SAND2015-6354C

Growth of BGaN Alloys on AlN

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

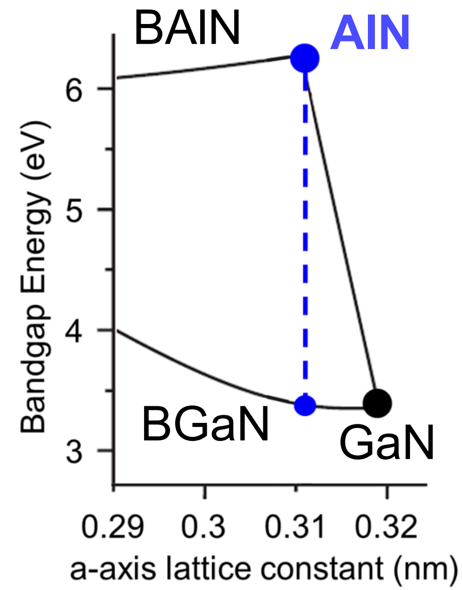
Sandia National Laboratories,
Albuquerque, New Mexico, USA, 87123

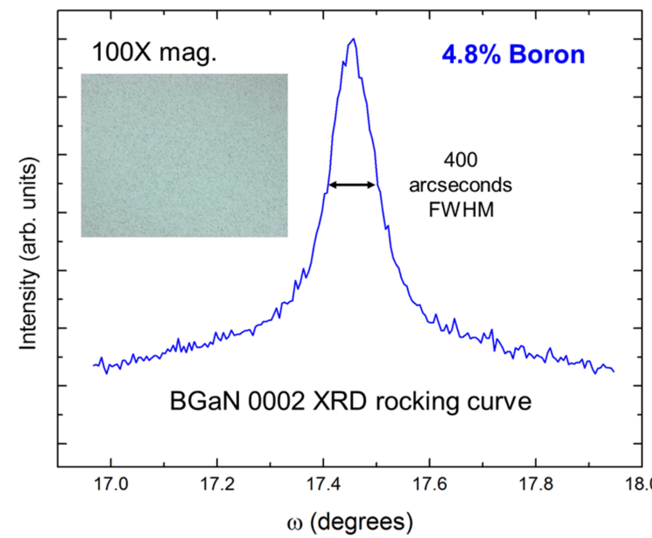
U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
LOCKHEED MARTIN
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear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

mwmosel@sandia.gov

Outline

- **Background**
  - Dislocation generation
  - Opportunities for lattice-matched epitaxy
- **Investigation of BGaN alloys**
  - Add TEB flow to GaN growth
  - Accurate calculation of B%
- **Explore effect of carrier gas**
  - Morphology
  - Crystal structure
- **Lower temperature/pressure growth**
  - 5% boron mole fraction

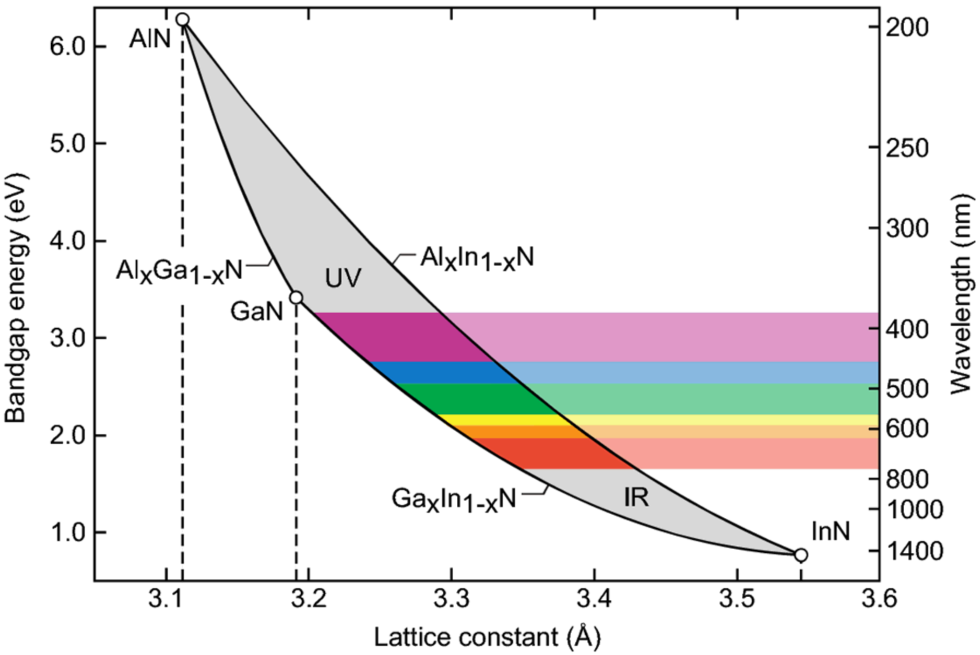




Group-III Nitrides - Challenges

Sandia National Laboratories

Substrate choice and trade-offs



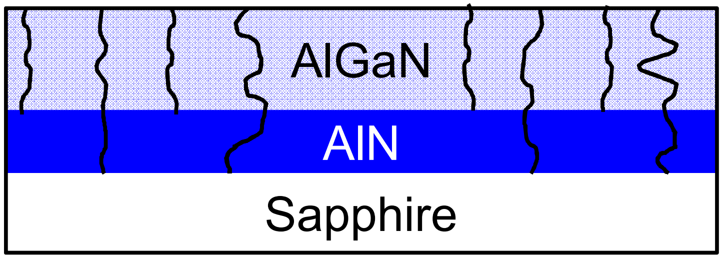
Substrate	Mismatch to GaN	Additional notes
Sapphire	14%	**Cheap**, electrically and thermally insulating
SiC	3.1%	**Expensive**, electrically and thermally conductive
Si (111)	17%	Cheap, mature, **forms amorphous SiN layer**
Bulk GaN/AlN	0%	**Expensive**, maturing technology

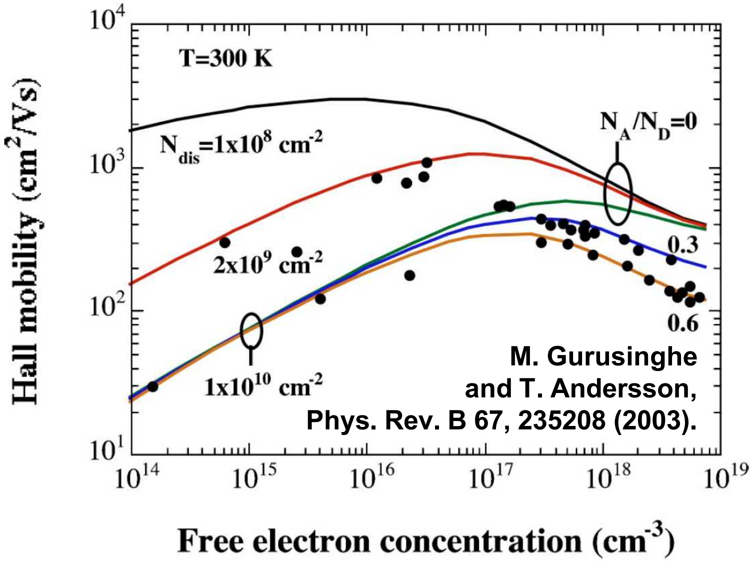
M. F. Schubert, Ph.D. Thesis, Virginia Polytechnic Institute and State University, 2009.
J. Wu, *J. Appl. Phys.* **106**, 011101 (2009)
G. Namkoong et al., *Appl. Phys. Lett.* **87**, 184104 (2005).
A. Janotti and C. G. Van De Walle, *Rep. Prog. Phys.* **72**, 126501 (2009).
G. Namkoong et al., *Thin Solid Films* ***517**, 6508* (2009).
L. M. Sorokin et al., *Tech. Phys. Lett.* **37**, 326 (2011).

No native substrate for AlGaN alloy growth

Group-III Nitrides - Dislocations

- **Dislocations generated from heteroepitaxy**
  - Lattice mismatch
  - Impact device performance
- **Act as compensating centers**
  - Scatter charge carriers
  - Reduce carrier mobility
  - Reduce minority carrier lifetime
- **Act as current leakage sites**
  - Premature breakdown voltages
  - Increases resistive losses





