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Lattice and Energy Band Engineering in AlInGaN/Ga Heterostructures

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Lattice and energy band engineering in AlInGaN/GaN heterostructures

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We report on structural, optical, and electrical properties of $\text{Al}_x\text{In}_y\text{Ga}_{1-x-y}\text{N}/\text{GaN}$ heterostructures grown on sapphire and 6H-SiC substrates. Our results demonstrate that incorporation of In reduces the lattice mismatch, Δa , between AlInGaN and GaN, and that an In to Al ratio of close to 1:5 results in nearly strain-free heterostructures. The observed reduction in band gap, ΔE_g , determined from photoluminescence measurements, is more than 1.5 times higher than estimated from the linear dependencies of Δa and ΔE_g on the In molar fraction. The incorporation of In and resulting changes in the built-in strain in AlInGaN/GaN heterostructures strongly affect the transport properties of the two-dimensional electron gas at the heterointerface. The obtained results demonstrate the potential of strain energy band engineering for GaN-based electronic applications. © 2000 American Institute of Physics. [S0003-6951(00)03909-7]

The past two years have witnessed impressive progress in the development of AlGaIn/GaN materials and devices for high-power, high-temperature applications. Record microwave power of 6.8 W/mm,¹ as well as high-temperature^{2,3} and low-noise performance⁴ of AlGaIn/GaN heterostructure field effect transistors (HFETs) have been demonstrated. The combination of superior electron transport in GaN⁵ with excellent thermal properties of SiC provides the key to enhanced current-carrying capability⁶ and reduced self-heating effects⁷ in GaN-based devices. However, the microwave power levels achieved are still far below what is expected from dc performance of GaN-based devices.

Further improvement of group III-N HFETs can be expected by increasing the Al molar fraction in the AlGaIn barrier layer. This increase should result in larger band offset and higher polarization charge (pyroelectric and piezoelectric) at the heterointerface and, thus, higher current-carrying capability of the devices. However, the development of high Al content AlGaIn/GaN HFETs is limited by fundamental properties of the system. The large lattice mismatch in a high x -value $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure decreases the critical thickness of a fully strained AlGaIn barrier, and results in uncontrolled local strain relaxation at the heterointerface via generation of misfit dislocations and cracks. These invariably degrade two-dimensional (2D) electron transport and increase noise. Therefore, the new approaches in developing

high Al molar fraction HFETs are necessary.

Recently, McIntosh and co-workers demonstrated the growth of AlInGaIn single layers on sapphire substrates.^{8,9} Use of this quaternary material should allow almost independent control of the lattice mismatch (and, as a consequence, “piezoelectric doping”^{10,11}) and the band offset in AlInGaIn-based heterostructures. This new heterostructure design should allow a significant increase of Al molar fraction in AlInGaIn barrier. Due to lattice matching, this design should also allow for keeping the built-in strain below the critical value for uncontrolled strain relaxation thereby increasing the critical thickness of the AlInGaIn barrier.

In this letter we report on the growth and characterization of structural, optical and electrical properties of AlInGaIn/GaN heterostructures over sapphire and SiC substrates. The epilayer structures used in this study were deposited on sapphire and n -type 6H-SiC substrates by low-pressure metalorganic chemical vapor depositor (MOCVD). The deposition of 0.2 μm of GaN on (0001) sapphire was followed by the growth of 0.2 μm of AlInGaIn. On SiC substrates, the growth of 100 nm of high-temperature AlN buffer was followed by the deposition of approximately 0.5 μm thick semi-insulating GaN, capped with a quaternary Al-InGaIn layer. In either case, the GaN layer was deposited using trimethylindium as a surfactant during growths.

The different In incorporation in our structures was

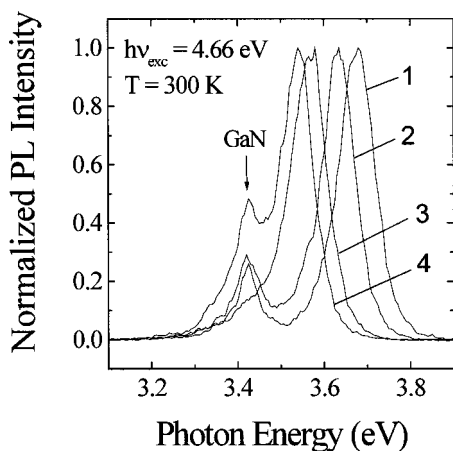


FIG. 1. Normalized room temperature photoluminescence spectra of AlInGaN with 9% of Al on GaN. Curve 1 corresponds to zero In flow, 2—25; 3—50; 4—75.

achieved by keeping constant triethylgallium (TEA) and triethylaluminum (TEG) fluxes and varying the flux of trimethylindium (TMI). The secondary ion mass spectrometry (SIMS) spectra exhibited an abrupt drop in In concentration near AlInGaN and GaN heterointerface. X-ray microanalysis of the samples showed that Al/Ga molar fraction in AlInGaN layers remained nearly constant. However, the In/Al and In/Ga mole fractions increased almost linearly with the TMI flux. We thus believe that under our growth conditions, In atoms replaced both Al and Ga atoms, proportionally, in the quaternary compound. The reflection high energy electron diffraction (RHEED) spectra indicated that all AlInGaN layers had a single crystal wurtzite structure.

