Materials Research Bulletin 45 (2010) 1581–1585

Contents lists available at ScienceDirect

Materials Research Bulletin

journal homepage: www.elsevier.com/locate/matresbu

Improved growth of GaN layers on ultra thin silicon nitride/Si (1 1 1) by RF-MBE

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ARTICLE INFO

Article history:
Received 25 May 2010
Received in revised form 15 July 2010
Accepted 23 July 2010
Available online 1 August 2010

Keywords:
A. Nitrides
B. Epitaxial growth
B. Luminescence
C. X-ray diffraction

ABSTRACT

High-quality GaN epilayers were grown on Si (1 1 1) substrates by molecular beam epitaxy using a new growth process sequence which involved a substrate nitridation at low temperatures, annealing at high temperatures, followed by nitridation at high temperatures, deposition of a low-temperature buffer layer, and a high-temperature overgrowth. The material quality of the GaN films was also investigated as a function of nitridation time and temperature. Crystallinity and surface roughness of GaN was found to improve when the Si substrate was treated under the new growth process sequence. Micro-Raman and photoluminescence (PL) measurement results indicate that the GaN film grown by the new process sequence has less tensile stress and optically good. The surface and interface structures of an ultra thin silicon nitride film grown on the Si surface are investigated by core-level photoelectron spectroscopy and it clearly indicates that the quality of silicon nitride notably affects the properties of GaN growth.

1. Introduction

GaN material system is gathering great interest from the viewpoint of its application to optical devices as well as electronic devices because of its wide band gap nature [1]. A number of studies have been performed successfully to grow GaN on different substrates such as Al_2O_3 [2], SiC [3], and Si [4]. Among these materials silicon is viewed as one of the most promising candidates for the GaN epitaxy because of its many advantages such as high-quality, large size, low cost and a well-known existing device technology [5]. However, three-dimensional (3D) island growth is unavoidable for the direct growth of GaN on Si (1 1 1) because of the extreme lattice and thermal expansion coefficient mismatch between the GaN and the Si substrate. Although some results have been reported on the successful growth of GaN on Si using AlN [6,7], SiC [8,9] and InGaN [10] buffer layers, but a defect-induced yellow luminescence (YL) was commonly present, which affects the optical properties of GaN greatly. On the other hand, it has been demonstrated that no YL was present when a silicon nitride buffer layer was used for the GaN growth [11–13]. The present work envisages a comparative study of the GaN growth by RF-MBE on Si (1 1 1) as a function of nitridation time and temperature. We have grown a high quality, less stressed and optically excellent GaN films using a new growth approach.

2. Experiment

The growth system used in this study was a RF-MBE system (OMICRON) equipped with a radio frequency (RF) plasma source. The base pressure in the system was below 1×10^{-10} mbar. The undoped Si (1 1 1) substrates were ultrasonically degreased in isopropyl alcohol (IPA) for 10 min and boiled in trichloroethylene, acetone and methanol at 70 °C for 5 min, respectively, followed by dipping in 5% HF to remove the surface oxide. The substrates were outgassed at 900 °C for 1 h in ultra-high vacuum. In sample (a)–(d) the nitridation of the substrate was carried out at 530 and 700 °C for nitridation times from 0 to 60 min as shown in Table 1. In sample (e) the new growth process sequence was employed in which the nitridation of the substrate was carried out at 530 °C for 30 min followed by annealing at 900 °C for 30 min and again nitridation at 700 °C for 30 min. For all samples, low-temperature GaN buffer layers of thickness of 20 nm were grown at 500 °C after nitridation, where the gallium (Ga) effusion cell temperature was kept at 950 °C and corresponding beam equivalent pressure (BEP) was maintained of 5.6×10^{-7} mbar. Afterwards, a GaN epilayers of thickness of 225 nm were grown on the buffer layer at 700 °C. Nitrogen flow rate and plasma power were kept at 0.5 sccm and 350 W, respectively for the nitridation, buffer layer and subsequent GaN growth. The structural characterization and surface

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doi:10.1016/j.materresbull.2010.07.025

Table 1
Growth process sequence for GaN on Si (1 1 1) substrate.

Name of samples	(a)	(b)	(c)	(d)	(e)
Thermal cleaning at 900 °C	60 min	60 min	60 min	60 min	60 min
Nitridation at 530 °C	–	–	–	60 min	30 min
Annealing at 900 °C	–	–	–	–	30 min
Nitridation at 700 °C	–	30 min	60 min	–	30 min
LT-GaN buffer layer	15 min	15 min	15 min	15 min	15 min
GaN growth	180 min	180 min	180 min	180 min	180 min

morphologies of the samples were carried out by high resolution X-ray diffraction (HRXRD) and atomic force microscopy (AFM), respectively. The samples were optically characterized by micro-Raman spectroscopy using 532 nm line of the Nd:YAG laser and the PL spectra were recorded at room temperature using He–Cd laser of 325 nm excitation wavelength with a maximum input power of 30 mW. The nature of silicon nitride film was investigated with core-level photoelectron spectroscopy.

