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Citation: J. Vac. Sci. Technol. B 16, 1275 (1998); doi: 10.1116/1.590087
View online: http://dx.doi.org/10.1116/1.590087
View Table of Contents: http://avspublications.org/resource/1/JVTBD9/v16/i3
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High mobility AlGaN/GaN heterostructures grown by gas-source molecular beam epitaxy

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(Received 22 December 1997; accepted 1 January 1998)

We report on the growth of high electron mobility AlGaN/GaN heterostructures on sapphire substrates by gas-source molecular beam epitaxy (GSMBE) using ammonia as the nitrogen source. Improvements in structural, electrical, and optical properties of GaN and AlGaN layers have been made to achieve this goal. For the growth of AlGaN layers, the reflection high-energy electron diffraction revealed a twofold surface reconstruction, indicative of atomic smoothness of the film surface. High mobility two-dimensional electron gas has been achieved in both unintentionally doped (by piezoelectric effect induced by lattice mismatch strain) and modulation doped AlGaN/GaAs heterostructures. The modulation-doped $n^+ - Al_{0.2}Ga_{0.8}N/1 - GaN$ heterojunction exhibited electron mobilities as high as 750 and 4070 cm$^2$/V s at 300 and 77 K, respectively. Both values are the highest ever reported for the AlGaN/GaN heterostructures grown by MBE techniques. © 1998 American Vacuum Society. [S0734-211X(98)06603-7]

I. INTRODUCTION

(Al, Ga)N is an ideal material system for both ultraviolet (UV) optical devices and high-power, high-temperature electronic devices due to its wide direct band gap tunable from 3.4 to 6.2 eV and high electron saturation velocities. In particular, with a small lattice mismatch and large band offset between AlGaN and GaN, the AlGaN/GaN heterostructure is suitable for developing heterojunction devices with improved performance. There have been numerous studies on growth of AlGaN/GaN heterostructures by metalorganic chemical vapor deposition (MOCVD)\textsuperscript{1,2} and molecular beam epitaxy (MBE),\textsuperscript{3} and two-dimensional electron gas (2DEG)\textsuperscript{4,5} and field-effect transistors (HFETs)\textsuperscript{6} were recently demonstrated. However, all of the AlGaN/GaN heterostructures with highest electron mobilities reported to date were grown by MOCVD and previous efforts on growth of similar structures using MBE were less successful, resulting in much lower 2DEG electron mobilities\textsuperscript{7} compared to those grown by MOCVD.

In this article, we report on the growth of high mobility AlGaN/GaN heterostructures on sapphire by gas-source MBE (GSMBE) using ammonia as the nitrogen source. The 2DEG in modulation-doped $n^+ - Al_{0.2}Ga_{0.8}N/i - GaN$ heterojunctions exhibited electron mobilities as high as 750 and 4070 cm$^2$/V s at 300 and 77 K, respectively. Both values are the highest ever reported for the AlGaN/GaN heterostructures grown by MBE techniques, and are comparable to the results reported for similar structures grown by MOCVD on sapphire substrates.

II. EXPERIMENTAL PROCEDURES AND RESULTS

The growth of the AlGaN/GaN heterostructures was performed in a Varian GEN-II MBE system equipped with an ammonia gas injector. Detailed system configuration has been previously reported.\textsuperscript{8,9} In this study, AlGaN/GaN heterojunctions were grown on highly resistive undoped buffer GaN layers 2–3 μm thick. The film quality of the undoped GaN buffer layers was found to play a key role in achieving high mobility 2DEG. The growth conditions for the GaN buffer layers were optimized: growth temperatures around 800 °C with growth rates around 1 μm/h. High ammonia flow rates of 40–70 sccm were used and found instrumental to reduce the level of unintentional $n$-type doping generated by nitrogen vacancies. GaN films with significantly improved overall quality in structural, electrical, and optical properties have been achieved. Figure 1 shows the photoluminescence (PL) spectrum at 10 K for a typical high-quality GaN film. The FWHM of the main peak at 3.478 eV, which is attributed to the neutral-donor-bound exciton ($D^0X$), was as narrow as 3.8 meV, whereas in the higher energy region a free A exciton peak at 3.483 eV was clearly observed; the yellow band emission was also absent in our samples. From van der Pauw Hall measurements, the as-grown undoped GaN films exhibited a resistivity of larger than 10$^3$ Ω cm with an electron mobility of 150 cm$^2$/V s and a doping level of 1 × 10$^{17}$ cm$^{-3}$. The FWHM of the x-ray diffraction rocking curve of the as-grown GaN films was as narrow as 101 arcsec for the symmetric (002) and 104 arcsec for the asymmetric (102) directions, respectively, indicative of the high structural quality of the films.

