

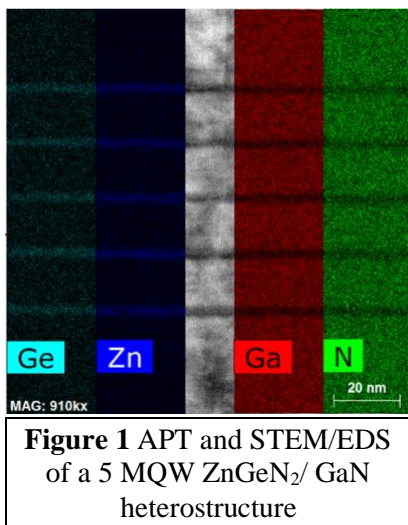
Structure and Chemistry of ZnGeN₂ Quantum Wells in GaN for use in Green LEDs

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Hybrid II-IV-N₂/III-N heterostructures, based on current commercialized (In,Ga)N light-emitting diodes (LEDs), are predicted to significantly advance the design space of highly efficient optoelectronics in the visible spectrum, specifically in the green to amber regions where LED efficiencies are orders of magnitude lower than other colors. Yet, there are few epitaxial studies of II-IV-N₂ materials. ZnGeN₂, a ternary analogue of GaN, is explored as a potential green-to-amber emitter which can be integrated into existing GaN LED heterostructures due to structural similarity. ZnGeN₂ is wurtzite when disordered, and is structurally and electronically similar to GaN, possessing a lattice mismatch of ~0.8%. Previous work by this group has demonstrated epitaxial growth of ZnGeN₂ on GaN and AlN via molecular beam epitaxy (MBE) [1-2]. Here we present the growth of abrupt quantum wells (QW) of ZnGeN₂ within GaN by nitrogen plasma-assisted MBE, including successful five-layer multiple quantum well (MQW) structures.



Detailed structural and elemental analysis of the heterostructures was performed, including X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), energy dispersive X-ray spectroscopy (STEM-EDS), and atom probe tomography (APT). These methods demonstrate high-quality and abrupt interfaces in the heterostructures after multiple repeating heterointerfaces and some compositional nonidealities in each layer. Through changes in growth methodology, we demonstrated methods to improve unintentional impurities including associated improvements in structural quality. We also investigated conduction band offset using X-ray photoelectron

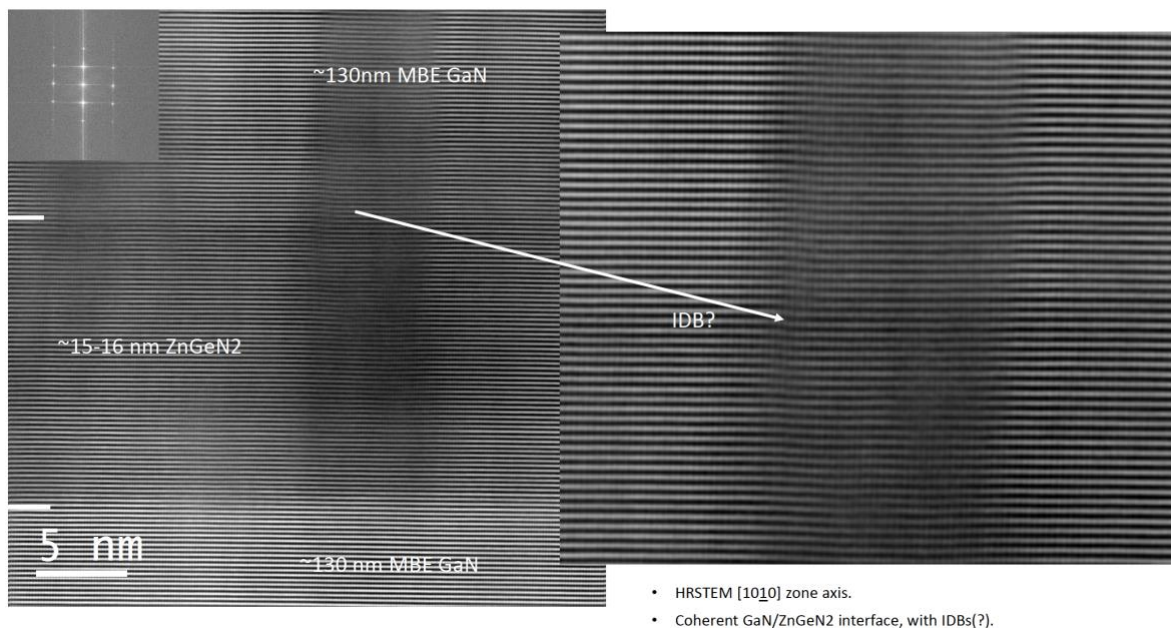
spectroscopy (XPS) in the GaN/ZnGeN₂ heterostructures, important for LED design. Together, these data demonstrate both the promise of heteroepitaxially integrated hybrid ternary/binary nitride systems along with the challenges associated with growing such systems, including an outlook on methods to improve the materials and eventual devices.

[1] M. B. Tellekamp et al 2020, Crys. Growth Des. 20, 3, 1868–1875.

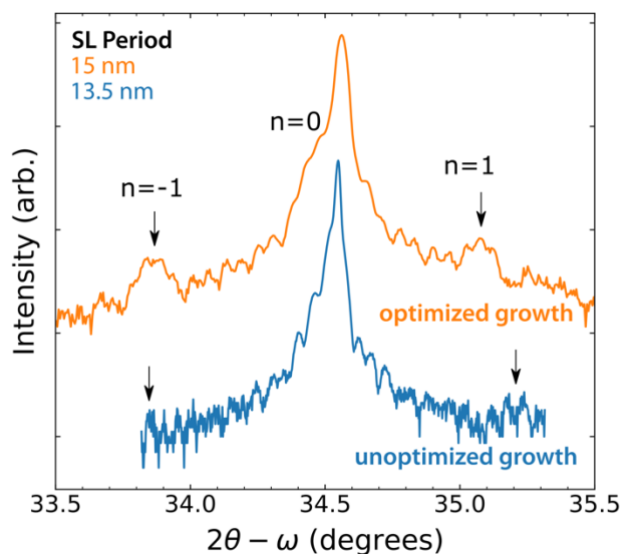
[2] M. B. Tellekamp et al 2022, Crys. Growth Des. 22, 2, 1270–1275.

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Supplementary Pages



S- Figure 1: High-resolution transmission electron microscopy along wurtzite $[10\bar{1}0]$ zone axis, along with an FFT (inset) for a single ZnGeN₂ QW within GaN. Shows abrupt and coherent interfaces without misfit dislocations. However, a large concentration of inversion domains are formed at the interface.



S- Figure 2: Symmetric XRD around GaN (0002) for unoptimized and optimized multiple quantum well structure of five repeating units of ZnGeN₂ and GaN. Optimized sample shown to have superlattice peaks and higher coherency.