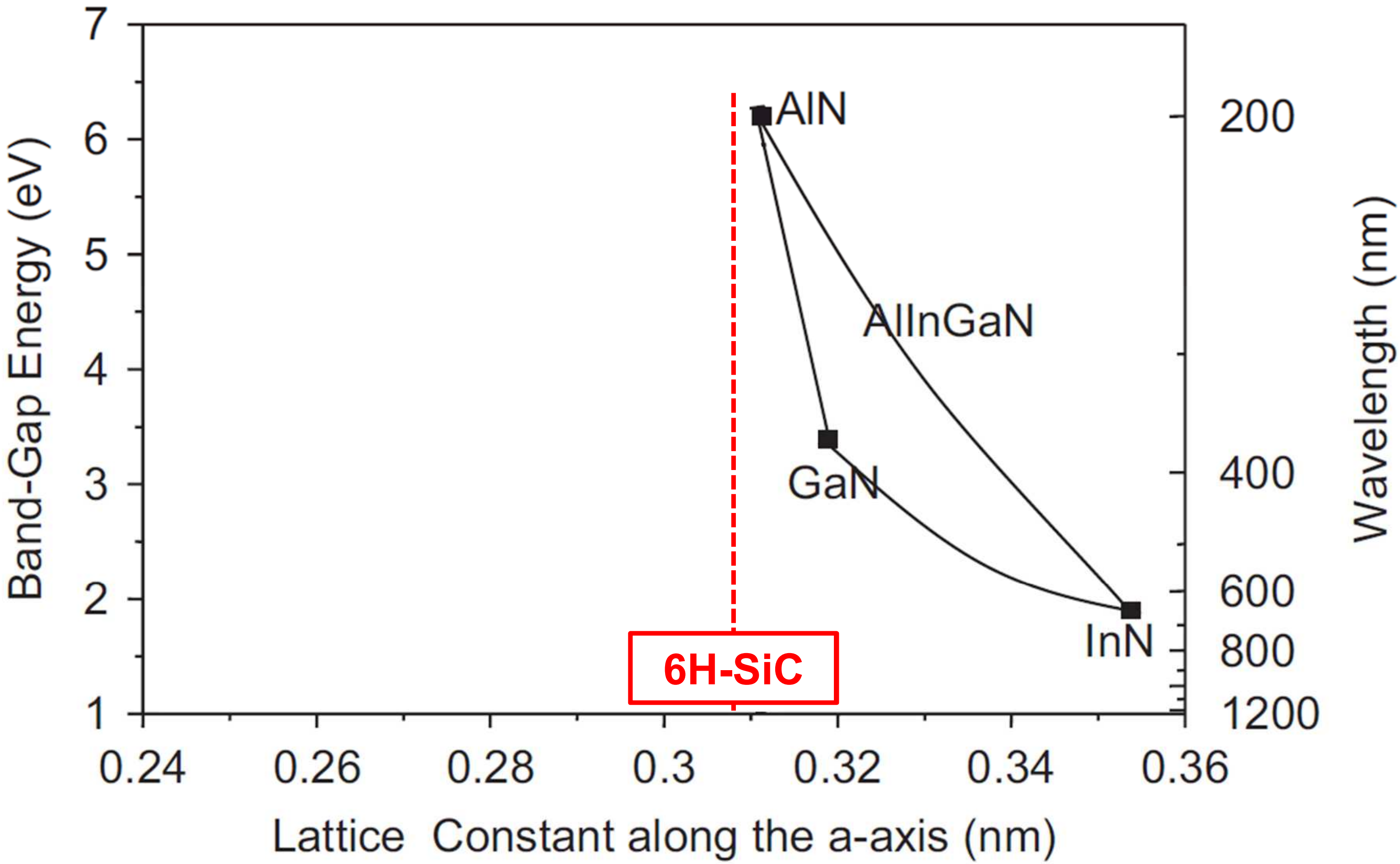
Can we prevent dislocations via novel materials?

A. Wickenden et al., Growth **260,** 54 (2004).
M. Khan et al., PESC 2005, pg 15 (2005).
Z. Bandić et al., Appl. Phys. Lett. **74,** 1266 (1999).
S. W. Kaun et al., Appl. Phys. Express **4,** 024101 (2011).

AlInGaN materials system

Sandia National Laboratories

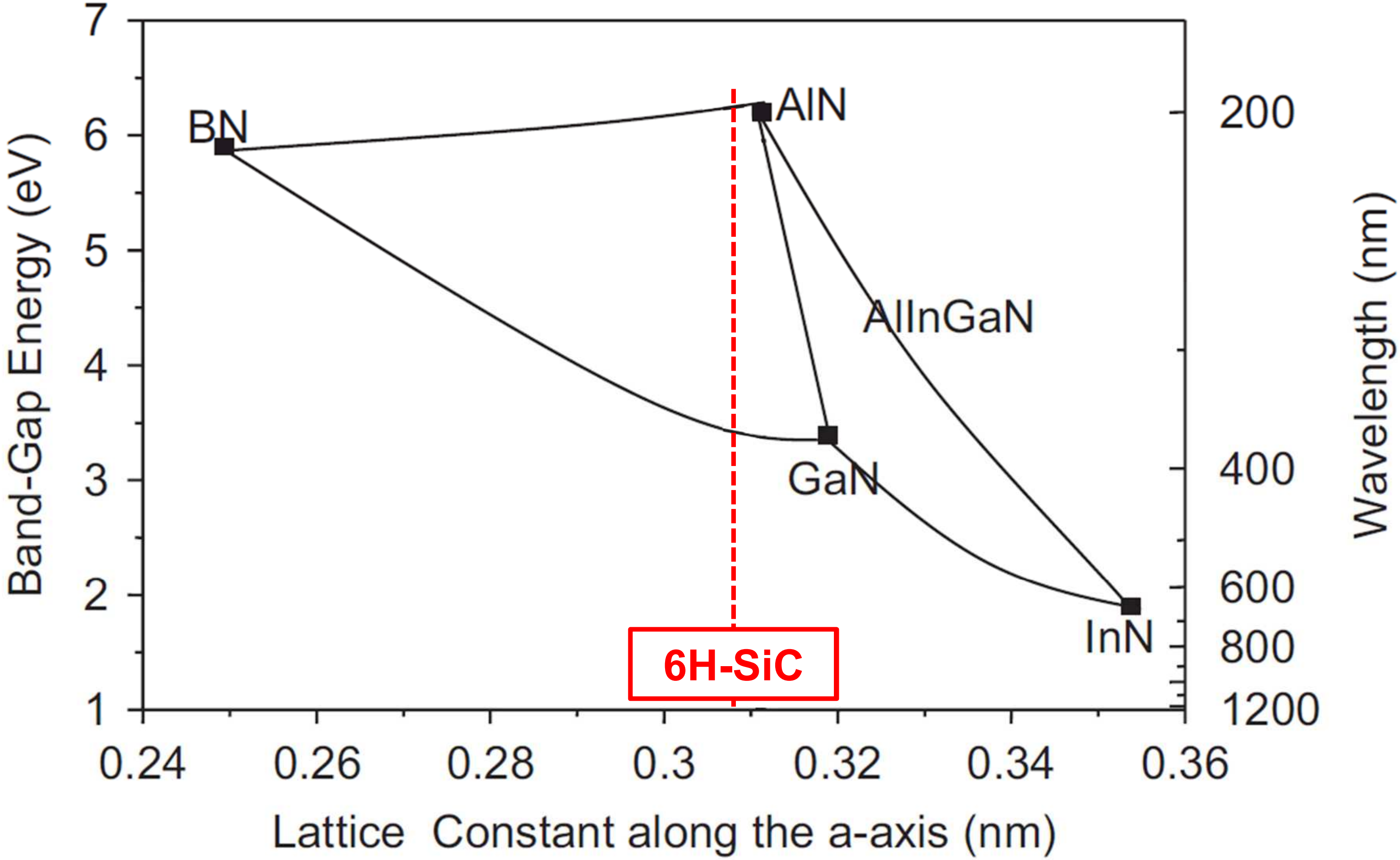
Familiar territory, well explored



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

Boron-containing nitride alloys

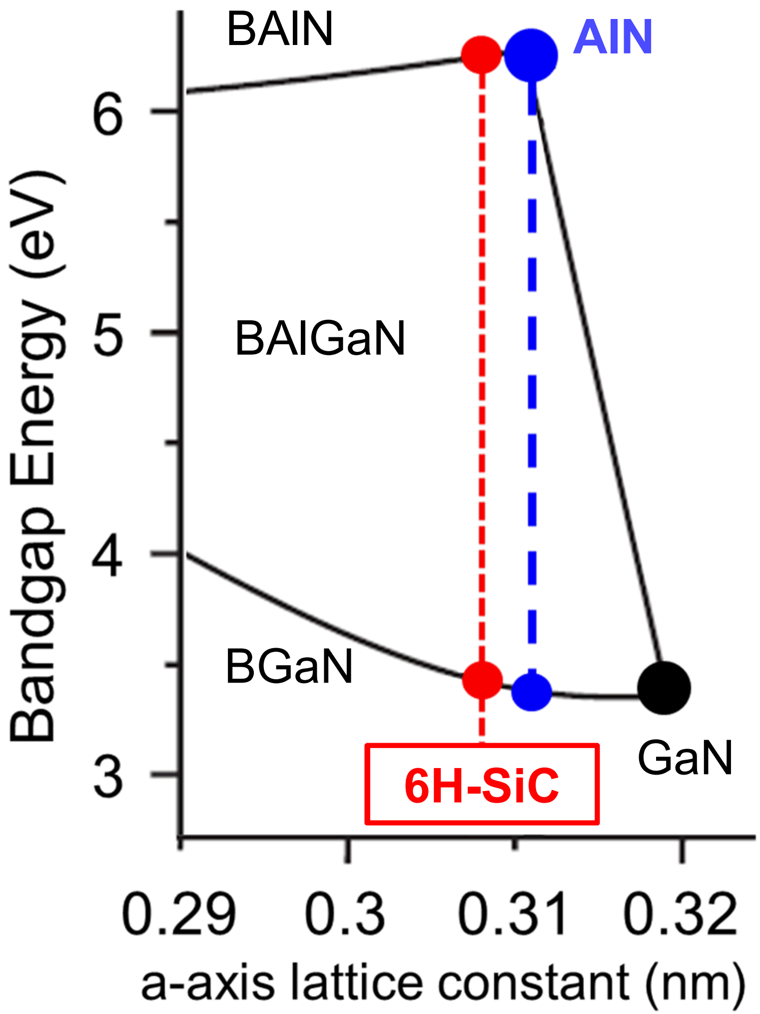
New opportunities for wide-bandgap lattice engineering!



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

BGaN and BAlN

Expanded view:

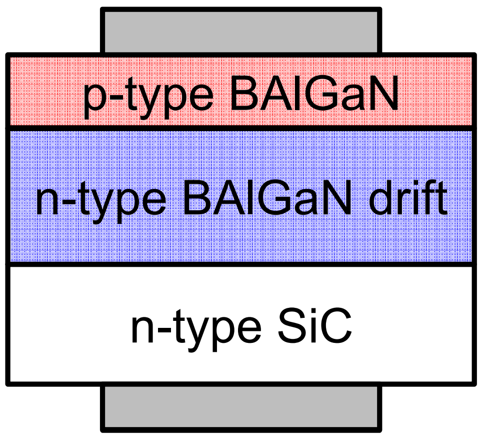


after Ougazzaden, J. Cryst. Growth (2007).

