

Growth of GaN film on Si (1 1 1) substrate using AlN sandwich structure as buffer

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ABSTRACT

A single high temperature AlN (HT-AlN) buffer has been used to relieve the stress in the growth of GaN epilayers on Si (1 1 1) substrates, but the growth of crack-free GaN on Si is still difficult due to the large mismatch of the lattice and coefficient of thermal-expansion (CTE) between GaN and Si. In this paper, we report the growth of 1.2 μm thick crack-free GaN epilayers on 2 in. Si (1 1 1) substrates using the AlN sandwich structure as a buffer. The surface morphologies of the samples were observed using a microscope and AFM. Further analysis shows that the crack-free sample is closely correlated to the introduction of the AlN sandwich structure as the buffer. To better understand the relationship between the cracks and the stress, Raman scattering has been used to study the stress in the samples. The results indicate that the sandwich structure with top AlN and bottom AlN can more effectively accommodate the strain energy caused by CTE mismatch stress.

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1. Introduction

GaN and related group-III nitrides grown by metal–organic chemical-vapor deposition (MOCVD) can be applied to the construction of high power and high frequency electronic devices as well as light emitting diodes (LEDs) and laser diodes. Due to the limited availability of bulk GaN substrates for homoepitaxial growth, GaN films are mainly grown heteroepitaxially on sapphire, SiC, and Si substrates. GaN growth on a Si substrate has attracted considerable attention 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. However, for the large lattice mismatch (16.9%) and the large coefficient of thermal-expansion (CTE) mismatch between GaN ($\alpha_a = 5.59 \times 10^{-6} \text{ K}^{-1}$) [3] and Si ($\alpha_a = 3.77 \times 10^{-6} \text{ K}^{-1}$) [4], the GaN epitaxial layers grown uniformly on Si substrates suffer from randomly distributed cracks, which are mostly caused by CTE mismatch. This is obviously a critical issue for nitride based electronic devices. There are many efficient ways of controlling the geometrical distribution of the thermal cracks [5–8], such as a high temperature AlN (HT-AlN) buffer, an $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /GaN superlattice buffer, graded $\text{Al}_x\text{Ga}_{1-x}\text{N}$ buffer, patterned silicon substrate, and so on. In these methods, the AlN buffer layer grown on Si (1 1 1) is necessary, which cannot only prevent the diffusion of silicon, but also be beneficial to the growth of the following layers. Based on the theory, this paper presents a sandwich structure AlN/composite

buffer/AlN as the buffer. The key point to note here is that previous studies only consider bottom HT-AlN as an individual part; instead, we consider bottom HT-AlN and top HT-AlN as systems that can more effectively accommodate the strain energy caused by CTE mismatch stress. The major characteristics of this system is that both top AlN and bottom AlN grow under the same experimental conditions as compared with those reported by Raghavan et al. [9].

Raman scattering has been extensively used to study III-nitrides and is a proven method for studying stress. Stress is an important factor that can influence the vibrational properties. Because the E_2 (TO) phonon frequency is sensitive to strain, it has been extensively used in GaN to quantify stress [10–12]. The phonon–stress relationship is extremely important because it would allow one to measure compressive or tensile stress in GaN and AlN on Si (1 1 1) substrates. In this paper, using the Raman scattering technique, we have investigated stress state and strain state in cracked GaN without top AlN and crack-free GaN with top AlN.

2. Experiment

Three samples were grown by metalorganic chemical vapor deposition (MOCVD) on 2 in. Si (1 1 1) substrates. The Si substrates were degreased using hot H_2SO_4 solutions for 5 min, $\text{NH}_3 \cdot \text{H}_2\text{O}$: H_2O_2 : H_2O (1:1:5) solutions for 5 min, and HCl : H_2O_2 : H_2O (1:1:5) solutions for 5 min in this order, and then etched with HF (2%) for 0.5 min to remove the surface oxide layer. This procedure results in an oxide-free, hydrogen-terminated Si surface. Trimethylaluminum (TMA), trimethylgallium (TMG), and ammonia were used as Al, Ga, and N sources, respectively. H_2 was used as a carrier gas.

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After preparation, the Si (1 1 1) substrates were heated under H_2 ambient at 1060 °C for 3 min to clean its surface prior to growth. Pre-deposition of Al was used to prevent the formation of SiN_x . In the initial stages of growth, a 60 nm thick HT-AlN layer was grown, which is used as the nucleation layer, and then a composite buffer layer, including 60 nm $Al_{0.25}Ga_{0.75}N$ and 20 periods of the AlN/GaN (2 nm/3 nm) superlattice, was grown. For sample A, 1.2 μm GaN was grown directly on the composite buffer layer, while for samples B and C another 30–40 nm HT-AlN layer was grown following the composite buffer layer. Finally, for samples B and C, GaN with thicknesses of 1.2 and 1.6 μm were grown, respectively. Fig. 1 shows a schematic diagram of the layer structure for samples A–C.

