3.1 Publishable summary

3.1.1 Project description and objectives

Gallium nitride is a key material for our modern society. It is used in the highest performing light emitting diodes (LEDs) and in power electronics. A reduction in total electricity use, and thus CO_2 emissions, of 10% -15% associated with lighting and a further 10% associated with power electronics is possible with the widespread introduction of GaN technologies. The factors that need to be overcome in order to accelerate the widespread uptake of LEDs are in providing high quality light with a colour balance from the luminaire which is attractive to the consumer while delivering the light at an acceptable cost, and by further improving the conversion efficiency. While great inroads have been made, the LEDs currently on the market suffer from a reduction in their efficiency at higher currents, called droop, thus limiting the total amount of power from a single chip. Furthermore, the colour can change as a function of current and age as the white light is obtained using a down-converting phosphor leading to an energy loss. Therefore, a combination of colours including direct yellow emission would be desirable for higher efficiency and colour control. A solution to these issues can be obtained by basing the LEDs on semi-polar planes where there is a reduction of the polarization fields. However, the necessary semi-polar substrates are difficult to engineer resulting in them being costly and having limited wafer size.

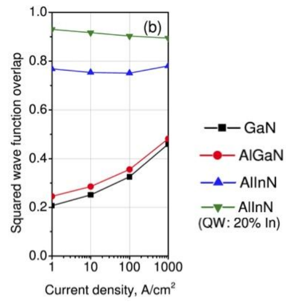
The ALIGHT project has assembled a consortium to investigate new approaches to large area of up to 100 mm diameter wafer, low defect density, semi-polar (11-22) GaN substrate technologies based on structured r-plane (10-12) sapphire and structured (113) silicon substrates. This required fundamental modelling of the surface chemistry. Extensive work is taking place on growth processes along with detailed material characterisation. Using these template substrates, highly efficient blue and yellow light emitters are being designed and the epitaxial processes developed. This work is supported by a thorough fundamental investigation of the composition dependent properties of InAlGaN materials.

The major material challenges are in the details of the patterning of the wafer structures, achieving growth processes for the generation and coalescence of semi-polar planes while obtain low stacking fault density (BSFs $<10^5$/cm) and low dislocation density (TDDs$\sim10^6$/cm^2). To address this, the influence of substrate fine orientation and growth parameters have been investigated and their influence assessed by detailed X-ray measurements, luminescence and atomic scale imaging. Scaling of the substrates is being addressed by both Metal-Organic Vapour Phase Epitaxy (MOVPE) and Hydride VPE (HVPE) techniques. Quantum wells were utilised as the active light emitting material and the spatial distribution of emission is assessed by detailed microscopy.

3.1.2 Description of work and key results

Modelling of AlInGaN materials and devices

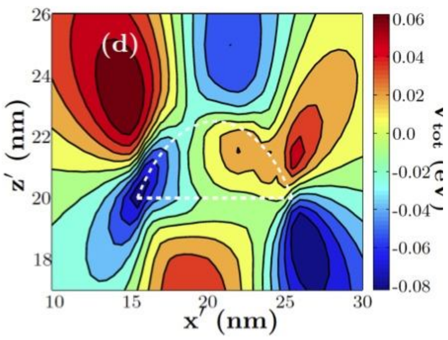
The bandgaps of AlInGaN alloys were studied at a fundamental level and a deep understanding of their properties was obtained. We showed that the incorporation of indium has an important role in creating localised states which strongly perturb the band structure leading to the breakdown of the virtual crystal approximation. Using the localized states in the conduction and the valence bands of AlInN for low In content leads to an accurate description of the composition dependent bandgap. The bandgap, valence and conduction band-offsets, and strain dependence of the AlInGaN alloys were incorporated into a commercial drift-diffusion software allowing us to design novel quantum well LED structures on semipolar planes. Particularly, we could compare the wave function overlap as a function of current density for c-plane, non-polar and different semi-polar planes and show how to compensate the residual build in field in (11-22) quantum wells.



