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High Quality AlN and GaN Grown on Compliant Si/SiC Substrates by Gas Source Molecular Beam Epitaxy

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Epitaxial layers of AlN and GaN were grown by gas source molecular-beam epitaxy on a composite substrate consisting of a thin (250 nm) layer of silicon (111) bonded to a polycrystalline SiC substrate. Two dimensional growth modes of AlN and GaN were observed. We show that the plastic deformation of the thin Si layer results in initial relaxation of the AlN buffer layer and thus eliminates cracking of the epitaxial layer of GaN. Raman, x-ray diffraction, and cathodoluminescence measurements confirm the wurtzite structure of the GaN epilayer and the c-axis crystal growth orientation. The average stress in the GaN layer is estimated at 320 MPa. This is a factor of two less than the stress reported for HVPE growth on 6H-SiC(0001).

Key words: Si/SiC, substrate, composite, AlN, GaN

INTRODUCTION

One of the problems in the epitaxy of nitrides is the lack of a suitable substrate material on which lattice-matched group III-nitride films can be grown. The large lattice mismatch of most of the available substrates leads to high interfacial strain between the substrate and the epitaxial layer, resulting in three-dimensional (3D) growth and formation of misfit dislocations.[1] Growth on compliant substrates offers a way of minimizing such interfacial strain.[1–6] The idea is to produce a free-standing thin layer by placing the layer on a bulk substrate with frictionless glide on each other.[7] There are additional advantages of bonding the compliant layer to a polycrystalline substrate. More specifically, polycrystalline SiC substrate offers an excellent match of thermal expansion coefficient to GaN. Low cost, large diameter polycrystalline SiC substrates are commercially available, offer high thermal conductivity (300 W/m·K), and can be made electrically conducting or insulating (>5000 ohm-cm), an important feature for optical devices and microwave power applications. The concept of a strain-relaxed compliant substrate and the behavior of epitaxial films grown on such substrates are well known.[2] However, the influence of the free-standing layer thickness and its plasticity on the subsequent growth of AlN and GaN are still under study.

This work describes preparation of AlN and GaN on a thin (250 nm) Si(111) film that is wafer bonded to a 100 mm diameter polycrystalline SiC substrate. We also discuss the investigation of growth mechanisms, stress relaxation, and optical properties of epitaxial AlN and GaN layers.

EXPERIMENTAL DETAILS

AlN and GaN films were grown by gas source molecular beam epitaxy (GSMBE) with ammonia on a thin (250 nm), chemically-mechanically polished (CMP) silicon (111) layer that was bonded to a polycrystalline SiC substrate. The poly-SiC substrates were polished using the technology developed previously for SiC mirrors, which makes wafer bonding possible.[8] Atomic force microscopy (AFM) of the top Si layer shows a RMS roughness of 0.2 nm.

The influence of growth conditions on the structure and homogeneity of the epitaxial layers of AlN and GaN was studied using 10 kV reflection high energy electron diffraction (RHEED), x-ray diffraction (XRD), Raman spectroscopy, and cathodoluminesence (CL).

Ammonia was introduced into the growth chamber through a mass-flow controller operating in the range of 30 sccm. The substrate temperature was measured by a pyrometer, corrected for the emissivity of the

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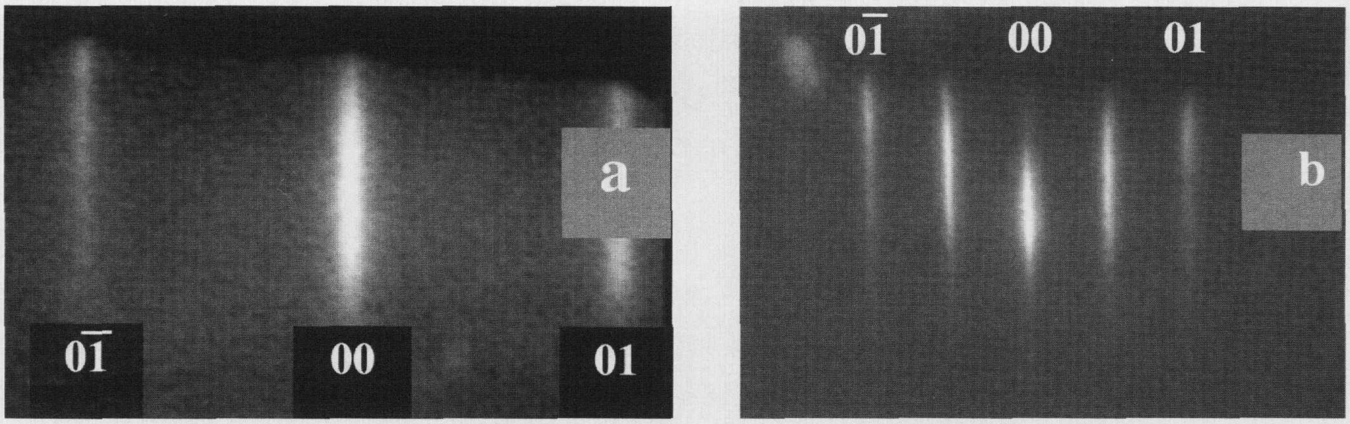

