SAND2016-6503C

Sandia National Laboratories

Phase Degradation in $B_xGa_{1-x}N$ Films Grown at Low Temperature by Metalorganic Vapor Phase Epitaxy

Brendan P. Gunning,
Michael W. Moseley, Daniel D. Koleske,
Andrew A. Allerman, Stephen R. Lee

Sandia National Laboratories
Albuquerque, New Mexico, USA, 87123

UWBG ULTRAWIDE BANDGAP POWER ELECTRONICS

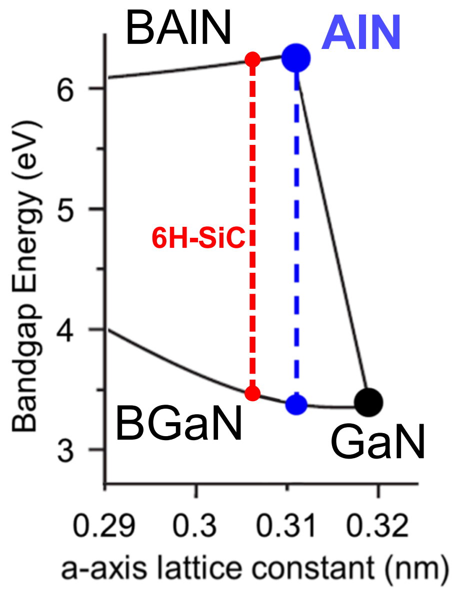
U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration LOCKHEED MARTIN

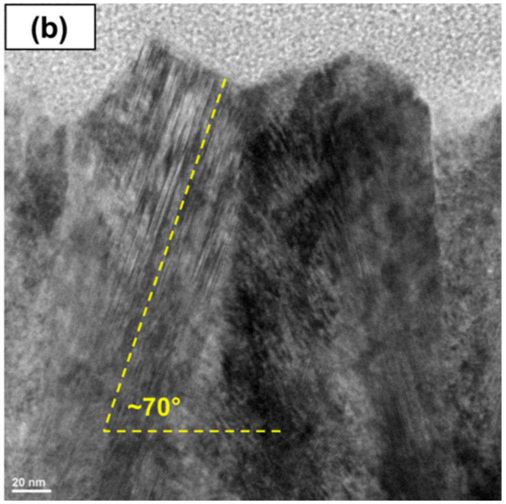
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

bpgunni@sandia.gov

Outline

- **Background**
  - Dislocation generation
  - Opportunities for lattice-matched epitaxy
- **Preliminary BGaN growth study**
  - Low-temperature growth
  - Low-pressure, no H_2
- **Deep structural characterization**
  - XRD phase analysis
  - TEM microstructure
- **Investigate phase degradation**
  - Effect of TEB

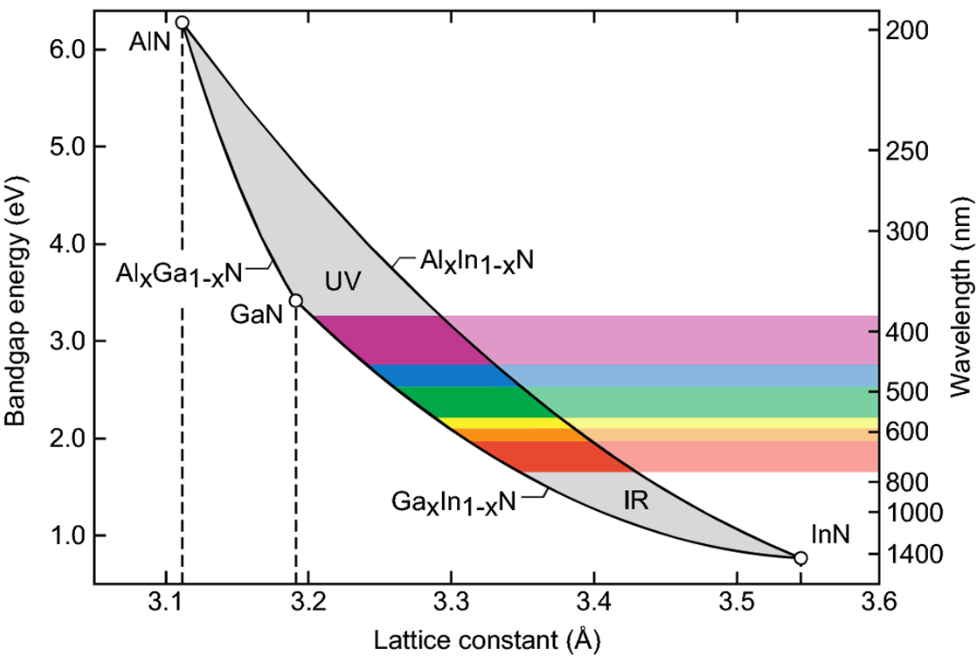




III-Nitride Challenges

Sandia National Laboratories

Substrate choice and trade-offs

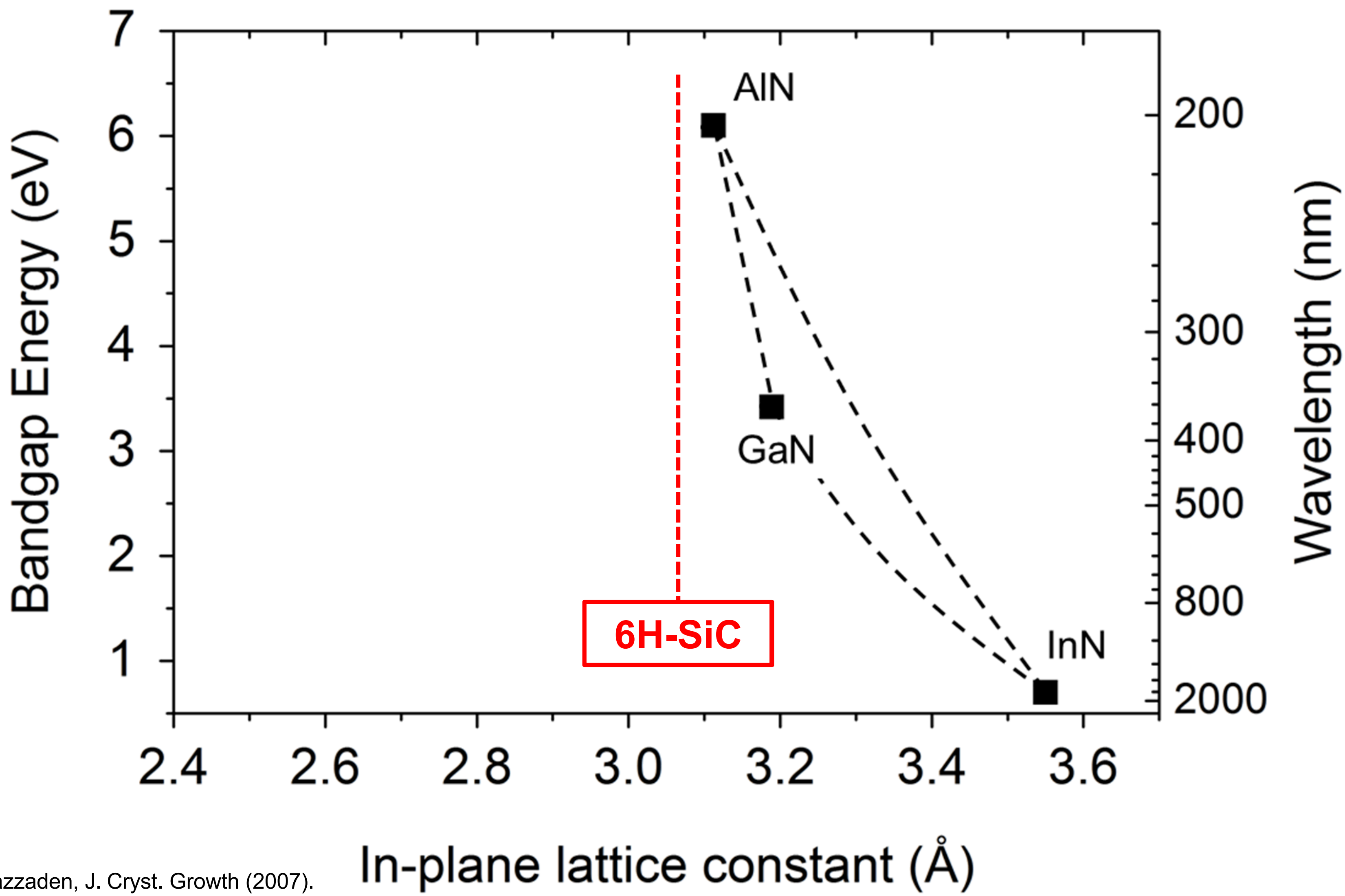


M. F. Schubert, Ph.D. Thesis, Rensselaer Polytechnic Institute (2009).

Substrate	*Mismatch vs. GaN*	*Additional notes*
Sapphire	14%	**Cheap**, electrically and thermally insulating
SiC	3.4%	**Expensive**, electrically and thermally conductive
Si (111)	17%	Cheap, mature, **forms amorphous SiN layer**
Bulk AlN	2.4%	**Expensive**, maturing technology
Bulk GaN	0%	**Expensive**, maturing technology