Semipolar $In_{0.17}Ga_{0.83}N$-based LED designed for blue emission (450 nm): Calculated ground state electron and hole wavefunction overlap for structures containing GaN, AlGaN and AlInN barriers.

Modelling of quantum dot emission on (11-22)

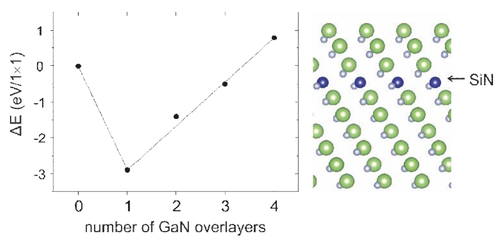
A detailed theoretical analysis of the electrostatic built-in field and the electronic structure of polar and semi-polar dot-in-a-well system was carried out based on a multi-band $k \cdot p$ model parameterized by the incline angle to the wurtzite c-axis, that accounts fully for the three-dimensional quantum dot structure. The built-in fields in isolated (11-22) quantum dots are strongly reduced compared to an equivalent c-plane structure. The electron and hole ground state wave-function overlap is larger in the (11-22) dot-in-a-well systems when compared with its polar counterpart. By increasing the InN content in the quantum dot up to a critical value leads to an increase in the ground state electron and hole wave-function overlap which can be attributed to changes in the built-in potential profile inside the (11-22) quantum dot. Such quantum dots could be efficient yellow emitters.



Built-in potential V_{tot} in a semipolar (11-22) InGaN quantum dot. V_{tot} is shown for a slice through the centre of the structure

Modelling of the effect of a Si layer on (11-22) GaN surfaces

A highly doped silicon nitride interlayer is very important in the growth of (0001) GaN due to its anti-surfactant behaviour where it blocks the growth and leads to rougher surfaces. This effect is in turn exploited during epitaxial lateral overgrowth to reduce the density of extended defects. We investigated the atomistic mechanisms underlying the anti-surfactant behaviour of Si in the growth of (0001) GaN surfaces, and we performed calculations on the effect of Si on (11-22) GaN surfaces. Based on Density Functional Theory (DFT) calculation of the total energy and forces we derived the phase diagram of these surfaces under the influence of Si

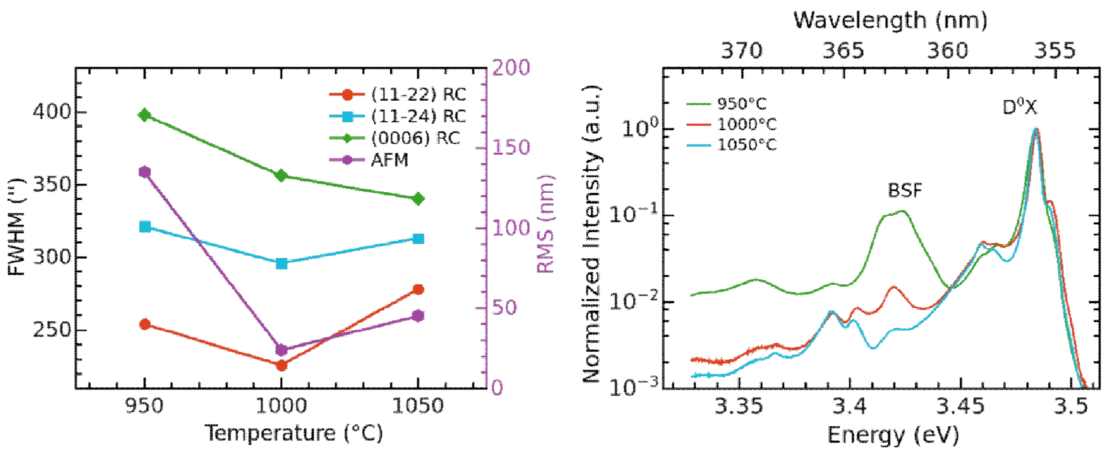


Right: Surface energies versus number of GaN layers grown above the SiN layer. The energies are referenced with respect to the SiN terminated surface. The dashed line is a guide for the eye. Left: Schematic ball and stick representation of a SiN layer with 3 GaN overlayers. Green, blue, and gray balls indicate Ga, Si, and N atoms, respectively.

and we confirmed and explained the Si anti-surfactant effect on (11-22) surfaces.