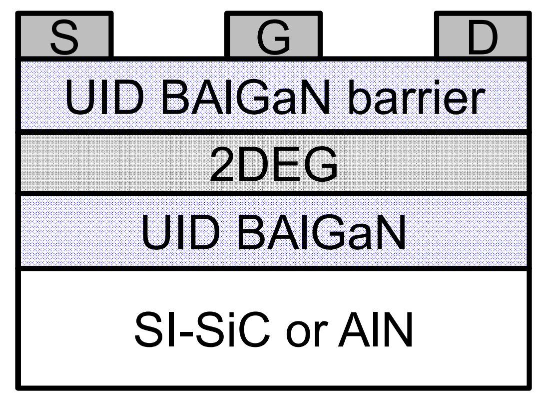
Lattice-matching opportunities:

$B_{0.08}Ga_{0.92}N$ on AlN
$B_{0.17}Ga_{0.83}N$ on 6H-SiC
$B_{0.05}Al_{0.95}N$ on 6H-SiC

Device prospects:



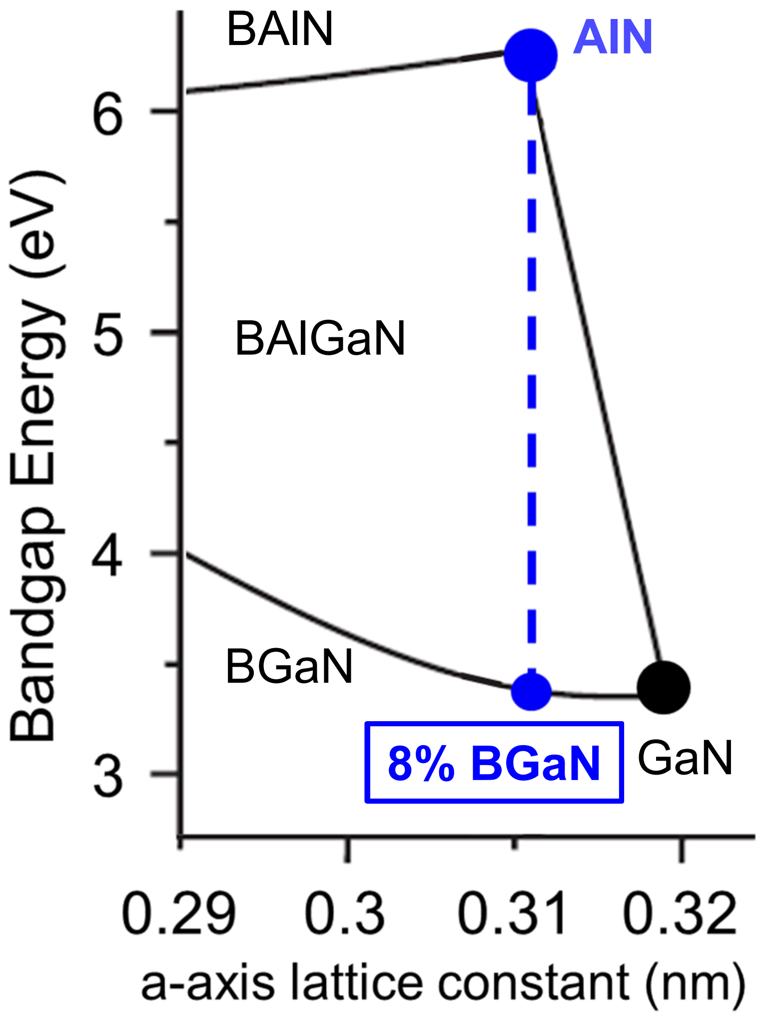
Two-terminal vertical device



Three-terminal lateral device

BGaN and BAlN

Expanded view:



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

Lattice-matching opportunities:

$B_{0.08}Ga_{0.92}N$ on AlN ←
$B_{0.17}Ga_{0.83}N$ on 6H-SiC
$B_{0.05}Al_{0.95}N$ on 6H-SiC

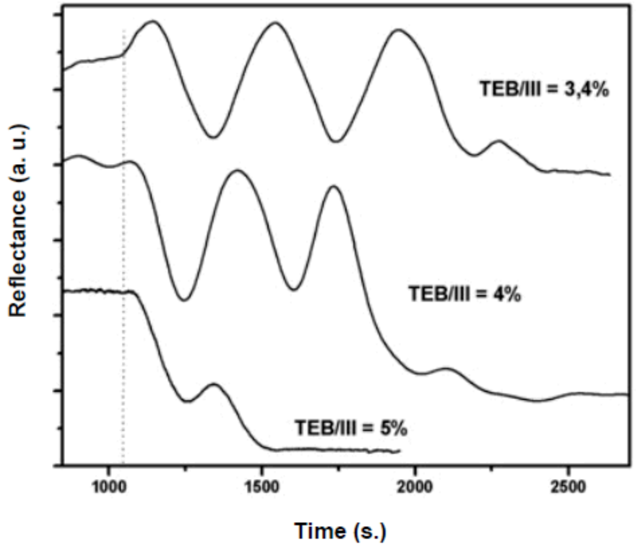
Growth structure:

0.1 – 1 µm BGaN overgrowth
1.4 µm AlN buffer layer
Sapphire

Challenges

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 and pitted surfaces



Growth temperature incompatibility

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

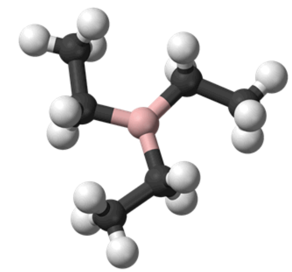
Potential obstacle with incomplete miscibility of B in GaN

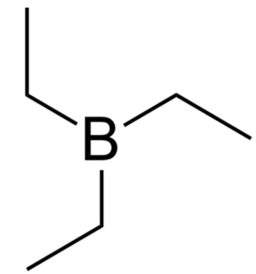
T. Malinauskas et al., Phys. Status Solidi B **252,** (2014).
S. Gautier et al., J. Cryst. Growth **312,** 641 (2010).
S. Gautier et al., J. Cryst. Growth **315,** 288 (2011).
T. Takano et al., J. Cryst. Growth **237,** 972 (2002).
A. Polyakov, et al., Journal of Elec Materi **26,** 237 (1997).
S. Majety et al., Appl. Phys. Lett. **101,** 051110 (2012).
C. Wei and J. Edgar, J. Cryst. Growth **208,** 179 (2000).
L. K. Teles et al., Physica E **13,** 1086 (2002).
V. Ravindran, Thesis (2013).

Goals

Goal: 8% BGaN lattice-matched to AlN

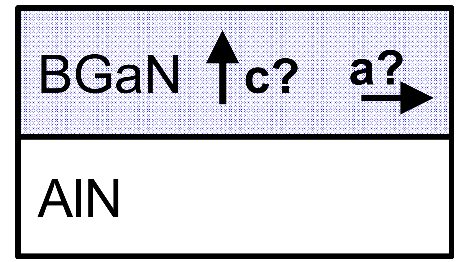
- Less than 8%, compressive strain
- Use triethylboron (TEB)
- Start investigation with GaN conditions + TEB
- 800 °C, 75 Torr





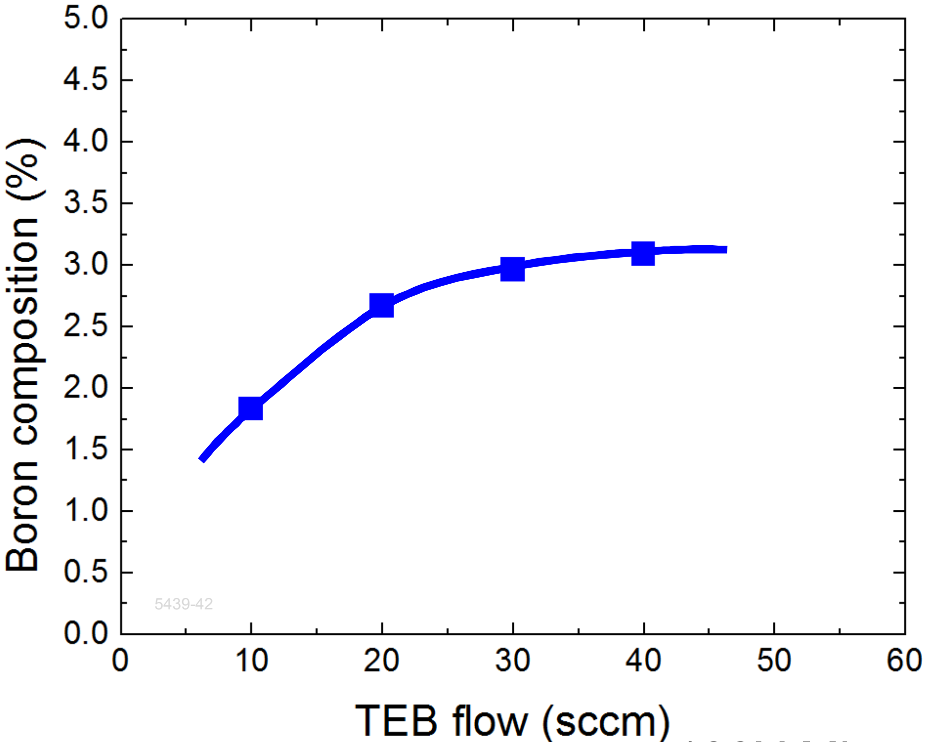
Develop accurate calculation of B% via XRD

