Polarization-free integrated gallium-nitride photonics

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ABSTRACT

Gallium Nitride (GaN) materials are the backbone of emerging solid state lighting. To date, GaN research has been primarily focused on hexagonal phase devices due to the natural crystallization. This approach limits the output power and efficiency of LEDs, particularly in the green spectrum. However, GaN can also be engineered to be in cubic phase. Cubic GaN has a lower bandgap (~200 meV) than hexagonal GaN that enables green LEDs much easily. Besides, cubic GaN has more isotropic properties (smaller effective masses, higher carrier mobility, higher doping efficiency, and higher optical gain than hexagonal GaN), and cleavage planes. Due to phase instability, however, cubic phase materials and devices have remained mostly unexplored. Here we review a new method of cubic phase GaN generation: Hexagonal-to-cubic phase transition, based on novel nano-patterning. We report a new crystallographic modelling of this hexagonal-to-cubic phase transition and systematically study the effects of nano-patterning on the GaN phase transition via transmission electron microscopy and electron backscatter diffraction experiments. In summary, silicon-integrated cubic phase GaN light emitters offer a unique opportunity for exploration in next generation photonics.

Keywords: polarization, cubic, light emitting diode, Gallium Nitride, Silicon

1. INTRODUCTION

Lighting technologies have been developed to substitute for sunlight and have been pivotal in the development of mankind. Over the past 200 years, lighting has evolved from being a by-product of burning a medium, such as a candle or an oil-based lamp, to first the incandescent lamp (that generates light by heating a filament), and then the fluorescent lamp (that generates light by heating mercury or a halogen source). All such lighting forms have limited efficiencies in the <25% efficiency range at best, which means 75% of the input power is mostly lost as heat. During the past 50 years, new lighting technologies have been investigated to break the 50% efficiency barrier for ***generating more light than heat***. The resulting technology, **solid state lighting (SSL)**, is based on **light emitting diodes** (LEDs) and can drastically reduce the energy consumption to help lower greenhouse gas emissions.

The awarding of the 2014 Nobel Prize in Physics to GaN-based "blue" LEDs has pushed fundamental research and development of the GaN-based LEDs forward. Today, light-emitting diodes based on $In_XGa_{(1-X)}N$ alloy are the most promising candidates for fulfilling the green gap. InGaN is a direct wide bandgap semiconductor with an emission that can span the useful visible spectrum from 400 nm up to 700 nm via increasing the indium content (x) of the $In_XGa_{(1-X)}N$ alloy. Basically, the alloy is precision engineered for light emission at a target wavelength and incorporated into the LED structure as the active layer. Although phosphor-converted blue LEDs are ready available for green spectrum emission, curling and delamination of phosphor prevents employment of such emitters for extended periods of time and for high power lighting applications. Comparing the existing (i.e. color-mixing vs. phosphor-converted) white color generation approaches, color-mixing approach promises: (1) More natural white light spectra, and (2) Higher efficiency lighting technology than any other white lighting means. The color-mixed approach will only realize its potential advantage over the phosphor-converted alternatives when green LEDs can be achieved with power conversion efficiencies in the 60 to 70 percent range (whereas today their efficiencies are ~30%). Many scientists have been working in this area more than two decades, and contributed significantly to this body of research which has led directly to technological breakthroughs

