Growth of Non-Polar Cubic GaN on Common Si

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By some accounts group-III nitride may be the widest disseminated man-made compound semiconductors. Yet, what is it that makes it so successful? Maybe the wurtzite structure which allows for piezoelectric polarization? We know about the Stokes shift it induces and its associated troubles. So we rush to reduce polarization in non-polar growth. But how about the cubic form of GaN. Shouldn't that be free of polarization? Would it be the better light emitter even? To find out we prepare GaN and GaInN/GaN heterostructures in cubic lattice form. By virtue of some patterning we achieve cubic growth on the more common form of Si, the (001) orientation, which further allows for conceptional integration with the semiconductor of industry choice.

Group-III Structures and why their Structure Matters

The search for a wide bandgap semiconductor suitable for blue light emission has been a major motivation for the development of GaN and its related alloys with InN and AlN. Owing to a large bandgap of 3.42 eV it was kind of a conceptional stretch to consider it a semiconductor. Yet, with achievement of high crystalline GaN layers in heteroepitaxy on sapphire by help of low-temperature-deposited buffer layers, doping both, n- and p-type was enabled.\textsuperscript{1} Then, alloying with even the slightest amounts of InN in GaInN layers, tremendous light emission efficiency was achieved leading to the rapid development of powerful blue LEDs which then could be used to pump suitable phosphor material to produce LEDs of white light perception. A theoretical description, let alone prediction of the electronic bandstructure of the group-III nitrides, however, proved a bit more challenging since the group-III nitride preferentially crystallize in the hexagonal wurtzite crystal structure, unlike all conventionally utilized semiconductors of the time being described in the cubic zincblende structure. A simple first approximation to describe a wurtzite lattice in the zincblende structure is imposing a superlattice onto zincblende along the (111) direction with a superlattice period of twice the layer spacing in that direction. This lifts the inversion degeneracy and allows for piezoelectric polarization. It also induces a zone folding leading to rather low lying secondary
conduction band minimum in Γ, thought to lie about 2 to 3 eV above the direct bandgap defining the conduction band minimum in Γ. The possibility of piezoelectric polarization is not necessarily observed in first principles calculations in finite atom cell models. To manage calculation effort and memory requirements periodic boundary conditions are frequently applied which essentially eliminate the polarization. It was not until it was specifically considered that huge polarization charges were quantified theoretically. Early findings in the bias voltage dependence of GaInN/GaN quantum wells\(^3\) hinted at their resulting huge electric fields across the GaInN/GaN heterointerface. Recognizing their dominant role in the description of the electronic bandstructure we directly quantified the effective fields from direct observation of Franz Keldysh oscillations to reach 0.83 MV/cm in the (0001) layered wells of Ga\(_{0.82}\)In\(_{0.18}\)/GaN multiple quantum well structures.\(^3\)

Such large electric fields turn the QWs transition effectively spatially indirect. The dipole matrix element responsible for radiative emission drops rapidly with increasing well width, while at the same time increasing otherwise forbidden transitions. The resulting increase in dynamical carrier lifetimes leads to high densities of transient carriers accumulating in the well and thereby increasing the probability of carrier-carrier interactions such as no-radiate Auger recombination. The latter is one of the currently favored models for efficiency droop in LEDs under high injection current. Non-radiative Auger recombination should also be enhanced if the electron excitation path leads to the above mentioned low-lying zone-folded second conduction band.

**Opportunity of Cubic Group-III Structures**

Recognizing all those effects so characteristic for the wurtzite structure of the group-III nitrides, it must be deemed a priority to analyze its twin brother, the less stable zincblende cubic polytype.\(^4,5\) With such a direct comparison of heterostructures in wurtzite and cubic bandstructure a relevant test for the above models will become possible. Moreover, in the absence of such strong piezoelectric polarization, potentially higher preforming LEDs and laser diodes might become possible. In particular for the longer wavelength emitters of green, amber, and red, the cubic polytype offers the additional benefit of a smaller electronic bandgap, an advantage that can help overcome some of the challenges of incorporation of high InN fractions into the GaInN alloys.

**Formation of cubic GaN structures**

Recognizing the simple stacking difference between zincblende and wurtzite structure we coalesce easily grown wurtzite structure at the proper angle to force a stacking transition that accommodates both initial growth fronts to further progress along the only symmetrically open third direction. This transition amounts to the exact stacking fault that distinguishes cubic from the wurtzite structure and the joint growth front therefore progresses in cubic structure growth. As a growth template we choose conventional Si (001) V-grooved to expose opposing pairs of (111) planes. Those planes form a close match to GaN nucleating in the wurtzite structure. In order to prevent etch back melting of the Si in the NH\(_3\) growth environment, a thin protective layer of AlN is deposited first. Upon coalescence, the wurtzite layers turn cubic and progress to fill the V-groove with stripes of cubic GaN.\(^6,7\) Layer size thereby can reach a few µm in width while their length is limited only by the size of the substrate, a couple of cm in our experiments. Such
structures could prove ideal as a laser stripe and according development work is underway in our laboratories.

With the substrate of conventional Si (001), rather than more frequently utilized Si (111), we are in line with the mainstream semiconductor industry implying Si (100) technology. Devices such as high blocking voltage diodes, power transistors, and the channels of high frequency transistors could thereby directly integrated with conventional and industry scale semiconductor technology. For the purpose of high brightness light emitters, removal of the absorbing Si substrate however, seems advisable. In this way we have grown test structure comprising green emitting GaInN/GaN multiple quantum wells embedded within a cubic structure pn-junction, metalized the top layers and etched back the Si for a free standing LED chip. Future work aims at analyzing electron transport properties and diode characteristics.

Summary

In summary, work to explore the uniqueness of wurtzite structure GaInN/GaN and its role as LED in energy efficient solid state lighting, as diode and transistor in high power electronics is being analyzed by developing its win brother in cubic structure which does not allow for such polarization charges. The approach thereby allows for a direct one to one comparison of the role of polarization in the remaining challenges of the group-III nitrides for their ever wider application field. In the process, we also develop a potent candidate for the direct emission in the longer wavelength visible spectral range for the green amber and red light emitters.

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References

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