

AlGaIn/GaN heterostructures on insulating AlGaIn nucleation layers

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A single temperature process using AlGaIn nucleation layers has been developed that produces device-quality, GaN-based materials with bilayer step surfaces. The AlGaIn nucleation layer is deposited by flow modulation organometallic vapor phase epitaxy at temperatures in excess of 1000 °C, where GaN and AlGaIn films can be subsequently grown. We have optimized this process on both sapphire and SiC substrates, where the conditions for nucleation are found to be quite different. For growth on SiC, aluminum mole fractions ranging from 6% to 35% result in featureless surfaces. Optimizing the alloy composition and thickness of the nucleation layer on SiC allows the deposition of GaN buffer layers exceeding 5 μm without the formation of cracks. A minimum of 15% aluminum in the nucleation layer is required for smooth growth on sapphire substrates. High room temperature two-dimensional electron gas mobilities of 1575 and 1505 cm^2/Vs with sheet charge densities of 1.0×10^{13} and $1.4 \times 10^{13} \text{ cm}^{-2}$ are observed in undoped AlGaIn/GaN structures placed on insulating AlGaIn nucleation layers on sapphire and SiC, respectively. © 1999 American Institute of Physics. [S0003-6951(99)03325-2]

Gallium nitride and related alloys have demonstrated great potential for short-wavelength optical devices¹ and high frequency electronics.² The lack of suitable GaN substrates for homoepitaxy makes the growth of device-quality heterostructures in this material system difficult. Efforts have been directed towards producing nucleation and buffer layers on mismatched substrates such as sapphire and SiC. Hexagonal GaN growth is accomplished by a two-step process consisting of a thin low temperature GaN³ or AlN^{3,4} nucleation layer followed by a thick high-temperature GaN buffer. The high-temperature GaN initially grows three dimensionally as islands which eventually coalesce into a planar thin film. Although the individual GaN islands may be free of defects,⁵ when they coalesce structural and native defects form at the meeting surfaces contributing to a high background free carrier concentration in the range of 10^{16} – 10^{18} cm^{-3} .^{3,6,7} This defect-rich part of the GaN buffer is often thicker than 5000 Å, resulting in excess of 10^{12} cm^{-2} unintentional sheet electron concentrations with low electron mobility. This charge forms a parasitic current path which is not accessible by reasonable gate bias on laterally conducting, high electron mobility transistors (HEMTs).⁸

We have developed a high temperature process using $\text{Al}_x\text{Ga}_{1-x}\text{N}$ films as nucleation layers on both sapphire and SiC which results in insulating buffer layers. This process simplifies the growth by eliminating large temperature ramps, while producing device-quality GaN-based films with low background carrier concentrations ($\leq 10^{13} \text{ cm}^{-3}$). The introduction of aluminum in the high temperature nucleation layer aids in the uniform wetting of the substrates as opposed to three dimensional growth observed at high temperatures with GaN. In this letter, we present the optical and electrical properties of undoped AlGaIn/GaN based HEMT structures grown on insulating AlGaIn nucleation layers.

Undoped AlGaIn/GaN heterostructures were grown on either *c*-plane sapphire or SiC (both 4H semi-insulating and 6H n^+) substrates, by flow modulation organometallic vapor phase epitaxy at 76 Torr.⁹ Substrates were degreased in acetone and methanol, with the SiC additionally cleaned by the RCA method. All substrates were then subjected to a 1100 °C anneal for 10 min under H_2 just prior to growth. Deposition temperatures were monitored by an optical pyrometer and fixed at 1040 °C for sapphire and 1010 °C for SiC. Reactant species used were triethylgallium, trimethylaluminum, and NH_3 with H_2 as the carrier gas.