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that have transformed LEDs into a lighting solution. **Based on this available body of research, six major fundamental barriers in LEDs have been identified** (Fig. 1).
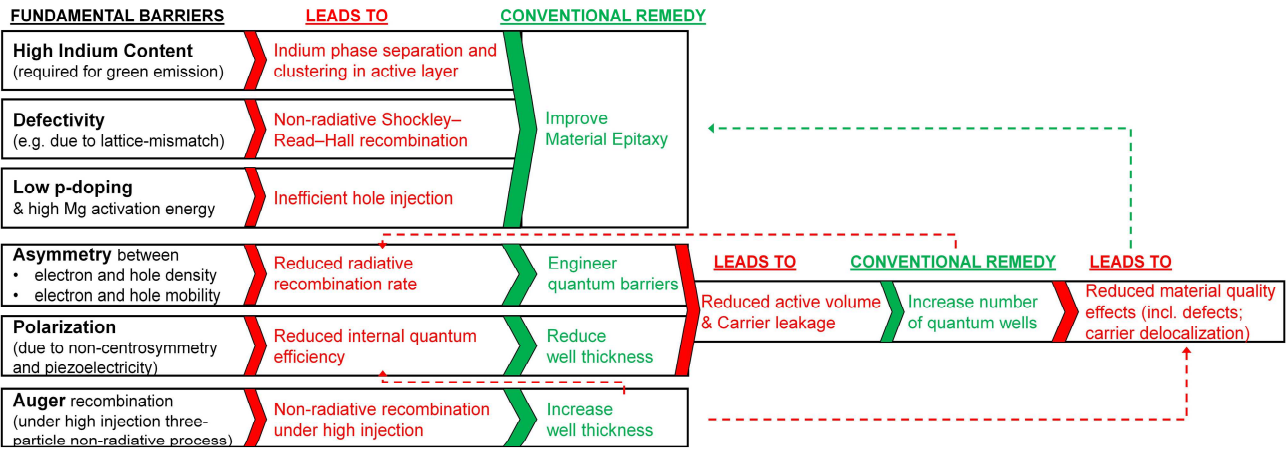

Figure 1 | *Fundamental barriers (i.e. High Indium Content; Defectivity; Low p-doping; Asymmetry; Polarization; Auger) in today's III-nitride green light emitting diodes and conventional remedies. Despite the best efforts, all visible LEDs are bottlenecked by these six barriers. Across the visible spectrum, green LEDs are the most affected and have the (1) Lowest efficiency (< 20%) and (2) Lowest power (< 10mW) under 35A/cm2 injection at 25 °C, far from theoretical potential.*

Almost without exception, all green emitting LEDs employ hexagonal phase GaN materials and suffer from **high-indium content** (due to required high indium content for green emission and miscibility gap of InGaN in these high-In content layers), **defectivity** (due to employment of lattice- and thermal- mismatched growth on non-native substrates), **low p-doping** (due to large (e.g. > 200 meV activation energy of Mg impurity)), **asymmetry** between electron and hole density/mobility (due to difference between p-dopant Mg and n-dopant Si activation energies(i.e. 200 meV vs 30 meV), **polarization** (due to non-centrosymmetry and inherit piezoelectricity of the hexagonal lattice), and **Auger** non-radiative recombination (under high (> 10 A/ cm^2)injection densities) (Fig. 1). Hence, addressing the "green gap" problem requires a technological breakthrough. Polarization-free GaN photonic research has been one of the pathways in doing so.
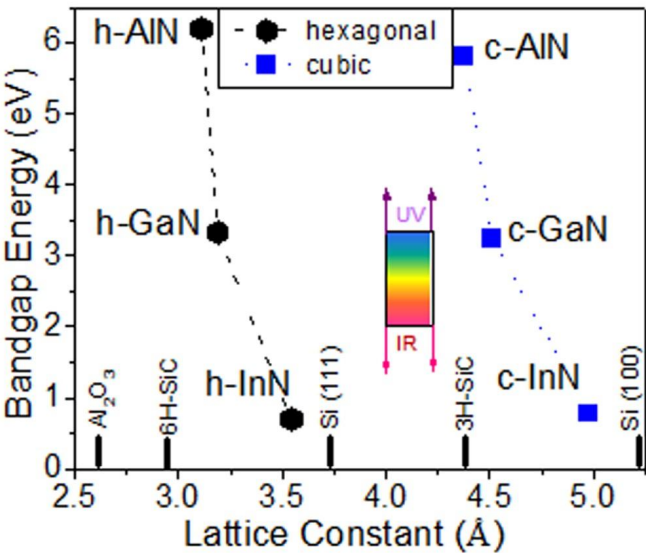

Figure 2 | *Cubic phase III-nitrides might enable a new era for "green" LEDs thanks to their ~0.2 eV lower bandgap than their hexagonal counterparts.*

