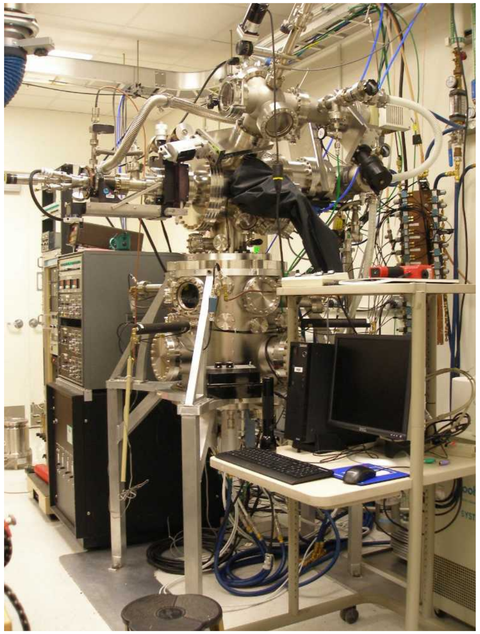
Epitaxial Oxides for GaN and AlGaN Power Electronics

SAND2016-2058PE



9 March 2016

Jon Ihlefeld,[1] Elizabeth Paisley,[1] Michael Brumbach,[1] Christopher Shelton,[2] Jon-Paul Maria,[2] Andrew A. Allerman,[1] David R. Wheeler,[1] Albert Baca,[1] Robert Kaplar,[1] and Stanley Atcitty[1]

[1] Sandia National Laboratories

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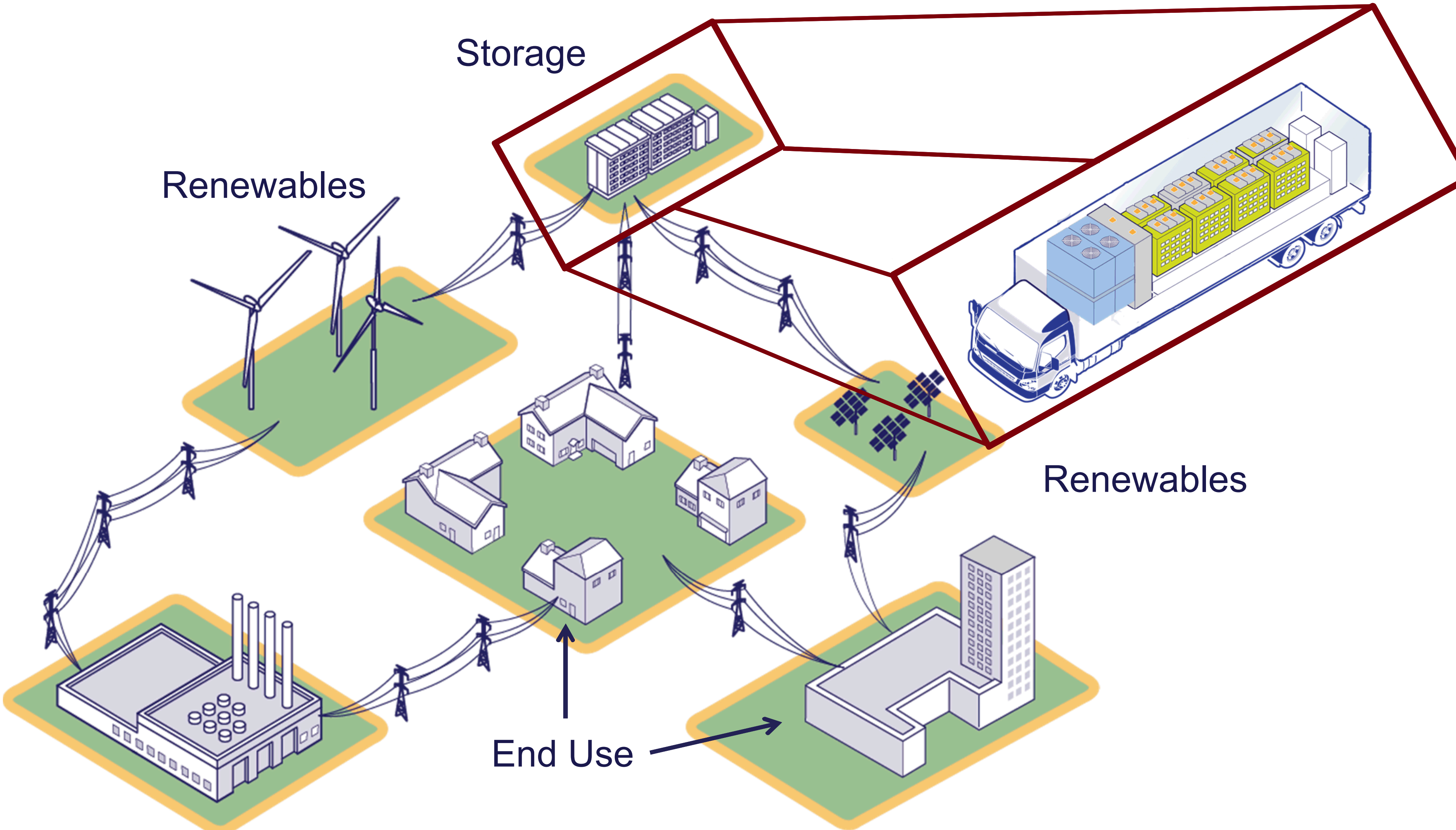
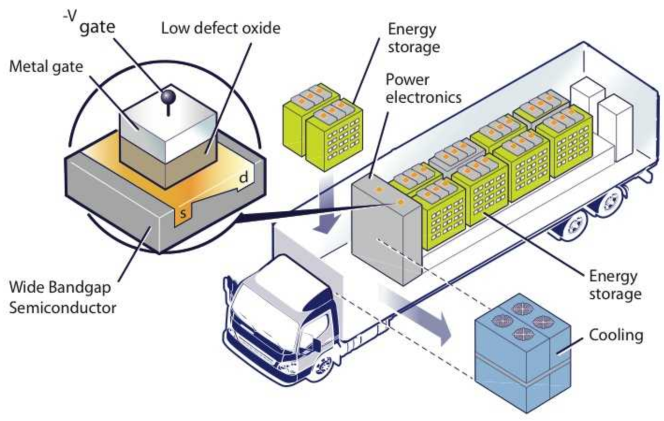
Power Electronics for the Electrical Grid



Semiconductors for Power Electronics



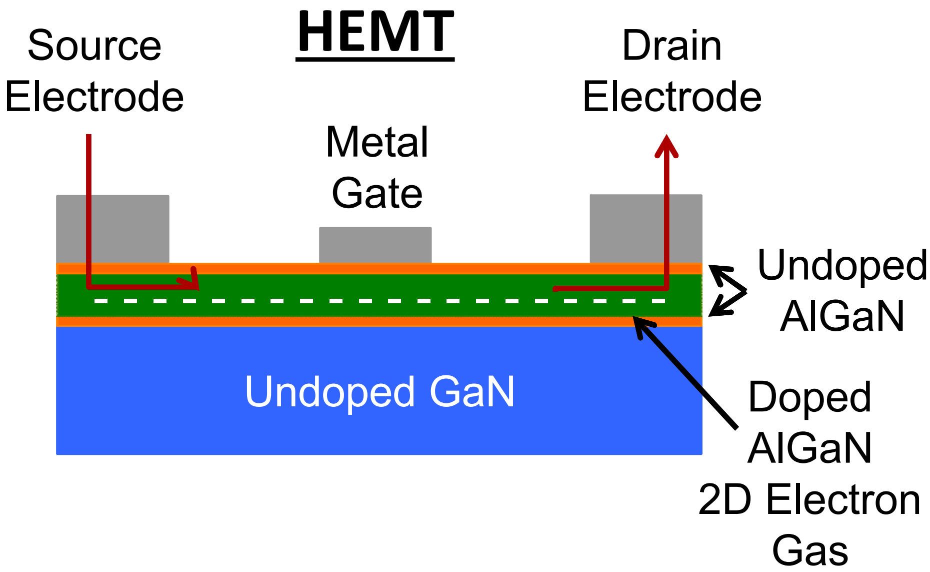
	Silicon	4H-SiC	GaN
Bandgap (eV)	1.1	3.2	3.4
T_{max} (°C)	300°C	600°C	700°C
Mobility (cm^2/Vs)	1500	260	1500
Breakdown Field (MV/cm)	0.3	3.5	2.0

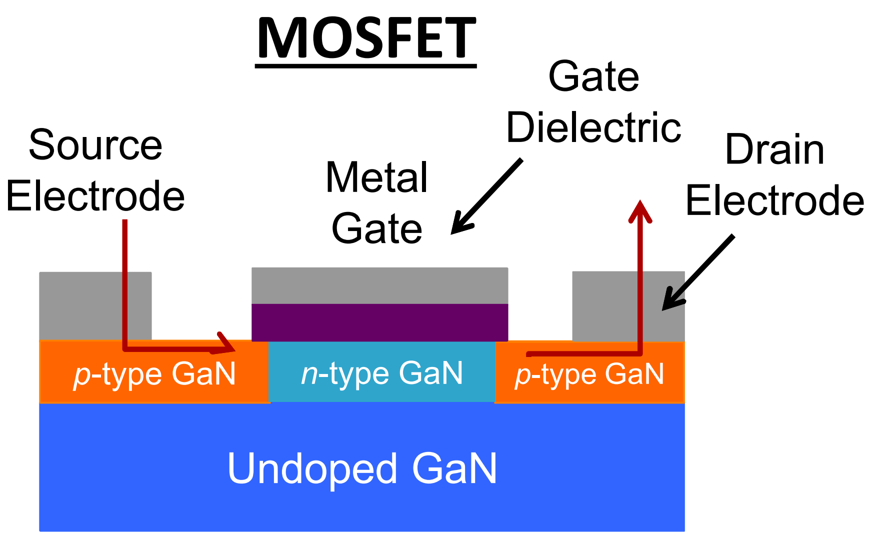
Data adapted from: R.S. Pengelly, *et al. IEEE Trans. M.T.T.*, **60** (6) (2012)

- Power electronics are necessary for energy modulation and introduction of storage on the electrical grid
- Leading technology today is Si-based IGBTs
  - Si-based devices are limited in operating temperature and electric field
- Costs and low mobility associated with SiC technology makes GaN devices attractive
  - Particularly useful for 600 V applications

GaN Devices

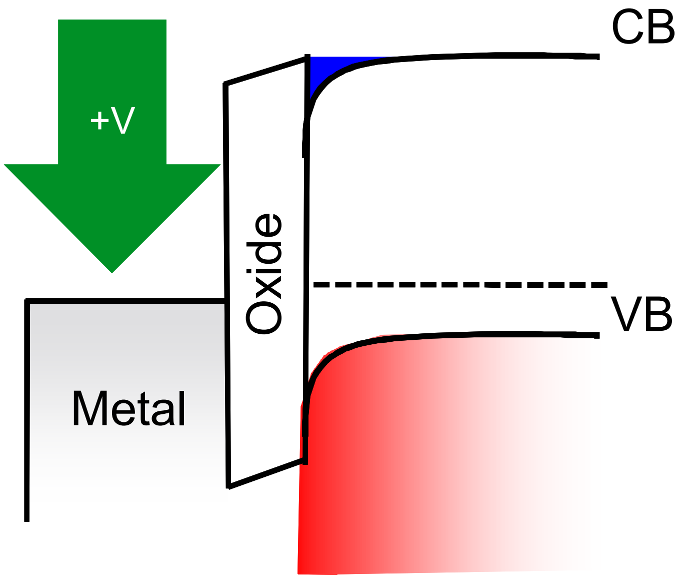
- “Ideal” GaN Device
  - Voltage Controlled
    - *Smart Grid* compatible
  - Film Embodiment
    - Inexpensive compared to SiC
  - Enhancement Mode (nominally off)
    - Existing HEMTs are typically always on
    - Safety issue
  - MOSFETs (or MOSHEMTs) would be advantageous