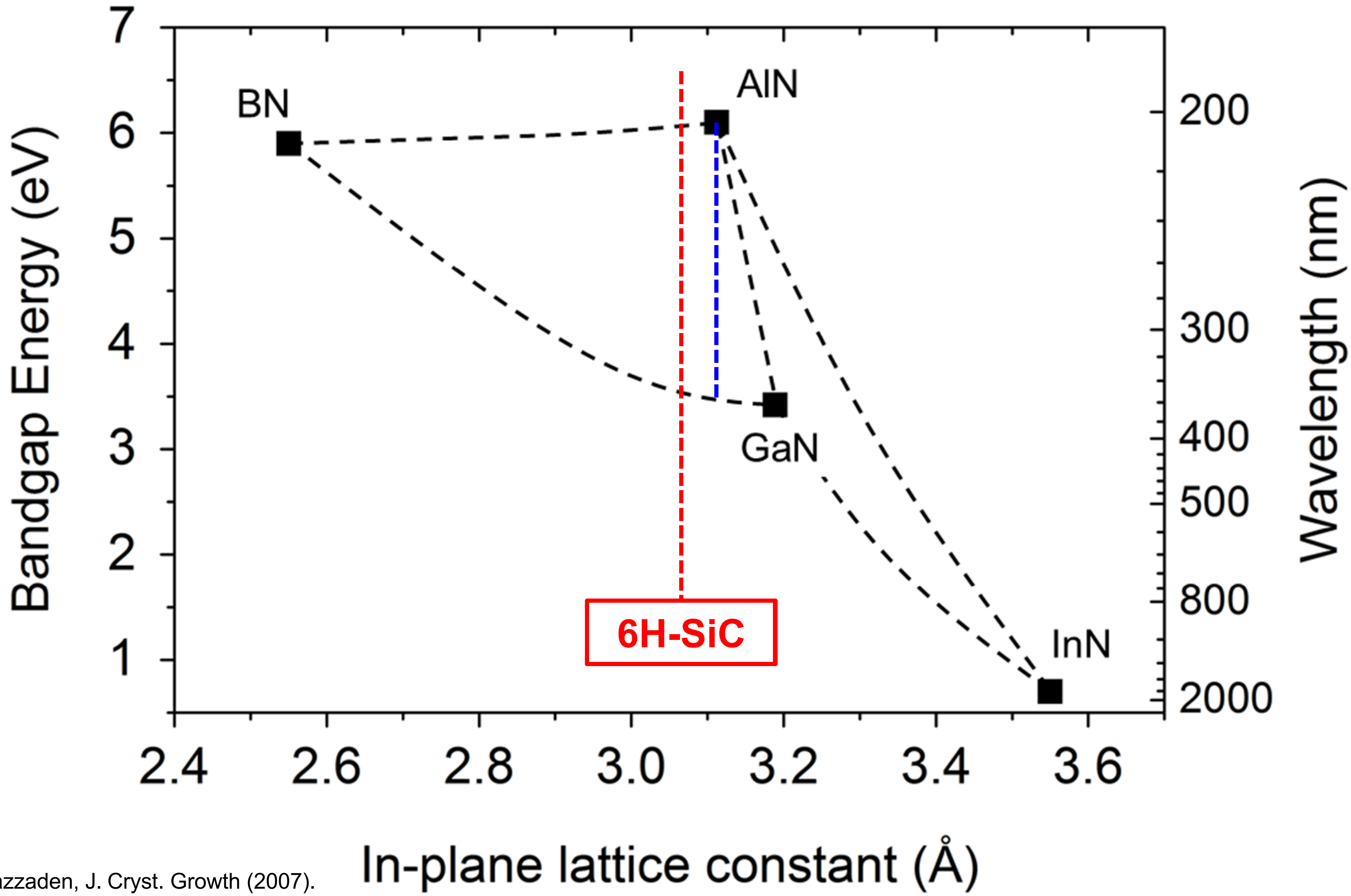
No native substrate for AlGaN alloy growth

InAlGaN materials system



after Ougazzaden, J. Cryst. Growth (2007).

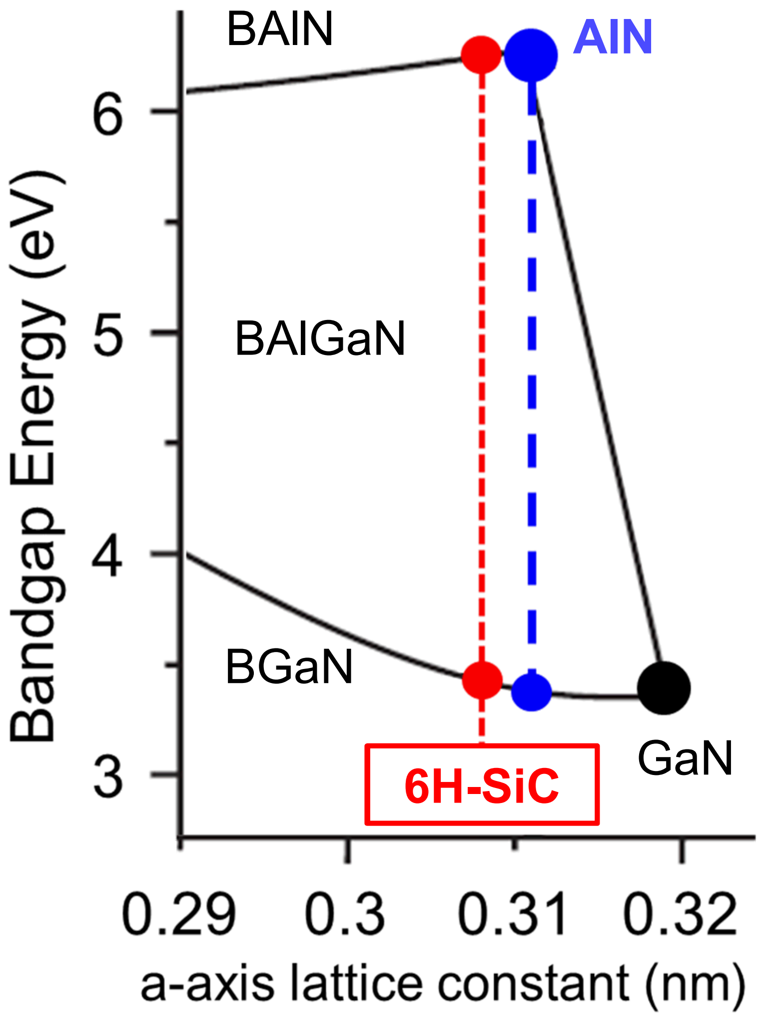
Boron-containing nitride alloys



after Ougazzaden, J. Cryst. Growth (2007).

BGaN and BAlN

Expanded view:



after Ougazzaden, J. Cryst. Growth (2007).