3. Results and discussion

Figs. 1 and 2 show the HRXRD 2θ-ω scans and rocking curve (ω-scans) of the GaN films grown on Si (1 1 1) substrate. The samples (b)–(d) were obtained with substrate nitridation and sample (a) was without substrate nitridation, whereas sample (e) corresponds to present new growth process sequence. From the figures it can be seen that except the substrate peak, only a strong (0 0 0 2) GaN diffracted peak at $2\theta = 34.59^\circ$ and a weak (0 0 0 4) peak at $2\theta = 73^\circ$ are present, indicating the epitaxial GaN thin film to be highly oriented along the [0 0 0 1] direction of the wurtzite GaN.

The crystalline quality of GaN epilayers grown on Si (1 1 1) substrate was determined by full width half maximum (FWHM) of HRXRD rocking curves of (0 0 0 2) symmetry planes of GaN epilayers, as shown in Fig. 3. The XRD peaks for all the samples grown on nitridated substrates show lower FWHM values, indicating improved crystalline structures compared with that of the sample without substrate nitridation. Fig. 3 also summarizes the FWHM of the GaN (0 0 0 2) plane as a function of nitridation temperature at a fixed nitridation time of 60 min. The GaN grown on the Si (1 1 1) by using a new nitridation process achieves the lowest FWHM. The FWHM value of GaN grown by new nitridation method is relatively poorer, as compared to the film grown on Al_2O_3 [2] and SiC [3] substrates, but found better than that grown on Si (1 1 1) using silicon nitride buffer layer [11,12] and comparable to AlN buffer layer [6,7].

Fig. 4(a)–(e) shows 3 μm × 3 μm AFM images of the GaN films for samples (a)–(e), respectively. The root mean square (RMS) roughness of the GaN films is drastically decreased from 23.752 to 5.989 nm when the nitridation time was changed from 0 to 60 min. Fig. 3 shows the dependence of the RMS values of the GaN surface on the nitridation time and temperature. When the nitridation period was increased from 0 to 30 min and to 60 min, the grains gradually coalesced and the number of big-sized grains decreased, reflecting the transition from three-dimensional growth mode to two-dimensional like growth mode during growth. It suggests that the surface of GaN on Si (1 1 1) would be covered over by coalescence of GaN grains preferentially formed at initial growth stage by the substrate nitridation for the long period. As can be observed in samples (c), (d) and (e), nitridation temperature can also significantly affect the surface morphology of the GaN epilayer at a fixed nitridation time of 60 min. The RMS value of surface roughness decreases from 5.989 to 5.332 nm when the nitridation temperature was changed from 700 to 530 °C for a fixed nitridation time of 60 min. However, The GaN grown on the Si (1 1 1) by using new nitridation process achieves the lowest RMS value of

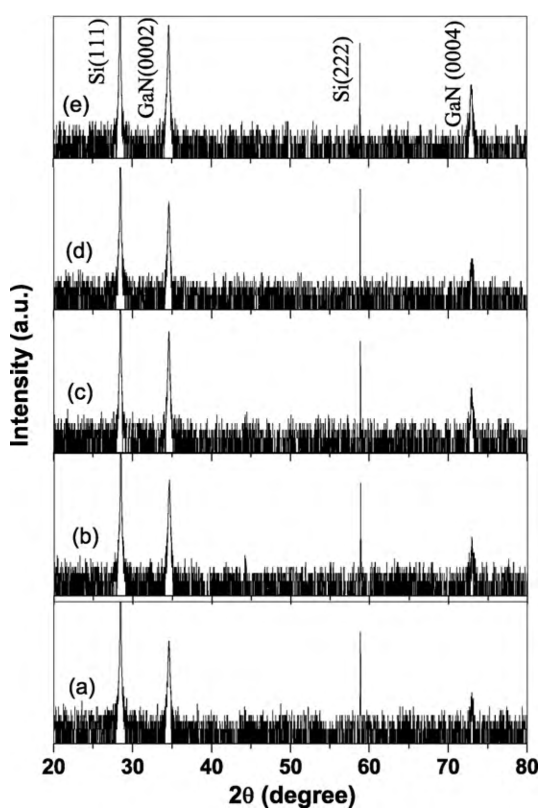

Fig. 1. HRXRD 2θ-ω scans of GaN on Si (1 1 1) substrate.

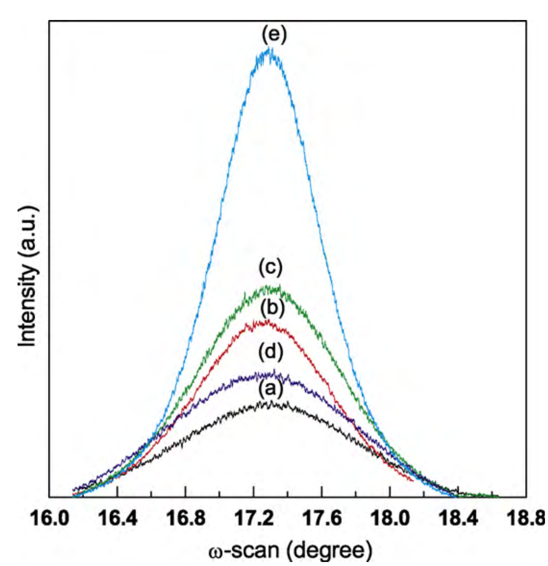

Fig. 2. The HRXRD rocking curves obtained from the GaN film grown on the Si (1 1 1) substrate for all samples.