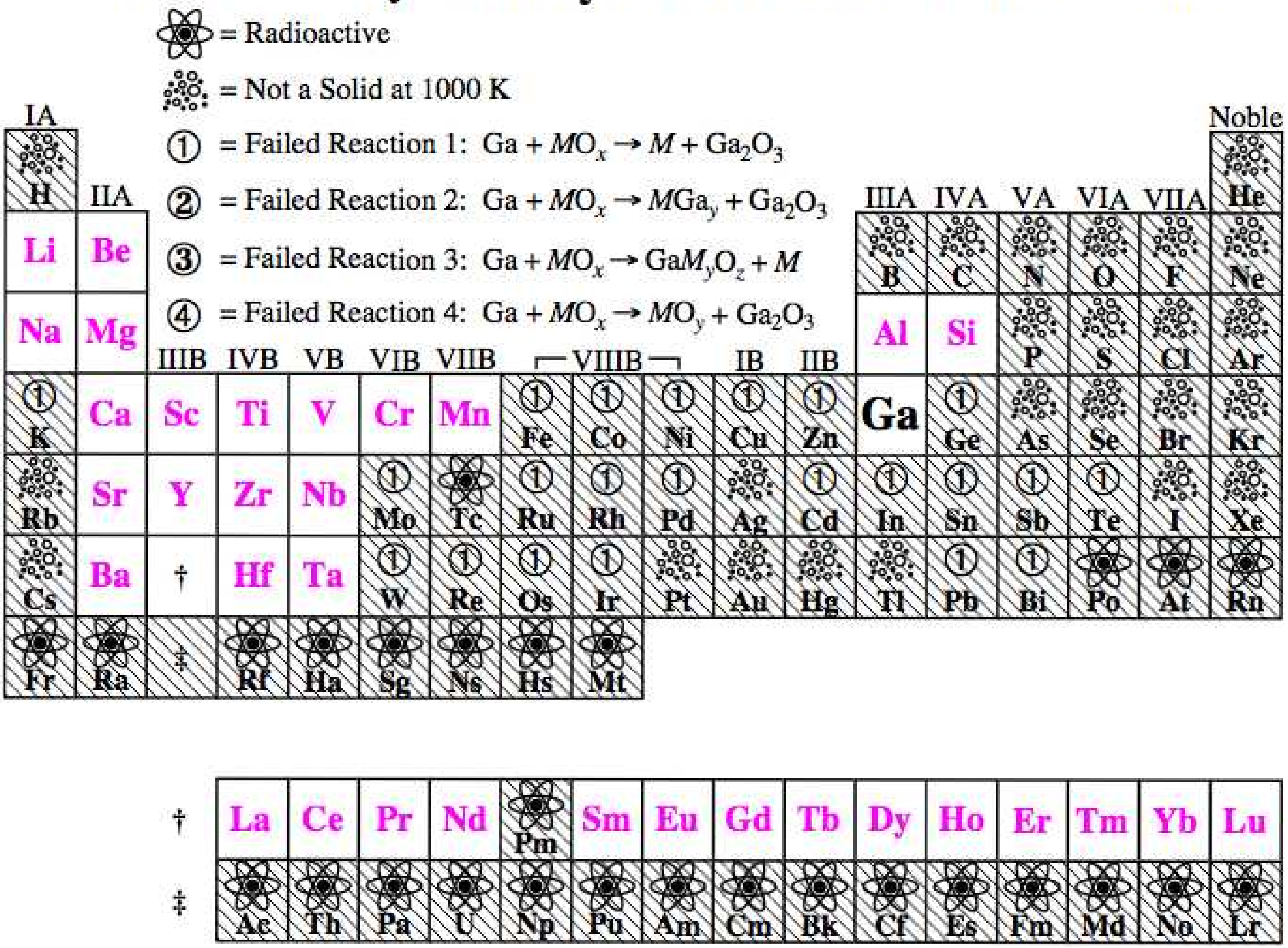
GaN Devices

- Oxide requirements for MOSFETs:
  - Large bandgap
  - Band offsets > 1 eV with semiconductor
  - Chemically compatible
  - Grows as a smooth film on GaN
  - Low interface defect density



- Our strategy:
  - Identify chemically compatible wide bandgap oxides that may have acceptable offsets with WBG and UWBG semiconductors
  - Utilize epitaxy to form well-controlled interfaces

Oxides Thermodynamically Stable in Contact with Gallium



Insufficient Thermodynamic Data to Complete Calculations **Experimentally Demonstrated**

Lanthanide Oxides: Candidate Materials

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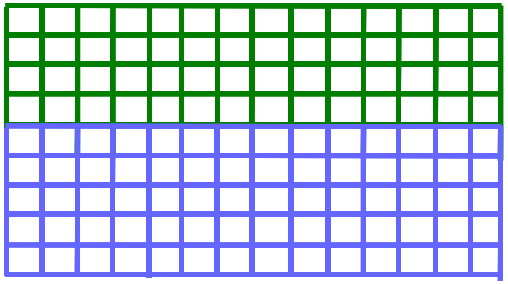
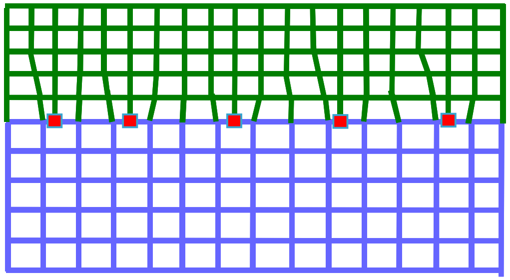
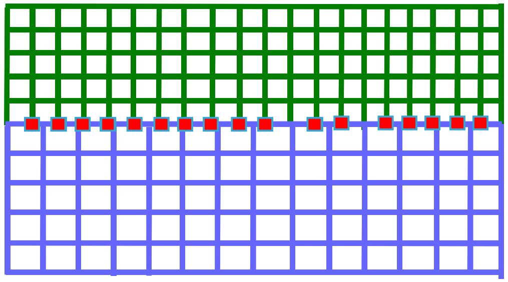
0% Strain
Coherent Interface
Satisfied Bonds



~< 10% Strain
Pseudomorphic
With Dislocations



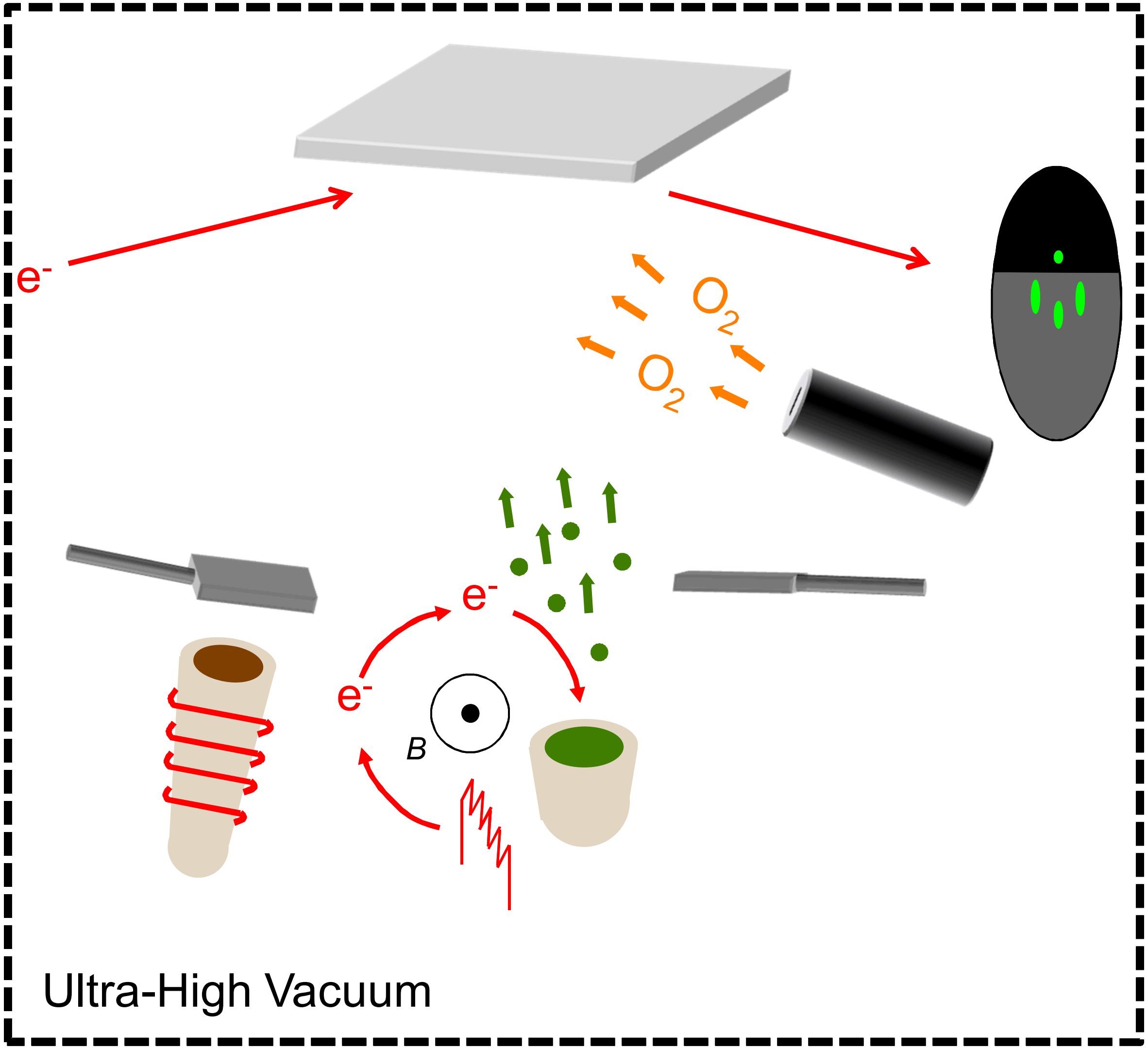
~>10% Strain
Incoherent
With Dislocations



Ln_2O_3	La	Nd	Sm	Gd	Dy	Ho	Er	Tm	Yb	Lu
ε_{cub}	0.7%	-10%	-3%	-4%	-5.4%	-5.9%	-6.4%	-6.9%	-7.4%	-7.7%
ε_{hex}	19.1%	16.9%	-	-	-	-	-	-	-	-
E_g	5.5	4.7	5	5.4	4.9	5.3	5.3	5.4	4.9	5.5
K	20-30	10	11	12	12	12	14	-	13	9

Data from: G-Y. Adachi and N. Imanaka, *Chem. Rev.* (1998)
J-P. Maria in *High Dielectric Constant Materials* (2005).

Oxide Molecular-Beam Epitaxy

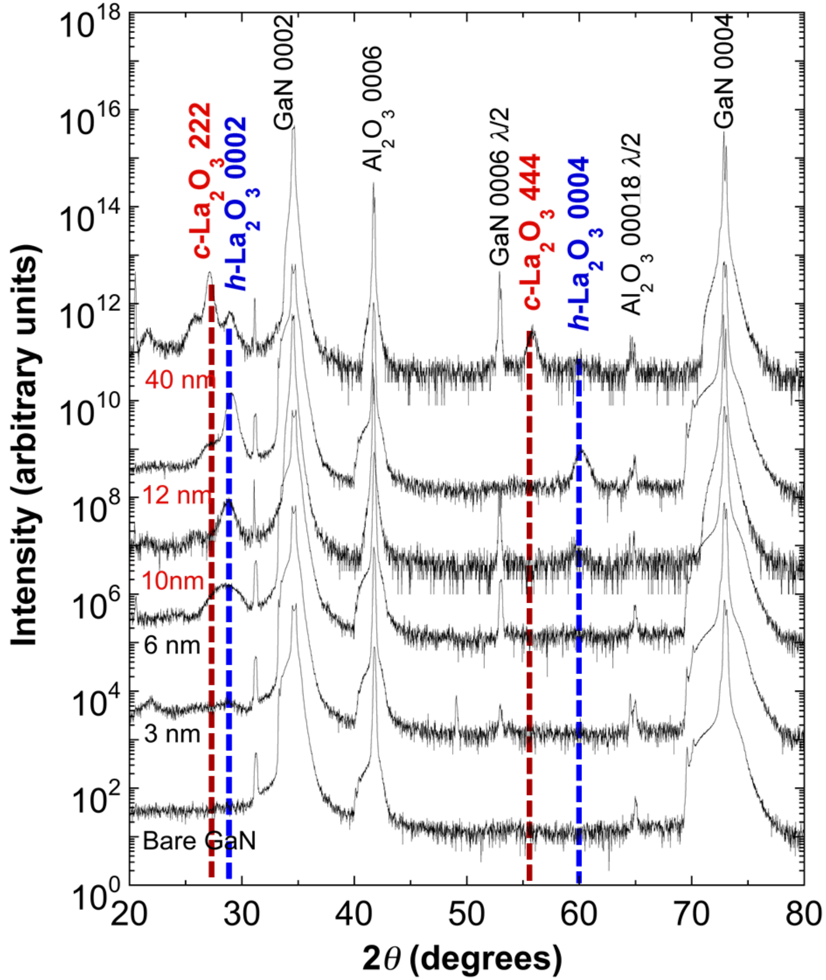


Reactive MBE

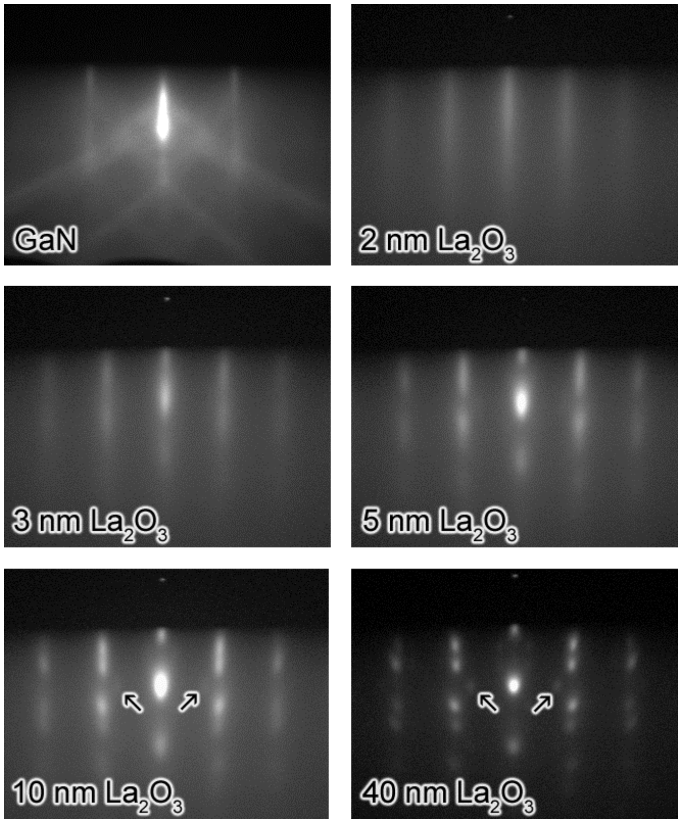
- Metallic La and Gd sources
- E-beam evaporation
- O_2 oxidant
- *In situ* RHEED
- Growth rates 0.5-1 Å/minute
- $5x10^{-7}$ Torr O_2
- 550-600° C substrate temperature