To date, polarization-free LED efforts primarily focused on switching the growth plane from inherently polar ones to inherently polarization-free (a.k.a. nonpolar) ones. Practically, the most common nonpolar substrate is the m-plane freestanding GaN one (i.e. making 90° with the respect to <0001> direction) that is sliced along {1100} planes out of GaN boules grown along <0001> direction. Hence, m-plane substrates are small in area (~ cm^2) and are expensive. Moreover, (1) high quality epitaxial regrowth of GaN on nonpolar surfaces is challenging due to low surface energy of nonpolar planes, and (2) alloying (such as $In_XGa_{(1-X)}N$) is significantly degraded for nonpolar structures limiting the promise of such substrates in LEDs and laser diodes (LDs) applications [1]. An alternative method of enabling polarization-free GaN devices is switching to the cubic phase GaN materials (Fig. 2) that are completely free of spontaneous and piezoelectric polarization along the common <001> direction. Moreover, the optical gain of a cubic phase GaN/InGaN quantum well is larger than that of hexagonal one because of its smaller electron and hole effective masses as well as its weaker TE-polarization on account of the small spin-orbit splitting energy [2]. Our simulation results suggest significant improvement (more than two orders) in the overlap integral when a cubic phase material is used rather than a hexagonal material phase (Fig. 3a) meaning more than four orders of magnitude larger radiative recombination rates. The understanding of fundamental cubic phase material behavior in alloying and investigating alloyed cubic phase InGaN material will enable a more accurate prediction of polarization-free photonic devices, a necessary requirement for enabling high efficiency high power vertical devices. Moreover, due to the cubic GaN possessing a lower bandgap, cubic InGaN active layers are expected to have ~10% less indium content (Fig. 3b) [3] and possess no miscibility gap for green emission [4] – making cubic phase InGaN active layers ideal for green emitters.
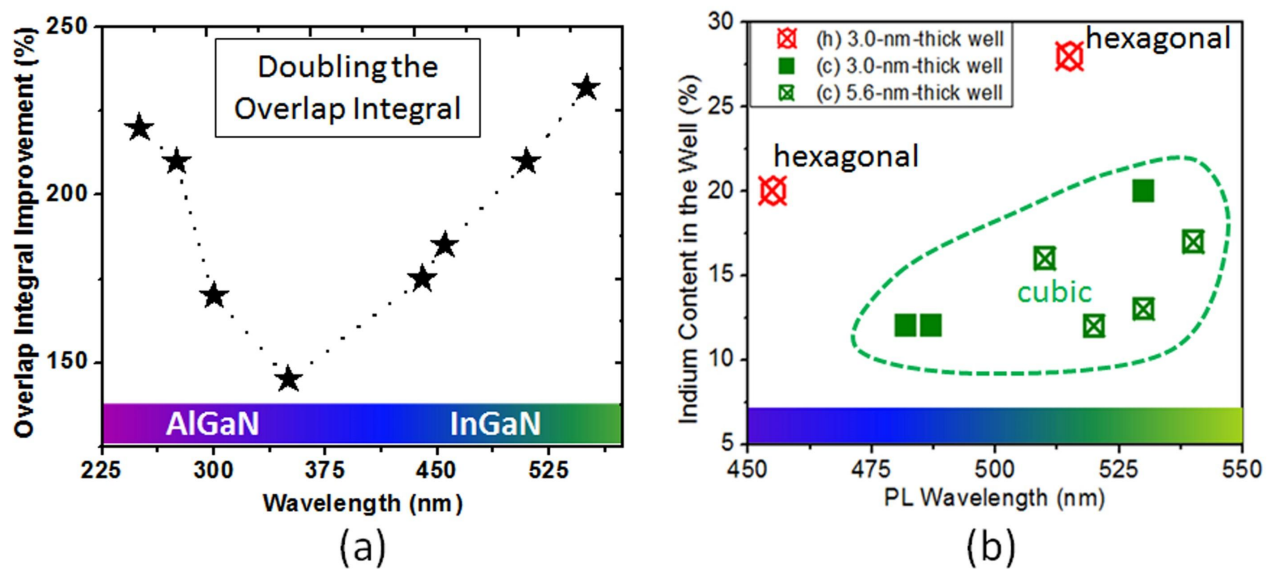