Undoped ternary AlGaN layers of typically 2000 Å thick were also studied. C-plane sapphire substrates were used for the growth, and the standard two-step deposition method was followed.\textsuperscript{10} A thin AlN nucleation layer of 200–300 Å was first deposited at 500 °C and then the substrate temperature was increased to high temperatures for the growth of the main layers. AlGaN was either directly deposited on the low-temperature-grown AlN buffer or on a 1 μm thick GaN layer. The AlGaN was grown at 800 °C at a growth rate of...
0.7 μm per hour. An NH₃ flow rate of 50 sccm was used, ensuring a N-rich condition. The Al beam flux was varied between $8 \times 10^{-8}$ and $2 \times 10^{-7}$ Torr for various Al compositions. The RHEED showed a very streaky (1 × 1) pattern during the growth of AlGaN, indicating a smooth layer-by-layer two-dimensional growth mode. As the substrate temperature was lowered to below 500 °C after the growth, a sharp 2 × RHEED reconstruction pattern was clearly observed along the $(\overline{1}1\overline{2}0)$ azimuth, as shown in Fig. 2. We believe it was a result of the changed surface structure corresponding to increased group V coverage. This is the first observation of twofold surface reconstruction for AlGaN growth. The morphology of as-grown AlGaN films was examined by Nomarski microscopy and scanning electron microscopy (SEM). The films exhibited a mirror-like featureless morphology without cracks or textured patterns. The structural properties of the AlGaN films were characterized by x-ray diffraction. Figure 3 shows the (0002) plane x-ray rocking curve of an AlGaN/GaN heterostructure with 2000 Å AlGaN grown on a 2 μm GaN layer. It can be seen that the diffraction peaks for both AlGaN and GaN are well resolved, and the FWHMs of the peaks are as narrow as 95 and 120 arcsec for GaN and AlGaN, respectively, indicating the high structural quality of the AlGaN/GaN heterostructure.

With the capability of growing high-quality GaN and AlGaN, undoped and modulation-doped AlGaN/GaN heterostructures were grown on a high-quality highly resistive undoped GaN layers. First, thin AlGaN layers of 300 Å were deposited on GaN buffer layers of different thickness, from 0.5 to 3 μm, to investigate the effects of the underlying GaN buffer layers. It was revealed that the undoped GaN buffer layers had to be above a certain thickness to obtain high mobility 2DEG in AlGaN/GaN heterostructures. This observation can be explained by the reduced threading dislocation density near the AlGaN-GaN interface with increased thickness of the GaN buffer layers. In the present work, a GaN thickness of at least 2 μm was found to be necessary. The Al composition of AlGaN was calibrated by Vegard’s law from x-ray diffraction data. In the 2DEG study described below, an Al composition of $x = 0.2$ was chosen for all AlGaN layers. The AlGaN/GaN heterostructures consisted of an undoped $i$-GaN layer of 2–3 μm, followed by a 250 Å AlGaN layer, either undoped or doped with Si to a level of $2 \times 10^{18}$ to $6 \times 10^{18}$ cm⁻³. An undoped AlGaN spacer layer of 30–80 Å was inserted between the $i$-GaN and the $n^+$-AlGaN for the latter case. Van der Pauw Hall measurements were performed at 300 and 77 K to characterize the electrical properties of the as-grown samples. We have studied ohmic contacts to both $n$- and $p$-type GaN. Indium makes excellent practical ohmic contacts to both $n$-type and $p$-type GaN with linear $I–V$ characteristics and thus apparently without significant barriers to carrier transport. The detail mechanisms are not completely understood yet. This indicates that for routine sample characterizations using van...
under Pauw Hall measurements, the complicated procedures of evaporating Al on n-type and Au on p-type GaN as ohmic contacts are not necessary. In this study, In dots were soldered to the surface of the as-grown samples to make ohmic contacts for measurements. For the undoped AlGaN/GaN sample, an electron mobility of 583 cm$^2$/V·s was found at room temperature, and 2070 cm$^2$/V·s at 77 K. These enhanced mobilities, compared to those for bulk GaN, were clear indications of 2DEG. We have previously reported an observation of the 2DEG generated by the strain-induced piezoelectric field in a similar AlGaAs/GaAs/InGaAs system,12 with which our effect is expected to play a more important role in the formation of 2DEG in the AlGaN/GaN system,13 with which our experiments exhibit good agreement. For modulation-doped samples, the 2DEG mobility was 753 cm$^2$/V·s at room temperature and 4070 cm$^2$/V·s at 77 K. Figure 4 shows the temperature-dependent Hall mobility and sheet carrier density for the modulation-doped sample. Electron mobilities reach 4070 cm$^2$/V·s and became constant at temperatures below 100 K, clearly indicating the existence of a 2DEG. Our results represent the highest reported 2DEG mobilities for AlGaN/GaN heterostructures grown by MBE techniques. These mobility values are comparable to the best published data for the 2DEG in AlGaN/GaN grown on sapphire by MOCVD.4,5 The sheet carrier density of these samples was in the range $1 \times 10^{13} \text{--} 4 \times 10^{13}$ cm$^{-2}$, depending on such structure parameters as the doping level of the AlGaN barrier and the thickness of spacer layer.

III. SUMMARY

High electron mobility AlGaN/GaN heterostructures have been grown on sapphire substrates by GSMBE using ammonia as the nitrogen source. Significant improvements in structural, electrical, and optical properties for GaN and AlGaN layers have been made to achieve this goal. For the AlGaN growth, a 2 $\times$ RHEED reconstruction pattern was observed for the first time, indicative of an atomically smooth surface of the layer. A 2DEG has been observed in both unintentionally doped and modulation-doped AlGaN/GaN heterostructures. The modulation-doped $n$ + -Al$_{0.2}$Ga$_{0.8}$N/−-GaN heterojunctions exhibited electron mobilities as high as 750 and 4070 cm$^2$/V·s at 300 and 77 K, respectively. Both values are the highest ever reported for AlGaN/GaN heterostructures grown by MBE techniques.

ACKNOWLEDGMENTS

The work of L.K.L., J.A., and W.I.W. was supported by DARPA (Dr. Anis Husain) and ONR (Dr. Colin Wood and Max Yoder). The work of D.C.L. and D.C.R. was performed at the Avionics Directorate, Wright Laboratory, Wright-Pattson AFB under Contract No. F33615-95-C-1619.