La_2O_3 Growth Characteristics

X-ray Diffraction



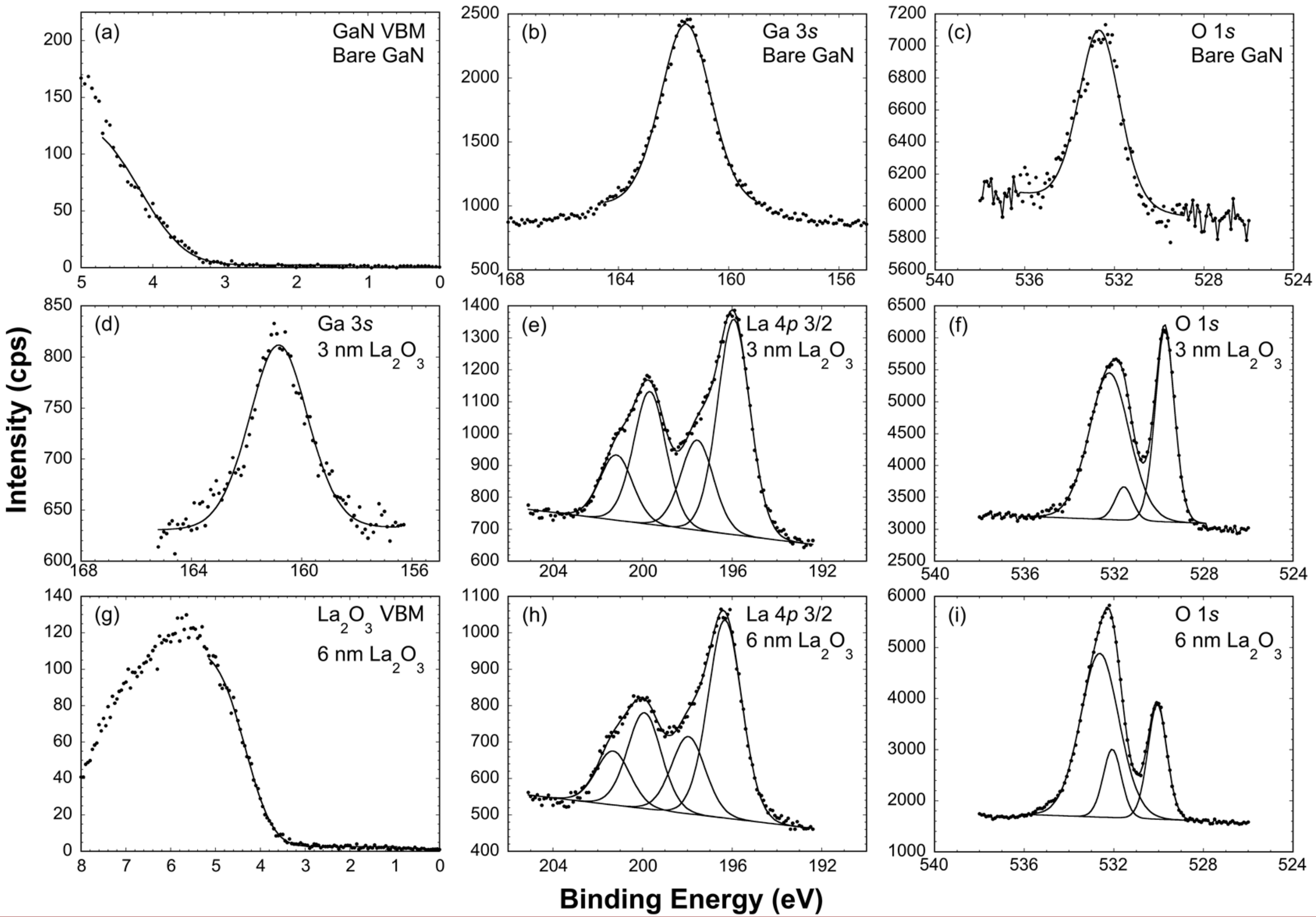
RHEED



- Hexagonal growth observed for thicknesses of ≤ 6nm
- Transitions to rough cubic phase for thicknesses > 6nm

J.F. Ihlefeld, M. Brumbach, and S. Atcitty, *Applied Physics Letters*, **102**, 162903 (2013)

XPS Determination of Band Offsets



La_2O_3/GaN Band Alignments

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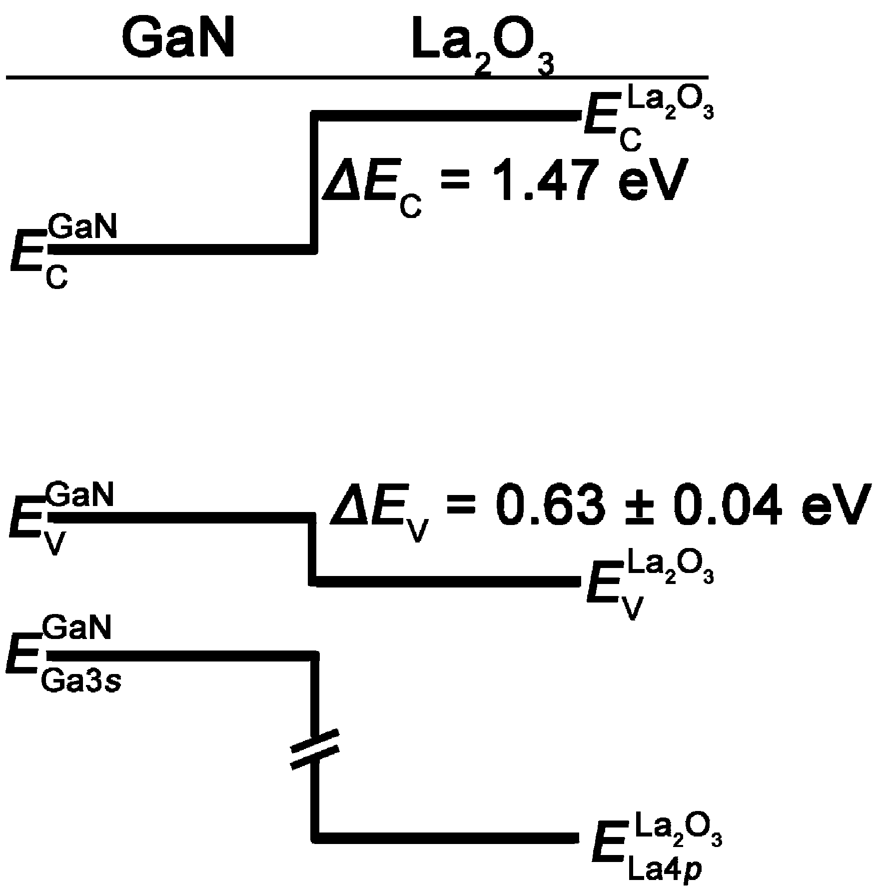

- Valence band offset of 0.63 eV measured at the La_2O_3-GaN interface (La 4*p* & Ga 3*s*)
  - 0.64 ± 0.04 eV (La 4*p* & Ga2*p*)
  - 0.60 eV (O 1*s* & Ga 3*s*)
  - 0.68 eV (O 1*s* & Ga 2*p*)
- Ideally want band offsets >1 eV to maximize performance and reliability
- Conduction band offset of 1.47 eV
- ***Low valence band offset may limit applications***

J.F. Ihlefeld, M. Brumbach, and S. Atcitty, *Applied Physics Letters*, **102**, 162903 (2013)

Gd_2O_3 as Gate Dielectric

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COMMUNICATION

ADVANCED MATERIALS www.advmat.de

Nanometer-Thick Single-Crystal Hexagonal Gd_2O_3 on GaN for Advanced Complementary Metal-Oxide-Semiconductor Technology

By *Wen Hsin Chang, Chih Hsun Lee, Yao Chung Chang, Pen Chang, Mao Lin Huang, Yi Jun Lee, Chia-Hung Hsu,* J. Minghuang Hong, Chiung Chi Tsai, J. Raynien Kwo,** and *Minghwei Hong**

phys. stat. sol. (a) **188**, No. 1, 239–242 (2001)

Gadolinium Oxide and Scandium Oxide: Gate Dielectrics for GaN MOSFETs

B.P. Gila[1]) (a), J.W. Johnson (b), R. Mehandru (b), B. Luo (b), A.H. Onstine (a), K.K. Allums (a), V. Krishnamoorthy (c), S. Bates (a), C.R. Abernathy (a), F. Ren (b), and S.J. Pearton (a)

(a) Department of Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA

(b) Department of Chemical Engineering, University of Florida, Gainesville, FL 32611, USA

(c) Uniroyal Optoelectronics, Tampa, FL 33619, USA

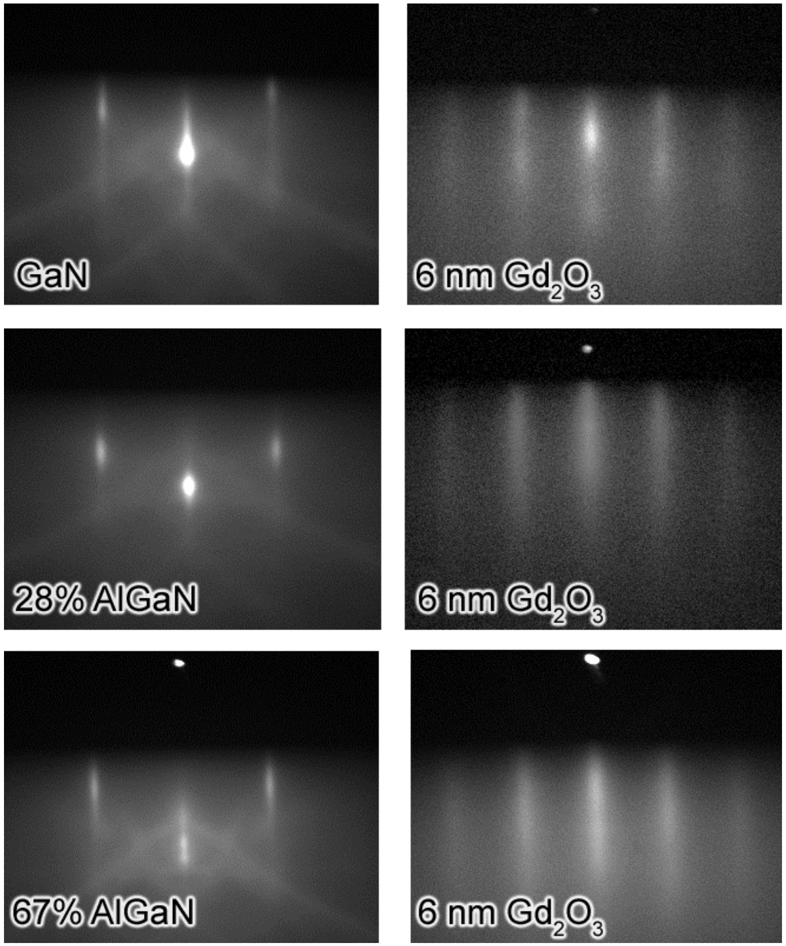
(Received June 23, 2001; accepted August 4, 2001)

Subject classification: 68.55.Jk; 68.55.Ln; 73.20.At; 77.55.+f; 81.15.Hi; S7.14; S10.1

- High temperature stable oxide gate
- High permittivity in hexagonal phase (24)
- Other reports of a 1 eV valence band offset
- Potential for low interface trap density

Gd_2O_3 on AlGaN Growth

RHEED



- Films grown at 600° C
- 5 x 10^{-7} Torr O_2 atmosphere
- 7 Å/minute growth rate
- All films grow smoothly on different AlGaN composition substrates
- In-plane lattice spacing identical for each Gd_2O_3 film consistent with same phase independent of substrate

J.F. Ihlefeld, M. Brumbach, A.A. Allerman, D.R. Wheeler, and S. Atcitty, *Applied Physics Letters,* **105**, 012102 (2014)

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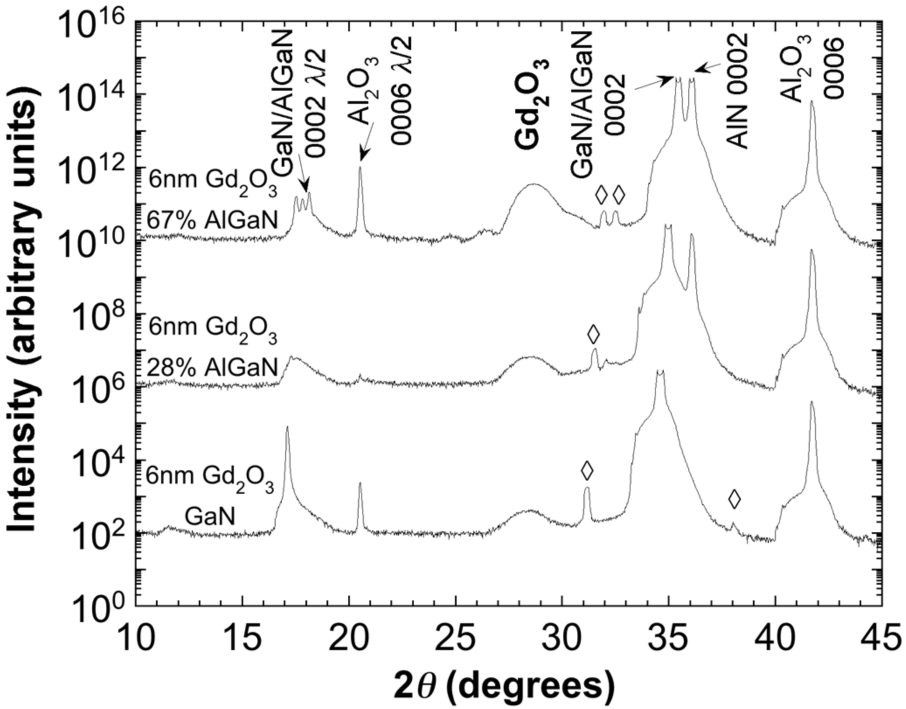
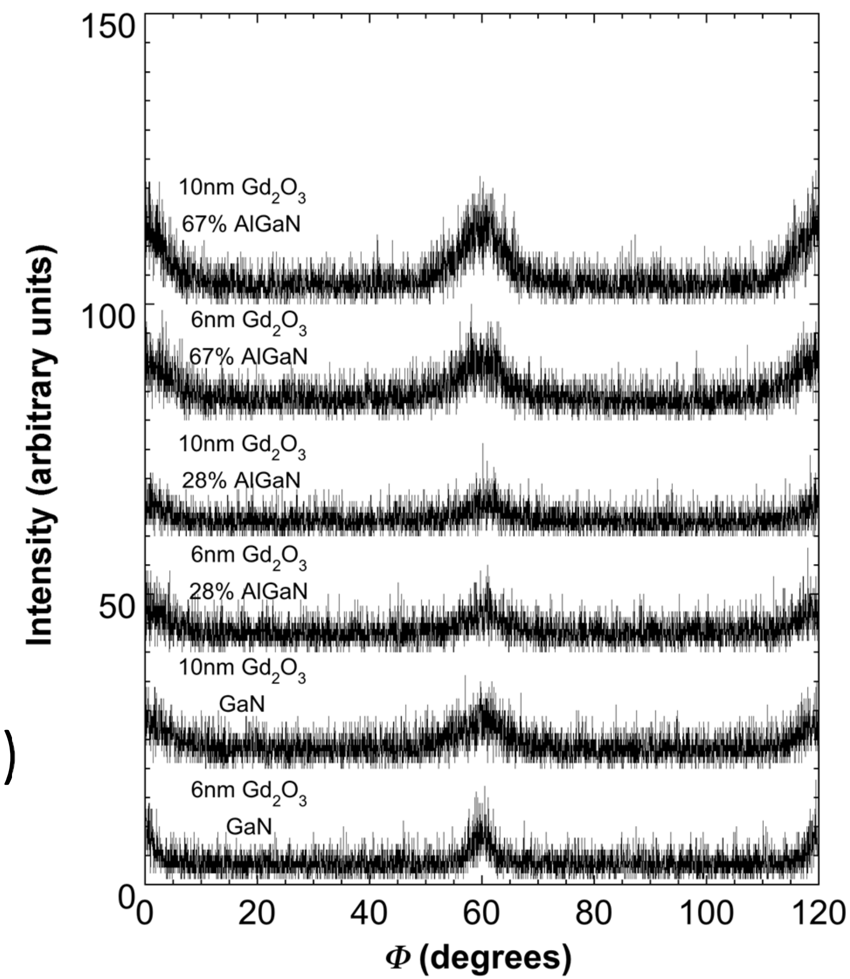