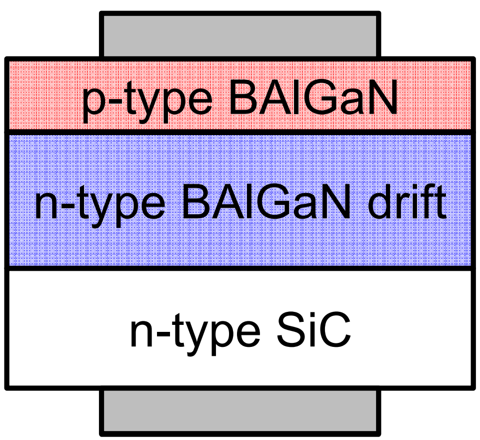
Lattice-matching opportunities:

$B_{0.12}Ga_{0.88}N$ on AlN

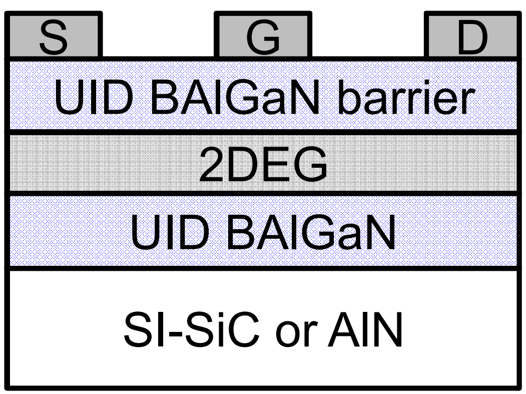
$B_{0.17}Ga_{0.83}N$ on 6H-SiC

$B_{0.05}Al_{0.95}N$ on 6H-SiC

Device prospects:



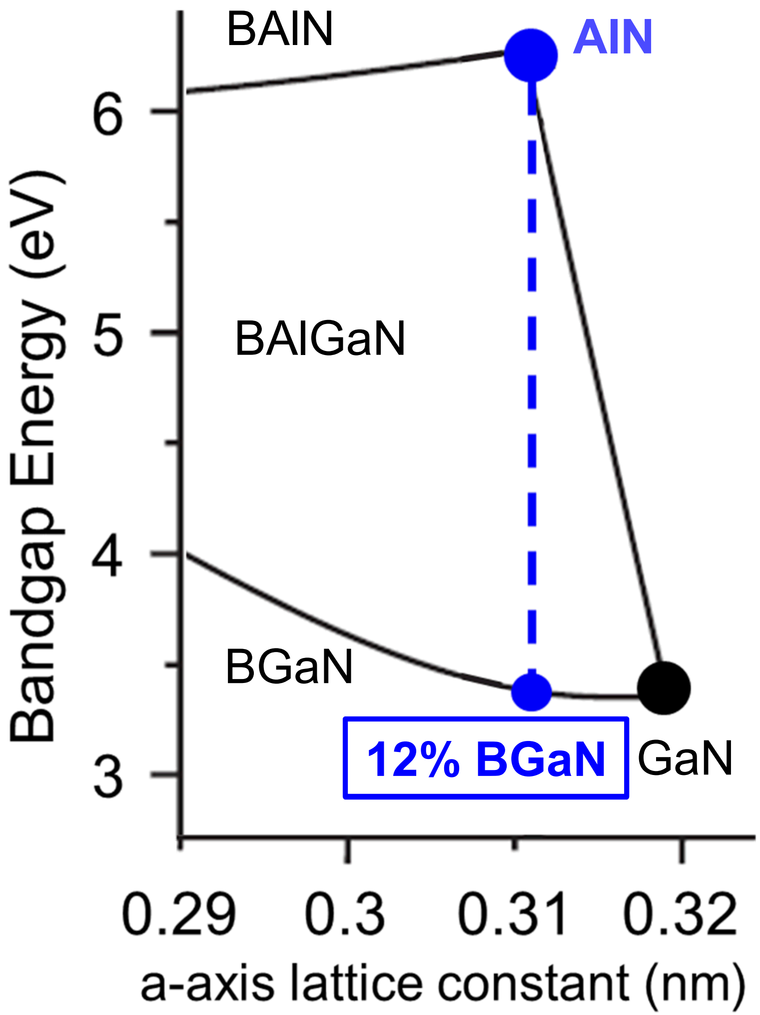
Two-terminal vertical device



Three-terminal lateral device

BGaN and BAlN

Expanded view:



after Ougazzaden, J. Cryst. Growth (2007).

Lattice-matching opportunities:

$B_{0.12}Ga_{0.88}N$ on AlN ←
$B_{0.17}Ga_{0.83}N$ on 6H-SiC
$B_{0.05}Al_{0.95}N$ on 6H-SiC

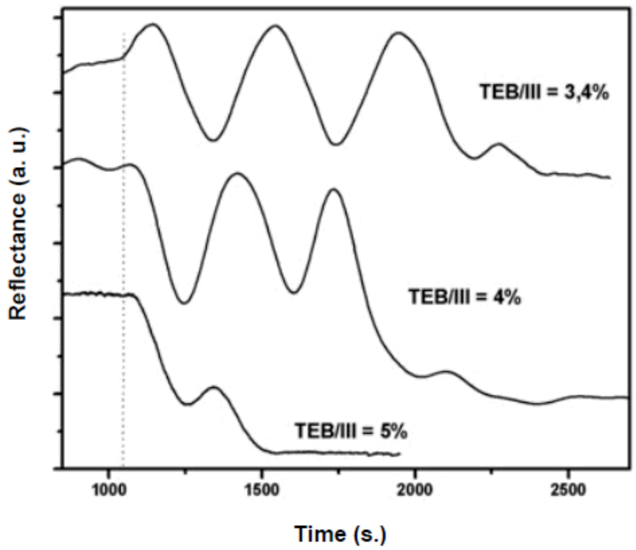
Growth structure:

0.01 – 1 µm BGaN film
1-3 µm AlN template layer
Sapphire

Challenges in BGaN Growth

Growth of BAlGaN alloys not yet extensively studied

- Few groups actively publishing on BGaN
- Typical B mole fractions **less than 5%**
- Simplistic calculations of B% in literature
- Rough surfaces, poor crystal quality



Growth temperature incompatibility

- Best boron nitride (h-BN) grown at >1300°C
- Best GaN grown at ~ 1050°C – GaN decomposes above 1000°C

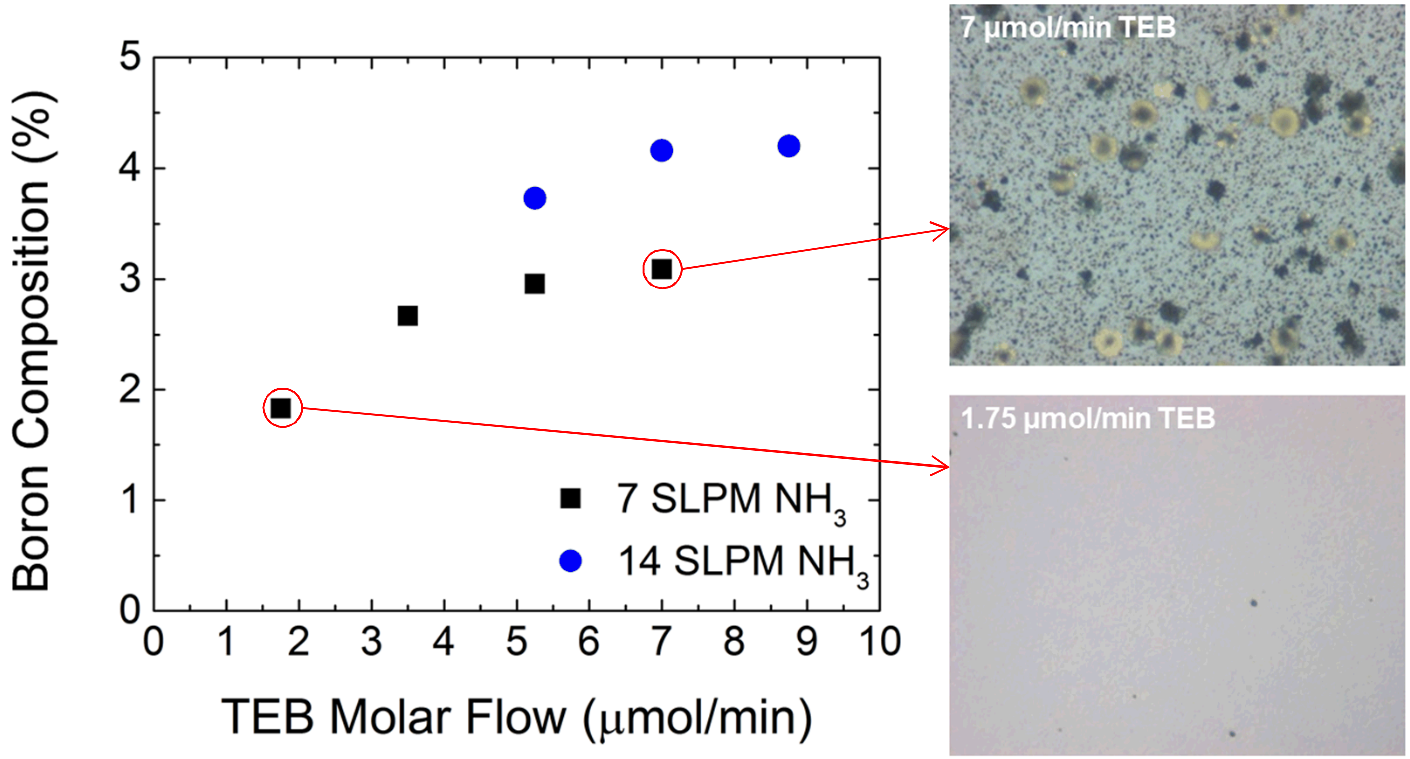
Potential obstacle with incomplete miscibility of B in GaN