Fig. 1. The (a) 1×1 and (b) 2×2 RHEED patterns related to 2D growth mode of AlN and GaN, correspondingly. The azimuth of the electron beam is parallel to the GaN [$\bar{1}\bar{1}20$]||Si[$1\bar{1}0$].

substrate. To increase the substrate heating efficiency Ti and Ni were used to coat the backside of the Si/poly-SiC. Layers of AlN were grown in the temperature range of 860±30°C.[9] Layers of GaN were grown at 780±20°C.[10]

RESULTS AND DISCUSSION

Epitaxial growth of AlN and GaN was performed using growth conditions similar to those described previously for bulk Si(111).[9,10–12] Formation of a thin film of AlN was monitored by RHEED. The growth process was carried out at a high temperature (>830°C), where formation of the Al-Si γ-phase is not possible due to the short residence time of Al atoms on Si. The growth was initiated by a brief exposure to NH_3. At this point, RHEED showed the presence of an ordered periodic structure on (111)Si, attributed to a strongly bound layer of chemisorbed N. Once the ordered structure was formed, the surface was exposed to the flux of Al. This resulted in the formation of Si-N-Al islands. This step was followed by alternating exposure to Al and ammonia, carried out several times, until a complete surface coverage with the Si-N-Al phase was obtained. After this step, the growth surface was free of amorphous SiN_x and epitaxial growth of AlN could be started. The surface periodic order examined by RHEED suggests that the nucleation of AlN occurs in a 2D mode. A typical 1×1 RHEED pattern due to the formation of AlN ordered surface structure is shown in Fig. 1a.

The best growth results were achieved for a NH_3/Al flux ratio near unity, in agreement with previous results obtained on bulk Si(111).[11] Thin (40 nm) AlN was used as a buffer layer for the subsequent growth of GaN. The initial formation of GaN on AlN layer showed 3D character. This could be explained by the large (~3%) lattice mismatch between GaN and AlN. The transition to 2D growth mode was observed after the growth of at most 10 nm of GaN. Once the 2D growth was reached GaN layers showed 2×2 surface reconstruction, presented in Fig. 1b.

In our experience on bulk Si (111), the strain energy of GaN can be reduced by a defect-blocking superlattice (SL) consisting of two to four pairs of $Al_xGa_{1-x}N$ (x ≈ 0.1–0.4) with GaN spacers.[10,13] The SL tends to accommodate the strain due to a large difference in thermal expansion coefficients between group-III nitride layers and Si. This strain is responsible for the formation of cracks in thick nitride layers (>0.1 μm). The use of the SL results in complete elimination of cracking in nitride layers thicker than 0.2 μm (see for details Ref. 10). However, in our growth experiments on Si(111)/poly-SiC substrates, the AlGaN/GaN superlattice was not needed. Formation of cracks was not observed for 0.5 μm thick layers of GaN grown on 40 nm thick AlN buffer layers. Such an outcome can be explained by

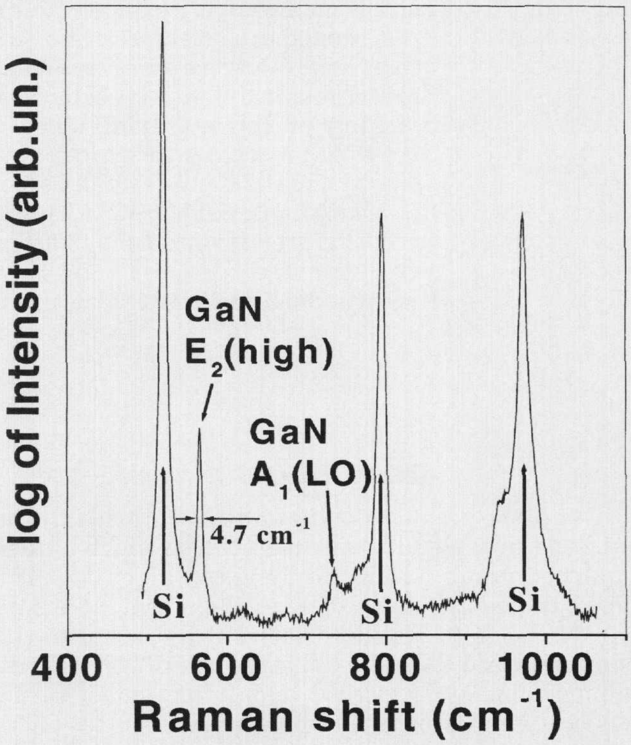

Fig. 2. Room temperature Raman spectra of GaN grown on Si/poly-SiC substrate. The intense bands at 520, 795 and 970 cm^{-1} are from the Si layer. E_2 phonon near 566 cm^{-1} is from GaN layer. A weaker A_1 optical band is observed at 735 cm^{-1}. This spectrum is characteristic of back scattering along the wurtzite GaN c = (0001) axis.