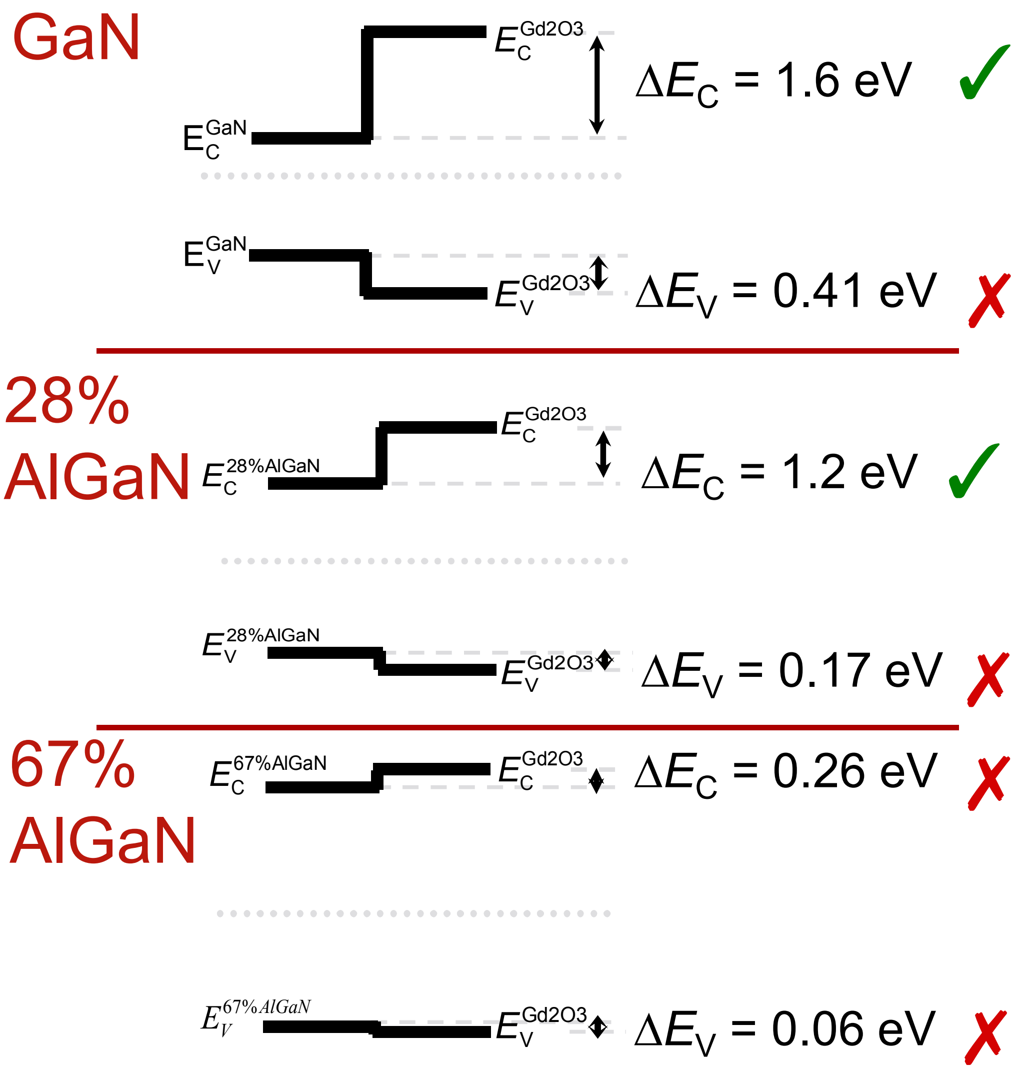


- All Gd_2O_3 films are cubic (bixbyite) regardless of thickness or substrate
- In-plane twins are present

400 reflection of cubic Gd_2O_3
(2θ = 33.2°, Ψ = 54.7°)

J.F. Ihlefeld, M. Brumbach, A.A. Allerman, D.R. Wheeler, and S. Atcitty, *Applied Physics Letters,* **105**, 012102 (2014)

Gd_2O_3 on AlGaN Band Offsets



- Band offsets are strongly semiconductor bandgap dependent
- All valence band offsets are < 0.5 eV
- ***Lanthanides may not work for UWBG devices***

J.F. Ihlefeld, Brumbach, Allerman, Wheeler, and Atcitty, *Applied Physics Letters*, **105**, 012102 (2014)

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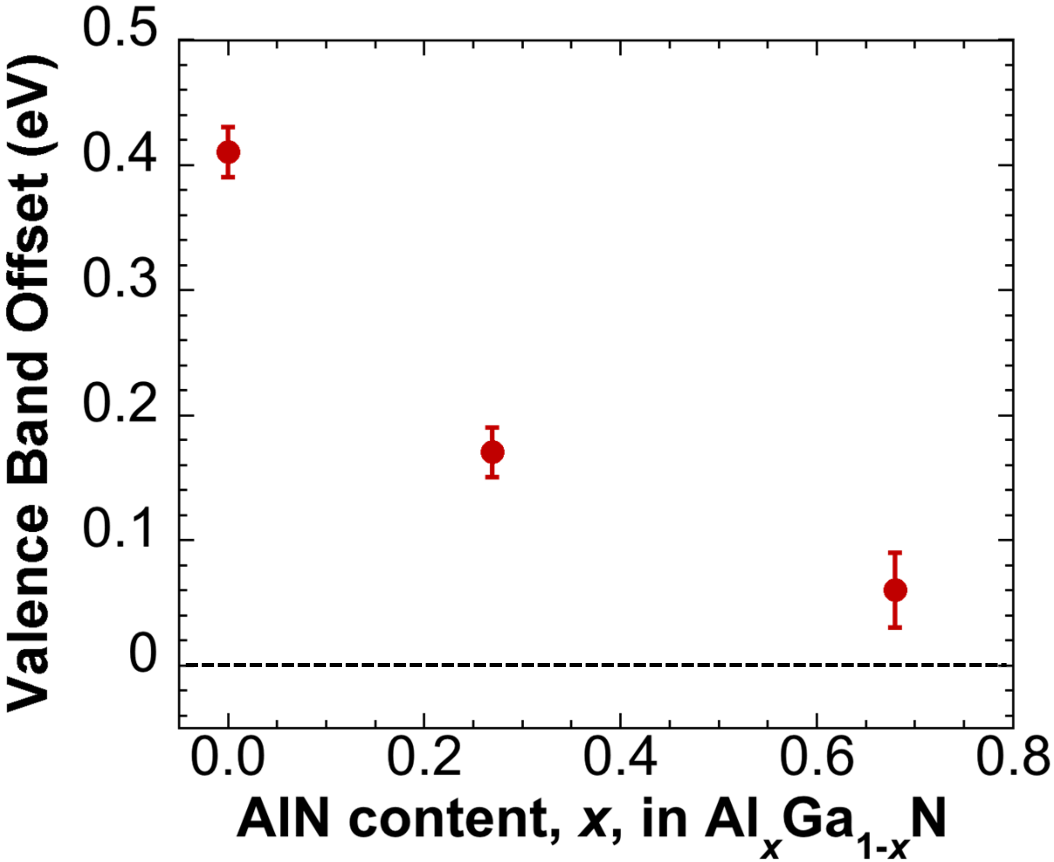

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Lanthanide Summary

- Lanthanide oxides possess some favorable attributes for use as a gate dielectric with GaN
  - Chemical compatibility
  - Large bandgaps
  - High dielectric constants
- ***Low band offsets, interfacial defects, difficult to control polymorphs may make lanthanide oxides poor choices for GaN and AlGaN gate dielectric applications***

Dielectrics for GaN Devices

- Oxide requirements for MOSFETs and MOSHEMTs:
  - Large bandgap
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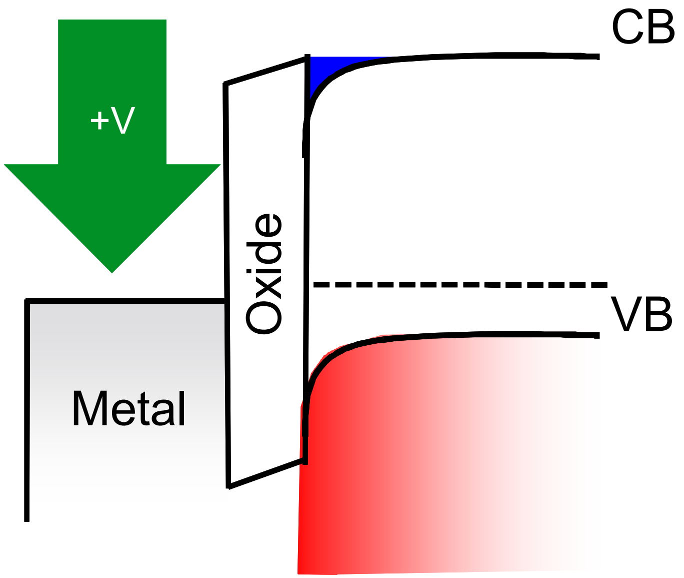