- Calculated miscibility gap beginning at ~5% B in GaN

V. Ravindran, Ph.D. Thesis, Georgia Institute of Technology (2013).

Initial BGaN Work at Sandia

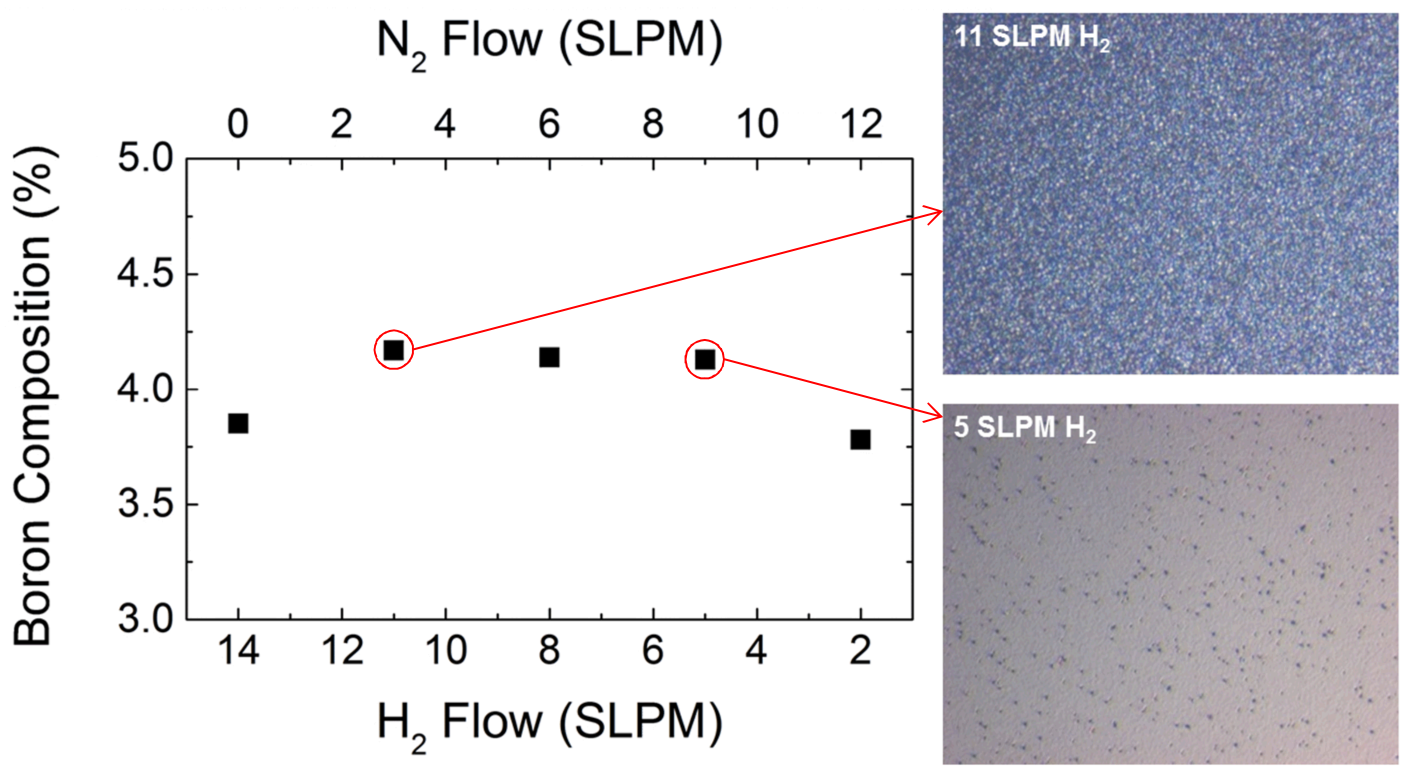
Sandia National Laboratories



Summary:

- Low temperature + high V/III ratio + low pressure
  - → Better B incorporation, better surfaces
- High TEB flow → rough, non-uniform surface and poor crystallinity

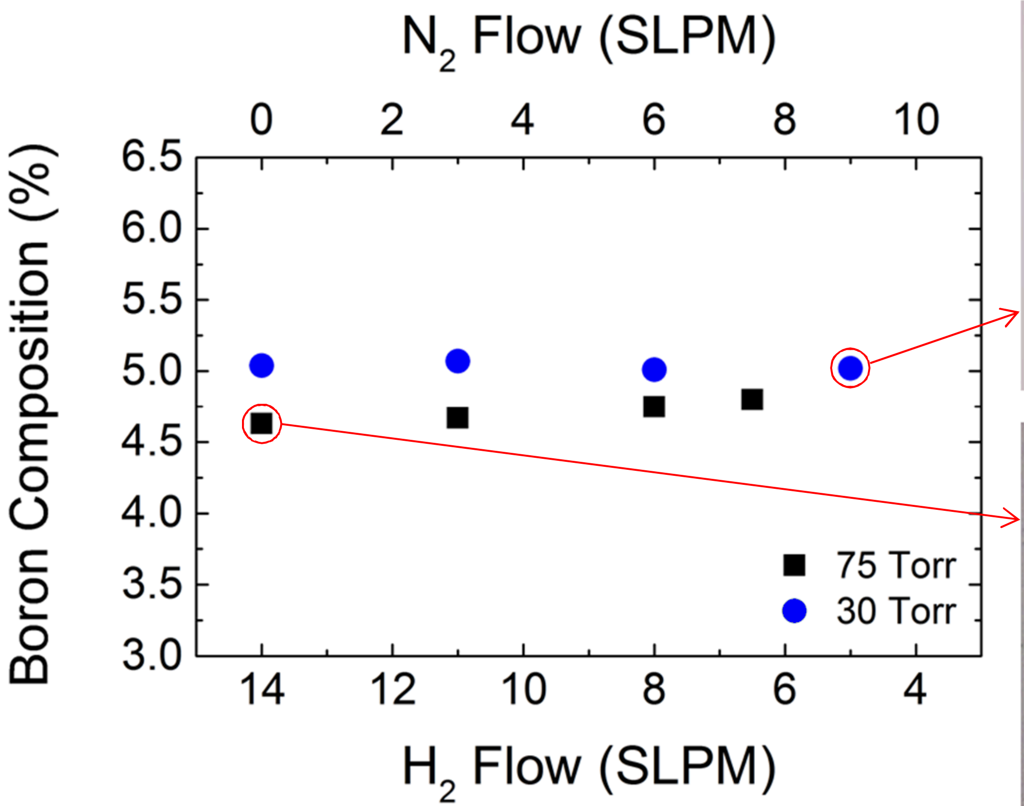
Initial BGaN Work at Sandia

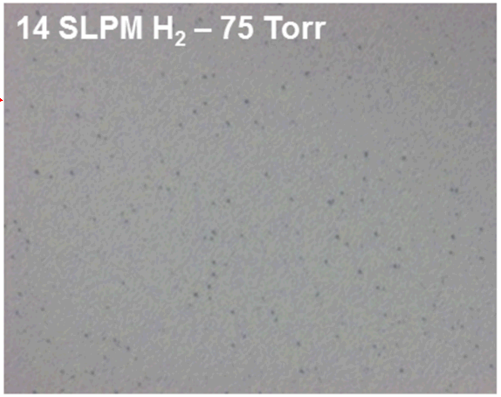


Summary:

- Low temperature + high V/III ratio + low pressure
  - → Better B incorporation, better surfaces
- High TEB flow → rough, non-uniform surface and poor crystallinity

Initial BGaN Work at Sandia





Final Conditions:

