

Green LEDs: The case for cubic GaN

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Green LEDs formed from cubic GaN can have lower Auger losses, higher hole carrier mobility, greater optical gain and increased p -doping efficiency

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The revolution in solid-state lighting is well underway. LEDs bulbs are now shipping in significant volumes, thanks to price tags that are far more competitive than they were just a few years ago.

However, if sales of this class of lighting are to continue to increase, it must not only get cheaper – it must also deliver higher powers and a better colour quality. And that means a fundamental change in the emission process.

The incumbent approach for generating white light involves using GaN-based, blue LEDs to pump phosphors that emit at longer wavelengths. But there are drawbacks with this: the phosphor can curl and delaminate, ruling out the use of such sources for extended periods of time and for providing high-power lighting.

A more promising approach is to colour-mix the emission from an AlGaInP-based red LED with green and blue LEDs made from the III-N material system. This can create a more natural white-light spectra and a higher wall-plug efficiency.

However, if this approach is to fulfil its promise, the green LED must produce a power conversion efficiency of 60 percent or more. Today it's just half that value, a problem described as the 'green gap'.

Researchers have been trying to find a solution to the green gap for more than two decades, and during that time six barriers to higher efficiency have been identified: a high-indium content, a high level of defectivity, low p -doping, carrier asymmetry, polarization and Auger.

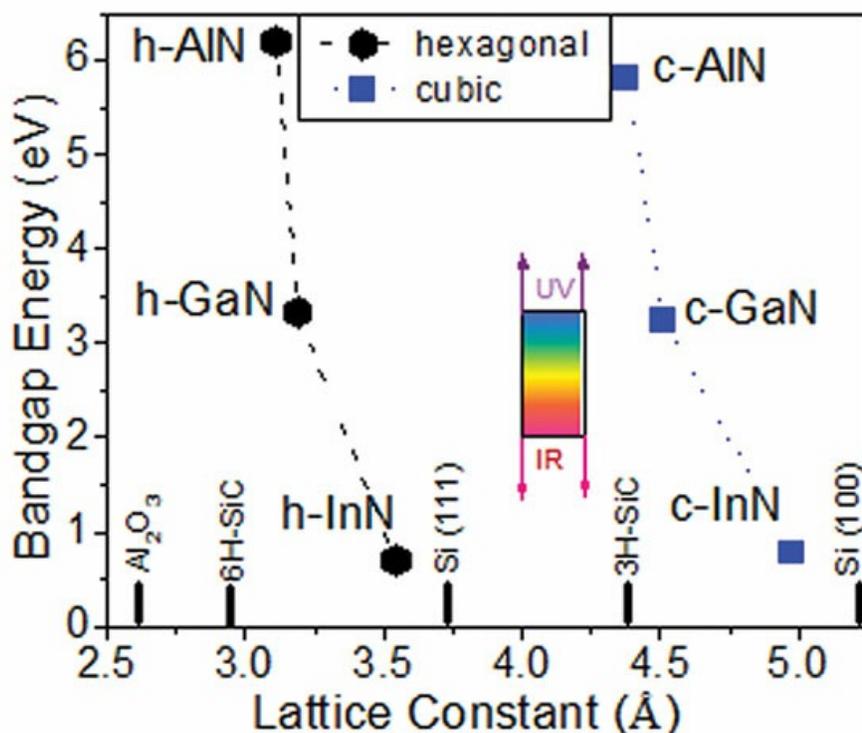


Figure 1. Cubic phase III-nitrides might enable a new era for ‘green’ LEDs, thanks to their ~0.2 eV lower bandgap than their hexagonal counterparts.

All of these six issues plaguing these conventional green LEDs, which employ the hexagonal phase of GaN, have been studied in significant depth. It is well known that the high indium content needed to ensure that InGaN quantum wells emit in the green LED hampers the efficiency of the device, due to a miscibility gap in this alloy; and that the epilayers are riddled with defects, due to lattice- and thermal-mismatch, which arise from growth on foreign substrates, such as sapphire and silicon. In addition, realising a high level of p -doping in nitrides is challenging, due to a high activation energy for the magnesium impurity (it is in excess of 200 meV); there is also a significant asymmetry between electron and hole densities and mobilities, stemming from the large difference between activation energies for p -type and n -type dopants; there are strong internal electric fields within the LED, associated with non-centrosymmetry and inherit piezoelectricity of the hexagonal lattice; and last, but by no means least, Auger non-radiative recombination suppresses efficiency at current densities beyond just 10 A cm^{-2} .