- Calculate in-plane and out-of-plane lattice constants



6	INPUT														
7	PARAMETERS	a	c	a/c	c13	c33	-2c13/c33						lambda		
8		(A)	(A)	(---)	(GPa)	(GPa)	(---)						(A)		
9	GaN:	3.1889	5.1852	1.62602	103	405	-0.5086						1.5405981		
10	AlN:	3.1113	4.9799	1.60058	108	373	-0.5791								
11	BN:	2.55	4.17	1.63529	74	1077	-0.1374								
12		epilayer	epilayer	epilayer	2theta (deg.)				h,k,m=					zero offset corrected:	
13	2-THETA	xrd	target	design		(000n)	(000n)	(000n)	1	(hk.m)	(hk.m)	(hk.m)	(hk.m)	(000n)	(hk.m)
14	MEASUREMENTS	peak	composition	thickness	n=	d	c	|K|	0	d	|K|	Kpara	a	2theta	2theta
15		id:	(---)	(um)	4	(A)	(A)	(1/A)	1	(A)	(1/A)	(1/A)	(A)	(degrees)	(degrees)
16	direct beam:		-------	-------	0.0000				0.0000						
17	peak 1:	AlN	-------	-------	76.3927	1.245717	4.9829	5.04383	37.9333	2.370022	2.6511	2.3320	3.1111	76.3927	37.9333
18	peak 2:	BGaN	-------	-------	73.2200	1.291657	5.1666	4.86444	36.9850	2.428581	2.5872	2.2835	3.1772	73.2200	36.9850
19															
20															
21				measured			measured	measured	pseudomorphic	measured				ITERATE "estimated alloy	
22	ANALYSIS	measured	measured	BN	unstrained	unstrained	parallel	perp	coh. strain	relaxation				estimated	computed
23	RESULTS	a	c	mole fraction	a0	c0	strain	strain	on AlN	on AlN				alloy	alloy
24		(A)	(A)	(---)	(A)	(A)	(---)	(---)	(---)	(%)				x	x
25	AlN	3.1111	4.9829	0.990	3.1121	4.9820	-0.00031	0.00018						1.0000	0.9899
26	BGaN	3.1772	5.1666	0.018	3.1772	5.1666	-0.00001	0.00001	-0.02080	99.9%				0.0183	0.0183

Initial results



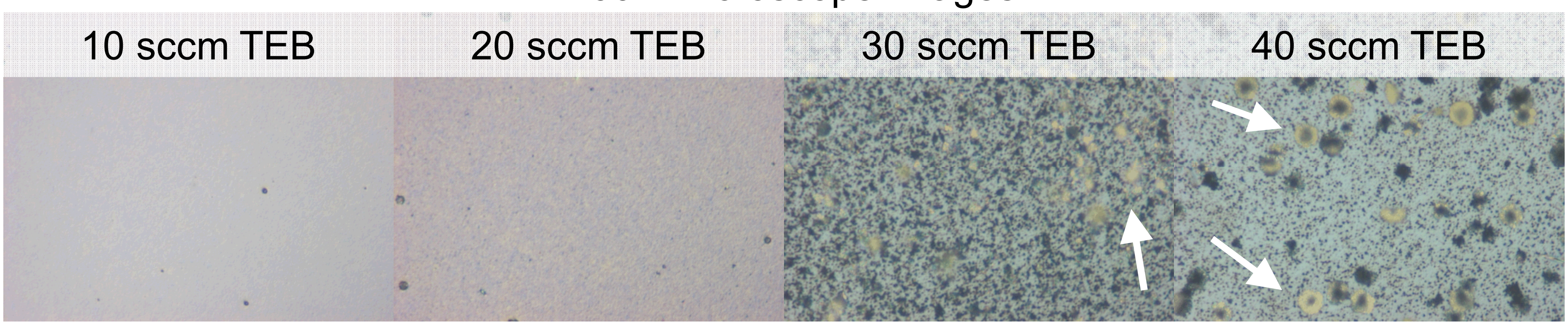
Observations

- Smooth surfaces with low TEB
- B% sublinear vs. TEB flow
- Some B not incorporated
- >4% B, but rough surfaces

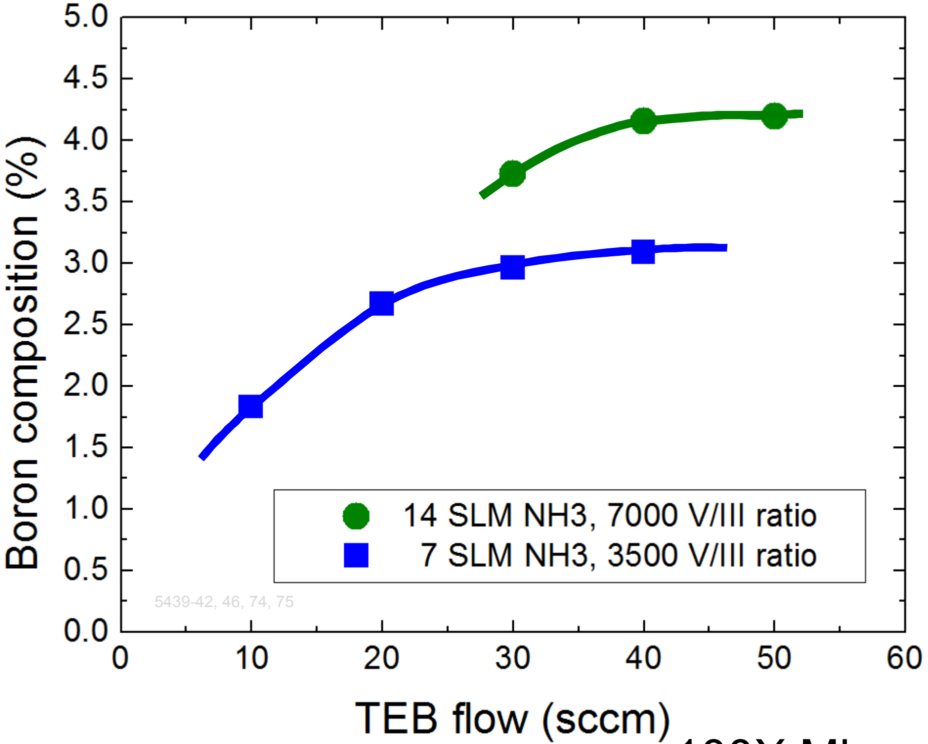
Yellowish clusters

- Excess boron?
- Increase in size with more TEB

100X Microscope Images



Initial results

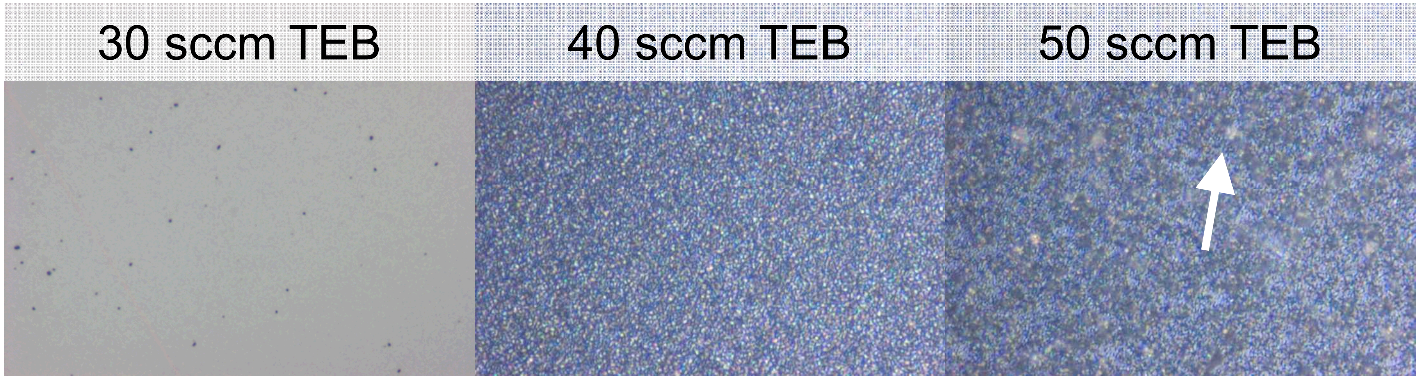


Higher V/III ratio

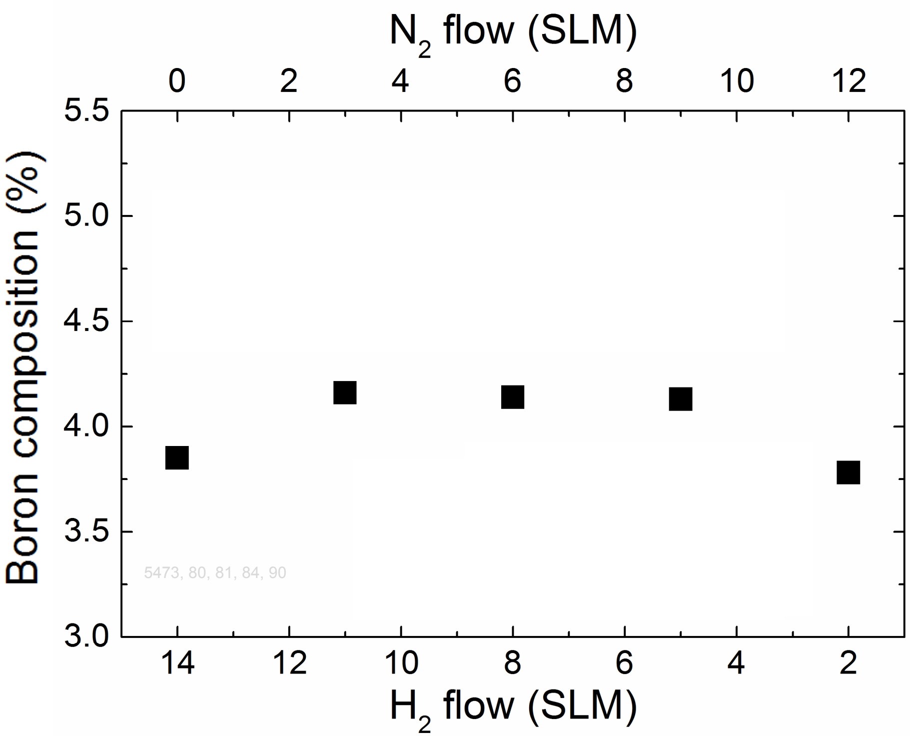
- More B incorporated
- Still sublinear
- Still exhibits yellow clusters
- >4% B, but rough surfaces