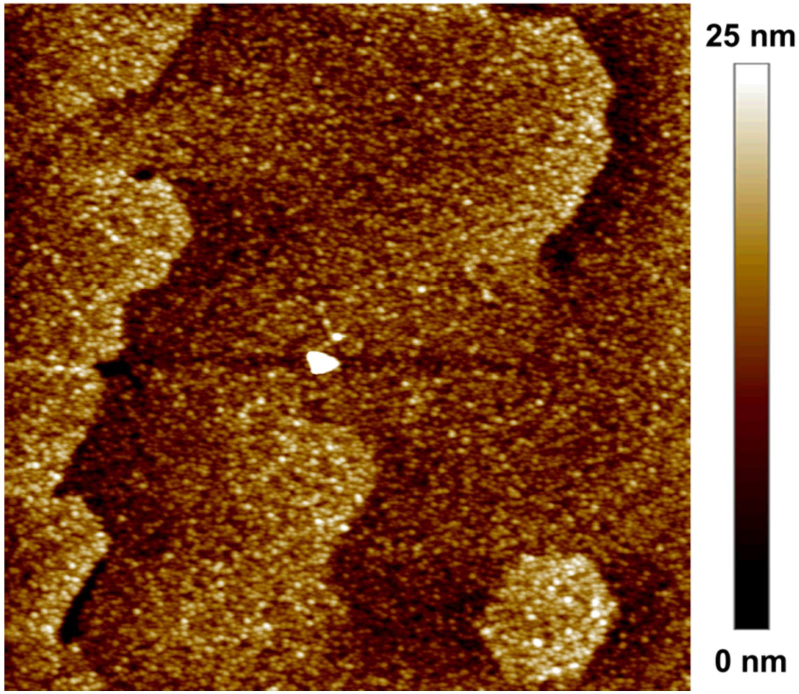
- Temperature: 750-800°C
- Pressure: 20 Torr
- NH_3 Flow: 14 SLPM
- N_2 carrier gas, no H_2

→ **B compositions ~3.5 – 5%**

BGaN Morphology

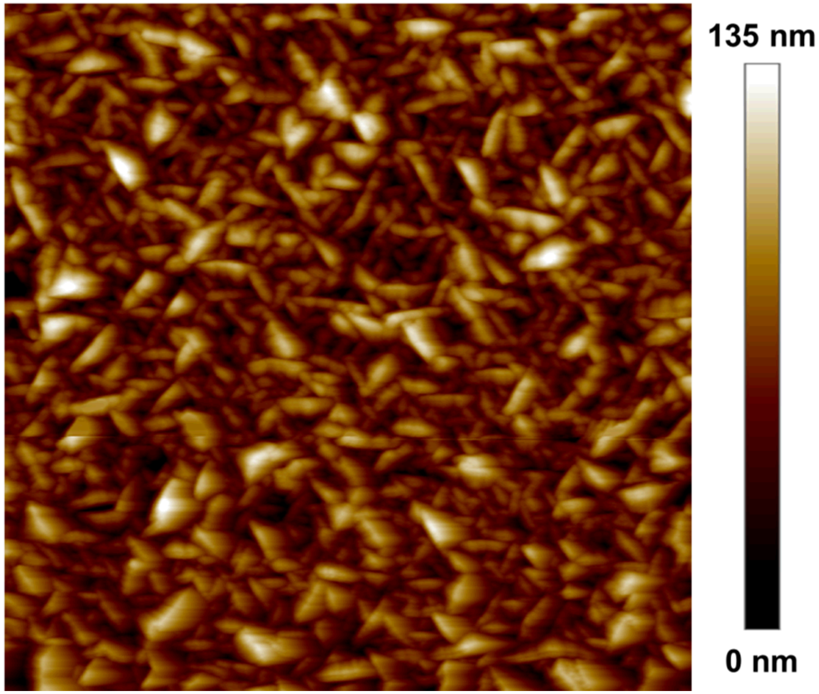
Boron composition ~3.7% (RBS-NRA)

~20 nm BGaN



~2.5 nm RMS

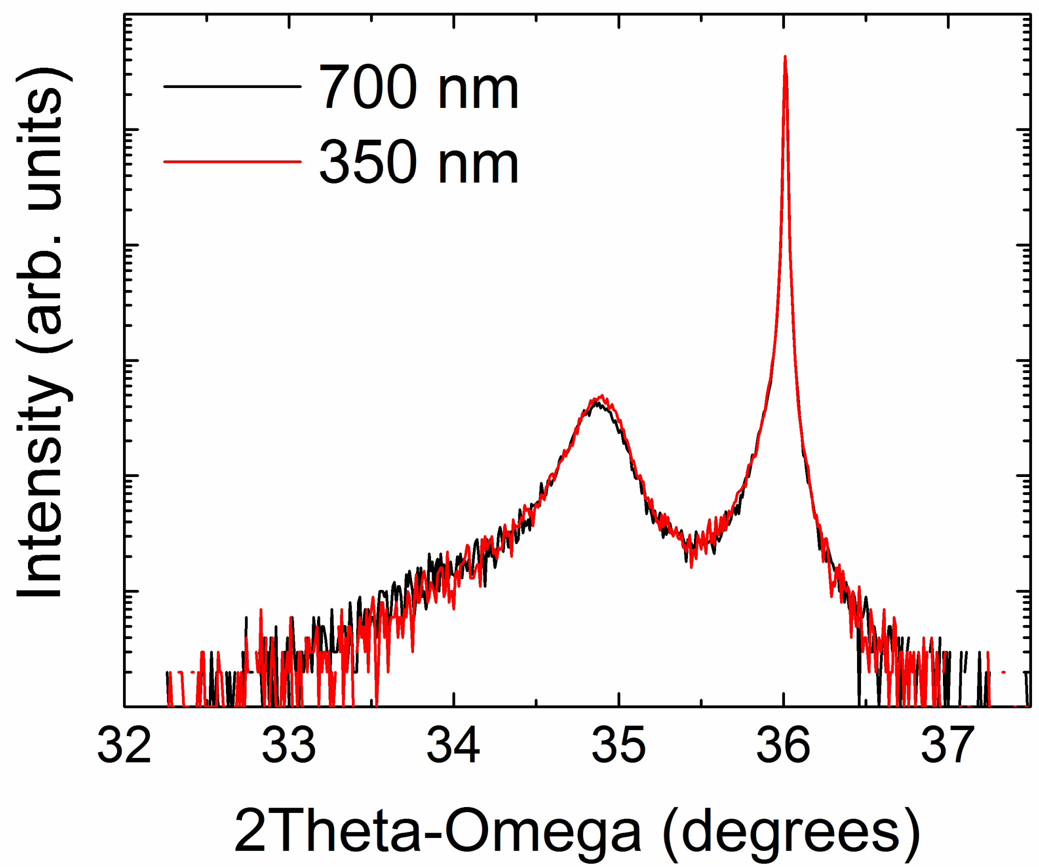
~700 nm BGaN



~20 nm RMS

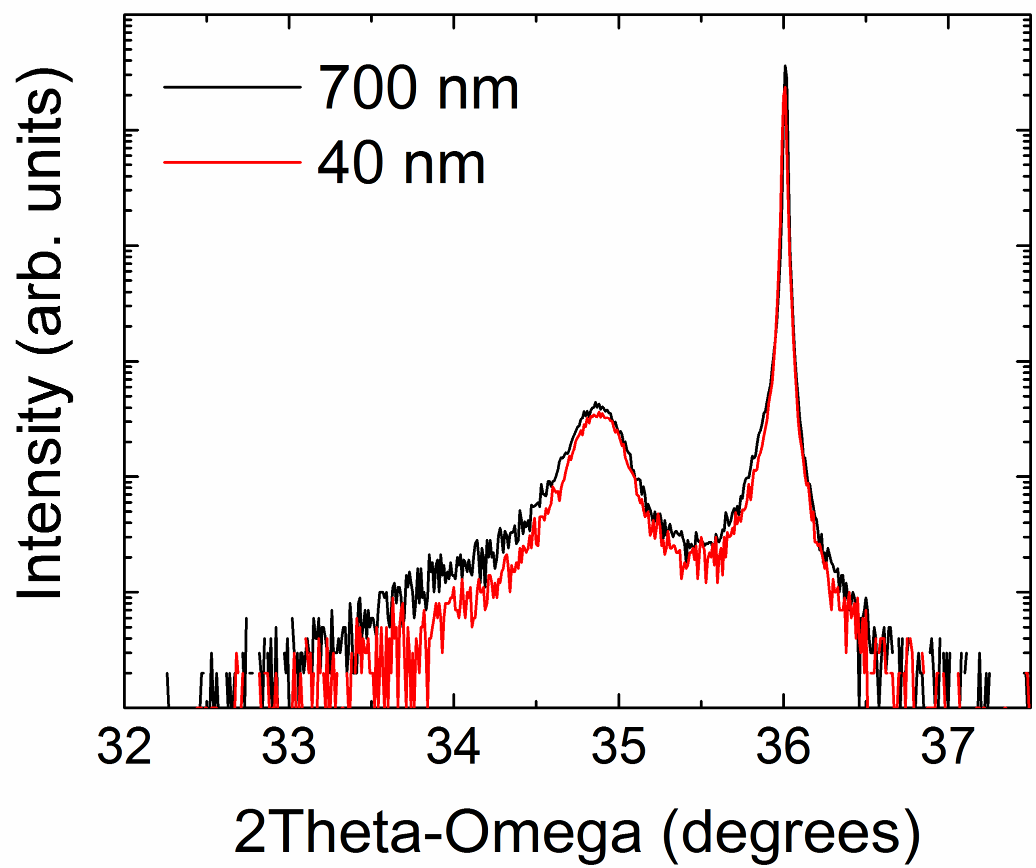
- Dramatic roughening with increasing thickness
- Possible crystallographic faceting (right)