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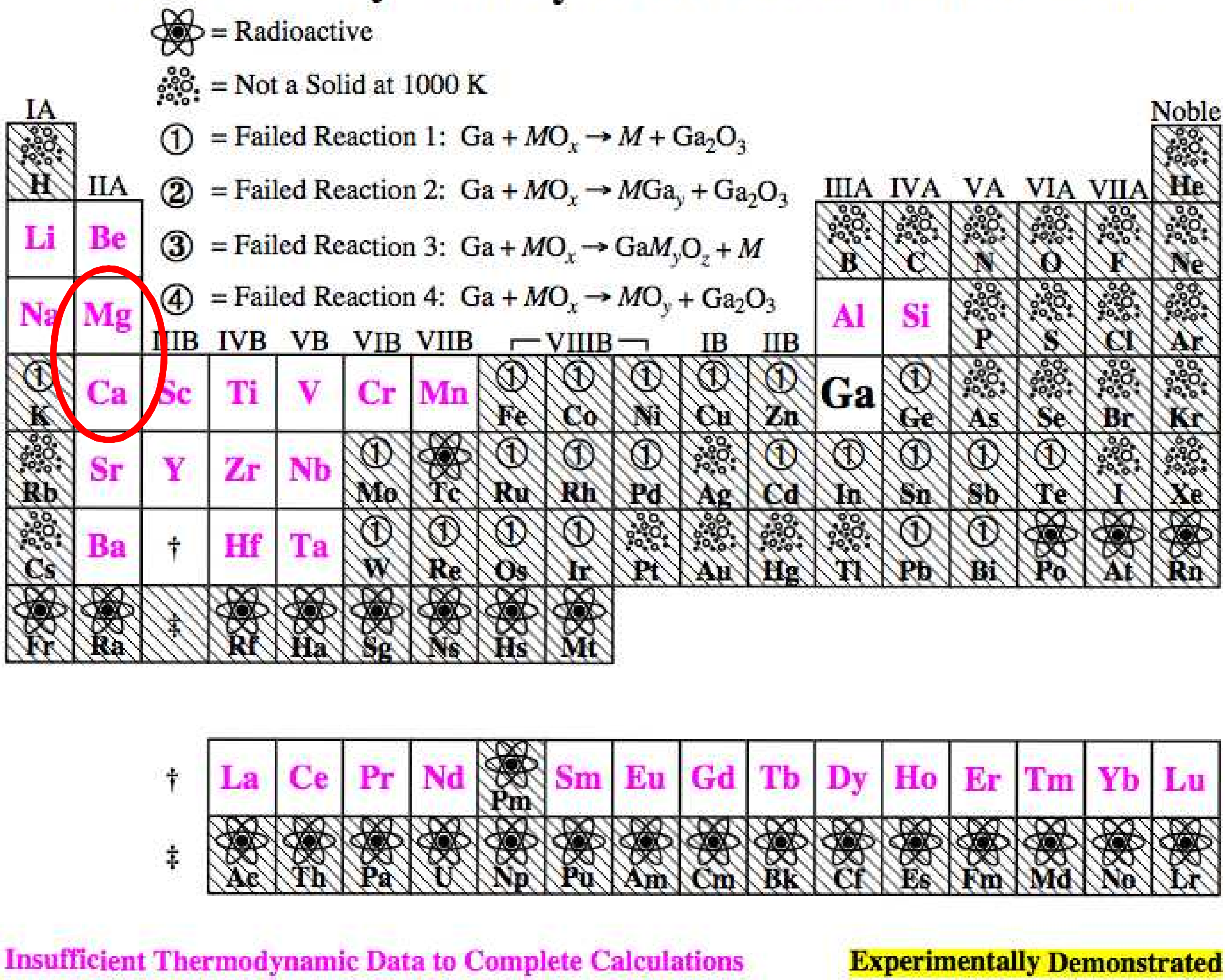
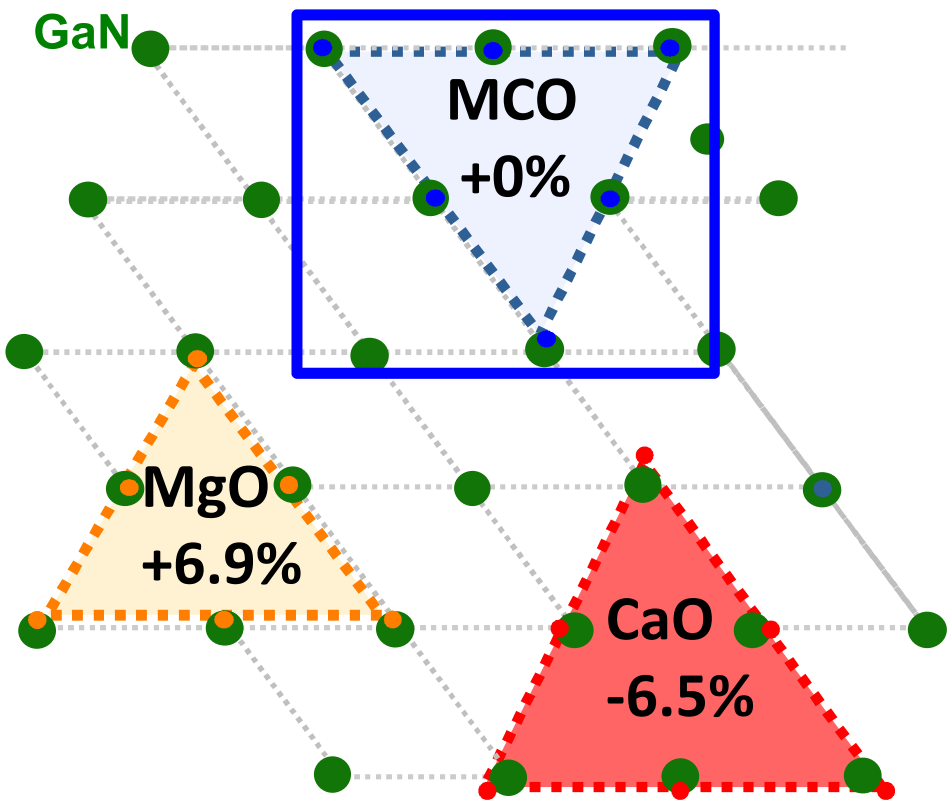


MgO-CaO/AlN-GaN growth compatibility

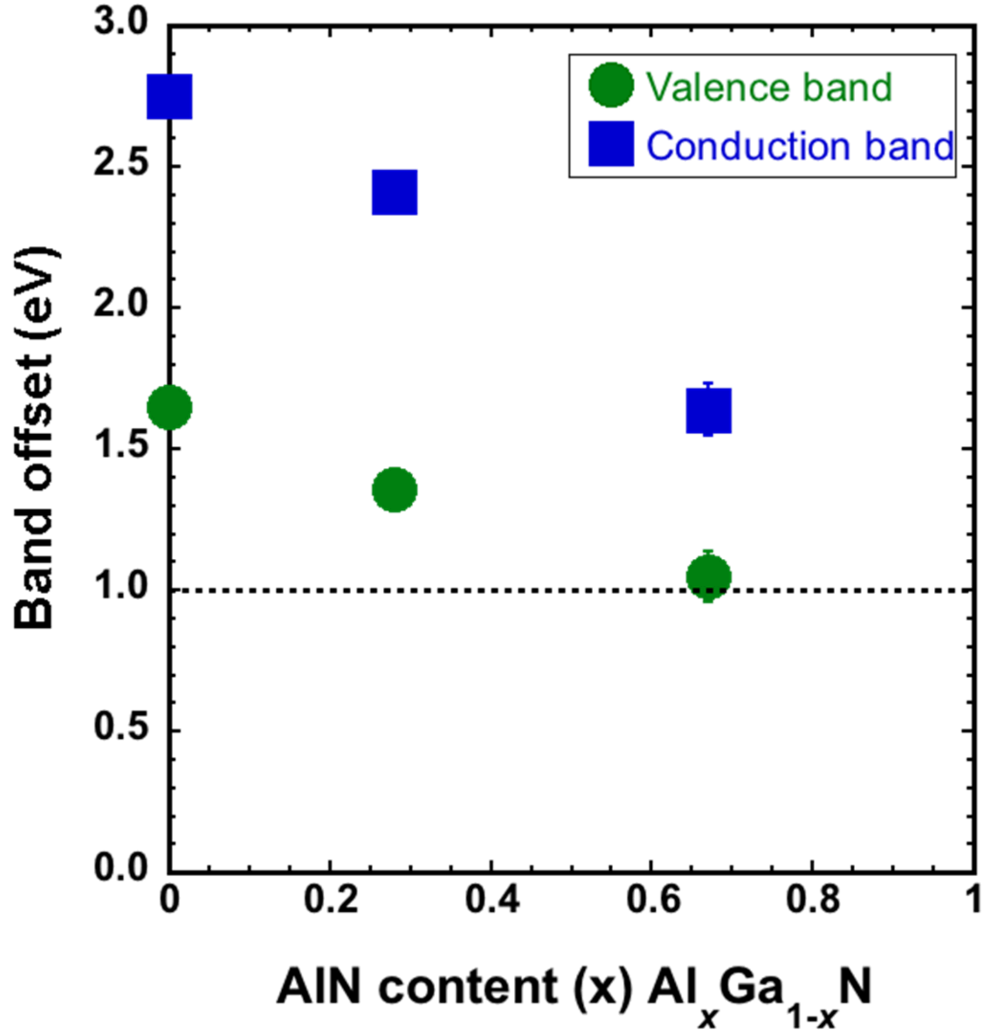
We can lattice-match to GaN through AlN…



- MCO/GaN: $Mg_{0.5}Ca_{0.5}O$
- MCO/67% AlGaN: $Mg_{0.63}Ca_{0.37}O$

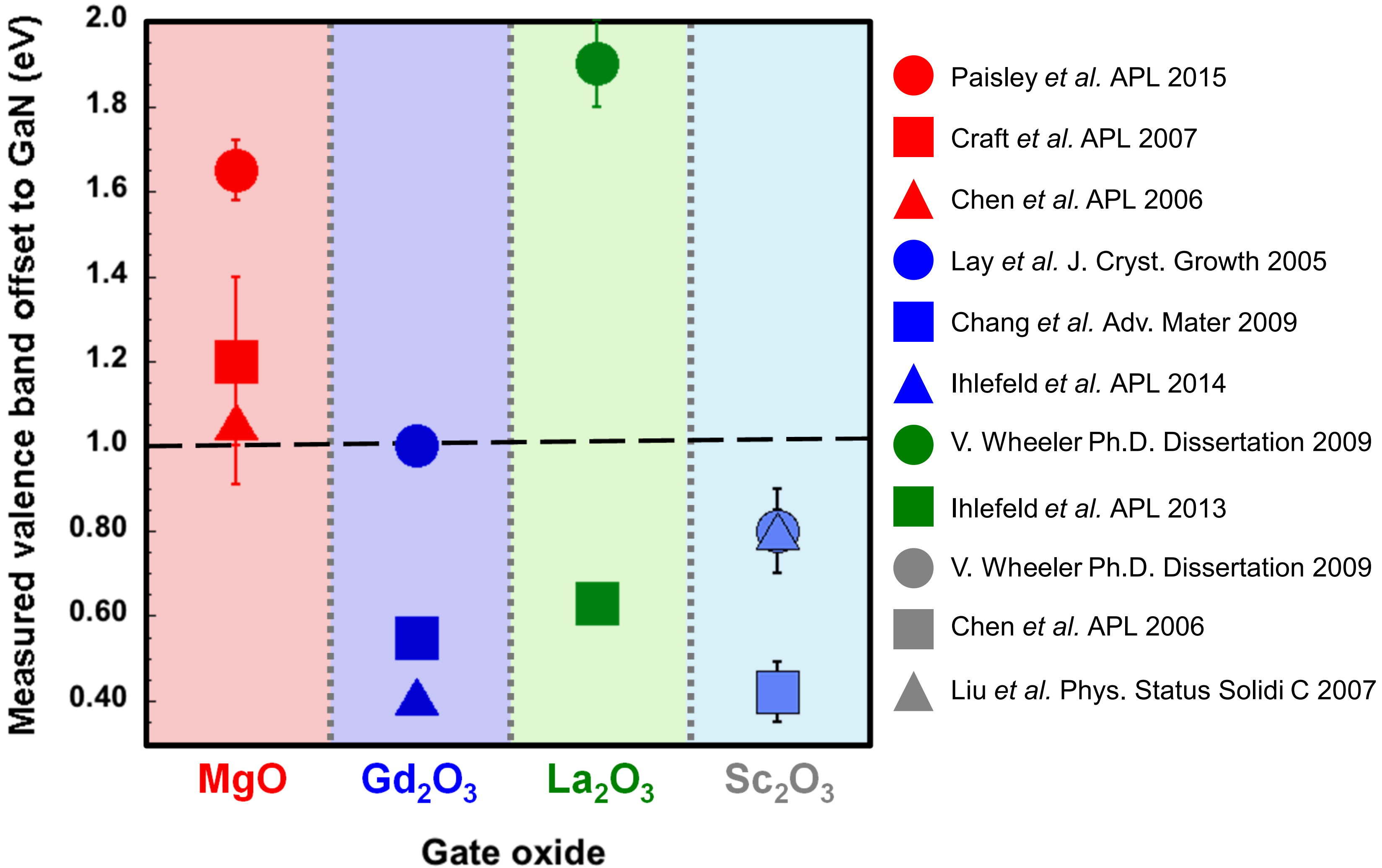
MgO/$Al_xGa_{1-x}N$ band offsets

- Band offsets measured on:
  - GaN: 3.4 eV
  - 28% AlGaN: 4.0 eV
  - 67% AlGaN: 5.2eV
- Band offsets are strongly semiconductor bandgap dependent
- Both ΔE_C and $\Delta E_V > 1$ eV
- ***MgO/CaO are viable as AlGaN gate dielectrics on the basis of band offsets***