Figure 3 | *Our preliminary investigation shows cubic phase quantum well (QW) structures being ideally suited for green LEDs thanks to improved electron-hole overlap and reduced indium content in the active layer. (a) Our preliminary calculations of the electron-hole wave function overlap integral in h- and c- QWs shows more than two-orders of magnitude improvement in the latter. (b) Comparison of c- and h- InGaN/GaN MQWs shows (i.e. for 3-nm-thick InGaN QW) cubic active layers needing (~10%) less indium in the InGaN well than hexagonal ones.*

In the literature, cubic phase GaN has first been realized via direct deposition on cubic phase substrates such GaAs [5], 3C-SiC [6], Si (100) [7], and MgO [8]. However, such direct deposition on non-native substrates suffers from high defectivity, structural metastability (i.e. phase-mixing), chemical metastability (i.e. tendency toward spinodal decomposition), and in some instances (such as GaAs) chemical incompatibility. Another approach to form cubic phase GaN is to mitigate hexagonal phase into a cubic one by impurity incorporation (such as Mn [9]). This technique relies on p-d orbital repulsion between the 3d impurity levels requiring a large density of impurity incorporation thus reducing the resulting material quality; it is thus unusable in device applications.

2. EXPERIMENT

Recently, we proposed a new method to enable cubic III-nitrides via U-shaped [Si{111}- Si{100}- Si{111}] groove structures [10, 11]. Based on the crystallographic fact that h-crystal <0001> direction and c-crystal <111> direction are equivalent, when two h-phase growth fronts merge with a degree of ~110° (i.e. the angle between the two Ga-N bonds in the hexagonal tetrahedral bonding), a c-phase would form after seam (Fig. 4). To realize, here we employ anisotropic nano-patterning of on-axis CMOS-compatible Si(100) substrates and create a novel U-shaped nano-pattern with a crystallographic angle of 54.74° between the (100) and (111)Si surfaces. Thanks to our proprietary growth conditions, we nucleate h-GaN selectively on the Si(111) surfaces. Thus, continuous growth leads to two h-GaN growth fronts meet in an apex angle (θ) of 54.74°$\times$2=109.48°, that is exactly the angle between the two Ga-N bonds in hexagonal tetrahedral bonding. Our novel technique enables transformation of the hexagonal (h-) GaN into a cubic (c-) GaN after seam (Fig. 5).
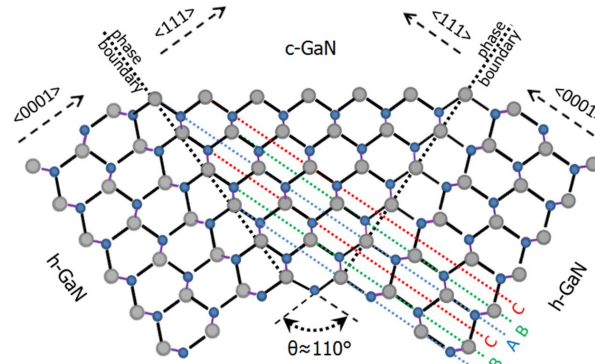