Both the composition and thickness of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ nucleation layer were separately optimized. It was discovered that a minimum aluminum content in the nucleation layer is required to create sufficient nucleation sites on the substrates to wet the entire surface, resulting in planar growth within several hundred angstroms. Compositions of at least 6% and 15% Al in the solid is required on SiC and sapphire, respectively, to achieve smooth GaN buffer layers. Figure 1 gives a typical atomic force microscopy (AFM) image of a 1- μm -thick GaN buffer layer on SiC, showing atomic steps with a root-mean-square (rms) surface roughness of $\leq 0.30 \text{ nm}$. GaN on sapphire gives similar images with a rms roughness of about 0.35 nm. Threading dislocation densities are estimated from AFM images to be in the mid 10^8 cm^{-2} and low 10^9 cm^{-2} for growth on SiC and sapphire, respectively. Higher Al contents (up to 35%) in the nucleation layer yielded optically smooth GaN buffers on both substrates but produced slightly poorer surface morphologies. In all cases, epitaxial growth on SiC substrates produced smoother surfaces than on sapphire.

Room temperature photoluminescence (PL) measurements of 1- μm -thick GaN buffers deposited with and without optimized Al content in the nucleation layers are shown in Fig. 2. Spectra of structures with optimized nucleation layers (dashed lines) are dominated by near-band edge re-

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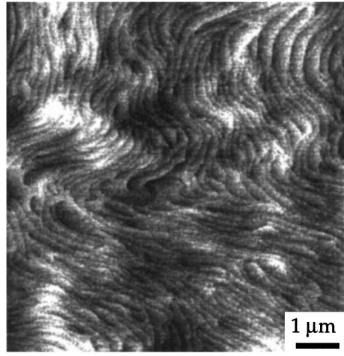


FIG. 1. Plan view AFM image of a 1 μm GaN buffer layer grown on SiC. The AlGa_xN nucleation layer had approximately 6% Al and was 1800 Å thick. The threading dislocation density is determined by counting dark circular features on the surface.

lated luminescence at 364.4 nm [full width at half maximum (FWHM)=32.7 meV] for SiC and 361.8 nm (FWHM=55.5 meV) for sapphire. The insets show spectra of optimized Al_xGa_{1-x}N nucleation layers (1800 Å thick) giving Al content of approximately 6% on SiC and 15% on sapphire. This Al fraction is determined by Vegard's law using a bowing parameter of 1.3 eV¹⁰ and assuming that the nucleation layers are relaxed. GaN layers on top of nucleation layers with Al compositions below the minimum required show higher defect related yellow-band (Y-B) luminescence as seen in Fig. 2 (solid lines). Increased Y-B emission is attributed to three-dimensional GaN growth, resulting from a nonplanar nucleation layer. The extended point of coalescence does not influence the final surface morphology or mobility of the two-dimensional electron gas (2DEG), but results in a buried charge layer.

Capacitance-voltage ($C-V$) profiling provides an effective means of detecting this defective buried charge layer within the GaN buffer. By varying the thickness of the AlGa_xN nucleation layer, the point of coalescence can occur before or after the nucleation layer is terminated. Thinner nucleation layers lead to incomplete coverage of the substrate surface, resulting in three-dimensional GaN growth. To illustrate this, two HEMT structures were grown on sapphire using the Al_{0.15}Ga_{0.85}N nucleation layer, one with a nucleation layer thickness of 150 Å, the other at 300 Å. These structures consist of a 1.6 μm GaN buffer capped with a 300-Å-thick Al_{0.30}Ga_{0.70}N barrier. Figure 3 gives the de-

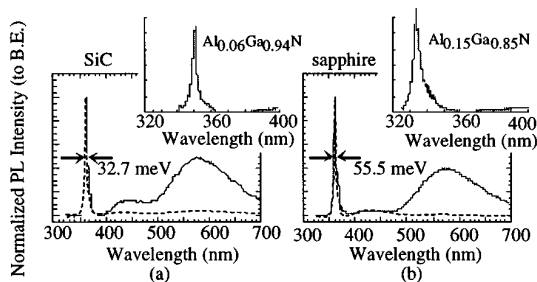


FIG. 2. Room temperature PL measurements of 1- μm -thick GaN epitaxial films with 1800 Å nucleation layers on (a) SiC and (b) sapphire substrates. Solid lines represent growth on nucleation layers below the required Al content. The insets are spectra of the AlGa_xN nucleation layer with the minimum alloy composition needed for growth of smooth epitaxial GaN buffers.