Optimisation of growth of (11-22) GaN on patterned r-plane sapphire

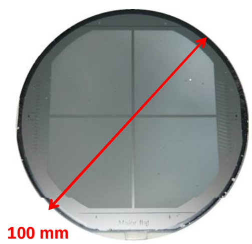
During this project, our approach to grow (11-22) GaN on patterned r-plane sapphire wafers by MOVPE has been thoroughly optimised. An optimisation of the trench patterning process helped to improve the surface smoothness of our semipolar layers. Moreover, we could experimentally confirm that an in-situ deposited SiN nanolayer indeed helps to decrease the penetration of defects (TDDs and BSFs)to the final semipolar GaN surface layer. A multi-step procedure was developed to improve the layer quality. By incorporating GaN:Si marker layers, we could successfully reduce the number of defects penetrating to the layer surface and therefore highly improve its crystal quality and smoothness. Particularly the variation of the growth temperature before stripe coalescence helped to get the best shape of the originally nucleating stripes, which has a huge influence on the quality of the coalesced layer. Under best conditions, a coalescence gap between stripes is formed which helps to stop BSFs in the –c-wing of the stripes from extending to the surface. This is confirmed by low-temperature photoluminescence spectra, which exhibit only a very weak peak related to such stacking faults at about 3.42 eV (~362.5 nm). Moreover, the marker layers helped investigating the formation of a commonly observed surface artefact known as “chevron” or “arrow-head”. This surface defect is formed by an uneven coalescence of one stripe growing over its neighbour in c-direction without flattening in the subsequent layers. Such optimized GaN templates with stacking fault densities below 10^3 cm^{-1} were subsequently overgrown by HVPE resulting in an improved layer quality. The achieved thickness of at least several 10s of µm allowed us to polish such substrates for the subsequent deposition of LED structures. HVPE layers with thicknesses above 1.5 mm have also been grown.



Left: FWHM of HRXRD rocking curves and surface roughness measured by AFM against growth temperature of the pre-coalesced stripe. Right: Low temperature (T=15K) PL spectra.

Growth of (11-22) GaN on structured silicon

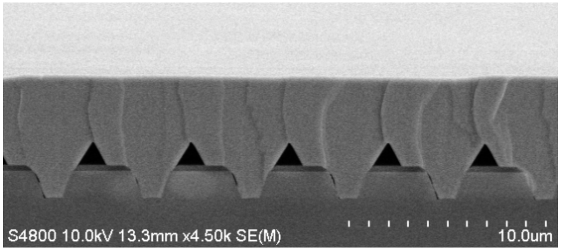
We developed a growth sequence for (11-22) GaN on patterned (113) Si. We successfully demonstrated crack-free nucleation and growth on a 100 mm silicon wafer. However, the pattern orientation on the (113) Si turns out to be extremely critical. The resulting surfaces were frequently very rough, and the onset of cracking at around a growth thickness 5.5 µm prevented smoothing by overgrowth to 7 µm or more in thickness.

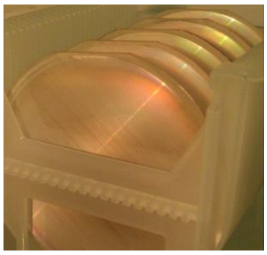


100 mm patterned (113) Si wafer with 4.5 µm of un-cracked semi-polar GaN.

Low defect density, large area (11-22) GaN templates

We successfully realised high-quality (11-22) GaN templates grown on 100 mm diameter patterned r-plane sapphire in a multiwafer MOVPE reactor. Trench patterning was performed by plasma etching using a slanted SiN_x mask that is formed by a resist reflow process and subsequent dry etching. Epitaxial overgrowth by MOVPE was optimized with the aid of in-situ monitoring to monitor the GaN coalescence behaviour and surface morphology. Wafer curvature at the growth temperature exceeds typical values of c-oriented GaN, whereas room-temperature bow is spherical and comparable to polar material. The morphological and structural properties compare well with published data on 2 inch substrates. TDDs of about $2x10^8$ cm^{-2} and BSF densities in the order of $1x10^3$ cm^{-1} were deduced from cathodoluminescence studies. Low residual impurity concentrations ([O, Si] < $1x10^{17}$ cm^{-3}) were verified.