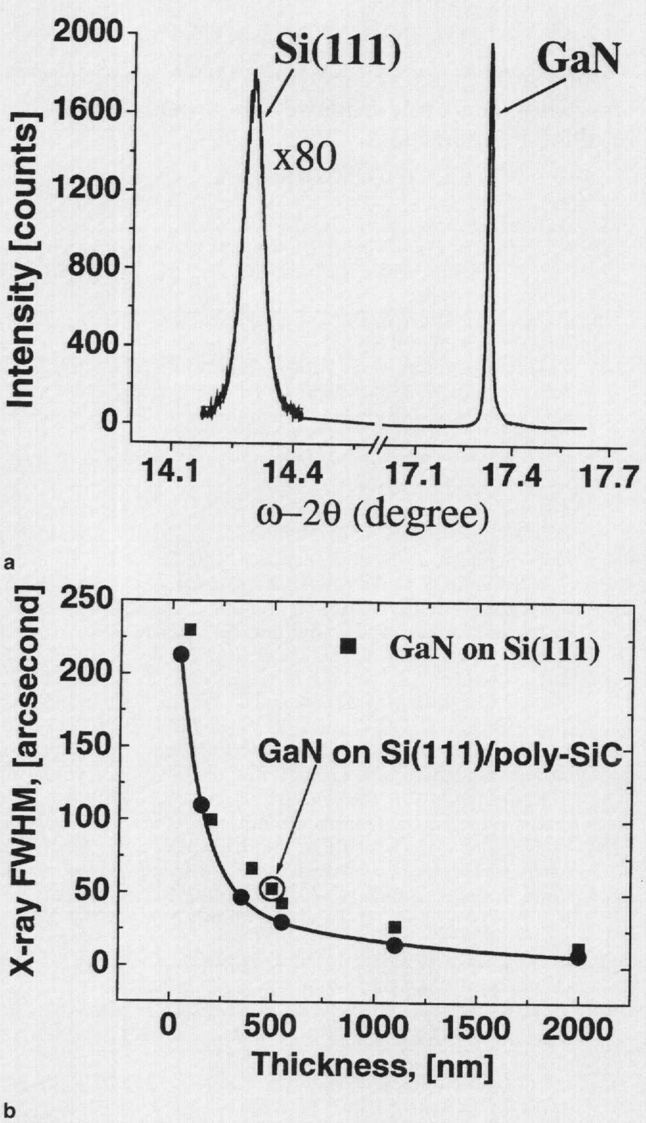

Fig. 3. Results of an x-ray diffraction (XRD) study. (a) XRD-pattern of wurtzite GaN film grown using a thin AlN buffer layer on a thin Si(111) layer that is wafer bonded to a polycrystalline SiC substrate; (b) x-ray linewidth (FWHM) measured for GaN layers as a function of thickness. Black squires correspond to GaN grown on bulk Si(111). Circled square corresponds to GaN grown on Si/poly-SiC. The solid line shows the FWHM calculated for an ideal crystal (see Ref. 18).

the high degree of relaxation of the initial lattice mismatch at the AlN/Si hetero-interface. We believe the reduction in stress occurs through the plastic deformation of the thin Si layer bonded on poly-SiC.

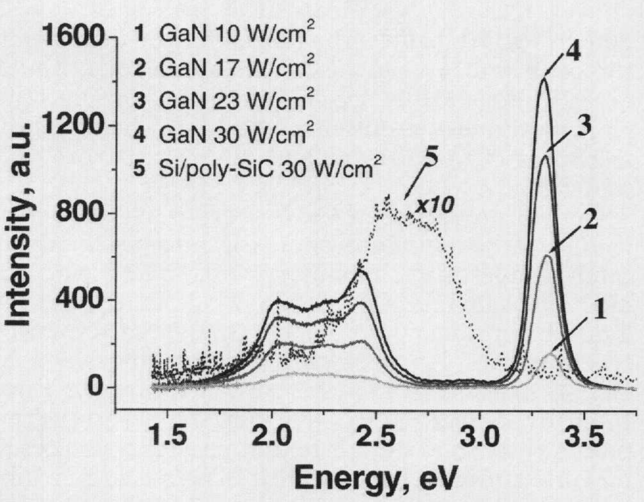

Fig. 4. Room temperature CL of GaN grown on Si/poly-SiC. The symbols 1–4 represent GaN peaks for different excitation power. The spectrum, labeled 5, corresponds to the SiC substrate.