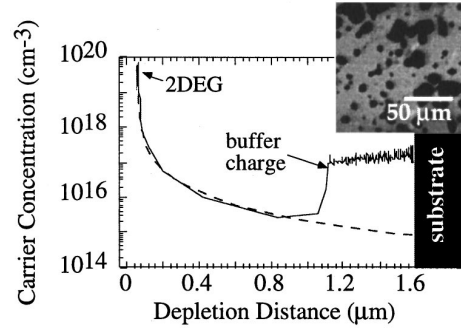


FIG. 3. Carrier concentration profile derived by $C-V$ profiling technique. The solid and dashed lines are of AlGa_xN/GaN HEMT structures grown on a 150- and 300-Å-thick AlGa_xN nucleation layer, respectively. The inset is a micrograph of the GaN surface within the defect rich region close to the nucleation layer.

rived carrier concentration obtained by $C-V$ measurements on these structures. Growth on 150-Å-thick nucleation layer clearly shows a buried charge layer extending approximately 0.5 μm into the GaN layer with a charge density in the low 10^{17} cm^{-3} . The inset shows a Nomarski micrograph of the GaN surface with growth suspended in the charge region where voids appear indicating incomplete coalescence of the film. If the growth is allowed to continue, the film planarizes and becomes atomically smooth. Nucleation layers thicker than 150 Å are coalesced, providing a planar surface in the initial stages of GaN growth and structures which are free of buried charge.

Although thin nucleation layers produce regions of atomically smooth GaN on SiC, large defects originating from surface scratches on the substrates propagate throughout the buffer layer. These defects can be eliminated by increasing the thickness of the nucleation layer to 1800 Å. However, increasing the nucleation layer thickness increases the stress applied to the GaN buffer, resulting in film cracking for nucleation thickness exceeding ≈ 2500 Å. An 1800-Å-thick nucleation layer on SiC resulted in crack-free GaN films exceeded 5.25 μm .

Despite the absence of intentional doping in the HEMT structures, high sheet carrier concentrations ($n_s > 10^{13} \text{ cm}^{-2}$) forming a 2DEG are observed by $C-V$ at the AlGa_xN/GaN interface (Fig. 3). This is a consequence of piezoelectric and spontaneous polarization induced sheet charge σ at the interface.¹¹⁻¹³ For the growth in the (0001) orientation of pseudomorphic Ga-face AlGa_xN/GaN heterostructures, there will be a spontaneous polarization present in the wurtzite AlGa_xN and GaN layer and an additional piezoelectric polarization in the strained AlGa_xN barrier. The different polarizations in the AlGa_xN barrier and the GaN buffer will cause a positive sheet charge $+\sigma$ at the Al_xGa_{1-x}N/GaN interface.^{11,12,14} Electrons compensate the polarization induced sheet charge by forming a 2DEG with a maximum sheet carrier concentration that can be calculated by¹¹

$$n_s = \frac{\sigma}{q} - \left[\frac{\epsilon(x)}{q^2 d} \right] (q\phi_b + E_F - \Delta E_C), \quad (1)$$

where $\epsilon(x)$ is the dielectric constant of Al_xGa_{1-x}N, d is the width of the barrier, $q\phi_b$ is the Schottky barrier of the gate contact (for $x=0.3$, $q\phi_b \approx 1.4 \text{ eV}$), and $E_F - \Delta E_C$ is the en-

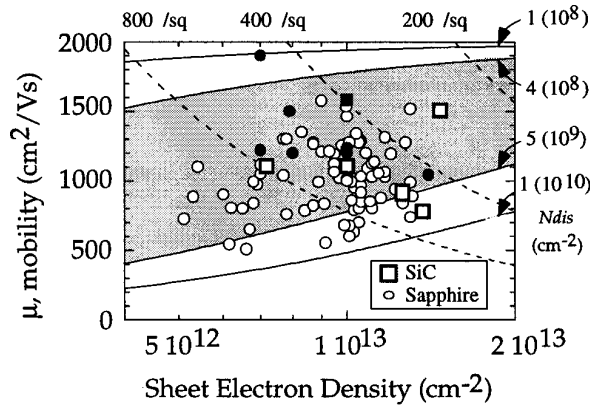


FIG. 4. Mobility vs 2DEG sheet carrier densities of AlGaIn/GaN heterostructures grown on SiC and sapphire substrates. Solid lines are defect density (cm^{-2}) contours and dashed lines are channel sheet resistivity contours.