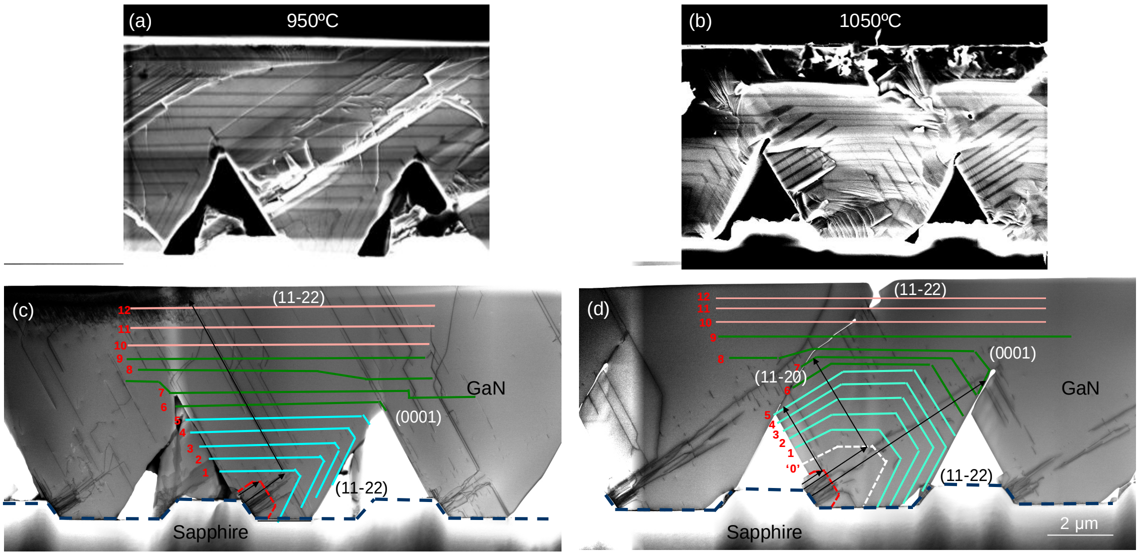




SEM image of coalesced layer of GaN producing a (11-22) surface and a batch of 100mm diameter (11-22) templates

Understanding how to reduce the defect density of GaN templates on pre-structured sapphire substrates using electron microscopy

An in-depth understanding of the growth of (11-22) GaN templates on patterned r-plane sapphire has been achieved by the use of a variety of characterisation techniques, particularly transmission electron microscopy (TEM). This has enabled a substantial reduction in the defect density as realized in WP2. To aid the microstructural analysis using TEM, a series of Si-doped GaN marker layers were deposited at different stages of the GaN growth, which provided key insights into the evolution of the GaN stripes, and hence into the complex shape of the GaN growth front, as a function of growth temperature. The cross-sectional secondary electron images (in a scanning electron microscope, SEM) and bright-field scanning transmission electron microscope (STEM) images were taken from samples with the GaN before coalescence grown at 950º and 1050ºC are shown below. Since the marker layers are invisible in the STEM images, their positions are redrawn corresponding to those in the SEM images. It is apparent that a low growth temperature promotes the appearance of a predominant (11-22) facet, which can bend dislocations originally propagating along the c-direction (0001) by 90º towards the [11-20] direction. In addition, dislocations propagating along the [11-20] direction (after bending) or still along the c-direction (no bending) may all be terminated during the coalescence process as a result of their association with a non-(11-22) facet. These findings allowed us to optimize the growth in order to substantially reduce the density of dislocations reaching the template surface.



