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Structural and optical characterization of hexagonal crack free GaN films grown on Si(111) by plasma-assisted molecular beam epitaxy (PAMBE)

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In this work, we report on the structural and optical characterizations of wurtzite structure GaN thin films grown on Si(111) substrate by plasma-assisted molecular beam epitaxy (PAMBE). X-ray diffraction (XRD), micro-Raman and micro-photoluminescence (PL) spectroscopies were used to evaluate the structural and optical properties of the GaN films. In order to examine the quality of the films, $\omega/2\theta$ scan of XRD rocking curves (RC) at (0002) plane were carried out. Two intense peaks corresponding to GaN(0002) and AlN(0002) diffraction peaks were observed at 17.29° and 18.12°, respectively. The full width at half-maximum (FWHM) values of these peaks were 936 arcsec and 432 arcsec, respectively. Micro-Raman results showed that all the allowed Raman modes of GaN were visible. For the micro-PL measurement, an intense and broad band edge emission peak of GaN was observed at 364.48 nm. We assign this intense band edge emission to the neutral-donor bound exciton (I_2). However, it is important to note that no discernible yellow emissions are observed in our PAMBE grown GaN epilayers although PL measurements were carried out at room temperature. This means that there are no detectable impurities from source materials or defects generated by energetic nitrogen ions from RF nitrogen source.

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1. Introduction

Wide band gap GaN and its related compounds have attracted considerable attention over the past few years because they are very promising materials for fabrication of optoelectronic devices such as light-emitting diodes, laser diodes, and detectors operating in the ultraviolet (UV) and blue spectral region [1-3].

Physical, chemical and other interesting properties of GaN and related nitride materials provide the basis for the design and development of optoelectronic devices. GaN and related nitride materials can grow both in the crystalline wurtzite as well as zincblede structures, but the wurtzite structure is more common. The lattice constant of GaN wurtzite structure is shorter than that of GaN zincblede (Yoder, 1996) [4]. GaN and related nitride materials are the wide bandgap semiconductors (WBGS) whose definition is that the bandgap energy of material is larger than 3 eV.

As GaN devices are usually made from hexagonal GaN epitaxial layers, Si(111) can provide the hexagonal template for AlN deposition. According to the literatures, X-ray diffraction (XRD) patterns showed that full width at half maximum (FWHM) of AlN(0002) peak grown on Si (111) substrates was smaller than in the case of layers grown on Si(100) substrates. XRD results also indicated that the preferred orientation of AlN films on Si(111) substrates is more easily controlled than those on Si (100) substrates. It can be attributed to the more matched lattice template with hexagonal structures of AlN films provided by (111) plane of silicon [5].

Vibrational characterization by Fourier transform infrared spectroscopy (FTIR) revealed that the stress in the AlN films deposited on Si (111) substrates was also smaller than AlN films eposited on Si (100) substrates. The lattices in AlN (0001) and Si (111) are both hexagonal, and thus Si (111) can provide matched template for AlN (0001) plane. For these reasons, the Si (111) substrate was used [1]. In this paper, we report on the structural and optical characterization of GaN thin films grown on (111) Si substrates. X-ray diffractometer (XRD), micro-Raman and micro photoluminescence (PL) spectroscopies were employed to characterize the structural and optical properties of the film.

2. Experimental procedure

In this work, the GaN epilayers with the wurtzite structure were unintentionally doped n-type and grown on Si substrates. The thickness of the GaN films was ~ 0.13 μm. The crystallographic *c* axis lays along the growth direction.

To evaluate the crystalline structure and the quality of the sample, high-resolution PANalytical X'Pert Pro MRD XRD system was used. The XRD symmetric rocking curve (RC) of (0002) plane measurements were performed in the ω/2θ mode.

Micro-Raman and photoluminescence (PL) measurements were performed at room temperature using Jobin Yvon HR800UV system. Argon ion (514.5 nm) laser and He-Cd (325.0 nm) laser were used as excitation sources for Raman and PL measurements respectively. To focus the laser on the sample surface, microscope objective lenses 100 × and UV40 × were employed for Raman and PL measurements respectively. The diameter of the laser spot on the samples was around 20 μm. The emitted light was dispersed by a double grating monochromator with 0.8 m focal length and equipped with 1800 grove/mm holographic plane grating. Signals were detected by a Peltier cooled charge-coupled-device (CCD) array detector.

3. Results and discussion

The structure of the thin films has been determined by means of conventional XRD ω/2θ scan. It is found that diffraction peaks from GaN(0002) and AlN(0002) were observed, along with reflections from Si peak. These results suggest that the GaN films were in wurtzite phase. In order to examine the quality of the films, ω/2θ scan of XRD rocking curve (RC) at (0002) plane was carried out. Figure 1 shows the ω/2θ scan of the XRD RC of (0002) plane for the GaN/AlN/Si. It can be seen that two intense peaks corresponding to GaN(0002) and AlN(0002) diffraction peaks are observed at 17.29° and 18.12° respectively. The full width at half-maximum (FWHM) value of these peaks is 936 and 432 arcsec, respectively.

