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Lattice and Energy Band Engineering in AlInGaN/Ga Heterostructures

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The past two years have witnessed impressive progress in the development of AlGaN/GaN materials and devices for high-power, high-temperature applications. Record microwave power of 6.8 W/mm, as well as high-temperature and low-noise performance of AlGaN/GaN heterostructure field effect transistors (HFETs) have been demonstrated. The combination of superior electron transport in GaN with enhanced current-carrying capability and reduced self-heating effects 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 AlGaN 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 AlGaN/GaN HFETs is limited by fundamental properties of the system. The large lattice mismatch in a high x-value Al$_x$Ga$_{1-x}$N/GaN heterostructure decreases the critical thickness of a fully strained AlGaN 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 AlInGaN single layers on sapphire substrates. Use of this quaternary material should allow almost independent control of the lattice mismatch (and, as a consequence, “piezoelectric doping”) and the band offset in AlInGaN-based heterostructures. This new heterostructure design should allow a significant increase of Al molar fraction in AlInGaN 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 AlInGaN barrier.

In this letter we report on the growth and characterization of structural, optical and electrical properties of AlInGaInN/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 AlInGaN. 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-In-GaN layer. In either case, the GaN layer was deposited using trimethylindium as a surfactant during growths.

The different In incorporation in our structures was...
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 $0.2\mu m$. The molar fraction of Al in Al$_x$Ga$_{1-x}$N/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:Nd$^{3+}$ 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 AlGaN) to approximately $13 \mu$mol/min. All four spectra had a sharp maximum at 3.42 eV associated with the GaN buffer. The measured data illustrate that AlInGaN layers 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. Therefore 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 assuming that the 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 9% Al and approximately 1.5% In closely matches the lattice constant of In-free AlGaN with 9% Al. The estimated In to Al ratio for a close lattice match is about 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-

![Graph](image-url)
The transport properties of electron 2D gas at the AlInGaN/GaN interface were studied in. 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 the comparative study of sheet carrier density and electron mobility in strained AlGaN/GaN and nearly strain-free AlInGaN/GaN heterostructures we estimate the contribution of spontaneous polarization and piezoelectric doping to be of the order of $5 \times 10^{12}$ cm$^{-2}$ for the AlGaN barrier with 15% Al.

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