BGaN XRD Intensity Observation



2x thickness, but nearly identical XRD scan

BGaN XRD Intensity Observation

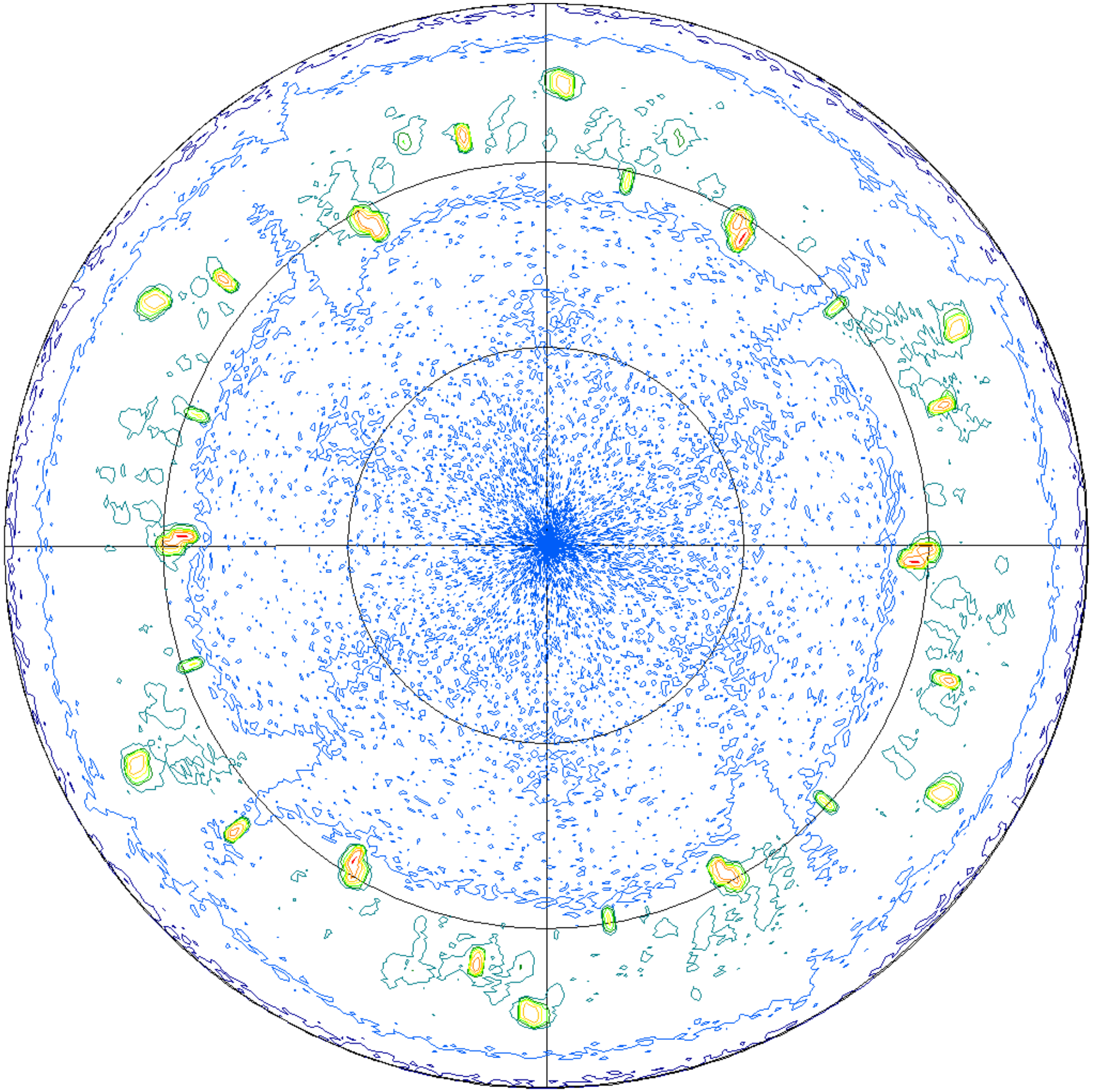


Nearly 20x thickness, but still minimal intensity change

X-ray Pole Figures

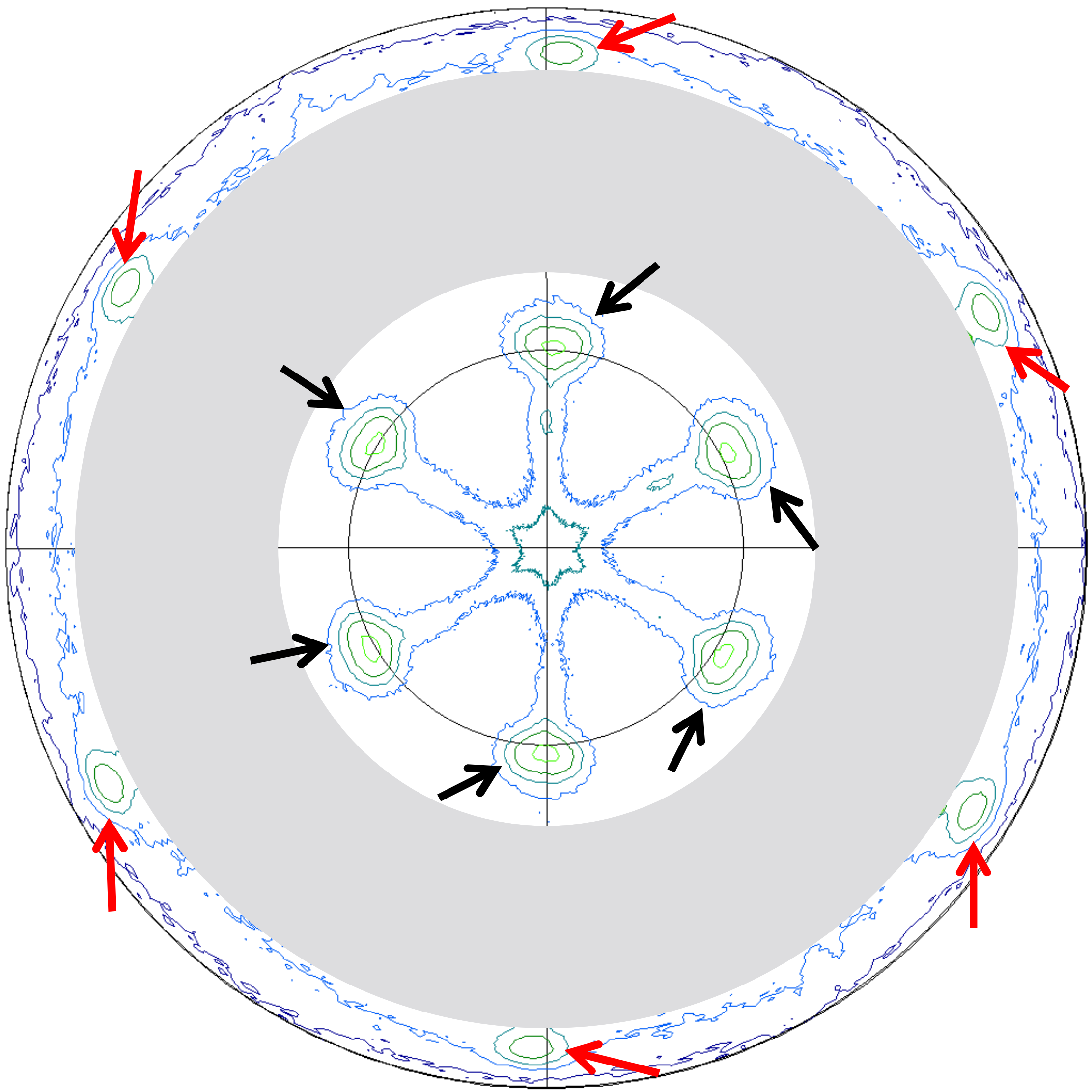
- Polar coordinate contour plot of intensity vs. Phi (Φ, 0-360°) and Chi (radius, 0-90°)
- Peaks from 55-76° related to wurtzite AlN reflections or sapphire substrate

