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INFLUENCE OF Al MONOLAYERS ON THE PROPERTIES OF AlN LAYERS ON Si (111)

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High-quality aluminum nitride (AlN) layers with full width at half maximum (FWHM) values of 11 arcmin were grown by plasma-assisted molecular-beam epitaxy on Si (111) substrates. AlN nucleation layers are being investigated for the growth of GaN on Si. Growth using AlN buffer layers leads to Al-polar films, with surfaces strongly dependent on the flux conditions used. Flat surfaces can be obtained by growing as Al-rich as possible, although Al droplets tend to form. Before starting the AlN growth, a few monolayers of Al are deposited on the substrate to avoid the formation of Si_3N_4. X-ray diffraction (XRD) techniques were employed to determine the surface and structural quality of the layers. XRD revealed that monocrystalline AlN was obtained. Best AlN films were obtained at high substrate temperatures (875°C) and III/V ratios close to stoichiometry.

Keywords: III–V nitrides; molecular beam epitaxy; XRD; AlN; Si (111).

1. Introduction

Group III nitrides have been recognized as one of the most promising materials for modern electronics, optoelectronics, and even spintronics devices.[1] GaN on silicon offers very attractive potential for the manufacturability and cost benefits for GaN optoelectronic and microelectronic devices. For the growth of crack-free, device-quality GaN on silicon, both the large lattice mismatch and positive thermal expansion coefficient difference must be overcome. The strong reaction between Si and Ga during the growth of LT-GaN results in poor crystal quality and morphology of the GaN film. Also, there is a strong tendency toward the formation of amorphous SiN_x, which will induce three-dimensional growth and polycrystalline GaN. GaN is therefore not well suited for direct epitaxial growth on silicon substrates. The use of AlN as an intermediate buffer layer is one of the most promising ways to achieve high quality of GaN on Si, and this approach has been widely studied in molecular-beam epitaxy (MBE) system. Since the buffer layer serves as the crystallographic and morphological template for subsequent GaN deposition, the microstructure and growth mode of this layer must be understood to achieve device quality GaN on silicon substrates.

Aluminum nitride (AlN), an important member of the group III nitrides with the highest bandgap of about 6.2 eV, has excellent thermal conductivity, good electrical resistance, high dielectric constant, large breakdown electric field, low dielectric loss, high piezoelectric response, and ideal thermal expansion, matching that of silicon. These properties are both physically interesting and technologically important.[2]

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 that grown on (100) plane of Si substrates. XRD results also indicate that the preferred orientation of AlN films on Si (111) substrates is more easily controlled than those on Si (100) substrates.[3] It can be attributed to the more matched lattice template with hexagonal structures of AlN films provided by (111) plane of silicon.

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 deposited on Si (100) substrates.[3] The lattices in AlN (0001) and Si (111) are both hexagonal, and thus Si (111) can provide matched template for AlN (0001) plane. The lattice mismatch between these two plane is 19% ($d_{\mathrm{Si}(111)} - d_{\mathrm{AlN}(0001)}/d_{\mathrm{Si}(111)}$, here $\mathrm{d}_{\mathrm{Si}(111)}$ refers to the Si lattice distance in Si (111) plane and $d_{\mathrm{AlN}(0001)}$ refers to the AlN lattice distance in AlN (0001) plane).

The lattice in Si (100) is square, which is unmatched with hexagonal lattice in AlN (0001) plane. The lattice mismatch between AlN (0001) and Si (100) is 42.7% ($d_{\mathrm{Si}(100)} - d_{\mathrm{AlN}(0001)}/d_{\mathrm{Si}(100)}$, here $d_{\mathrm{Si}(100)}$ refers to the Si lattice distance in Si (100) plane). The larger lattice mismatch between AlN (0001) and Si (100) is a main contribution to the larger strain in the formed films. In the case of GaN layers grown on AlN buffer layer, the crystalline quality is much improved because the lattice mismatch between GaN and AlN is only 2.5%. For these reasons, the Si (111) substrate was used.