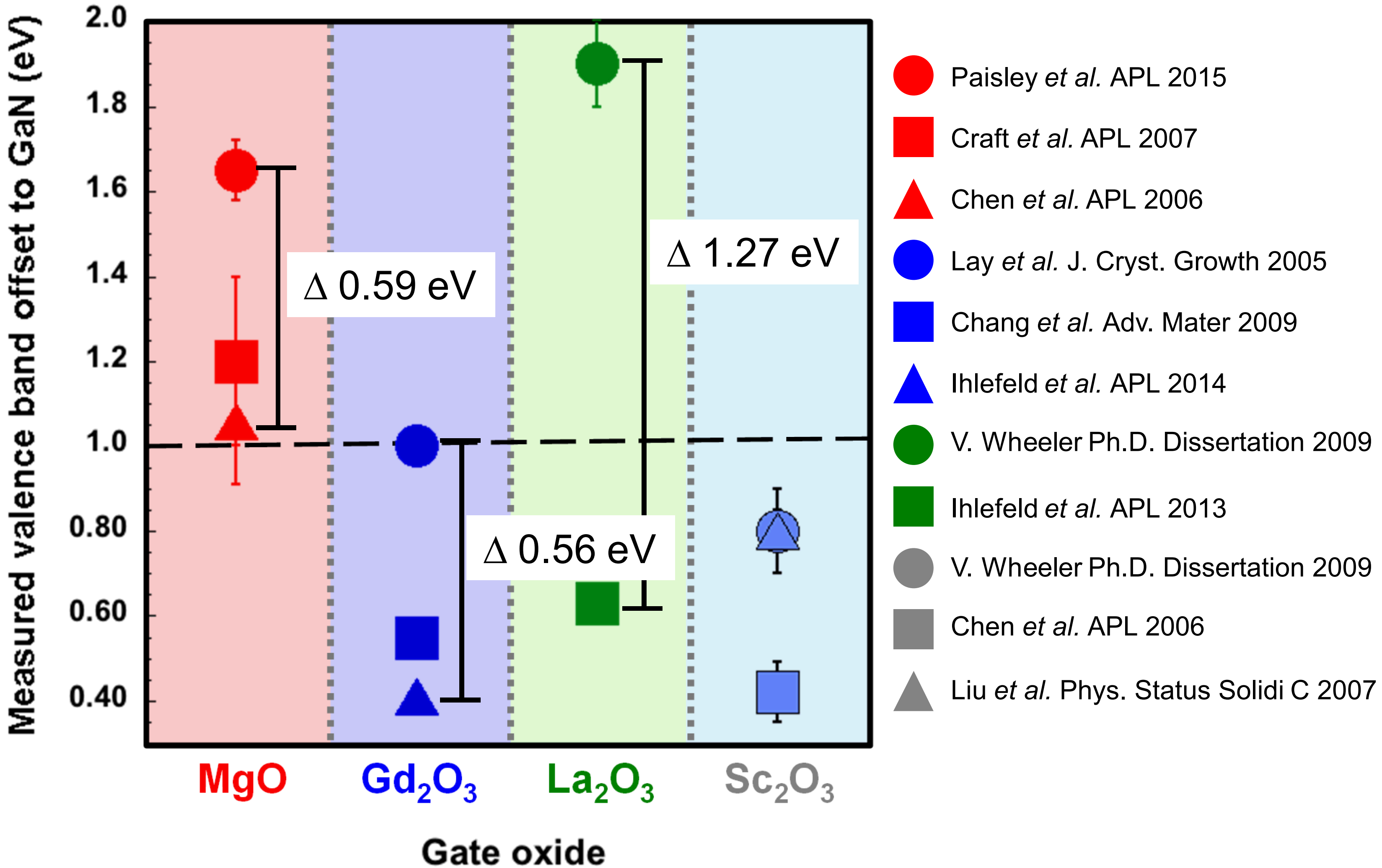
XPS by Michael Brumbach at SNL

The problem: Band offsets are wildly inconsistent



We want < 0.1 eV differences…

The problem: Band offsets are wildly inconsistent



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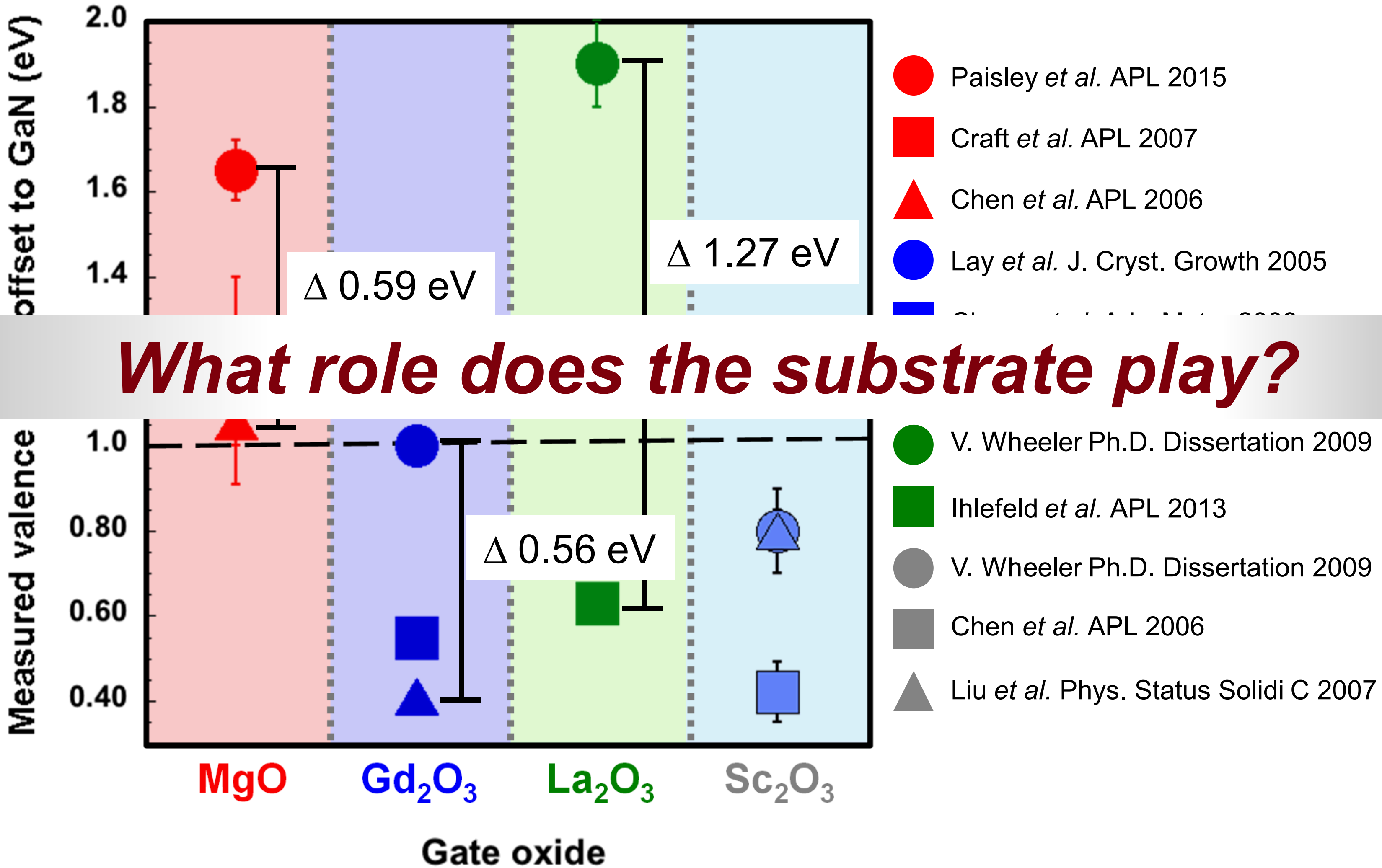


What role does the substrate play?

We want < 0.1 eV differences…

Band offset inconsistency experiment:

1. Acquire 5 GaN substrates: Lumilog, MTI, Sandia, and two from Maria group at NCSU
2. Clean substrates identically: acetone, methanol, UV-O_3, and HF dip
3. Grow MgO on top identically
4. Measure band offsets of MgO|GaN with XPS
   - M. Brumbach at SNL

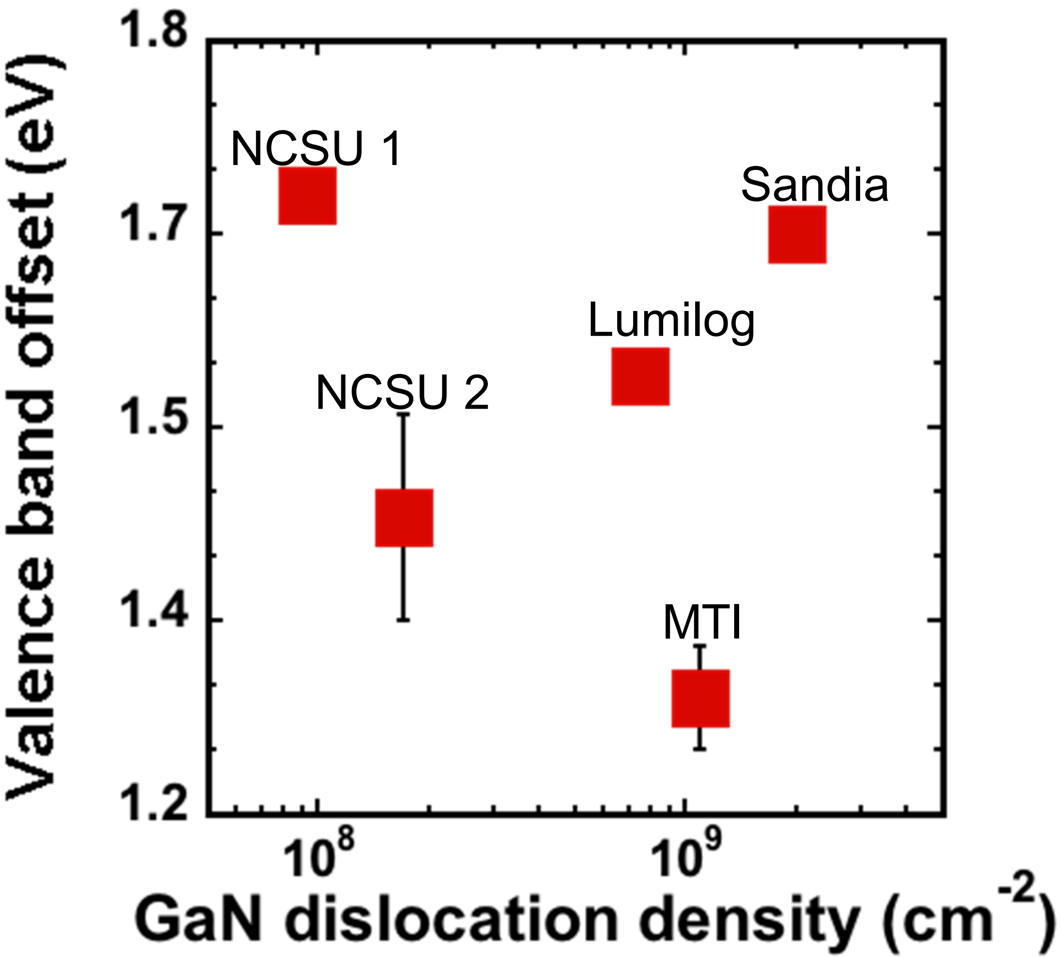
$$\Delta E_V = (Ga_{3d}\text{-}GaN_{VBM})_{GaN} - (G_{3d}\text{-}Mg_{2p})_{MgO/GaN} - (Mg_{2p}\text{-}MgO_{VBM})_{MgO}$$

Band offset inconsistency experiment:

Test what role the substrate plays in determining oxide/nitride band offsets:

1. **Dislocation density of GaN**
2. **Surface stoichiometry of GaN**

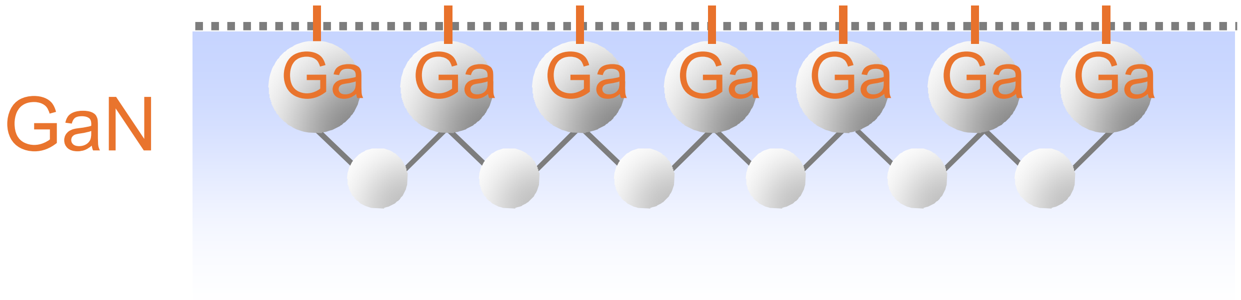
1. Dislocation density of GaN:



- Large changes in valence band offset across sample series
- No clear trend with dislocation density across the 5 substrates.
- Dislocations may matter, but the trend isn't obvious

2. Surface stoichiometry of GaN:

- When we epitaxially grow MgO on GaN along $[111]_{MgO}$:



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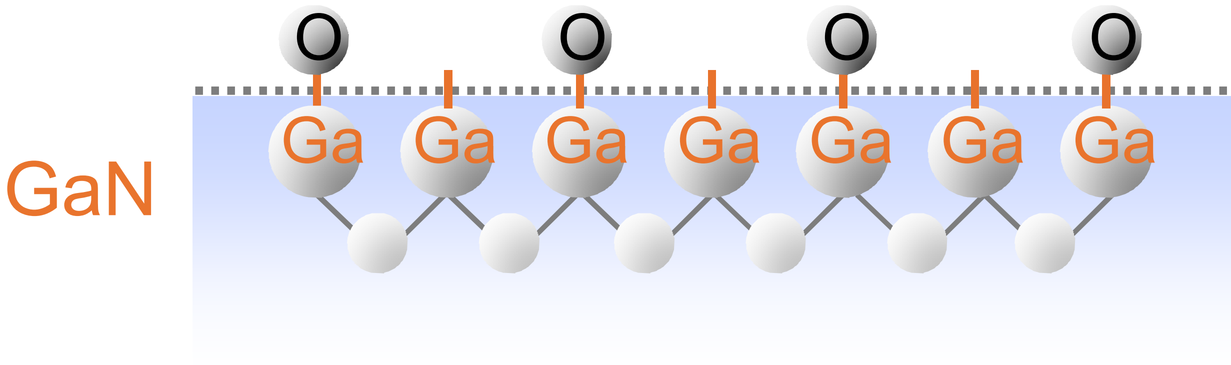

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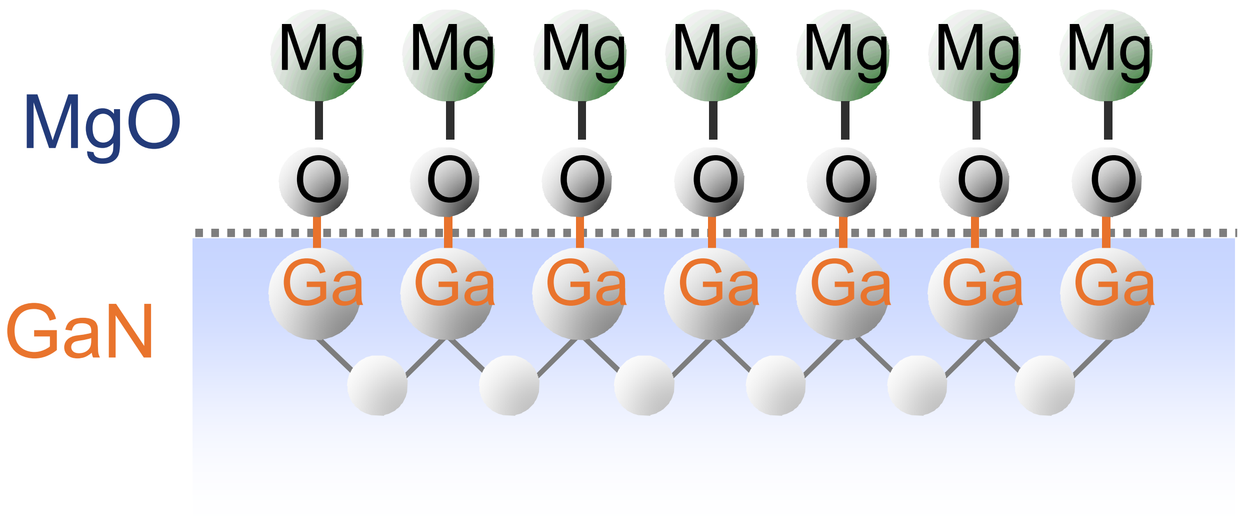

We expect abrupt MgO/GaN interfaces.

