

X-ray probes of local composition and structure near defects in InGaN multi-quantum wells

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Motivation

III-N nitrides are semiconducting materials with a wide range of band gaps for high power switches (AlN) and solid state lighting (GaN, InGaN LEDs).

There are no cost-effective, lattice matched substrates to make nitride thin films, so devices are limited by large defect densities. [1]

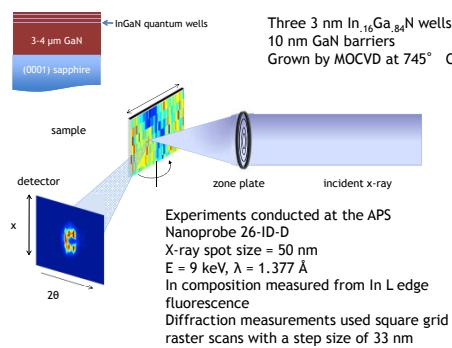
InGaN light-emitting devices (LEDs) consist of multiple thin InGaN layers separated by GaN barrier called a *multiquantum well* (MQW) structure.

In LEDs used in solid state lighting, high threading dislocation densities affect minority carrier concentration and recombination rates [2] within the InGaN MQW active regions of the devices, while compositional fluctuations are thought to localize carriers within the same region. [3]

Focused x-ray beams can be used to measure composition and structure at the same length scales as defects (see figure above).

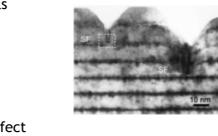
How do composition and structure vary near defects in InGaN MQW films?

Experiment



Parallel beam diffraction used to find MQW reflections.

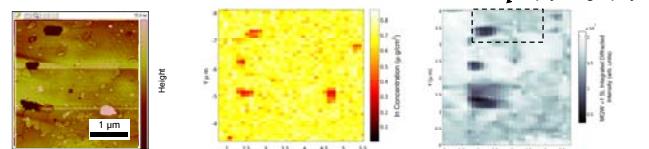
We used the SL +1 reflection for the microdiffraction experiments because it is well separated from the GaN (0002)



HRTEM image of 'v-defects' in InGaN/GaN MQWs. V-defects have stacking faults on (0001) planes that often originate above GaN threading dislocations. [4]

Microdiffraction from defects

Imaging v-defects

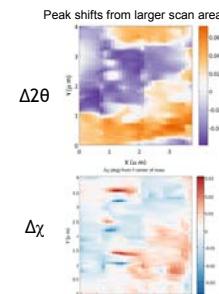
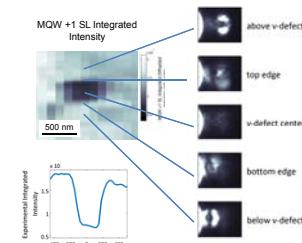


AFM: v-defects create large pits with triangular cross sections
XRF: v-defects have less In than surrounding film
XRD: integrated intensity of MQW reflections is lower in v-defects

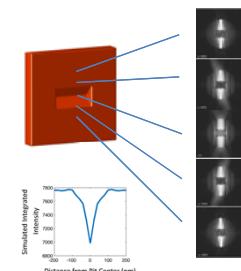
Indium content outside of defects is uniform.

Structural changes outside the defects are not related to compositional variations. Could be related to thinner MQW layers, increased roughness, strains, or rotations. To distinguish between potential causes, we quantified peak motions, simulated diffraction patterns from a pit, and used Bragg projection ptychography to reconstruct the sample.

Experimental MQW diffraction peak shifts at defect edges



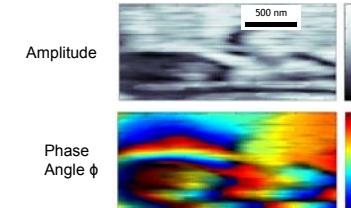
Simulated diffraction patterns from a defect



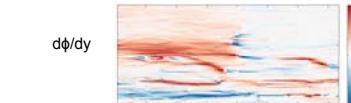
Simulation suggests that a pit in the film modifies the diffuse scattering, but does not shift the reflection's center of mass.

The shifts measured from the center of mass are not caused by the shape of the defect; they come from rotations and strains in the lattice.

Bragg Projection Ptychography



Phase Angle ϕ

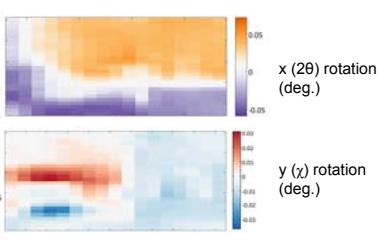


Peak Shifts from Center of Mass



Diffracted Intensity

Cannot measure phase experimentally



Bragg ptychographic reconstruction of the film was refined with the Ptychographic Iterative Engine [5-7].

Lattice rotations are related to the gradients of the phase, $d\phi/dx$ and $d\phi/dy$, which closely match the centers of mass of the experimental diffraction pattern at potentially higher resolutions compared with traditional scanning probe diffraction.

MQW (0002) planes are rotated near the defect edges, consistent with strain relaxation near a hole in the film.

Conclusions

AFM, x-ray fluorescence, and x-ray microdiffraction were used to image v-defects in InGaN MQWs.

Diffraction peak shifts indicate significant structural variations inside and outside of pits, independent of composition.

Lattice rotations measured independently from position of Bragg peak center of mass and derivatives of the phase retrieved from Bragg projection ptychography reconstruction are well correlated.

References

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Acknowledgements

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