ergy difference between the Fermi level and the conduction band offset (for $x=0.3$, $E_F - \Delta E_C \approx 0.5 \text{ eV}$).¹³ For $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$ HEMT structures we determine the positive polarization induced sheet charge and the maximum sheet carrier concentration of the 2DEG to be $1.67 \times 10^{13} \text{ cm}^{-2}$ and $1.51 \times 10^{13} \text{ cm}^{-2}$, respectively, without surface depletion. The calculated results are in good agreement with the sheet carrier concentrations of 1.1×10^{13} and $1.4 \times 10^{13} \text{ cm}^{-2}$ observed by C - V profiling for structures grown on sapphire and SiC, respectively.

The electron mobility in n -type GaN has been shown¹⁵ to be strongly dependent on the density of threading dislocations, which charge up and deplete nearby carriers. In the case of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures the mobility of the electrons in the 2DEG can be estimated analytically, assuming scattering from dislocations dominate along with the scattering by longitudinal polar optical phonons. In such a two-dimensional system, the scattering from the charged threading dislocations (and any ions) depends linearly on the average energy of the electrons being scattered. The scattering due to longitudinal polar optical phonons and piezoelectric effects predicts room-temperature mobility of around $2000 \text{ cm}^2/\text{Vs}$ for electrons confined near the AlGaIn/GaN interface.¹⁶ A measured room temperature value of electron mobility of $802 \text{ cm}^2/\text{Vs}$ occurs for a dislocation density of $5 \times 10^9 \text{ cm}^{-2}$ and a 2DEG density of $1.0 \times 10^{13} \text{ cm}^{-2}$. An ideal mobility contribution from the charged dislocations is $1339 \text{ cm}^2/\text{Vs}$ for $5 \times 10^9 \text{ cm}^{-2}$ dislocations at a sheet charge density of $1.0 \times 10^{13} \text{ cm}^{-2}$. Thus the room temperature mobility of a 2DEG in this undoped $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$ HEMT can be plotted, as shown by the solid lines in Fig. 4, from:

$$\frac{1}{\mu_{n\text{DEG}}} \approx \frac{1}{2000} + \frac{1}{\mu_{\text{dis}}}, \quad (2)$$

$$\mu_{\text{dis}} = 1339 \frac{\text{cm}^2}{\text{Vs}} \left(\frac{n_s}{1.0 \times 10^{13} \text{ cm}^{-2}} \right) \left(\frac{5 \times 10^9 \text{ cm}^{-2}}{N_{\text{dis}}} \right),$$

where n_s is the 2DEG density and N_{dis} is the dislocation density determined from AFM studies. The range of disloca-

tion defect densities from our AFM is shown by the shaded region. Data from our structures are plotted with open squares (Si-face SiC), and open circles (sapphire). Room temperature mobilities as high as $1505 \text{ cm}^2/\text{Vs}$ with a 2DEG sheet carrier density of $1.4 \times 10^{13} \text{ cm}^{-2}$ were measured on SiC, and $1575 \text{ cm}^2/\text{Vs}$ with a sheet carrier density of $1.1 \times 10^{13} \text{ cm}^{-2}$ on sapphire. The lower than expected mobility on SiC is attributed to both a high density of large point defects ($\approx 200 \text{ cm}^{-2}$) originating from the substrates and propagating throughout the epitaxial layers, and interface roughness in the higher 2DEG density case.^{13,16} Low channel sheet resistances of $275 \Omega/\text{square}$ on SiC and $325 \Omega/\text{square}$ on sapphire were measured.

In summary, we have grown insulating AlGaIn nucleation layers and GaN buffer layers at high temperatures on SiC and sapphire substrates. A simplified growth process produces device quality AlGaIn/GaN heterostructures with low free carrier concentrations in the GaN buffer layer on both substrates. By optimization of the alloy composition and the thickness of the nucleation layer, we have achieved low sheet resistances of $275 \Omega/\text{square}$, and $325 \Omega/\text{square}$ in undoped AlGaIn/GaN HEMT structures with sheet charge densities of 1.4×10^{13} and $1.1 \times 10^{13} \text{ cm}^{-2}$ on SiC and sapphire substrates, respectively.

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