Non-optimized conditions, warrants phase-space search

100X Microscope Images



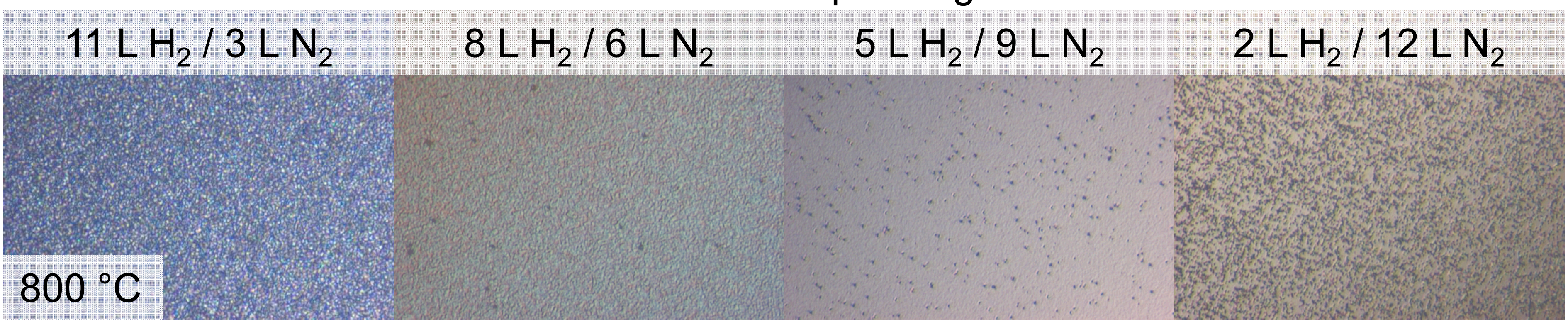
H_2:N_2 carrier gas ratio



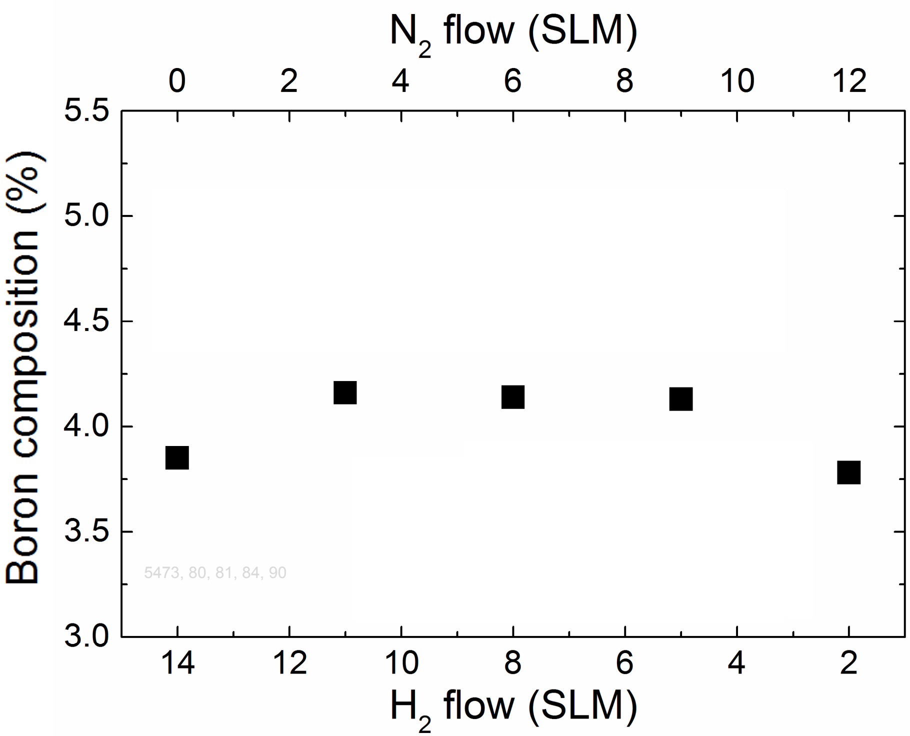
Morphology

- More H_2 → rough surface
- More N_2 → pitted surface

100X Microscope Images



H_2:N_2 carrier gas ratio



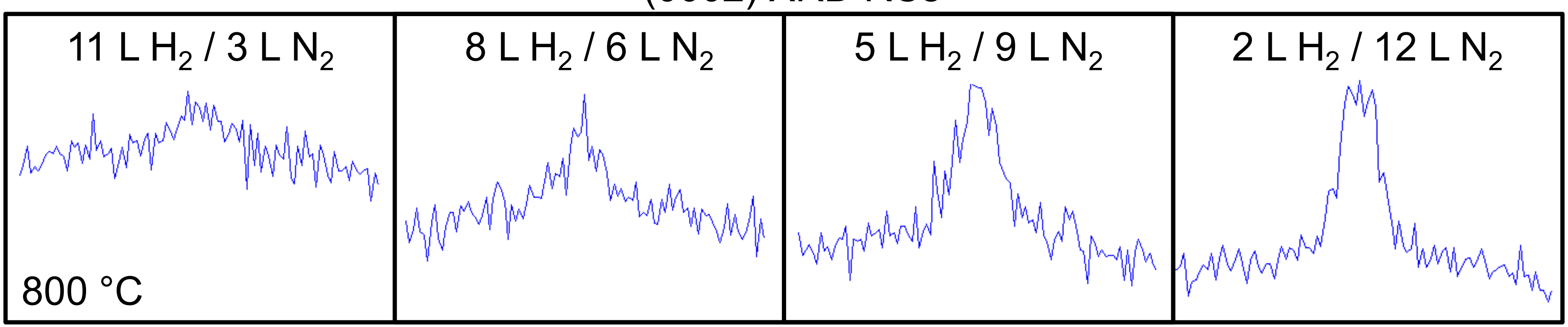
Morphology

- More H_2 → rough surface
- More N_2 → pitted surface

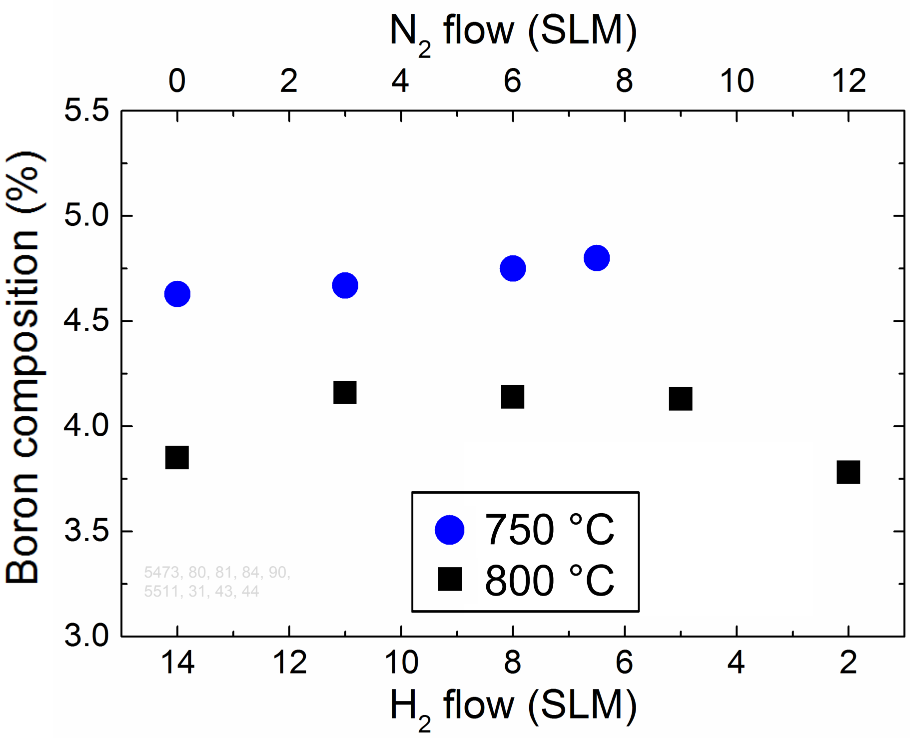
Crystal structure

- More H_2 → isolated, tilted grains
- More N_2 → coherent grains

(0002) XRD RCs



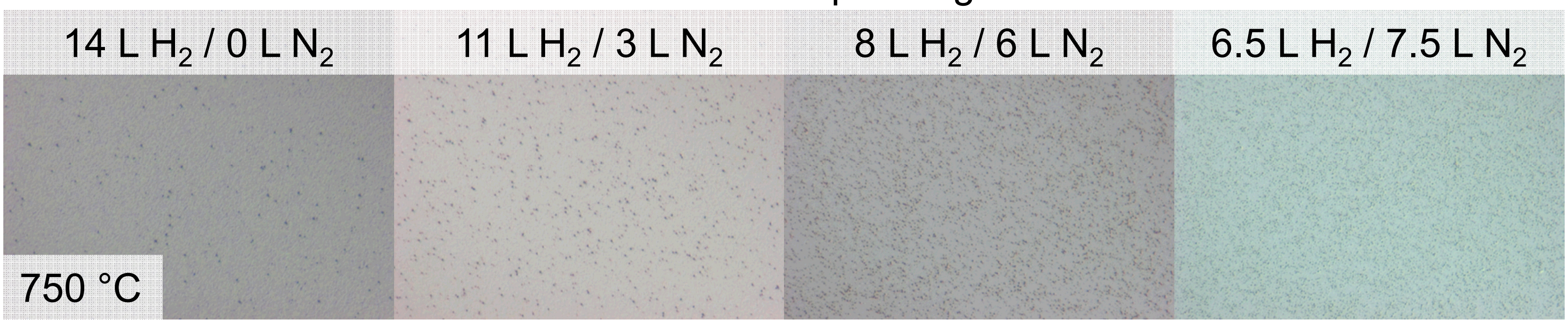
H_2:N_2 carrier gas ratio



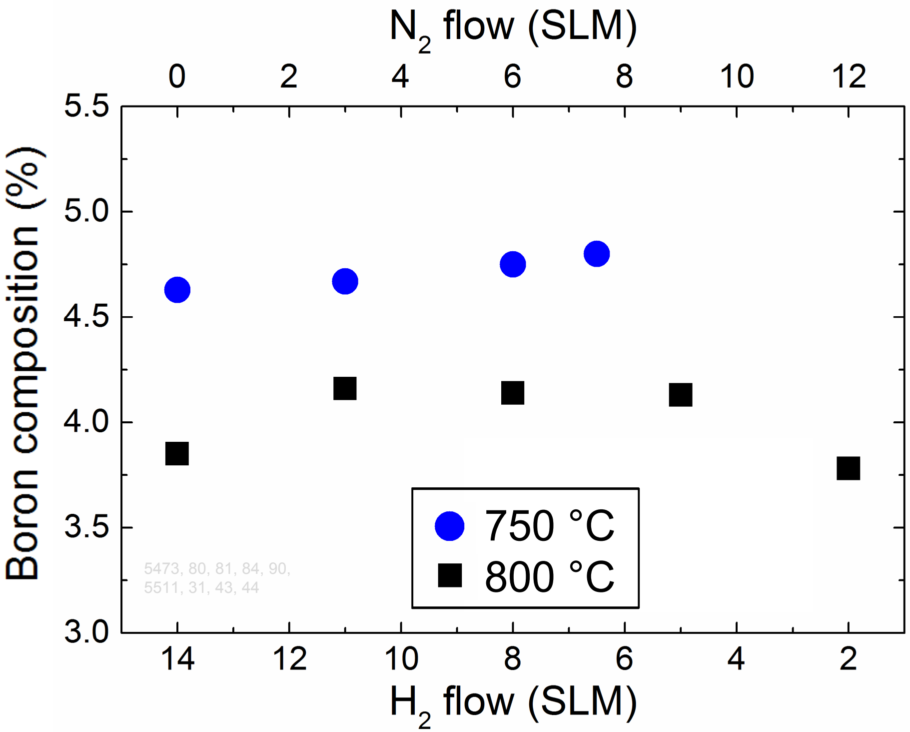