Bare AlN Template

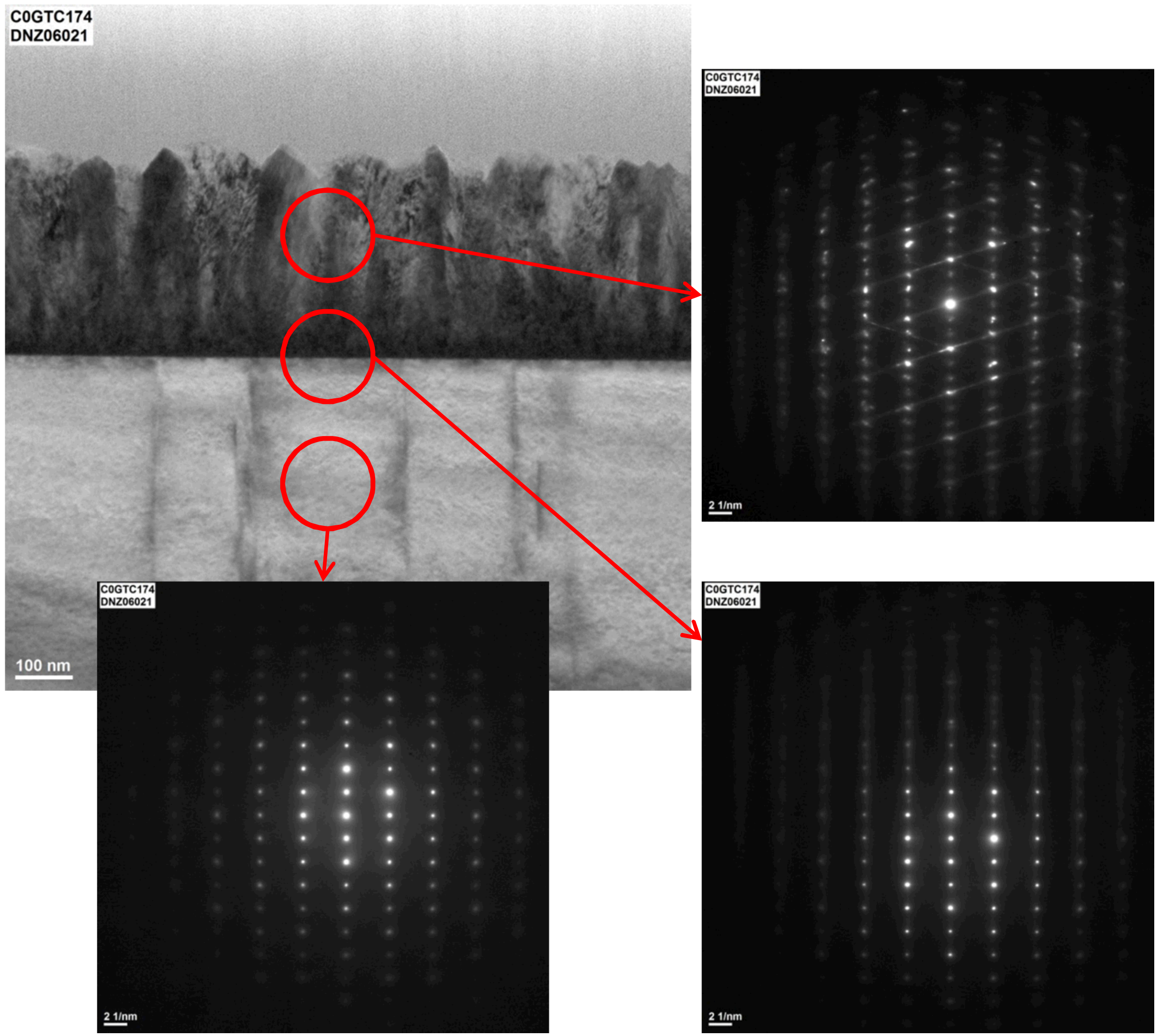


BGaN X-ray Pole Figures

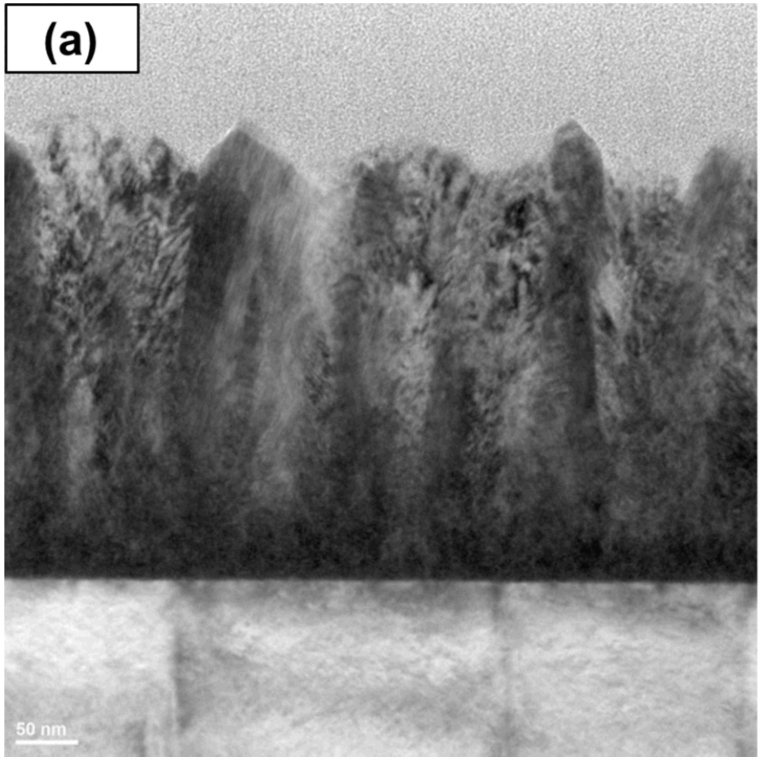
- Polar coordinate contour plot of intensity vs. Phi (Φ, 0-360°) and Chi (radius, 0-90°)
- Peaks from 55-76° related to wurtzite AlN/BGaN reflections or sapphire substrate
- Two sets of unidentified peaks with six-fold symmetry
  - ~31° → cubic (3 1 1)
  - ~81° → cubic (3 -1 -1)
  - Six-fold symmetry suggests twinning