In order to determine the In molar fraction and the energy band gap in AlInGaN, we measured PL and x-ray diffraction (XRD) for AlInGaN/GaN structures grown on sapphire substrates. The thickness of the top AlInGaN layer was 0.2 μm. The molar fraction of Al in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ and the band gap change in AlInGaN/GaN heterostructures with different In incorporation were extracted from the PL measurements using the fourth harmonic of YAG:Nd³⁺ laser (wavelength $\lambda = 266$ nm, pulse width $\tau = 10$ ns). Figure 1(a) shows the room temperature PL spectra for one set of AlInGaN/GaN heterostructures grown under TMI flux from zero (pure AlGaIn) to approximately 13 μmol/min. All four spectra had a sharp maximum at 3.42 eV associated with the GaN buffer layer, which was used as a reference. The PL spectra at zero In flow exhibited a maximum at 3.68 eV. The corresponding Al molar fraction in AlGaIn layer for this set of samples was approximately 9%. The incorporation of In resulted in a red shift of the PL peak by approximately 130 meV corresponding to a reduction of the band gap difference between AlInGaN and GaN from 260 meV (In=0) to 130 meV (In flow 13 μmol/min). A similar reduction of the band gap under the same In flow conditions was measured in AlInGaN/GaN heterostructures grown with 17% Al.

The lattice matching in AlInGaN/GaN heterostructures with different In incorporation was studied by measuring (0006) peaks from AlInGaN and GaN in the Θ -2 Θ x-ray diffraction spectra. The data for AlInGaN/GaN heterostructures with 9% of Al are shown in Fig. 2. The spectra have two double peaks corresponding to AlInGaN and GaN, re-

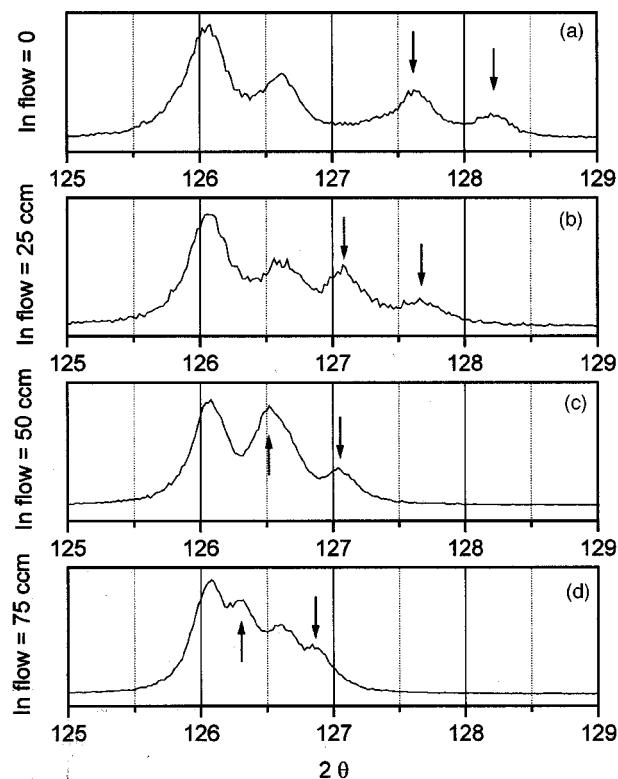


FIG. 2. Θ -2 Θ x-ray spectra of (0006) GaN and (0006) AlInGaN with 9% Al, deposited at different flow of In: (a) corresponds to zero In flow, (b) 25; (c) 50; (d) 75. Arrows mark peaks corresponding to AlInGaN layers with different In content. The other two peaks do not depend on In incorporation and correspond to GaN buffer. Samples were grown on (0001) sapphire substrates.

sulting from the $K\alpha_1$ and $K\alpha_2$ lines of the x-ray source. With an increase in In flow, the AlInGaN peaks shifted toward (and even exchanged positions with) the peaks corresponding to the GaN buffer. The measured data illustrate that AlInGaN with 9% Al and about 1.8% of In is closely lattice matched to GaN. We believe that AlInGaN layer is fully relaxed at low In fractions since the thickness of the layer is well above the critical value. At high In concentration the structure is practically unstrained due to lattice matching. Thus we speculate that all the XRD results correspond to relaxed structures. The measured peak shift was used for calculation of the lattice constant of a quaternary AlInGaN layer. The In incorporation was then estimated using the linear dependence of the lattice constant on In molar fraction extracted from XRD results under the assumption of fully relaxed quaternary layer. Figure 3 summarizes the data on lattice mismatch and energy band gap in AlInGaN/GaN heterostructures obtained from the PL and XRD measurements. As seen from Fig. 3(a), the reduction in lattice constant due to the incorporation of up to 1.8% In is nearly the same for AlInGaN layers with 9% and 17% Al. The lattice constant of AlInGaN with 17% Al and approximately 1.5% In closely matches the lattice constant of In-free AlGaIn with 9% Al. The estimated In to Al ratio for a close lattice match is about to 1:5, which is in good agreement with the expectations based upon Vegard's law. However, the band-gap reduction is significantly larger than expected from the same theoretical model. We speculate that the disagreement between experiment and theory may be caused by either more compli-