In this work, we present a study of the growth condition of the initial few monolayers of Al deposited on the Si (111) substrate prior to the growth of AlN layer by MBE with radio-frequency nitrogen plasma source. XRD techniques enable the assessment of the material quality. Optimization of the growth condition leads to high-quality AlN layers.

2. Experiments

The film growth has been performed in a Veeco Gen II MBE system using standard effusion sources for evaporation of Al and Ga. An optical pyrometer is used to determine the substrate temperature. The base pressure in the system was below 5×10^{-11} Torr. The RF plasma was operated at typical nitrogen pressure of 1.5×10^{-5} Torr under a discharge power of 300 Watts. Growth mode and surface superstructures have been monitored by a 15 kV RHEED system.

The growth of group III nitrides on 3-inch Si (111) substrate (resistivity > 0.005 ohm cm, n-type) 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. In the preparation chamber, the substrates were outgassed for 10 min at 400°C prior to growth. 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 SiO_2. Silicon substrate was heated to 750°C; then, a few monolayers of Ga were deposited on the substrate for the purpose of removing the SiO_2 by formation of GaO_2. Reflection high-energy electron diffraction (RHEED) showed the typical (111) plane of Si (7×7) surface reconstruction pattern with the presence of prominent Kikuchi lines, indicating a clean Si (111) surface.

Substrate temperature was then ramped up to 850°C, followed by the deposition of a few monolayers of Al prior to the AlN buffer layer growth. Care was taken to initiate the AlN nucleation layer growth on Si (111) without forming silicon nitride at the interface. This was done by avoiding exposure of the Si (111) surface to the RF nitrogen discharge alone, prior to growth of the nitrides. On the other hand, a way to avoid this amorphous Si_xN_y layer formation is to start the growth with an AlN nucleation layer, because the bond formation between Al and N atoms prevails over the Si–N one.

It has been found that an effective III/V ratio at the surface of the substrate during growth is the most critical parameter controlling the properties of the layer. This III/V ratio is highly affected by variations in the substrate temperature. For AlN layer deposition, silicon substrate was heated at 875°C; then, the deposition is started by opening both Al (cell temperature at 1120°C) and N cell shutters.

To determine the exact orientation relationship and the content of the sample, high-resolution

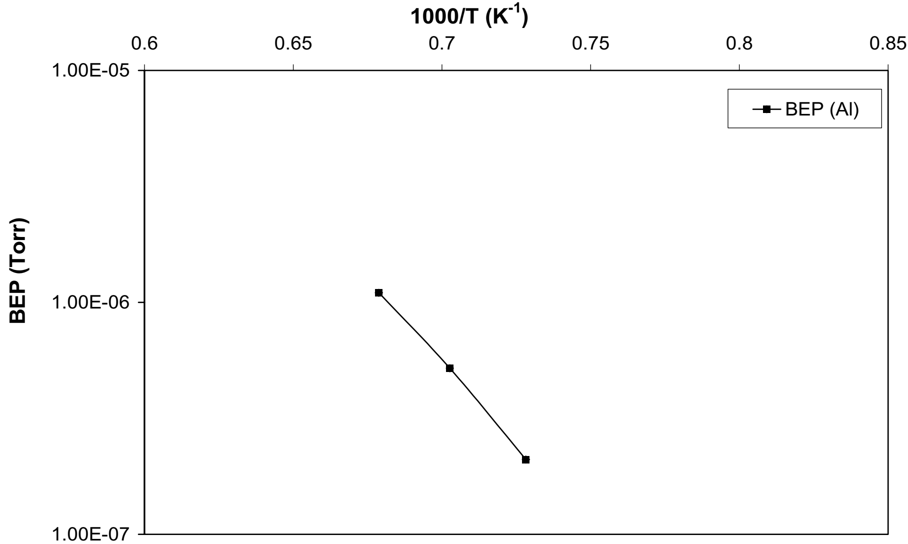

Fig. 1. Al flux (BEP) as a function of the reciprocal Al cell temperature.