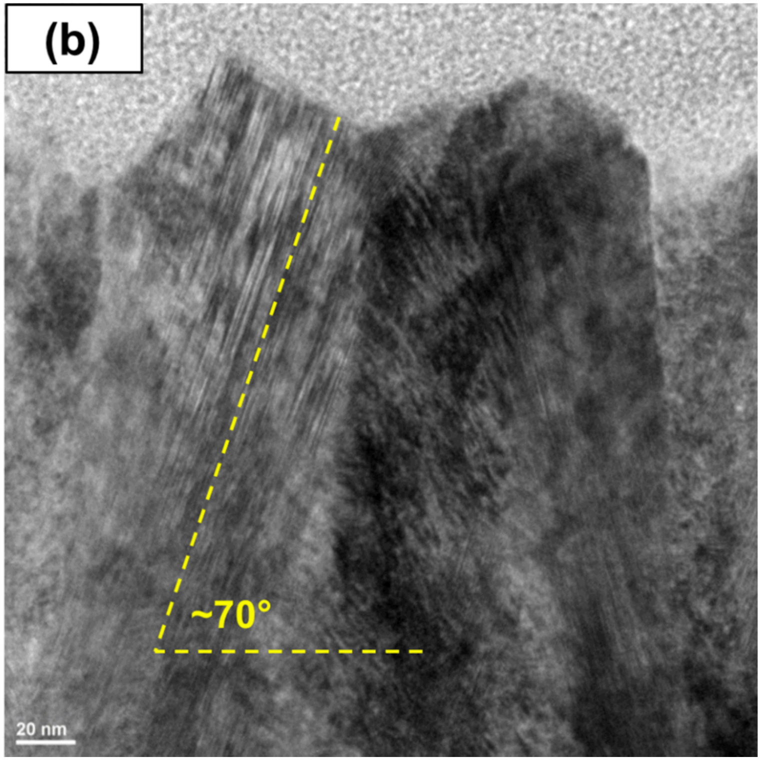


BGaN TEM & SAED



BGaN TEM – Cubic Phase Confirmation





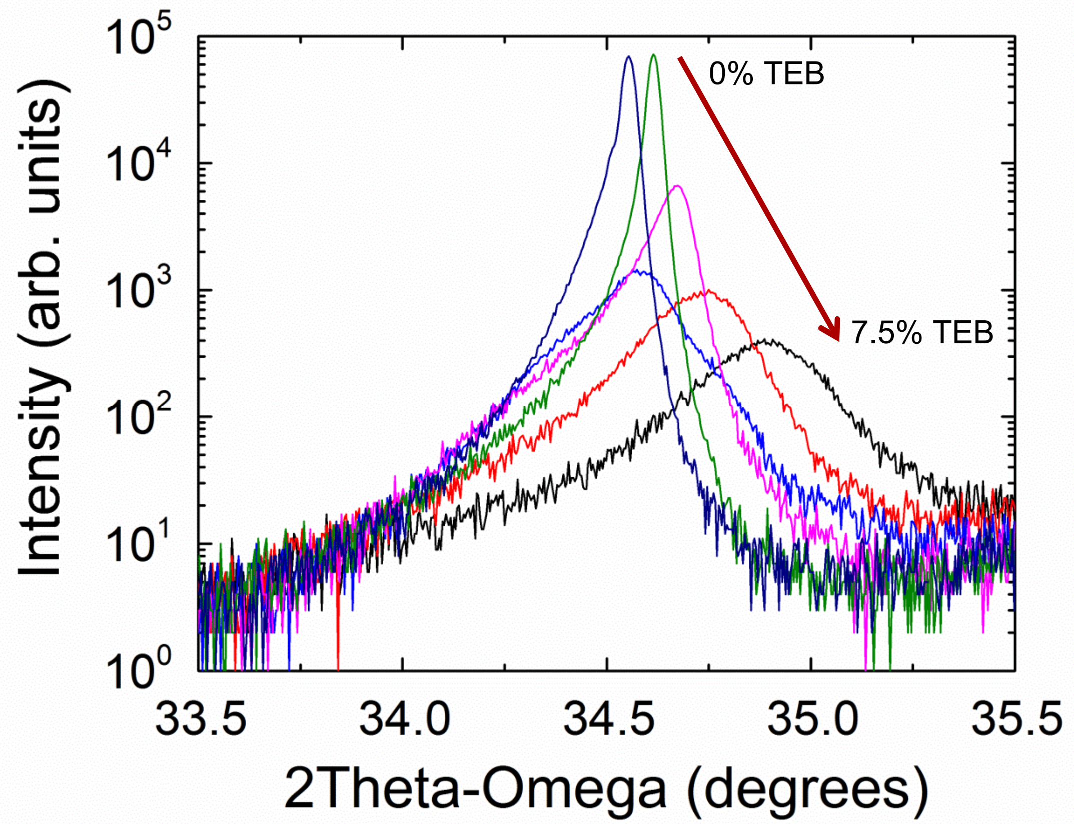
- Stacking faults tilted by ~70° relative to substrate
- <110> {111} slip system in zinc-blende crystal
  - → Basal plane stacking faults on equivalent (1 1 1) planes
  - → 70.5° angle between (1 1 1) and (1 -1 1) planes

XRD: Varied TEB

- Clear evolution from sharp, intense XRD peaks (<1% TEB) to broad, weak peaks (>1% TEB)

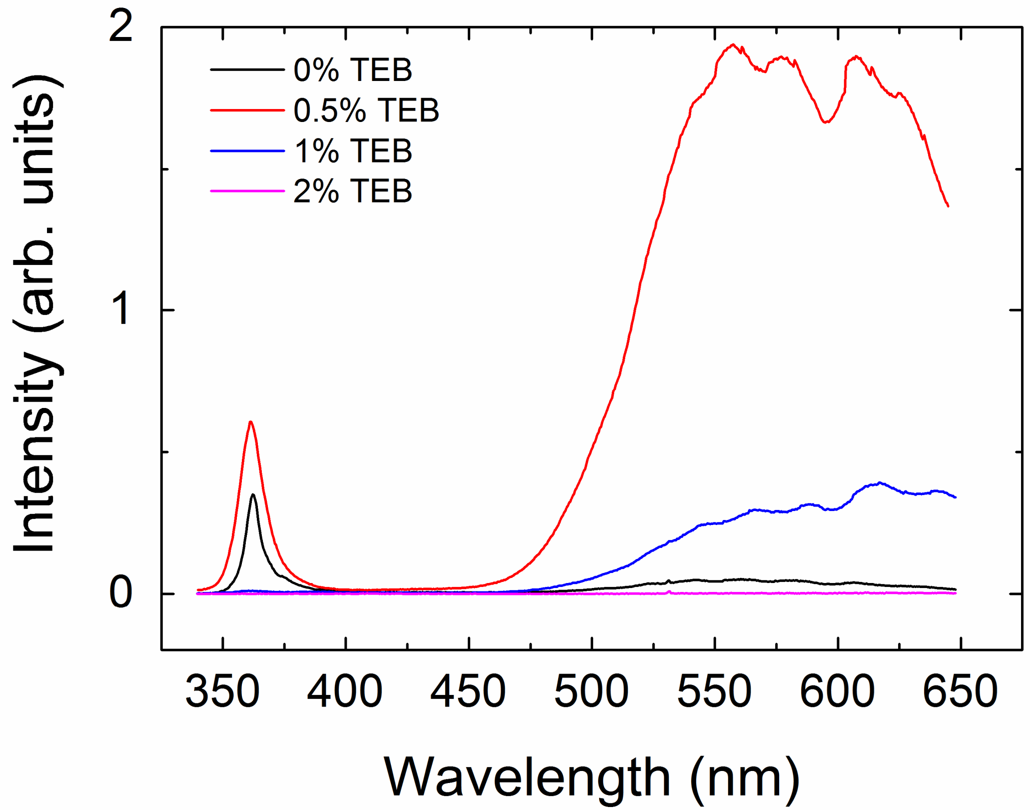
- Correlation with photoluminescence
  - 0% TEB → strong band-edge, weak deep-level
  - 0.5% TEB → band-edge, intense deep-level PL
  - 1% TEB → little/no band-edge, weak deep-level PL
  - >1% TEB → little/no PL

- Pole figures show cubic features in all cases except pure GaN (0% TEB)



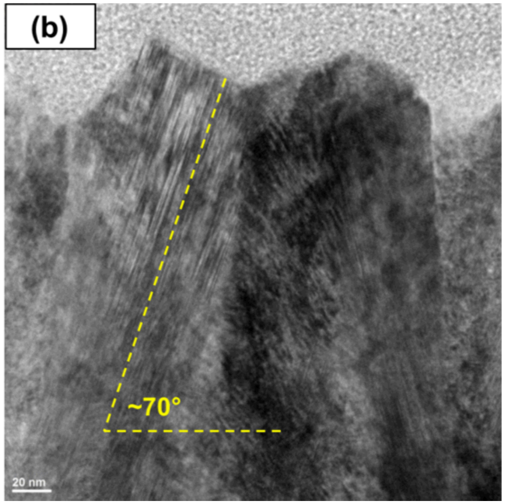
PL: Varied TEB

- Clear evolution from sharp, intense XRD peaks (<1% TEB) to broad, weak peaks (>1% TEB)
- Correlation with photoluminescence
  - 0% TEB → strong band-edge, weak deep-level
  - 0.5% TEB → strong band-edge & deep-level PL
  - 1% TEB → little/no band-edge, weak deep-level PL
  - >1% TEB → little/no PL
- Pole figures show cubic features in all cases except pure GaN (0% TEB)



Summary

- **Initial BGaN investigation**
  - GaN-like conditions → rough surfaces, poor boron incorporation
  - Low T, low P, N_2 carrier gas → up to 5% boron, specular surfaces
- **Deeper BGaN structural characterization**
  - Dramatic roughening with increasing thickness
  - Thicker films → saturated XRD intensity
  - Strong cubic contribution in x-ray pole figure
  - TEM confirms (111)-oriented twinned cubic structure



- **Investigate onset of cubic phase**
  - Wurtzite to cubic transition with increasing TEB flow
  - PL signal correlated with apparent wurtzite/cubic transition
  - Cubic phase present in all cases except for pure GaN

Phase Degradation in $B_xGa_{1-x}N$ Films Grown at Low Temperature by Metalorganic Vapor Phase Epitaxy

Brendan P. Gunning,
Michael W. Moseley, Daniel D. Koleske,
Andrew A. Allerman, Stephen R. Lee

Sandia National Laboratories
Albuquerque, New Mexico, USA, 87123

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration LOCKHEED MARTIN

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

bpgunni@sandia.gov