Given all these issues, it is clear that the addressing of the green gap requires a technological breakthrough. And one promising solution for this is to turn to polarization-free structures.

Preventing polarization

To date, efforts at developing polarization-free LEDs have focused on switching from an inherently polar growth plane to one that is inherently polarization-free – and also known as a non-polar plane. Practically, the most common non-polar substrate is the freestanding m -plane of GaN. This particular substrate is made by taking GaN boules that are grown along the $\langle 0001 \rangle$ direction and slicing them along $\{1100\}$ planes. It’s an expensive process, and the resulting substrates are limited to just a few square centimetres.

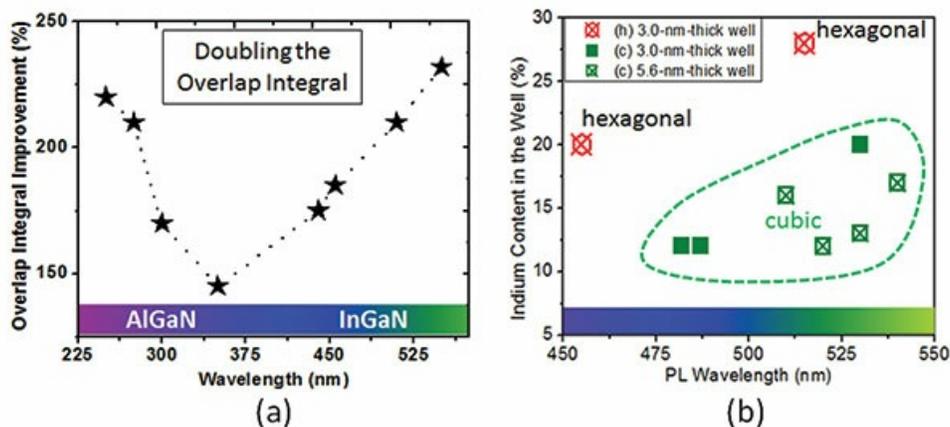


Figure 2. Preliminary investigations by a team from the University of Illinois at Urbana-Champaign show that cubic phase quantum-well structures are ideally suited for green LEDs, thanks to improved electron-hole overlap and reduced indium content in the active layer. (a) Calculations of the electron-hole wave function overlap integral in h - and c -quantum wells show a more than two-orders-of-magnitude improvement in the latter. (b) Comparison of c - and h -InGaIn/GaN multi-quantum wells shows that for the likes of 3 nm-thick InGaIn quantum wells, cubic active layers need about 10 percent less indium in the InGaIn well than hexagonal ones.

Making matters worse, the high-quality epitaxial regrowth of GaN on non-polar surfaces is challenging, due to the low surface energy of non-polar planes; and the quality of InGaIn alloys is inferior on this plane. So, in short, the m -plane platform is far from ideal for enabling polarization-free LEDs – and lasers – to fulfil their promise.

A better option for fabricating polarization-free GaN devices is the cubic phase of GaN (see Figure 1). Structures with this phase are completely free of spontaneous and piezoelectric polarization along the common $\langle 001 \rangle$ direction. What's more, the optical gain of quantum wells from the cubic phase of GaN/InGaN exceeds that of hexagonal variants, thanks to the combination of lower effective masses for the electron and hole; and weaker polarization in the transverse-electric direction, due to a small spin-orbit splitting energy.

Our team at the University of Illinois at Urbana-Champaign is evaluating the potential of cubic GaN LEDs. Our efforts have included simulations of carriers in quantum wells, which suggest an increase that exceeds two orders of magnitude in the overlap integral, compared to the hexagonal material phase (see Figure 2 (a)). That's a tremendous advantage, equating to a hike of more than four orders of magnitude in radiative recombination rates. Additional merits of cubic GaN are a lower bandgap than its hexagonal counterpart, so InGaN active layers can target the same wavelength while featuring a well with an indium content that is 10 percent lower, and freedom from the miscibility gap.

Of the handful of groups around the world that are developing cubic GaN devices, the majority form their structures via epilayer deposition on cubic phase substrates, such GaAs, 3C-SiC, silicon (100) and MgO. However, direct deposition on non-native substrates is not that successful, as it leads to: high defectivity; structural metastability, which is a form of phase-mixing; chemical metastability, such as a tendency toward spinodal decomposition; and in the case of growth on GaAs, chemical incompatibility.