Cross-sectional view of samples with theGaN layer before coalescence grown at 950ºC and 1050ºC. (a,b) SEM images, where the Si-doped GaN marker layers are visible. (c,d) STEM images with the marker layers redrawn corresponding to those in (a,b). The blue lines are associated with the GaN layer grown at 950ºC or 1050ºC. The surface of the pre-structured sapphire substrates is marked by dashed dark blue lines. The position of a SiN interlayer is marked by red dashed lines, which was deposited at an early stage of the growth to block the propagation of dislocations along the c-direction. The black arrows indicate the bending of dislocations when they meet the (11-22) facet.

Growth of semi-polar quantum well on chemical-mechanical polished GaNtemplates

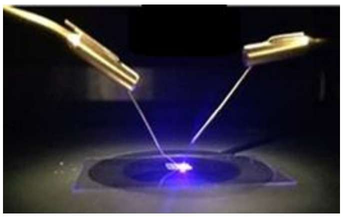
Chemical-mechanical polishing (CMP) of (11-22) GaN templates was performed to remove characteristic chevron shaped features which can otherwise lead to non-uniform emission in LEDs. InGaN multiple quantum well LEDs were subsequently grown on the polished template by MOVPE. By performing the initial GaN overgrowth under nitrogen ambient allowed us to maintain a smooth surface. The peak emission wavelength of the LEDs was varied from 445 nm to 550 nm. In contrast to simultaneously grown LEDs on unpolished templates, the LEDs grown on the polished templates have very smooth surface morphology, uniform luminescence and higher output power.

p-doped InGaN contact layer for low thermal budget

We investigated the growth of Mg-doped (11-22) InGaN layers for indium content from 0.3 to 11 % at growth temperatures from 750 to 875°C with different Mg/group-III ratios between 0.25 and 0.65%. Electrochemical capacitance voltage (ECV) measurements showed that Mg-doped layers are p-type for indium contents up to about 9.6%. The ionised acceptor concentration of the layers was found to be in the range of 10^{17} - 10^{18} cm^{-3} by ECV. The room temperature photoluminescence peak wavelength associated with the Mg emission line shifted from a blue band (435 - 440 nm) to a green band (500 - 545 nm) with increasing indium content. The green band was attributed to donor-acceptor pair recombination between nitrogen vacancies (donors) and substitutional Mg acceptors. The layers with about 6.5% indium content gave the best ohmic p-contacts. This result is significant for the fabrication of semi-polar devices with a long emission wavelength p-InGaN is grown at a low the growth temperature, thus preventing degradation of the InGaN quantum wells.

Semipolar LED Fabrication

Blue, green and yellow LEDs grown on patterned r-plane sapphire substrates were fabricated, incorporating chemical mechanical polishing to minimise epitaxy roughness and a novel p-metal contacting process that has led to exceptionally low forward voltages (<3.5V @ 20mA, from a 0.3x0.3mm^2 LED) and impressive light output (2.6mW in the blue and 0.6mW in the green at 100mA). Furthermore, ALIGHT has demonstrated the first free-standing semipolar LED employing laser lift-off to facilitate patterned substrate removal.



50μm thick free standing semipolar LED fabricated by laser lift-off that has demonstrated a 30% improvement in light output through the backside of the LED when compared to LEDs without substrate

Packaged green emitting (11-22) semipolar LED

3.1.3 Final results and impact

We have achieved our goal of low defect density, large area (100 mm diameter), (11-22) GaN templates and the realisation of LEDs on these substrates using wafer scale processing. The LEDs show excellent output power for this stage of their development, they show enhanced polarized emission and faster dynamics than c-plane LEDs. Freestanding LEDs have also been demonstrated. The work can be the basis of a new template production processes that can be taken on by European industry. This is an area where Europe is already strong with world-leading equipment manufacturers, substrate manufacturers and LED manufactures. Furthermore these templates have interesting possible uses as the basis for new opportunities in sensors and electronics. The resulting products can be used as LEDs for lighting, displays and data transfer with high efficiency. The technical achievements were the result of a strong and balanced collaboration among all the partners of the consortium. Many researchers – from students to professors - now have enhanced expertise in the physics and technology of semipolar templates and LEDs. A comprehensive range of publications describing the new knowledge are available in the peer reviewed scientific literature and can be accessed from the ALIGHT website.