Figure 4 | *Hexagonal-to-cubic phase transition. Sketch shows h-phase <0001> direction and c-phase <111> direction equivalency. When two h-phase growth fronts merge with a degree of ~110° (i.e. the angle between the two Ga-N bonds in the hexagonal tetrahedral bonding), a c-phase would form after seam.*
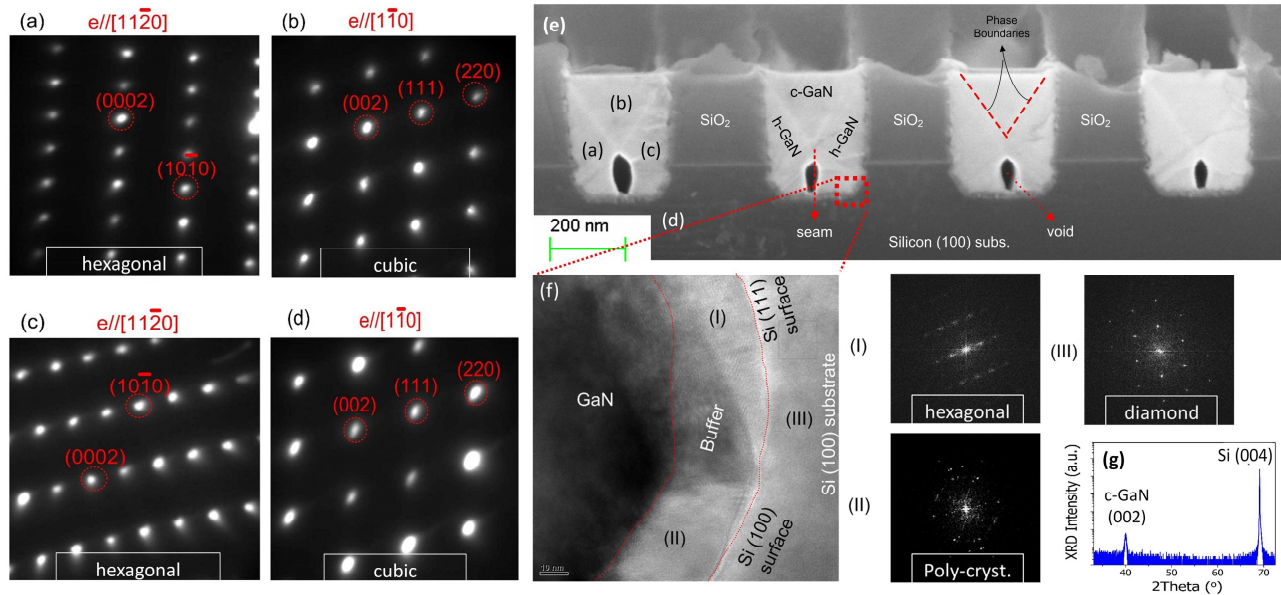

Figure 5 | *A new method of cubic phase synthesis: Hexagonal-to-cubic transformation. (a-e) Fast Fourier Transform (FFT) diffraction patterns in (a-d) belong to (a,c), (b), (d) regions shown in (e) corresponding to h-GaN, c-GaN, and Si (100), respectively. Electron beam is parallel to [11$\bar{2}$0] and [1$\bar{1}$0] zones of wurtzite and cubic phase GaN, respectively. (f) HR-TEM image of the GaN {0001}-Si{111} interface shows crystalline AlN buffer on Si{111} surfaces whereas poly AlN on Si{100}. FFT diffraction patterns from selected area regions (I), (II), and (III) are observed to be hexagonal single crystalline, polycrystalline, and diamond single crystalline. (g) Omega/2Theta XRD scan of GaN on a U-shaped nanopatterned Si (100) shows a clear cubic phase diffraction peak.*

3. RESULTS AND DISCUSSION

Our selective MOCVD scheme consists of four steps: (1) Ammonia-free heat up, (2) Prealuminization, (3) AlN buffer deposition, and (4) GaN layer deposition. Under selective MOCVD growth conditions, GaN regrowth is nucleated on the Si {111} family of planes rather than Si {100} ones. Thus, [SiO$_2$-Si{111}-Si{100}-Si{111}-SiO$_2$] groove structures have only two nucleation sites for GaN regrowth: Si (111) and Si $(\bar{1}\bar{1}1)$ surfaces. When GaN growth fronts initiated from facing directions meet, a void is formed in the middle where the seam forms. The size of the void depends on the groove period as well as the growth parameters.