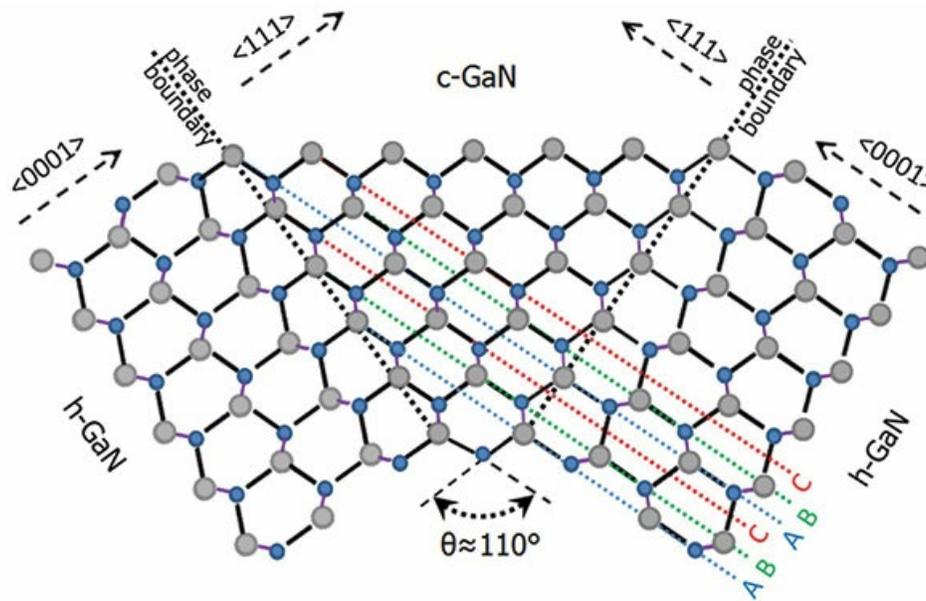


Figure 3. Hexagonal-to-cubic phase transition. The h-phase $\langle 0001 \rangle$ direction and c-phase $\langle 111 \rangle$ direction are equivalent. When two h-phase growth fronts merge with a degree of $\sim 110^\circ$, which is the angle between the two Ga-N bonds in the hexagonal tetrahedral bonding, a c-phase forms after the seam.

An alternative approach is to incorporate an impurity, such as manganese, into the growth. This transforms the hexagonal phase of GaN into a cubic one. However, as this technique relies on p - d orbital repulsion between the 3d impurity levels, success hinges on realising a high density of impurity incorporation. That's highly undesirable, because it degrades material quality to such an extent that it is unsuitable for device fabrication.

Groovy nitrides

We are exploring another avenue, forming cubic III-nitrides in U-shaped [silicon{111}- silicon{100}- silicon{111}] grooves. Our success hinges on the equivalence of the h -crystal $\langle 0001 \rangle$ direction and the c -crystal $\langle 111 \rangle$ direction.

This property means that when two *h*-phase growth fronts merge at $\sim 110^\circ$ – that is the angle between the two Ga-N bonds in the hexagonal tetrahedral bonding – a *c*-phase forms after the seam (see Figure 3).

To produce our cubic material, we apply anisotropic nano-patterning to on-axis CMOS-compatible silicon (100) substrates to create a novel U-shaped nano-pattern with a crystallographic angle of 54.74° between the (100) and (111) silicon surfaces. Thanks to our proprietary growth conditions, *h*-GaN nucleates selectively on the silicon (111) surfaces. This is followed by two *h*-GaN growth fronts meeting at an apex of 109.48° , which is exactly the angle between the two Ga-N bonds in hexagonal tetrahedral bonding. Cubic GaN forms after the seam (see Figure 4).

The growth process for forming cubic GaN is accomplished by MOCVD, and involves four steps: ammonia-free heat up, pre-aluminization, AlN buffer deposition and GaN layer growth. By employing selective MOCVD growth, GaN regrowth is nucleated on the silicon {111} family of planes rather than silicon {100} ones. Thus, [SiO₂-silicon{111}-silicon{100}-silicon{111}-SiO₂] groove structures have only two nucleation sites for GaN re-growth: silicon (111) and the silicon surfaces. When GaN growth fronts initiated from facing directions meet, a void appears in the middle, where the seam forms. The size of this void is governed by the groove period and the growth parameters.

