

The growth of AlN thin films on Si (111) substrate by plasma-assisted molecular beam epitaxy

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GaN-based materials received great deal of attention because of the potential applications for optoelectronic devices operating in the whole visible spectral range and in electronic devices such as high temperature, high power, and high frequency transistor. The III-nitrides form a continuous alloy system with direct band gap ranging from 6.2 eV (AlN) to 0.7 eV (InN) with 3.4 eV for GaN. Consequently, the growth and physics of GaN-based materials have attracted tremendous scientific attention. This article reports the use of plasma-assisted molecular beam epitaxy (MBE) to grow AlN on (111) Si substrate at 850 °C under UHV conditions for 15, 30, and 45 minutes. The films were characterized by high-resolution x-ray diffraction (HR-XRD) and micro-Raman spectroscopy. XRD phase analysis of (0002) plane of GaN exhibits two intense and sharp peaks, namely Si(111) and AlN(0002) diffraction peaks, at 28.4° and 36.1° respectively. Micro-Raman results show that all the allowed Raman modes of AlN and Si are visible.

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1. Introduction

GaN-based materials received great deal of attention because of the potential applications for optoelectronic devices operating in the whole visible spectral range and in electronic devices such as high temperature, high power, and high frequency transistor. The III-nitrides form a continuous alloy system with direct band gap ranging from 6.2 eV (AlN) to 0.7 eV (InN) with 3.4 eV for GaN. Consequently, the growth and physics of GaN-based materials have attracted tremendous scientific attention.

Aluminium nitride, AlN (wurtzite structure type) has specific physical properties such as high thermal conductivity (91-190 W/m-K), high electrical resistivity (10^{11} - 10^{14} Ωcm), high melting point and large energy gap [1-6]. Its applications as a component of refractory ceramics or buffer layers for GaN epilayers grown on sapphire are widely known. The detailed studies of nitrides may be helpful in design and improving the technologies involving aluminium nitride. In the last decade considerable interest arose in the use of thin films of AlN for various applications, from hard coatings and over coatings for magneto-optic media, to thin films transducers and GHz-band surface acoustic wave devices.

This article presents the growth of AlN on Si (111) substrate by using plasma assisted MBE (Veeco Gen II) for various deposition times. The structural and optical properties of grown AlN are then analyzed by a variety of characterization tools. High resolution x-ray diffractometer was used to assess and determine the crystalline quality. The optical quality of the film was investigated by micro-Raman spectroscopy.

2. Experiment

AlN was grown on Si (111) substrate using Veeco model Gen II MBE system. MBE system is based on ultra high vacuum (UHV) environment that is typically evacuated to less than 10^{-10} Torr. In our new MBE system, the background pressure of the MBE system was below 5×10^{-11} Torr (7×10^{-9} Pa). High purity material sources such as gallium (7 N), and aluminum (6 N5) were used in the Knudsen cells. Nitrogen with 7N purity was channeled to RF source to generate reactive nitrogen species. The plasma was operated at typical nitrogen pressure of 1.5×10^{-5} Torr under a discharge power of 300 W. The base pressure in the system was below 7×10^{-9} Pa. The nitrogen flux through plasma source, causing a nitrogen partial pressure in the MBE chamber of about 2.0×10^{-3} Pa during growth.

The growth of III-nitrides on 3-inch Si (111) substrate starts with the standard cleaning procedure by using RCA method. The substrate was then mounted on wafer holder and loaded into the MBE system. The Si substrate was outgassed in the load-lock and buffer chambers. After outgassing, the Si was transferred to the growth chamber. Prior to the growth of the epilayers, surface treatment of the Si substrate was carried out to remove the SiO₂. Si substrate was heated at 750°C, a few monolayers Ga was deposited on the substrate with the purpose to remove the SiO₂ by formation of GaO₂. Reflection high energy electron diffraction (RHEED) showed the typical Si (111) 7×7 surface reconstruction pattern with the presence of prominent Kikuchi lines, indicating a clean Si (111) surface.

Before the growth of nitride epilayers, a few monolayers of Al was also deposited on the Si substrate to

avoid the formation of Si_xN_y which is deleterious for the growth of the subsequent epilayers. The formation of such amorphous layer has been observed by many groups [7-8]. Calleja [8] reported that the growth of GaN epilayer on Si_xN_y will lead to polycrystal with full width at half maximum values from XRD measurements between 70 and 100 arcmin. The buffer layer or wetting layer, AlN was first grown on the Si substrate. It is well known that this buffer layer plays an important role in determining the crystalline quality of the thin film [9]. To grow AlN buffer layer, substrate temperature was heated up to 850°C, both of the Al (cell temperature at 1120 °C) and N shutters were opened simultaneously.

Three representative samples, article reports the use of plasma-assisted molecular beam epitaxy (MBE) to grow AlN on (111) Si substrate for 15, 30, and 45 minutes. To evaluate the crystalline structure and the quality of the sample, high-resolution PANalytical X'Pert Pro MRD XRD system was used. Micro-Raman measurement was performed at room temperature using Jobin Yvon HR800UV system. Argon ion (514.5 nm) laser was used as excitation sources for Raman measurement. Microscope objective lenses 100× were employed for Raman measurement to focus about the laser on the sample surface. 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 groove/mm holographic plane grating. Signals were detected by a Peltier cooled charge-coupled-device (CCD) array detector. A high quality single crystal silicon sample (with the zone-center-mode at 520.70 cm^{-1}) was used to calibrate the system before the micro-Raman. The full width at half-maximum (FWHM) of the Si Lorentzian peak width was $\sim 3 \text{ cm}^{-1}$. The essential parameters [peak position and full width at half maximum (FWHM)] of the Raman peak was determined by using curve fitting software with Gaussian and Lorentzian model.