Crystallographic relations between cubic and hexagonal phase of GaN and Si(100) are used to investigate optimum hexagonal-to-cubic phase transition parameters of opening width (t$_O$), oxide thickness (t$_{SiO2}$), and etch depth (t$_d$) that minimizes hexagonal incursions in cubic phase materials. For complete c-GaN surface coverage in these U-grooves, we have shown that the critical GaN deposition thickness (h$_c$) is obeying $h_c = (1.06p - 0.75t_d)/\left(1 - \frac{\tan\alpha}{0.71}\right)$, where p is the opening width of the U-groove at the dielectric/substrate interface, t_d is the silicon etch depth, and α is the dielectric sidewall angle [12, 13] (Fig. 6).
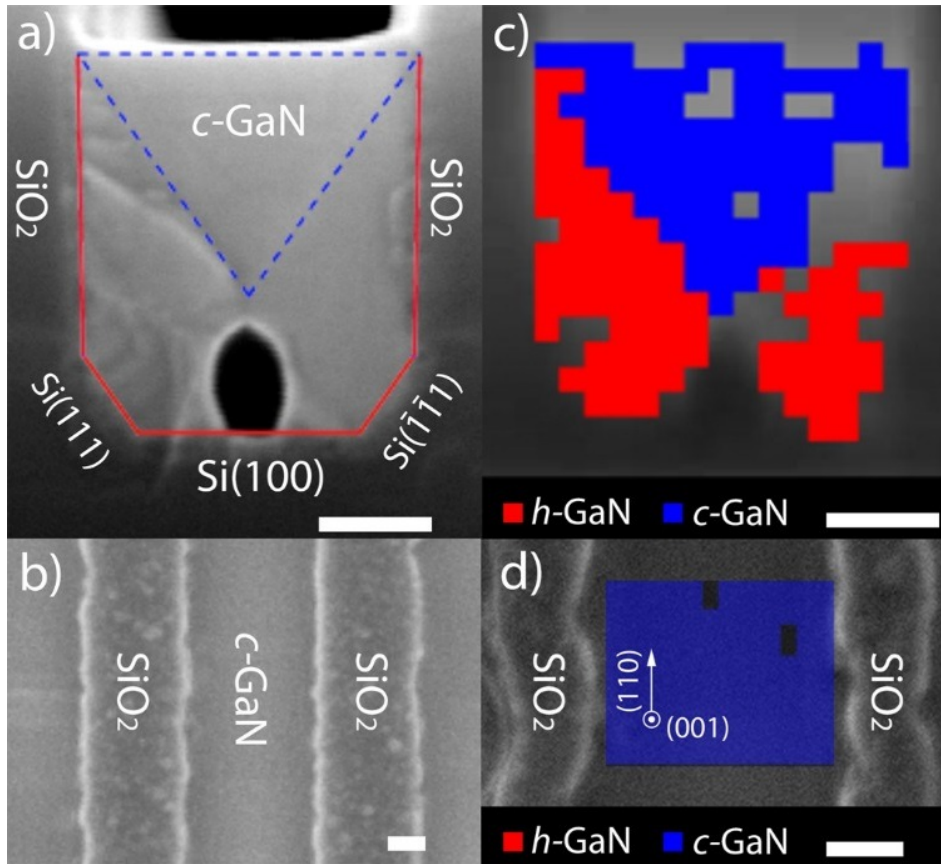

Figure 6 | **_A new method of cubic phase synthesis: Hexagonal-to-cubic phase transformation._** _The scale bars represent 100 nm in all images. (a) Cross sectional and (b) Top-view SEM images of c-GaN grown on U-grooved Si(100). (c) Cross sectional and (d) Top-view EBSD images of c-GaN grown on U-grooved Si(100), showing c-GaN in blue, and h-GaN in red._

4. CONCLUSION

In summary, nearly all of the 10,000+ articles in the GaN and related area utilize an inherently polar material referencing hexagonal (wurtzite) phase of GaN. This approach precludes the ability of the LED to have high radiative recombination rates, leading to degraded efficiency performance. Particularly, larger the indium content for green emission, larger is the lattice-mismatch and piezoelectric fields in a green LED. Thus, further In-content in the active layer for green emission lowers the LED efficiency. In addition, all GaN-based LEDs – without exception – have reduced light emission efficiency as injection current increases – a detrimental phenomenon known as "droop" – limiting the power output of GaN LEDs. The "droop" effect alone is shadowing the theoretical performance of LEDs, preventing the worldwide adoption of LEDs, and exists in every spectrum. The biggest contributors to "droop" effect in green LEDs are believed to be the high indium content, defectivity, low p-doping, asymmetry, polarization, and Auger**. A cubic phase LED shall address these current limitations with intrinsically more isotropic properties** (including smaller effective masses, higher drift velocity, higher carrier mobility, higher doping efficiency, higher optical gain, smaller Auger losses) than hexagonal counter parts, has no polarization, and requires at least ~10% less indium in the active layer (with respect to hexagonal ones) for the green emission.

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