Lower temperature

- H_2:N_2 trend still applies
- Smoother surfaces
- Higher maximum B% **(4.8%)**

100X Microscope Images



H_2:N_2 carrier gas ratio



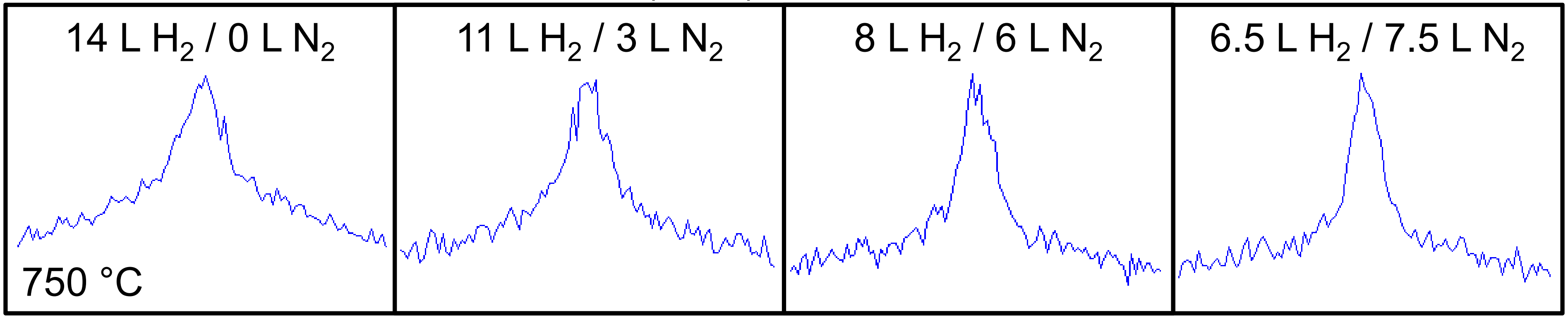
Lower temperature

- H_2:N_2 trend still applies
- Smoother surfaces
- Higher maximum B% **(4.8%)**

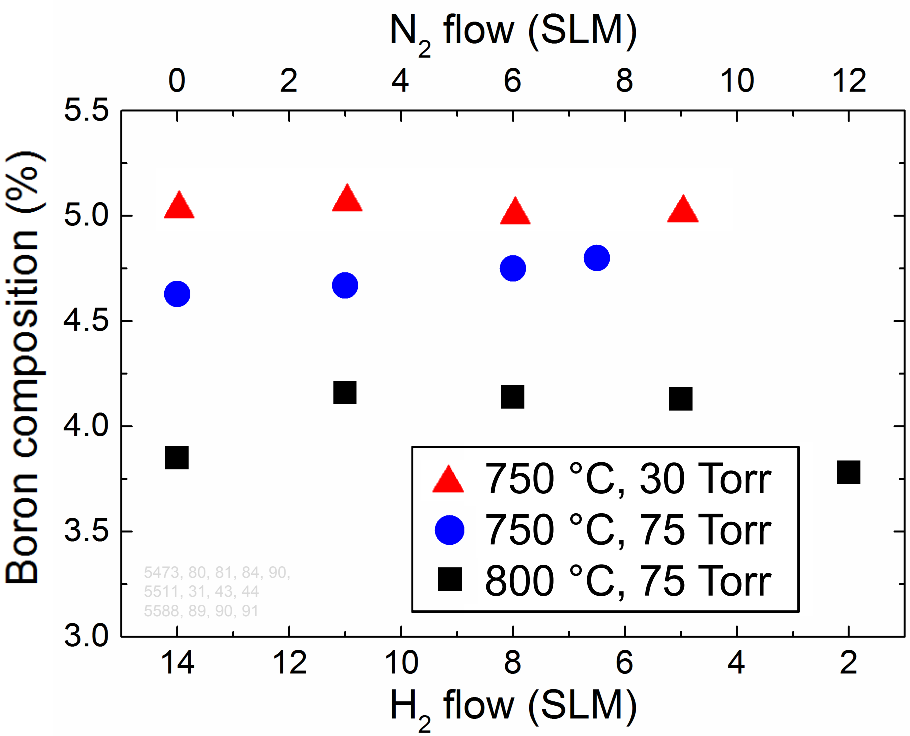
Crystal structure

- More coherent grains overall
- 400 arcsec (0002) RC FWHM

(0002) XRD RCs

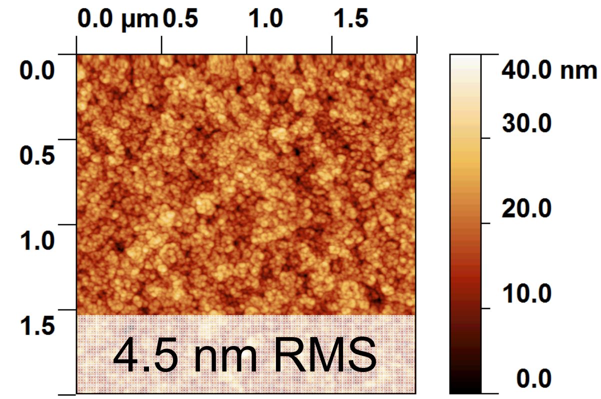


H_2:N_2 carrier gas ratio

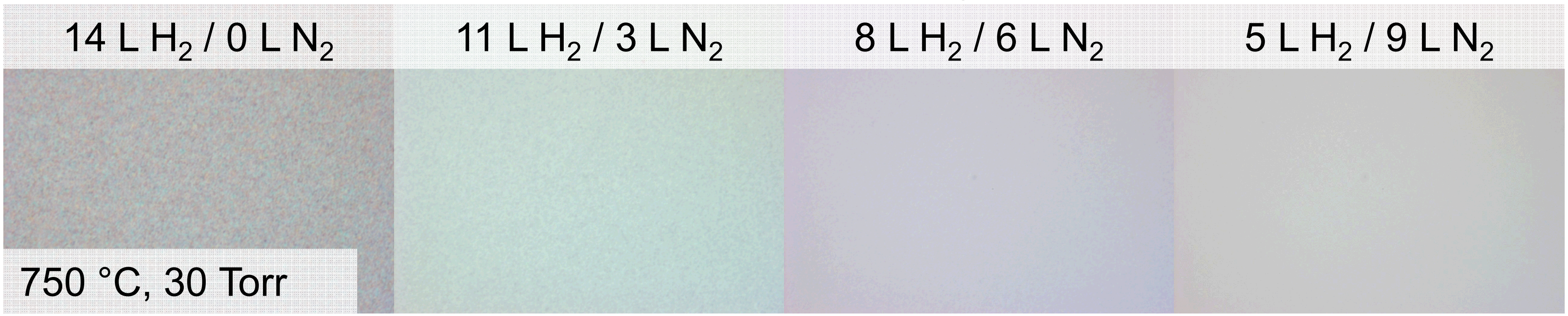


Lower pressure

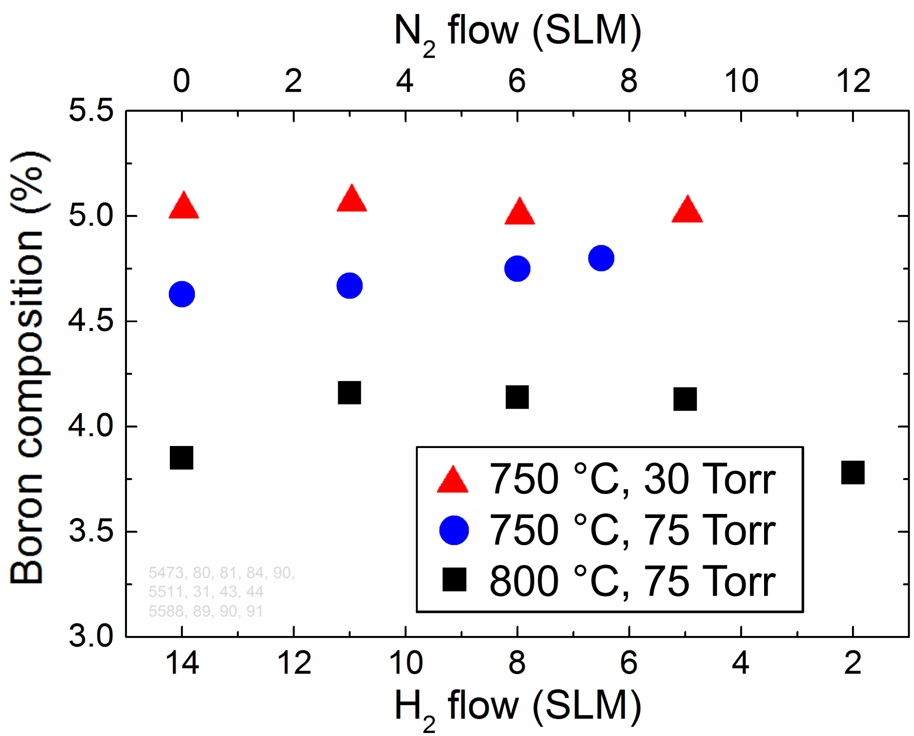
- 30 Torr vs 75 Torr
- Much smoother surfaces
- Higher maximum B% **(5%)**