3. Results and discussion

A high-resolution PANalytical X'Pert Pro MRD XRD system with a $\text{Cu-K}\alpha_1$ radiation source ($\lambda = 1.5406 \text{ \AA}$) was used to determine the exact orientation relationship and the content of the sample. The intensity data was collected in two dimensions by performing ω (sample angle) - 2θ (detector angle) scan at a range of different values. Fig. 1 shows the XRD phase analysis scan of AlN/Si. The peaks at about 28.4° and 36.1° correspond to diffraction peak of (111) Si and (0002) AlN film respectively. These results suggest that the AlN films were in wurtzite phase. However, the growth duration has no significant effect on the full width at half maximum (FWHM) of AlN peak (Fig. 2).

The 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 $(x, \text{unpolarized})$ refers to the polarization of the incident and scattered light. Under

this configuration, the allowed zone-center phonon modes of wurtzite GaN will be: $E_2(\text{low})$, $E_2(\text{high})$, and $A_1(\text{LO})$. The E_2 (high) modes in the Raman spectra can be used to estimate the stress, as it has been proven to be particularly sensitive to biaxial stress in samples.

Fig. 3 shows the corresponding room temperature micro-Raman spectrum of AlN on Si. It is found that all the allowed Raman phonon modes of AlN, i.e. the $E_2(\text{low})$, $E_2(\text{high})$, and $A_1(\text{LO})$ are clearly visible. The E_2 (high) phonon mode of AlN appears at 654.40 cm^{-1} and deviates from the standard value of 655 cm^{-1} for an unstrained AlN [10]. In addition, a peak from the silicon substrate is also seen at 520.33 cm^{-1} , and a band at 300 cm^{-1} due to the acoustic phonons of Si. There is no phonon modes related to the cubic phase AlN to be observed in Raman spectra of our AlN/Si. This gives a further confirmation together with XRD measurements on the wurtzite structural nature of our MBE grown AlN.

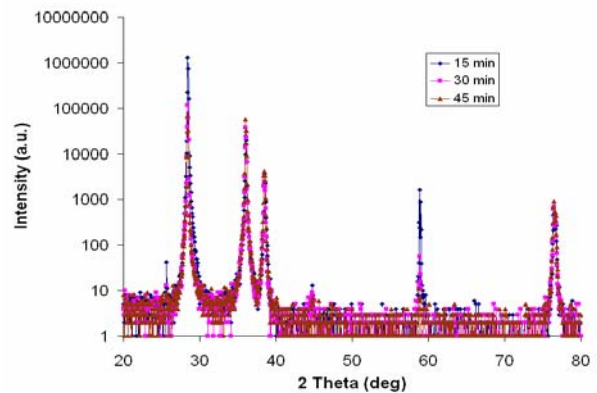


Fig. 1. XRD pattern of AlN thin film deposited on Si(111).

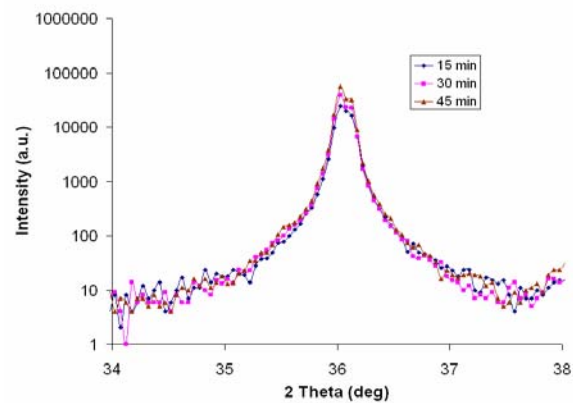


Fig. 2. XRD pattern of AlN thin film.

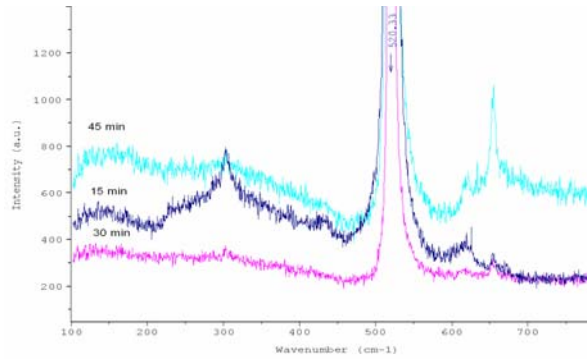


Fig. 3. Room temperature micro-Raman spectra of AlN grown on silicon substrate.

4. Conclusion

In summary, the growth of AlN on Si (111) substrate has been performed using plasma-assisted molecular beam epitaxy. The structural and optical properties of the thin film have been analyzed by HR-XRD and PL. The structural quality of the thin film is comparable to the reported values in the literature.

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