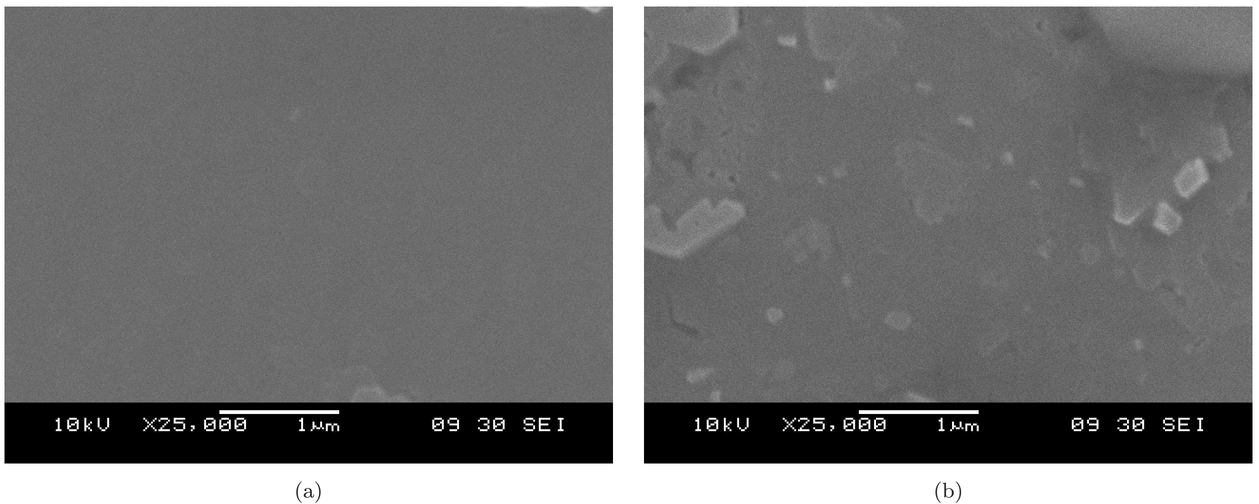

Fig. 2. SEM image of AlN thin film grown at different substrate temperatures: (a) 875°C and (b) 840°C.

PANalytical X'Pert Pro MRD XRD system with a Cu Kα_1 radiation source ($\lambda = 1.5406$ Å) was used. The XRD symmetric rocking curve (RC) of (0002) plane measurements were performed in the $\omega/2\theta$ mode.

3. Results and Discussion

In order to optimize the AlN buffer layer, the growth temperature and stoichiometry have to be carefully considered. Figure 1 shows the Al flux (beam equivalent pressure, BEP) as a function of the reciprocal Al cell temperature. Below this point, the growth proceeds under N-rich conditions and above it there is an Al-rich regime that may eventually lead to Al droplets formation. When the growth takes place near stoichiometry, optimum AlN buffers are obtained in terms of surface flatness and crystal quality, which correspond to growth temperatures around 875°C. Lower growth temperatures lead to an increasing surface roughness. Figure 2 shows SEM image of AlN thin film grown at different substrate temperatures.

The structure of the films has been determined by means of conventional XRD phase analysis $\omega/2\theta$ scan. The intensity data were collected in two