100X Microscope Images



H_2:N_2 carrier gas ratio



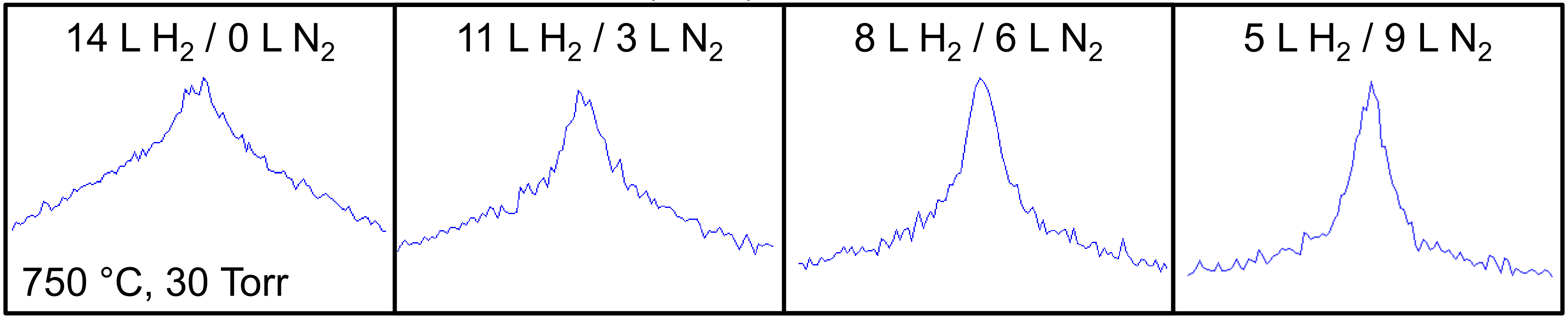
Lower pressure

- 30 Torr vs 75 Torr
- Much smoother surfaces
- Higher maximum B% **(5%)**

Crystal structure

- More coherent grains overall
- 370 arcsec (0002) RC FWHM

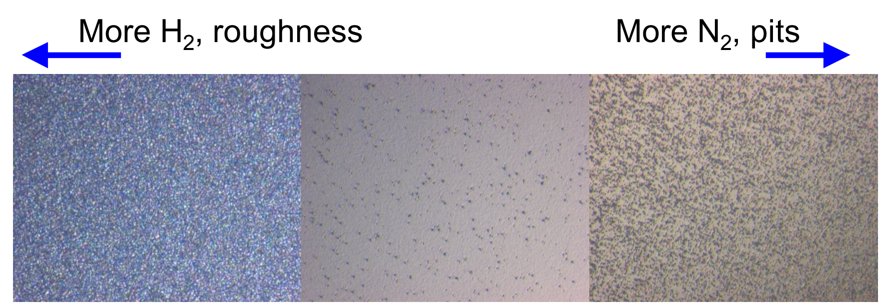
(0002) XRD RCs



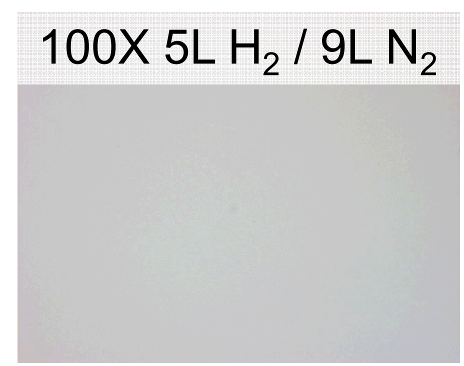
Summary

Growth of BGaN alloys on AlN

- **B mole fraction calculation**
  - Developed a more accurate B% estimation method
  - Initial work – 2-3% B
- **Explored effect of carrier gas**
  - H_2:N_2 ratio
  - More H_2 → rough, tilted grains
  - More N_2 → pitted, coherent grains



- **Reduced growth pressure and temperature**
  - Obtained 5% boron mole fraction
  - Smooth surfaces
  - Improving crystal quality



Growth of BGaN Alloys on AlN

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

Sandia National Laboratories,
Albuquerque, New Mexico, USA, 87123

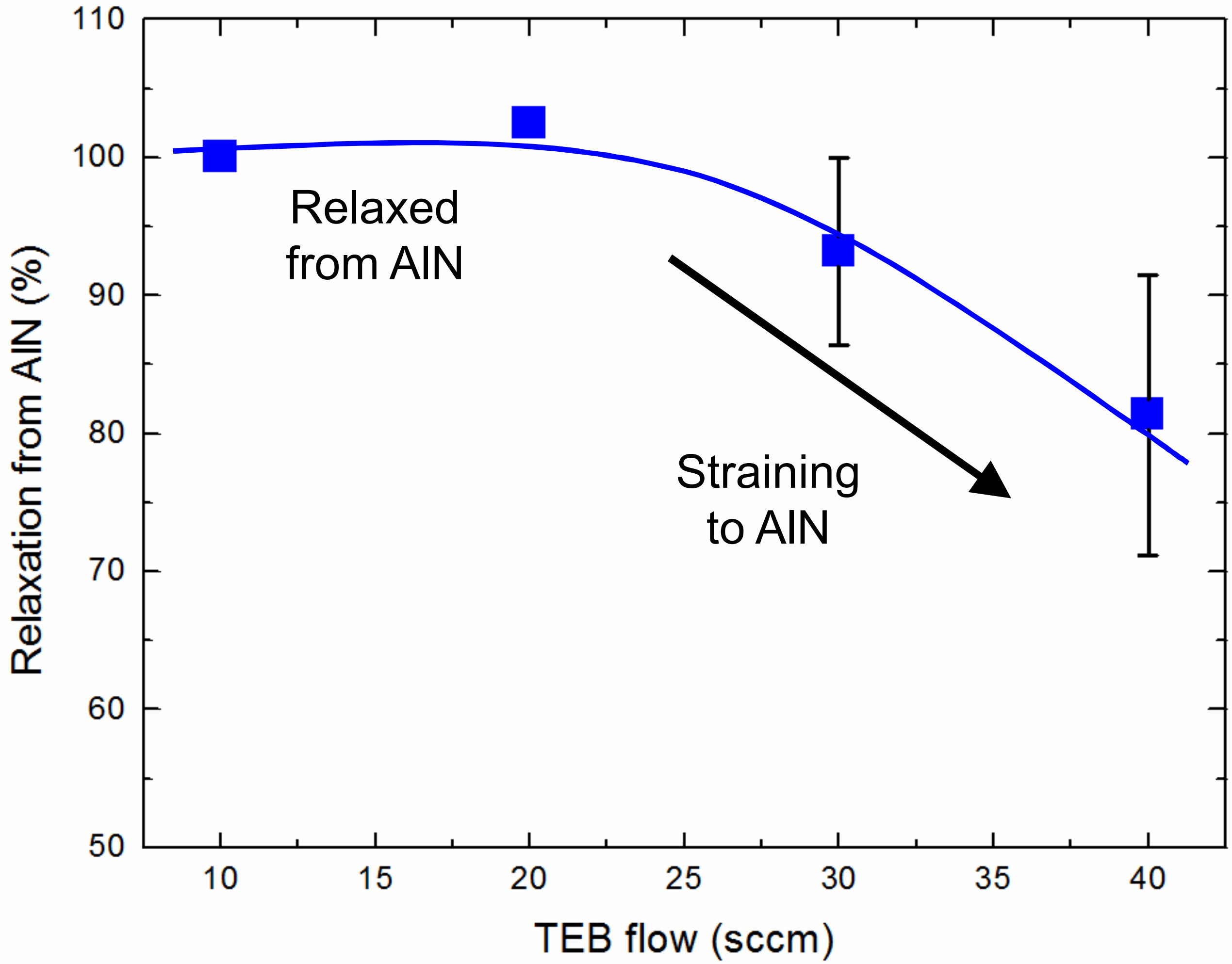
U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
LOCKHEED MARTIN