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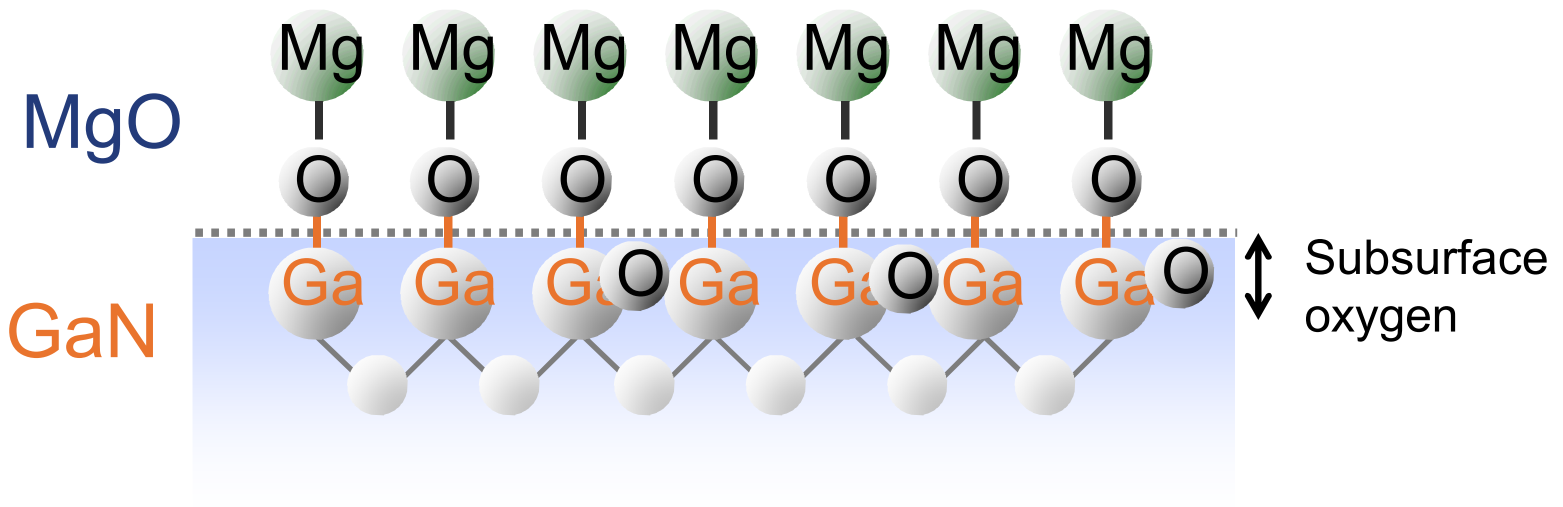

We expect abrupt MgO/GaN interfaces.
But, what about subsurface oxygen?

Baldereschi *et al.*, *PRB* 1991: "Tuning band offsets in GaAs/AlAs with Si intralayers"

Band offsets with (sub)surface oxygen:

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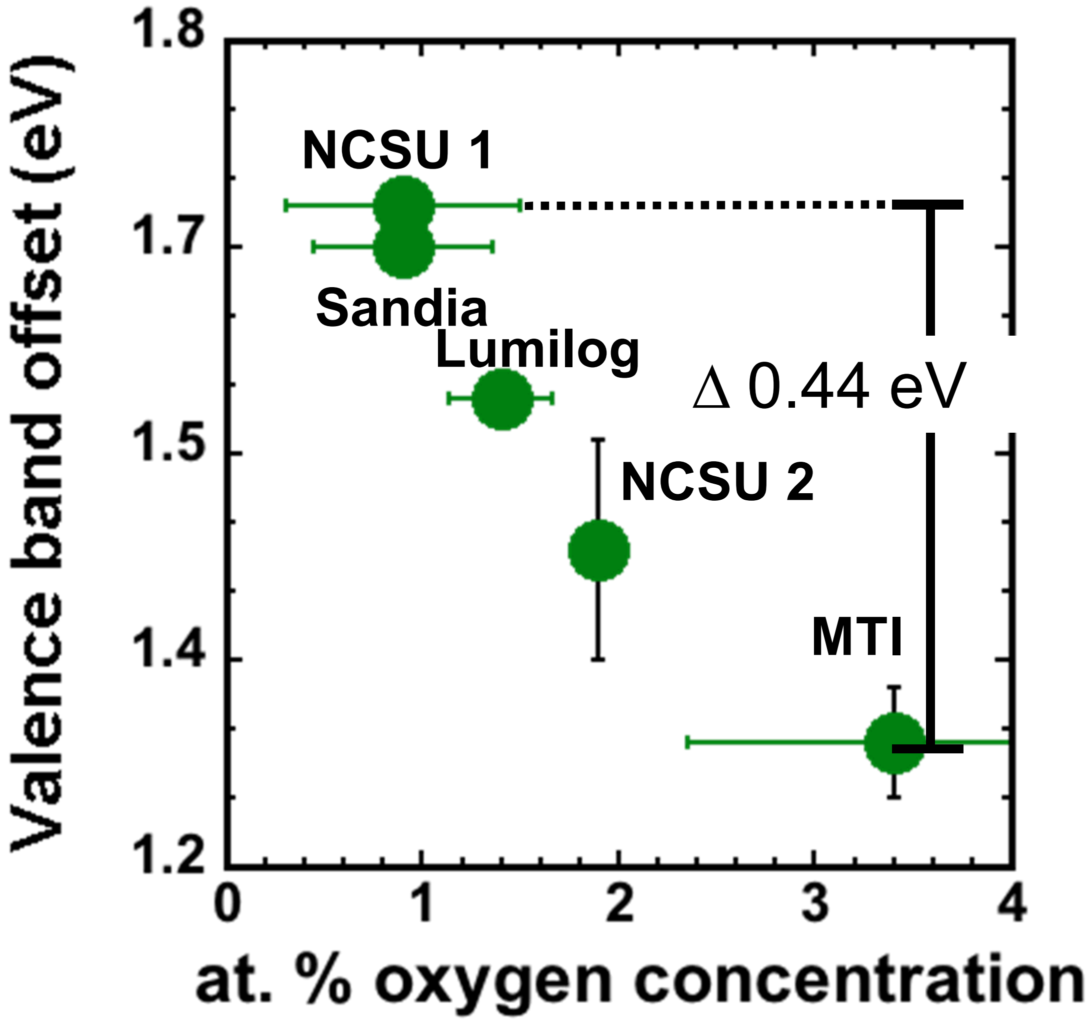
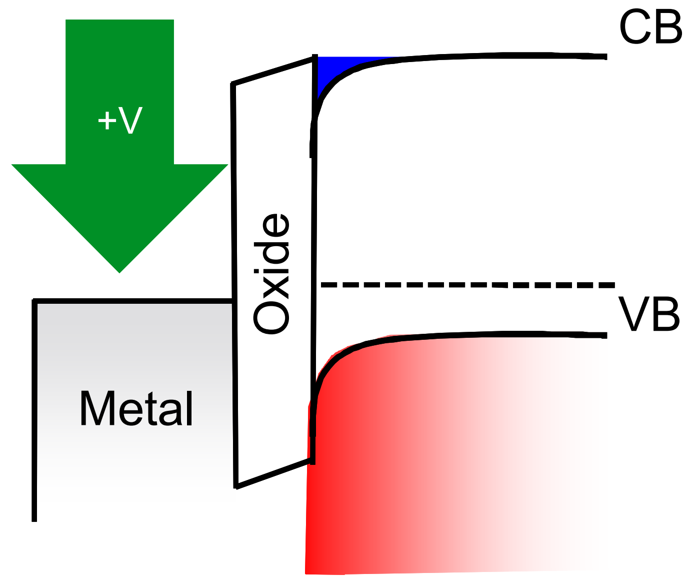


- Large change in band offsets has a clear trend with oxygen concentration in GaN
- Differences are similar to the magnitude of inconsistencies seen in the literature

Oxides for GaN Devices

- Oxide requirements for MOSFETs and MOSHEMTs:
  - **Large bandgap ✔**
  - **Band offsets > 1 eV with semiconductor ✔**
  - **Chemically compatible ✔**
  - Grows as a smooth film on GaN
  - ***Low interface defect density***



- Our strategy:
  - Identify chemically compatible wide bandgap oxides that may have acceptable offsets with WBG and UWBG semiconductors
  - Utilize epitaxy to form well-controlled interfaces

D_{it} measurements for oxides on GaN

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- We can extract D_{it} from Capacitance-Voltage analysis.
  - Several techniques are used to do this in literature.
- **Most techniques developed for silicon technology.**
- **These are not generally appropriate for wide bandgap devices:**
  - Low minority carrier generation rate
  - Require interface states with short emission times
  - Pyroelectric (temperature change results in surface charge)
- Many traditional techniques underestimate D_{it}.
- ***We will use Photo-assisted CV***

Photo-assisted CV analysis: MgO|GaN

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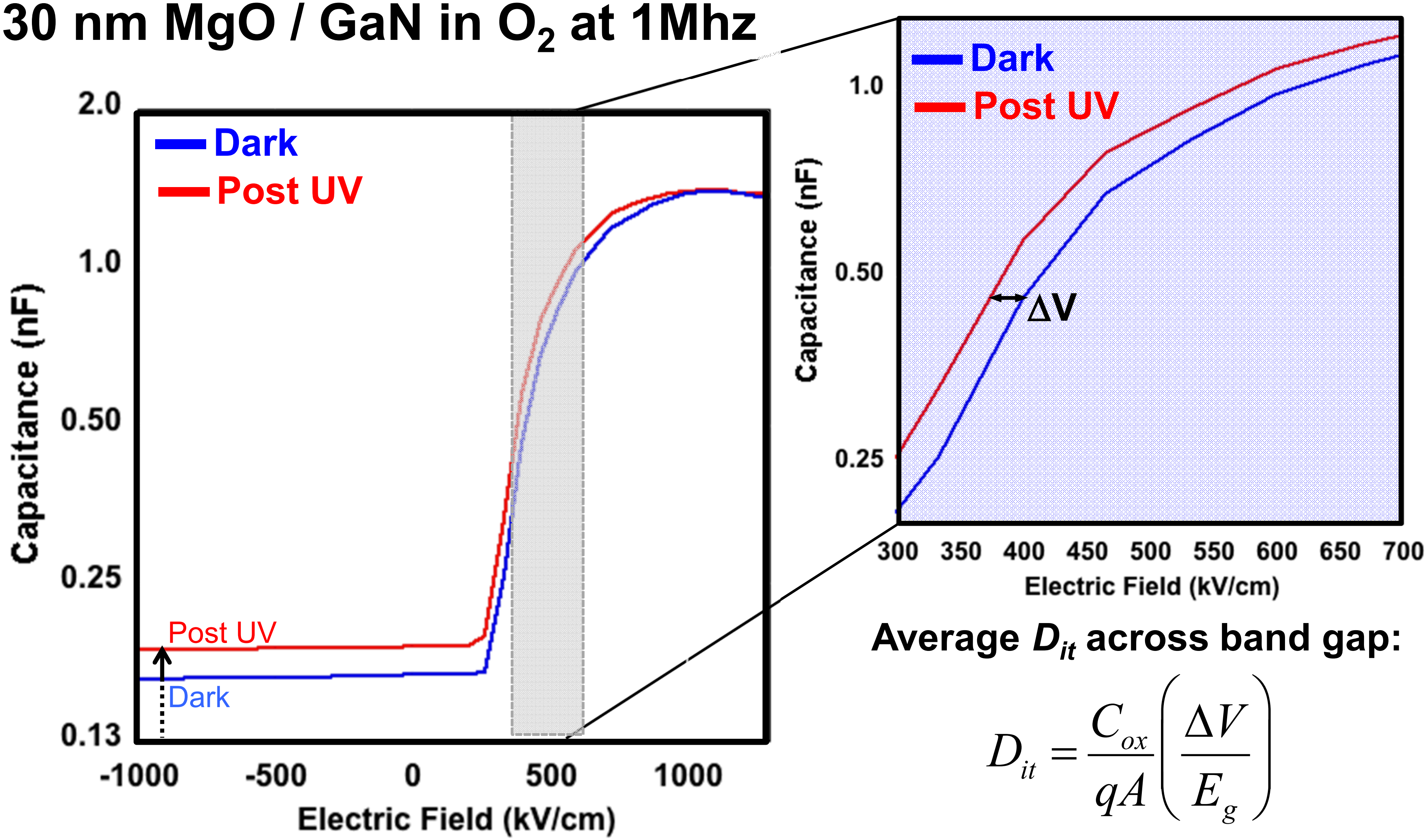
30 nm MgO / GaN in O_2 at 1Mhz