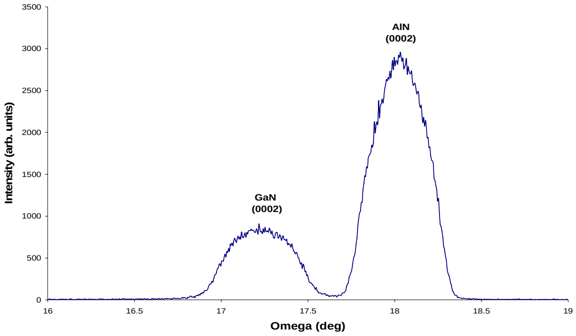

Fig. 1. RC of (0002) plane for GaN and AlN grown on Si substrate.

Micro-Raman scattering experiments were carried out in the $z(x, \text{unpolarized})\bar{z}$ scattering configuration. Here, the Porto's notation is used for scattering geometries with *z* to be parallel to wurtzite *c* axis, and (*x*, unpolarized) refers to the polarization of the incident and scattered light. Under this configuration, the allowed zone-center phonon modes that can be detected for wurtzite structure layer will be A_1(LO), E_2(Low), and E_2(High), unless there are some disoriented microstructures.

Fig. 2 shows the room temperature micro-Raman spectrum of GaN/Al/Si. The wurtzite crystal nature of our MBE-grown GaN materials on Si can be verified also via Raman scattering. A strong band is also shown at 520.39 cm^{-1} from Si(111) substrate, and a band at ~ 300 cm^{-1} due to the acoustic phonons of Si. There are no phonon modes related to the cubic phase GaN to be observed in the Raman spectra of our GaN/AlN/Si samples. These provide a further confirmation together with XRD measurements on the wurtzite structural nature of our MBE –grown GaN materials. However, the incorporation of the unintentionally doped (UID) has lead to high background intensities in the low wavenumber region.

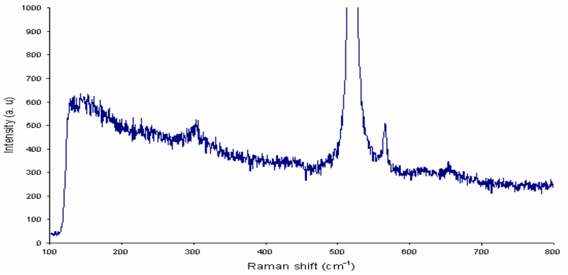

Fig. 2. Room temperature micro-Raman spectrum of GaN/Si.

The dominant E_2 (High) phonon mode of GaN appears at 565.81 cm^{-1}, which is nearly comparable to the result in the literatures [6,7]. However, the E_2(High) is considerably lower than that of strain-free bulk (568 cm^{-1}) [8] and this can be correlated to the thermal residual strain in the films. In general, compressive strain causes a red shift in phonon frequencies while tensile strain causes a blue shift. Consequently, this leads to suggest that the GaN films are subjected to a tensile biaxial thermal strain upon cooling down after growth due to the thermal expansion coefficient perpendicular to the Si which is smaller than that of GaN (5.59×10^{-6} $°C^{-1}$) [8]. The E_2 (high) phonon mode of AlN appears at 653.40 cm^{-1} and deviates from the standard value of 655 cm^{-1} for an unstrained AlN [9].

PL spectroscopy is a good characterization tool to identify the appearance of defect-related levels or defect induced luminescence in the sample. Fig 3 shows the room temperature PL spectrum of doped GaN/AlN/Si. A strong near band edge emission for the sample is observed at 361.25 nm which is attributed to the band edge emission of GaN. We assign this intense band edge emission to the neutral-donor bound exciton (I_2). However, it is important to note that no discernible yellow emissions are observed in our PAMBE grown unintentionally doped GaN epilayers although PL measurements were carried out at room temperature. This means that there are no detectable impurities from source materials or defects generated by energetic nitrogen ions from RF nitrogen source.

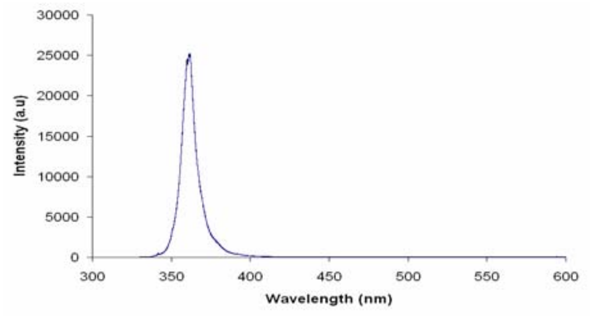

Fig. 3. Room temperature micro-PL spectrum of GaN on silicon.

4. Conclusions

In summary, we have investigated GaN films grown on Si(111) by plasma-assisted MBE. The GaN film quality was determined by X-ray rocking curve, photoluminescence (PL), and Raman spectroscopies measurements. The structural quality of the thin film is comparable to the reported values in the literature. Sharp and intense band edge emission of unintentionally doped GaN is observed in the PL measurement with the absence of yellow band emission which is an indication of good optical quality thin films.

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