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

mwmosel@sandia.gov

Backup figures

BGaN grown on AlN

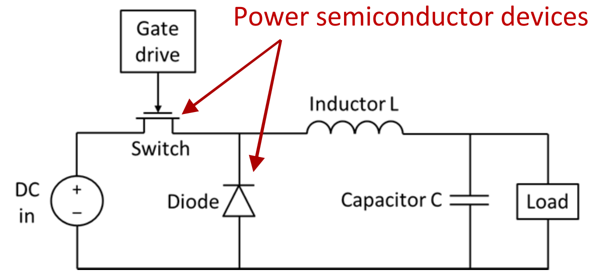


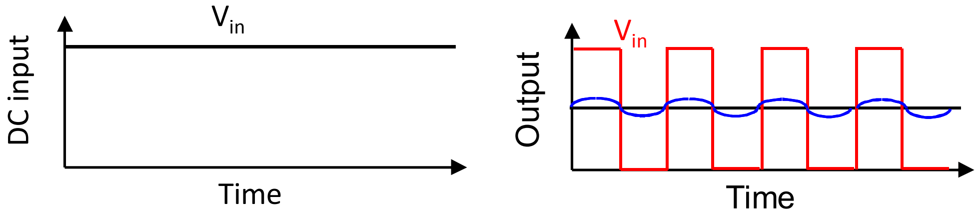
T_G: 800C
7 SLM NH3
~150 nm thick

III-Nitride Power Electronics

Application of solid-state electronics for routing, control, and conversion of electrical power

- **Impact**
  - Higher voltages
  - Higher frequency
  - Smaller size
  - Higher temperature
  - Reduce active cooling
  - Reduce passive components



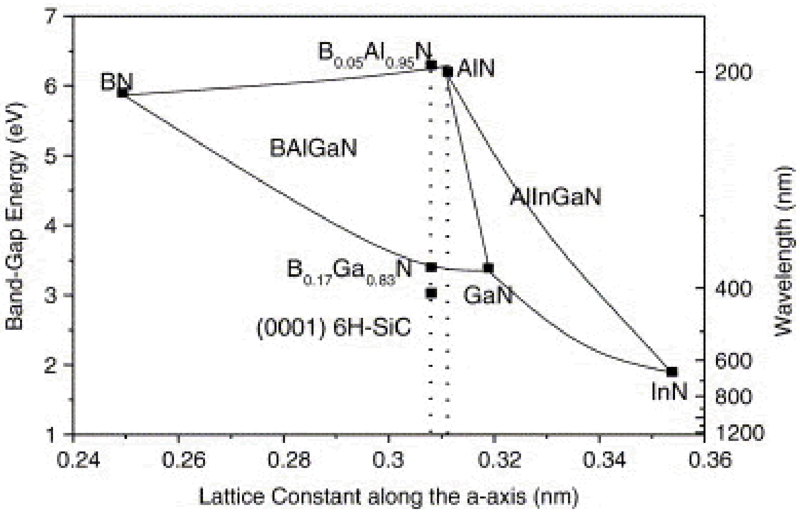


- **Applications**
  - Inverters, rectifiers, converters
  - Replace aging weapons components
  - Enable new systems and capabilities

S. Pearton, F. Ren, A. Zhang, and K. Lee, Mat. Sci. Eng. R **30,** 55 (2000).
U. K. Mishra et al., Proc. IEEE **96,** 287 (2007).

Group-III Nitrides - Solutions

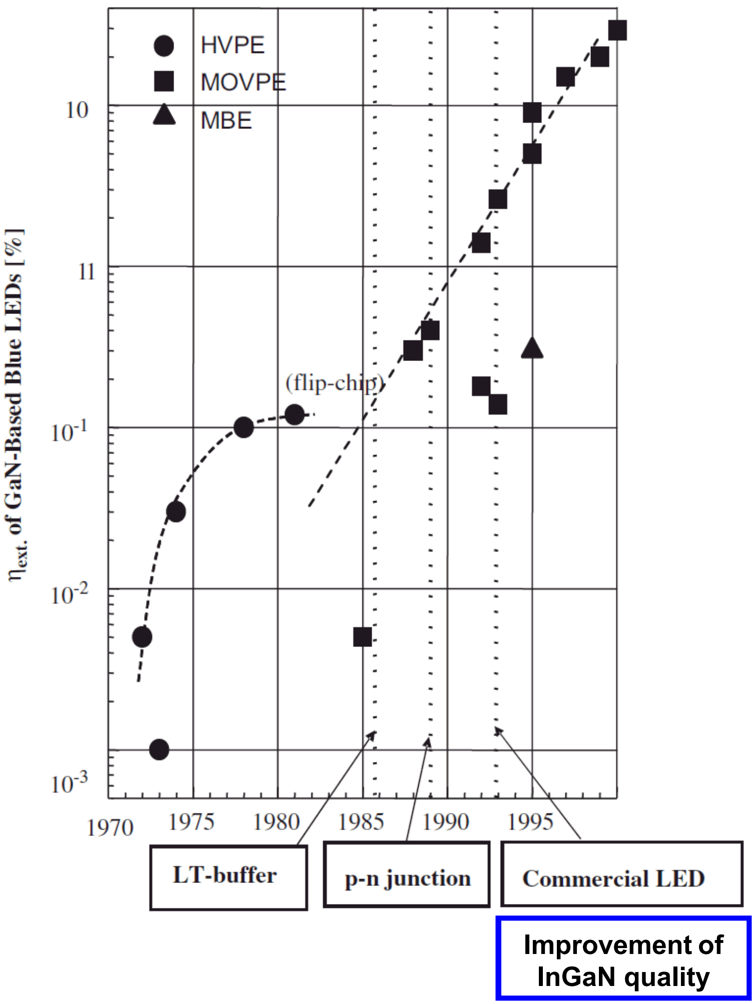
- **Investigate methods of dislocation density reduction**
  - Epitaxial lateral overgrowth
  - Dislocation annihilation
- **Circumvent mismatch by employing novel materials**
  - Boron-containing III-nitride alloys
  - Lattice match to SiC, AlN, and even AlGaN



D. Cherns and M. Hawkridge, (2006).
Allerman et al., (2014).
Ougazzaden et al., (2007).

Dislocation Density Reduction

III-nitrides – device improvement follows material improvement



Buffer/nucleation layer design

Lattice-constant engineering

- Novel substrates

Migration-enhanced epitaxy (MEE)

- Metal-modulated epitaxy (MME)
- Anion-modulated epitaxy (AME)
- Migration-enhanced metalorganic chemical-vapor deposition (MEMOCVD)
- etc.

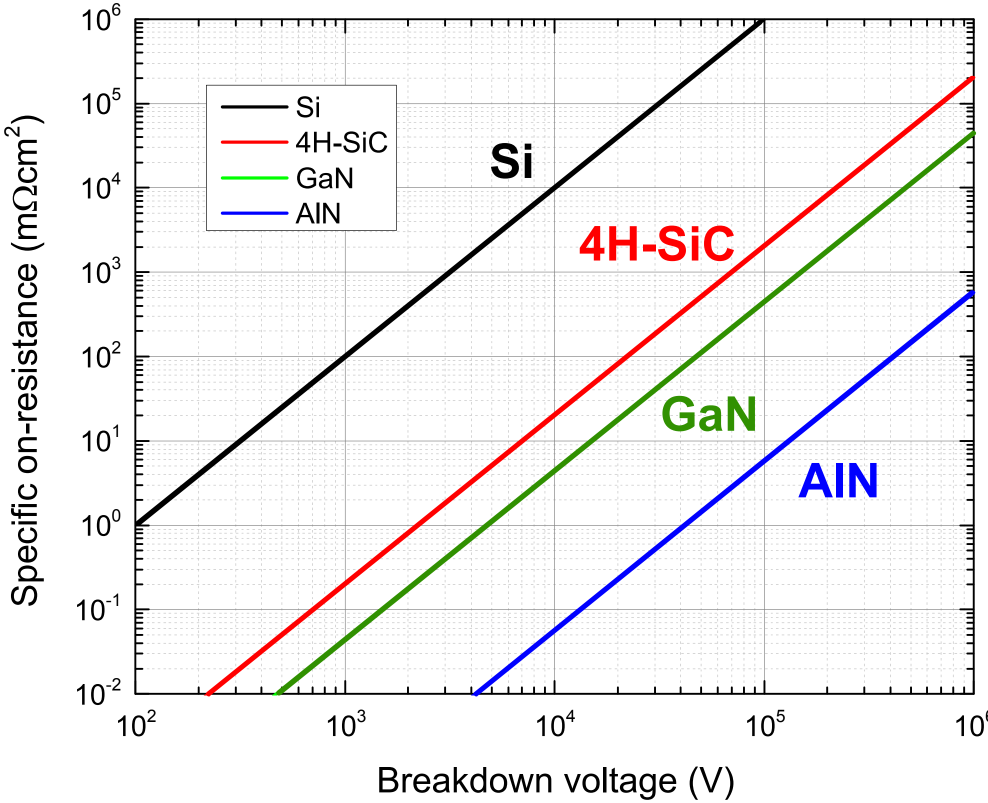
I. Akasaki, "Key inventions in the history of nitride-based blue LED and LD", *J. Cryst. Growth* **300**, 2 (2007).

Group-III Nitrides - Properties

Sandia National Laboratories

AlGaN materials system for power electronic applications

Unipolar Figure-of-Merit for Various Materials



Parameter	Si	GaAs	GaN	AlN
Bandgap, E_g [eV]	1.1	1.4	3.4	6.2
Breakdown electric field [MV/cm]	0.3	0.4	3.3	11.7
Thermal conductivity [W/cm K]	1.5	0.5	2	2.7
Saturated electron drift velocity [10^7 cm/s]	1.0	1	2.5	1.8

High breakdown electric fields

High thermal stabilities

High thermal conductivities

Radiation resistant

M. F. Schubert, Ph.D. Thesis, Virginia Polytechnic Institute and State University, 2009.
J. Wu, *J. Appl. Phys.* **106**, 011101 (2009).
L. Liu and J. H. Edgar, *Mater. Sci. Eng., R* **37**, 61 (2002).
T. P. Chow, *Microelectron. Eng.* **83**, 112 (2006).
D. I. Florescu et al., Appl. Phys. Lett. **77**, 1464 (2000).

Future work

- **Thicker films**
  - Enabled by lower pressure/temperature
- **n- and p-type doping**
  - Lower hole activation energy for Mg
- **Increase B% to lattice match to AlN**
  - Potential miscibility gap beyond 5%