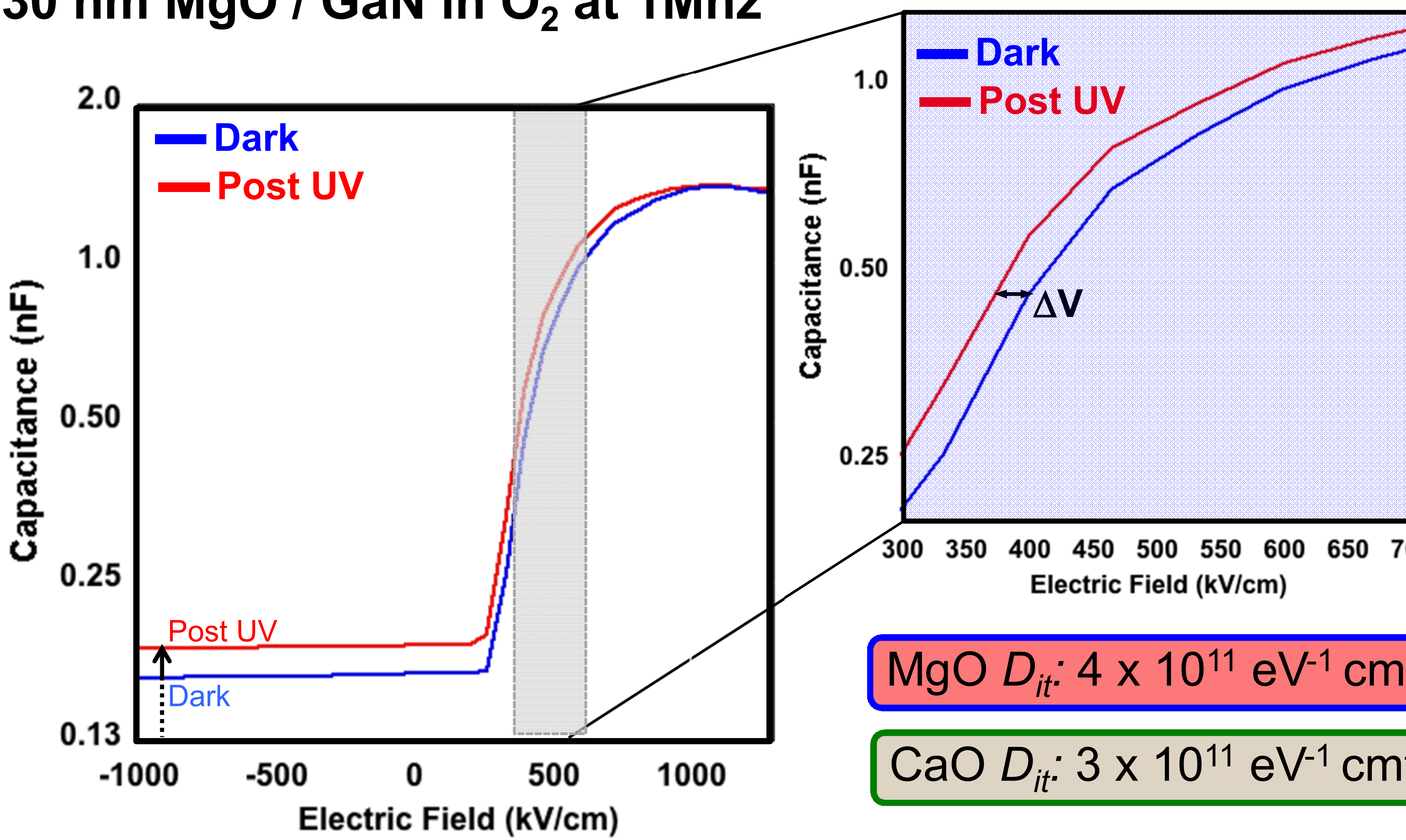
Average D_{it} across band gap:

$$D_{it} = \frac{C_{ox}}{qA}\left(\frac{\Delta V}{E_g}\right)$$

J. Tan *et al.*, APL **70** (1997)   Swenson and Mishra, J. Appl. Phys., **106** (2009)

Photo-assisted CV analysis: MgO|GaN

30 nm MgO / GaN in O_2 at 1Mhz

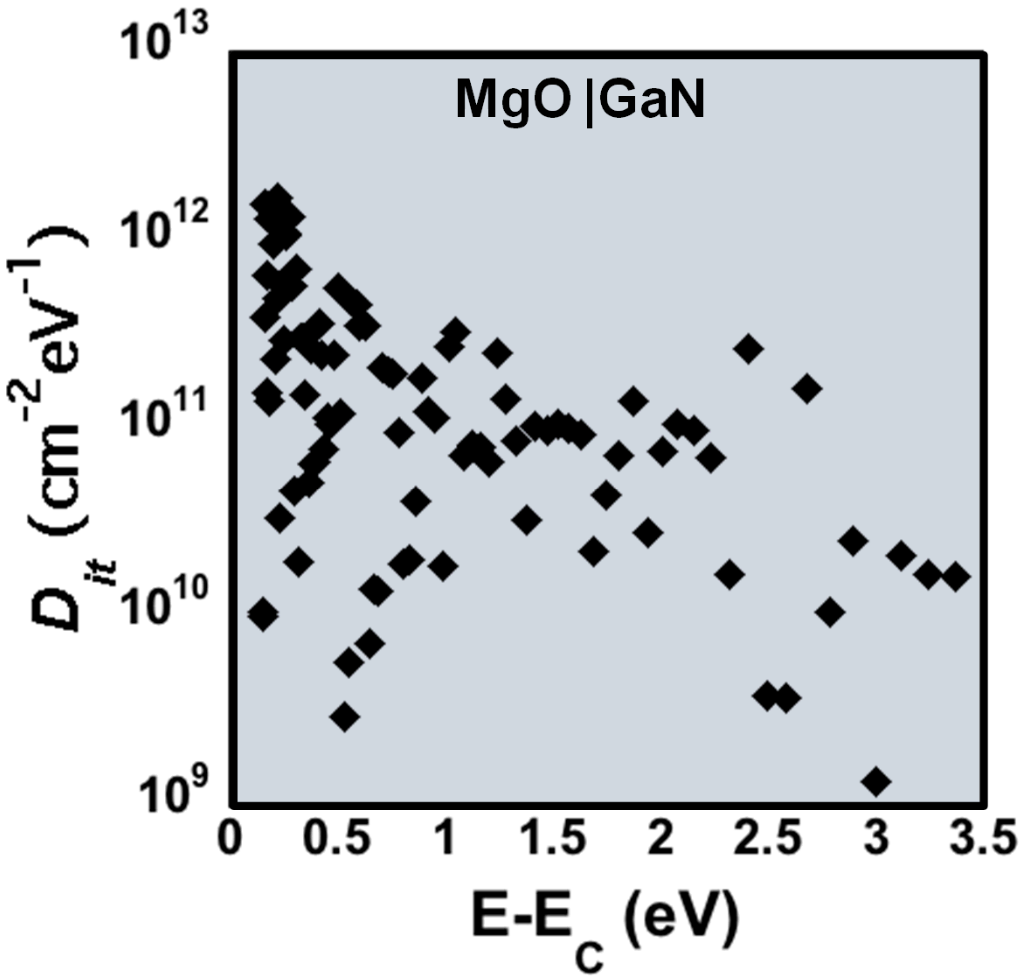


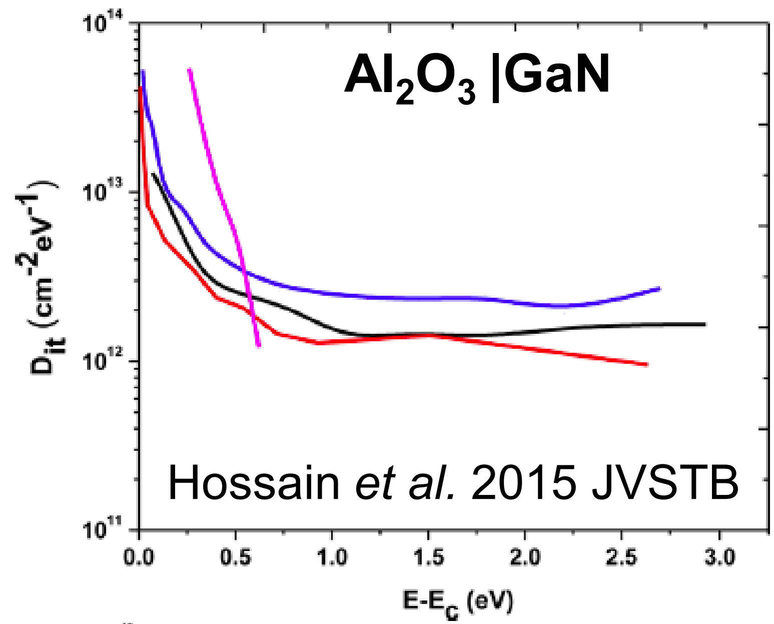
MgO D_{it}: 4 x 10^{11} eV^{-1} cm^{-2}

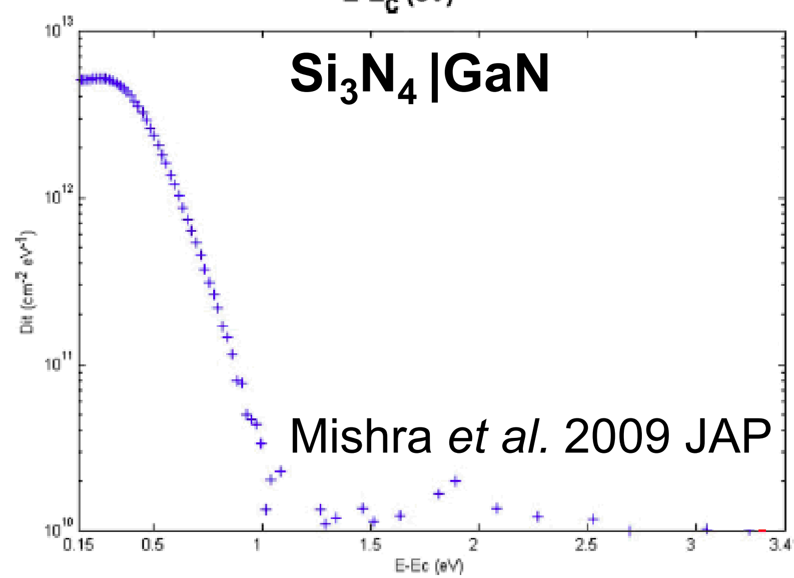
CaO D_{it}: 3 x 10^{11} eV^{-1} cm^{-2}

J. Tan *et al.*, APL **70** (1997) Swenson and Mishra, J. Appl. Phys., **106** (2009)

High quality interfaces with GaN:







Average D_{it}: 9 x 10^{10} cm^{-2} eV^{-1}

Comparison of dielectrics / GaN

- All measured with photo-assisted CV:

Dielectric / GaN	D_{it} (eV^{-1} cm^{-2})	Reference
La_2O_3	1×10^{12}	SNL
MgO	9×10^{10}	SNL
CaO	3×10^{11}	SNL
Ga_2O_3	4.2×10^{11}	[1]
Si_3N_4	5×10^{12}	[2]
Al_2O_3	3×10^{12}	[3]
Al_2O_3	5×10^{11}	[4]

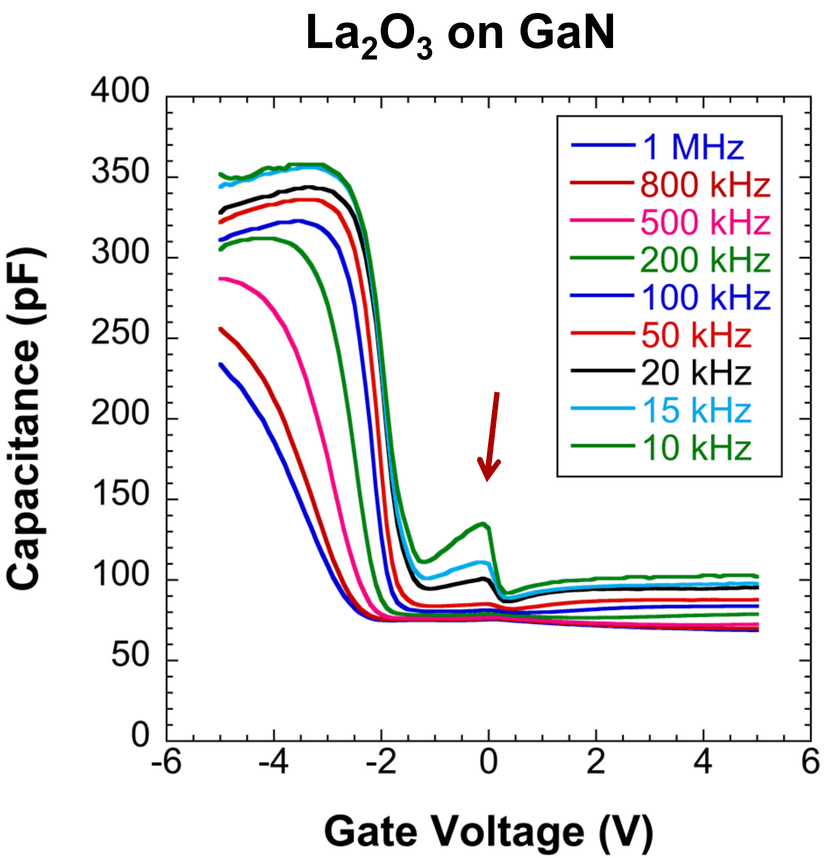
[1]Chiou, Y., Semicond. Sci. Technol. **25**, 2010.
[2]Mishra, U., J. Appl. Phys., **106**, 2009
[3]Ostermaier, C., Phys. Status Solidi C, **5**, 2008
[4]Wu, Y., Appl. Phys. Lett., **90**, 2007

Summary

- Enhancement mode GaN semiconductor devices are desirable for electric grid power management applications
- One candidate embodiment to achieve a normally off device is a MOSFET or MOSHEMT structure
- Lanthanides are probably not great candidates
- MgO/CaO epitaxial alloys may be excellent candidates
  - Chemical compatibility
  - Large bandgaps
  - Large band offsets
  - Low interface state densities
- ***Care must be taken to understand substrate growth and properties to reliably and repeatably prepare oxides on GaN***

La_2O_3/GaN Electrical Characterization

Sandia National Laboratories



- C-V curves enable identification of interface defects
  - Low frequency peak (red arrow) indicates presence of interface trap states
- I-V curves allow for measurement of leakage through gate insulator
- La_2O_3 looks great on paper, but does not work

Interface trap presence indicates performance limitation for this system

Background

- Few well characterized reports on gate oxides for WBG and UWBG semiconductors:
  - Most work is either poorly conducted (band offset characterization) or vague (interface trap density characterization)
- Important parameters:
  - Chemical compatibility
  - Band offsets
    - Available materials become increasingly limited as semiconductor band gap increases
  - Interface state density
- Our strategy:
  - Identify wide bandgap oxides that may have acceptable offsets with WBG and UWBG semiconductors
  - Utilize epitaxy to form well-controlled interfaces