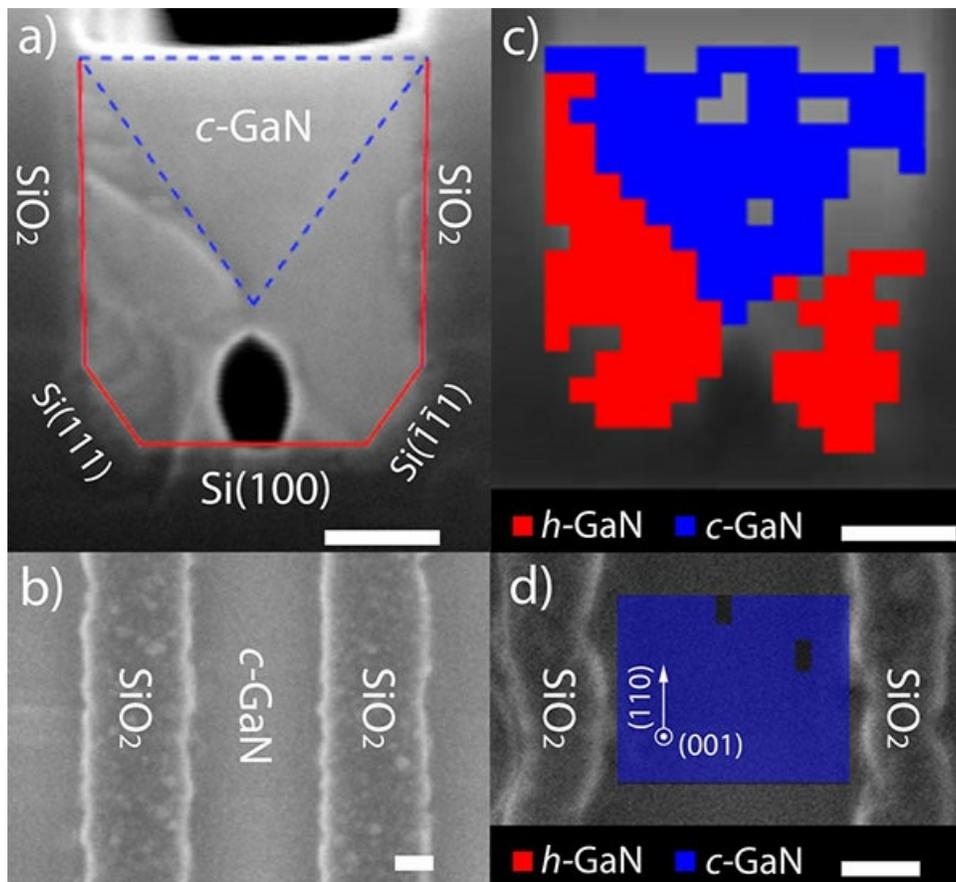


Figure 4. A new method of cubic phase synthesis: Hexagonal-to-cubic phase transformation. The scale bars represent 100 nm in all images. (a) Cross-sectional and (b) Top-view scanning electron microscopy images of *c*-GaN grown on U-grooved silicon (100). (c) Cross sectional and (d) Top-view produced by electron backscatter diffraction of *c*-GaN grown on U-grooved silicon (100), showing *c*-GaN in blue and *h*-GaN in red.

There are several ‘levers’ for optimising the transition between the hexagonal and cubic phases. Elimination of hexagonal incursions and minimizing defectivity in cubic phase material results from perfecting the opening width, oxide thickness and etch depth.

Our work lays the foundation for cutting droop in green LEDs. The biggest contributors to this malady in

conventional devices are high indium content, material defectivity, low p -doping, asymmetry, polarization, and Auger recombination. Switching to a cubic phase allow many of these weaknesses to be tackled head on – it enables smaller effective masses, higher drift velocity, higher carrier mobility, higher doping efficiency, higher optical gain, and smaller Auger losses. So it is clear that a promising route to efficient green LEDs – and ultimately efficient, high-quality LED lighting – is to use the cubic form of this material.

This work was carried out in the Micro and Nanotechnology Laboratory and Frederick Seitz Materials Research Laboratory Central Research Facilities, University of Illinois at Urbana-Champaign, IL, USA.

Further reading

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