The results of the growth experiments are supported by Raman and x-ray diffraction measurements. Raman measurements were carried out at room temperature using the 488-nm line of an Ar^+ laser. The scattered light was detected in back-scattering geometry of a micro-Raman system, as previously described.[14] Figure 2 shows a typical Raman spectrum of GaN(500 nm)/AlN(40 nm)/Si/poly-SiC sample taken in z (yy) z′ parallel polarization configuration. The most intense bands at 520, 795 and 970 cm^{-1} are from the Si layer. Because the epitaxial layer of GaN is very thin, its modes, E_2 (high) near 566 cm^{-1} and A_1(LO) band near 735 cm^{-1}, are weaker. The presence of these two modes is in good agreement with allowed polarization rules[15] and confirms both the wurtzite structure of the GaN epilayer and the c-axes crystal growth orientation. The observed 4.7 cm^{-1} FWHM for E_2 (high) is comparable to that obtained from bulk GaN, testifying to the high crystal quality.

The position of the E_2 (high) mode is red shifted with respect to the standard value for the bulk GaN. This reflects the presence of tensile biaxial stress in the GaN epilayer. Using the Raman stress factor of -6.2 cm^{-1}/GPa,[16] we obtained the average stress magnitude of 320 MPa. The stress variation across the wafer is ±10%. The 320 MPa tensile stress corresponds to the maximum stress value obtained in the GaN/Si system[10] and is a factor of two lower than the stress in GaN grown by HVPE on 6H-SiC(0001). This stress is below that of the breaking point of 400 MPa, for GaN under tensile stress.[17]

The results of x-ray diffraction studies are shown in Fig. 3a and b. The characteristic width of the x-ray rocking curve of GaN layer (500 nm thick) is in the region of 80 arcsec (ω/2θ scan). These results confirm the high quality of the GaN layers grown on the wafer bonded layer of Si(111) and are similar to those obtained for GaN grown by GSMBE on bulk Si(111) and sapphire.[10,12] Figure 3b plots the x-ray diffraction linewidth, full width at half maximum (FWHM), of the (0002) peak of GaN grown on bulk Si(111) (black squares) and on Si/poly-SiC(circled square), measured as a function of the layer thickness. Figure 3b also shows the FWHM curve calculated for ideal crystalline layers as a function of thickness.[18] A comparison of measured and calculated FWHM shows that our GaN layer grown on Si/poly-SiC is almost completely coherent in the growth direction.

A considerable increase in the FWHM of the thin Si layer, shown in Fig. 3a, was observed after the growth of GaN. The linewidth of the 250 nm thick Si(111) layer was about 180 arcsec, while the FWHM of the Si(111) layer prior to growth of GaN was about

100 arcsec. We believe the reason for the increase in the peak width is plastic deformation of the thin Si layer. This could also account for the relaxation of the GaN layer and elimination of cracking. The optimum thickness of the Si layer and its plasticity are still under study.

Optical properties of GaN layers were characterized by cathodoluminescence (CL) measurements at room temperature. Samples were excited with an electron beam in the range of 1–9 keV, at a current of 1 mA. Excitation power density was changed from 10 to 30 W/cm^2. The resulting spectra are shown in Fig. 4. At the low excitation intensity, curve 1, an intense peak at 3.336 eV (~368 nm) was observed. The peak's position is similar to that previously reported for GaN grown on bulk Si(111).[13] The red shift exhibited with higher excitation intensities is attributed to sample heating. On the other hand, the FWHM of 110 meV is larger than the 40–80 meV observed in samples grown on bulk Si (111).[10,19] This difference may be due to the limited thickness of the GaN layer. Weak emission in the range of 2–2.5 eV was also observed. The relative intensities of the two bands change with the excitation intensity, confirming the deep level nature of the broad emission peak. At the excitation level of ~20 W/cm^2 the intensity of the deep emission level begins to saturate.

In addition to the GaN-related features, we observed, at high incident voltages, a band originating in the SiC substrate. The origin of this band, labeled 5, was confirmed by CL measurement on substrates prior to growth. The presence of SiC-related feature distorts the shape of GaN "yellow" emission band by producing a peak at ~2.4 eV.

In summary, we describe the growth of high quality AlN and GaN on a thin silicon (111) layer wafer bonded to a polycrystalline SiC substrate. Raman measurements show the average stress magnitude of 320 MPa, similar to the values measured in GaN layers grown on bulk Si (111), and about a factor of two lower than the stress in GaN grown on 6H-SiC(0001) by HVPE. X-ray diffraction measurements suggest that the strain is transferred from the epitaxial GaN layer to the thin Si layer bonded to the SiC substrate. Epitaxial layers grown on the composite substrate are completely coherent in the growth direction.

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