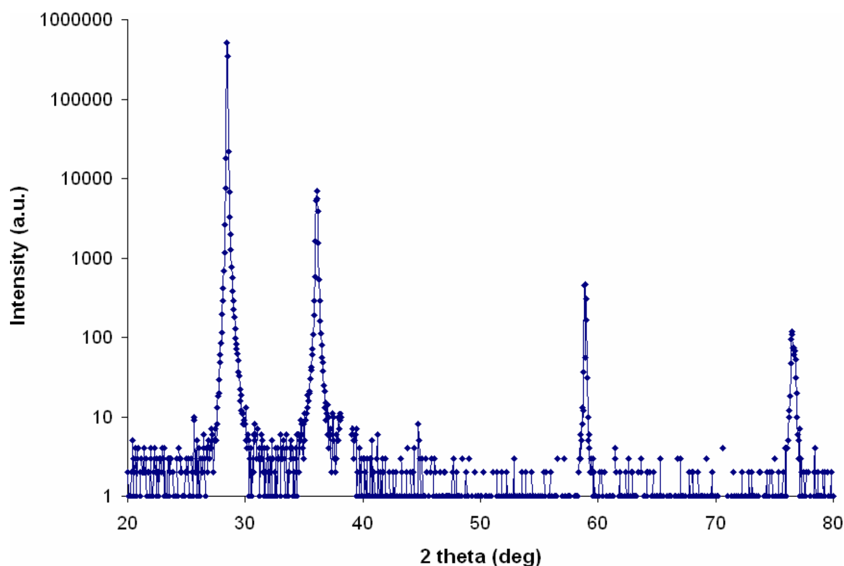

Fig. 3. XRD scan of AlN on silicon.

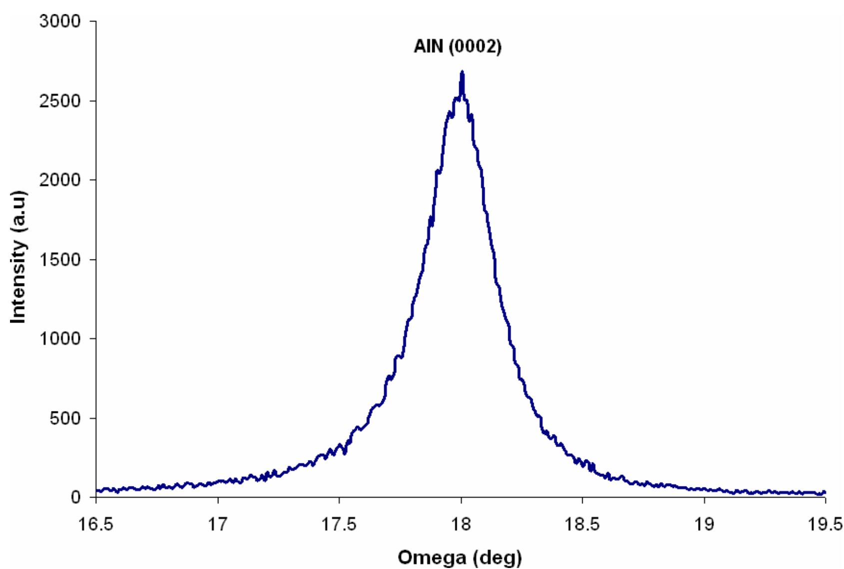

Fig. 4. X-ray diffraction (XRD) rocking curve (RC) of a 90 nm AlN buffer on Si (111) at 875°C.

dimensions by performing ω (sample angle) — 2θ (detector angle) scan at a range of different values. Figure 3 shows the XRD phase analysis scan of sample grown at 875°C. These results suggest that the AlN films were in wurtzite phase. It is found that only diffraction peaks from AlN (0002) were observed, along with reflections from Si (111) peak. The double-peak structure shown in the diffraction spectra is due to the $K\alpha_1$ and $K\alpha_2$. In order to examine the quality of the films, $\omega/2\theta$ scan of XRD RC at (0002) plane was carried out. Figure 4 shows the $\omega/2\theta$ scan of the XRD RC of (0002) plane for the AlN. The main result from Figure 4 (11 arcmin XRD-FWHM) has to be compared with previous reports by Stevens *et al.* (26 arcmin),[5] by Meng and Perry (51 arcmin),[6] and by Yasutake *et al.* (55 arcmin),[7]

which used the same approach of Al coverage prior to the AlN buffer growth.

4. Conclusion

In summary, good quality AlN layers were grown on silicon (111) substrates by optimizing the nucleation growth conditions. III/V ratios close to stoichiometry and high substrate temperature (around 875°C) lead to a best value of FWHM of 11 arcmin. The structural quality of the thin film is comparative to the reported values in the literature. No amorphous Si_xN_y layer was observed at the interface and AlN films with good epitaxial crystalline quality were obtained.

Acknowledgments

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