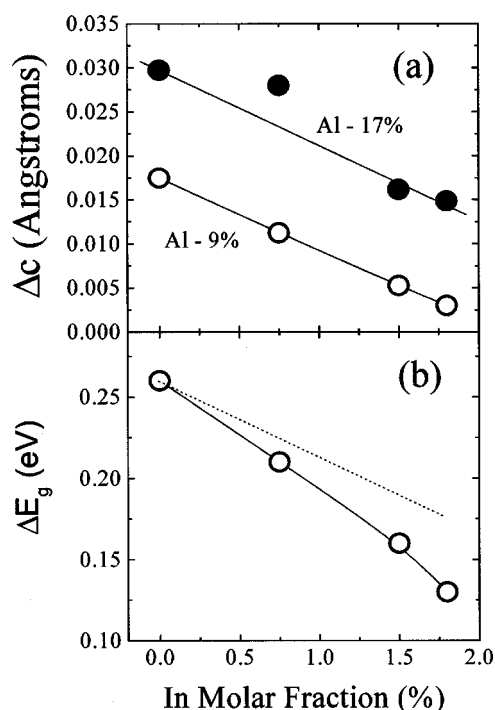


FIG. 3. (a) Lattice mismatch in AlInGaN/GaN with 9% of Al (open circles) and 17% of Al (solid dots) vs In molar fraction; (b) energy band-offset in AlInGaN/GaN with different In content. Dashed line shows calculated band-offset dependence assuming that In replaces Al in the AlInGaN layer.

cated AlInGaN band gap dependence on In molar fraction or by the fluctuations of In content near the layer surface, which does not change the x-ray data but strongly affects PL spectra. Also, the peak positions of PL spectra are known to demonstrate a significant shift with respect to the actual band gap; thus the band gap reduction deduced from PL measurement might be not accurate enough. The results of more detailed experiments to establish the actual band gap–In fraction dependence, such as PL excitation measurements, will be published elsewhere.

The incorporation of In changes the electrical characteristics of AlInGaN/GaN heterostructures. The effect of AlInGaN barriers on the structural and transport properties of HFET structures was investigated further for barrier thickness ranging from 14 to 17 nm. Figure 4 shows cross-section transmission electron micrographs (TEMs) of AlInGaN–GaN heterostructures with 9% Al and 1.8% In in the barrier layer. From the TEM data, we conclude that the nearly lattice-matched quaternary AlInGaN layer is of high crystallinity. The interface was atomically smooth and abrupt to within a monolayer. Addition of In to the barrier layer did not result in the generation of any new defects at the heterointerface. From the cross-section electron micrographs the thickness and hence, growth rate of the AlInGaN barrier layers were determined. The results obtained showed that the addition of up to 1.8% indium reduced the AlInGaN growth rate by approximately 15%–20%.

The transport properties of electron 2D gas at the AlInGaN/GaN interface were studied in.¹⁰ It was found that both sheet carrier density and electron mobility depend strongly on band offset and polarization at the heterointerface, and hence, on the In composition in the barrier. From

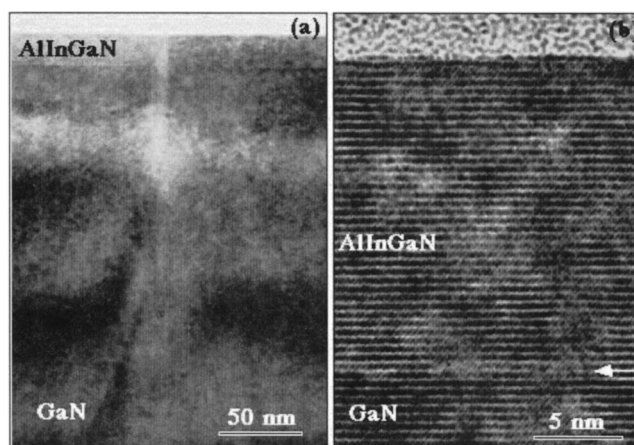


FIG. 4. Cross section electron micrographs for AlInGaN–GaN heterostructure with 15% Al and 2.8% In, grown on 6H–SiO substrate.

the comparative study of sheet carrier density and electron mobility in strained AlGaIn/GaN and nearly strain-free AlInGaIn/GaN heterostructures we estimate the contribution of spontaneous polarization and piezoelectric doping to be of the order of $5 \times 10^{12} \text{ cm}^{-2}$ for the AlGaIn barrier with 15% Al.

In conclusion, we demonstrated the potential of In-based strain energy band engineering in AlInGaIn/GaN heterostructures. Our data show that by incorporating In we can vary the energy band structure and built-in strain in the structures, which strongly affect 2D electron characteristics near AlInGaIn/GaN heterointerface. This approach should enable us to significantly increase the sheet carrier density in high power AlInGaIn/GaN HFETs and restrict the built-in strain below the critical values in order to prevent the degradation of device characteristics.

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