The samples were investigated by XRD rocking curve measurements, and the surface morphology was observed using a microscope and an atomic force microscope (AFM). Raman scattering experiments were carried out in a backscattering geometry with a combination of

instruments of a monochromator equipped with 1800 lines/mm grating. In the room-temperature Raman scattering experiments, the 514 nm line gas laser was employed as the excitation light.

3. Results and discussion

The surface morphologies of samples A–C are shown in Fig. 2. The photograph shown in Fig. 2 reveals good quality mirror-like surface of sample B. No pits and cracks were observed on the film over the entire area of the Si substrate. But the surface of sample A without a top AlN layer and sample C with thicker GaN epilayers than sample B distribute significant cracks. To investigate the surface of sample B precisely, AFM measurements were performed. As shown in Fig. 3, the surface is extremely smooth. Atomic steps are detected and regularly distributed. The root-mean-square (rms) roughness is only 0.5 nm in a $1 \times 1 \mu m^2$ scan area.

1.2 μm GaN	1.2 μm GaN	1.6 μm GaN
	HT-AlN	HT-AlN
AlN/GaN 20 periods	AlN/GaN 20 periods	AlN/GaN 20 periods
$Al_{0.25}Ga_{0.75}N$	$Al_{0.25}Ga_{0.75}N$	$Al_{0.25}Ga_{0.75}N$
HT-AlN	HT-AlN	HT-AlN
Si(111)	Si(111)	Si(111)
Sample A	Sample B	Sample C

Fig. 1. Schematic of MOCVD grown sample structures.

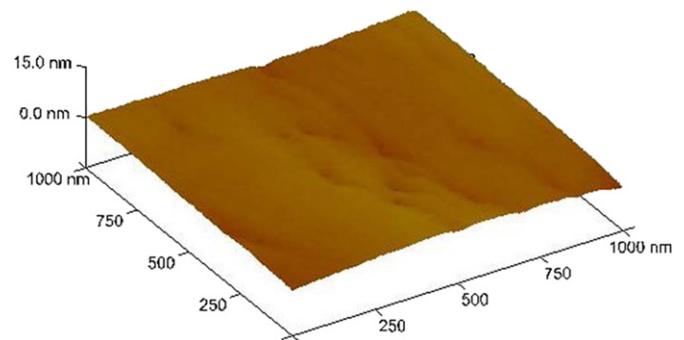


Fig. 3. 3D AFM images ($1 \times 1 \mu m^2$ scan) of sample B grown with AlN sandwich structure as buffer.

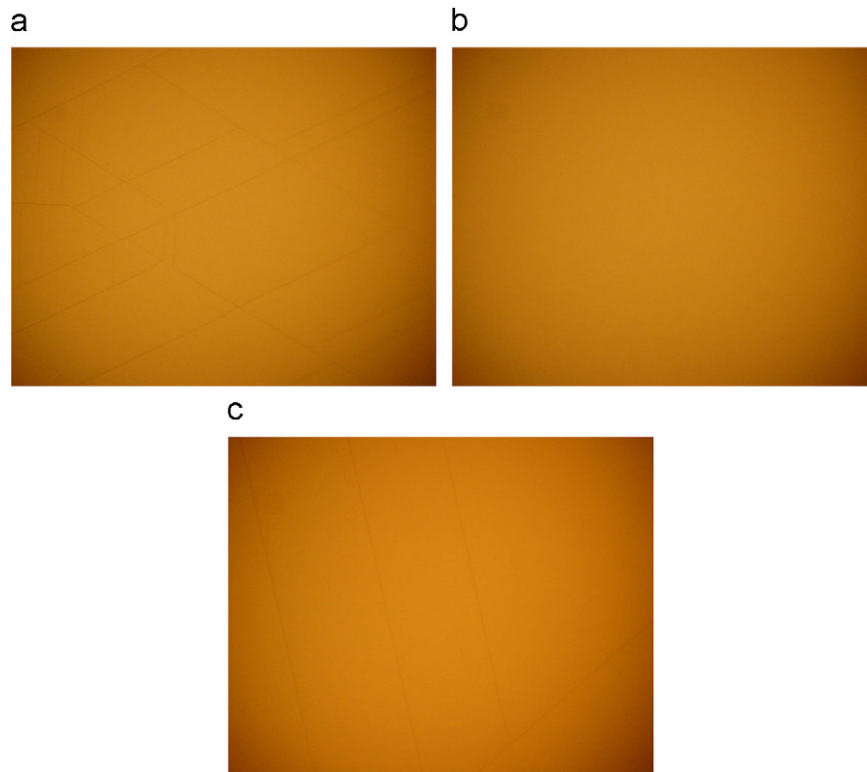


Fig. 2. $0.5 \times 0.5 mm^2$ optical microscope images of the surfaces of (a) sample A, (b) sample B, and (c) sample C.

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