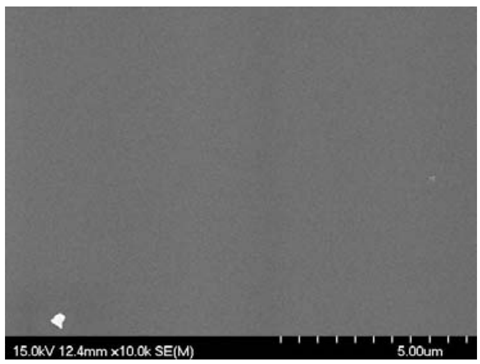

Fig. 5. SEM surface image of the GaN with AlN/α-Si_3N_4 structure.