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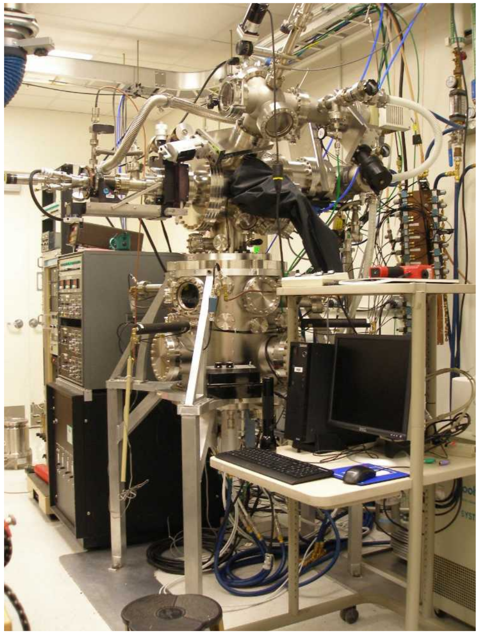

Growth and Band Offsets of Epitaxial Lanthanide Oxides on GaN and AlGaN

22 January 2015

Jon Ihlefeld, Michael Brumbach, Andrew A. Allerman, David R. Wheeler, and Stanley Atcitty

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Exceptional service in the national interest

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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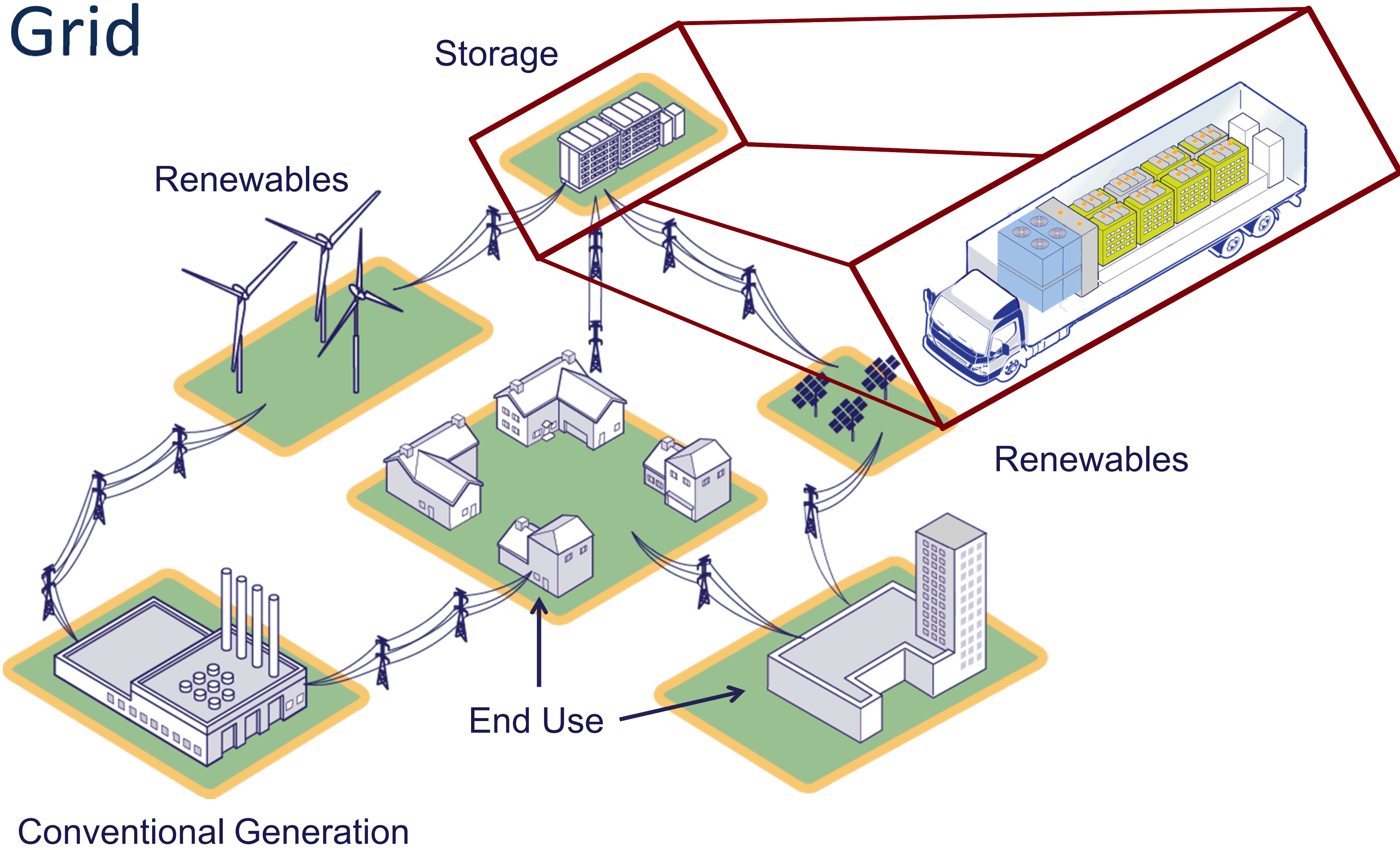
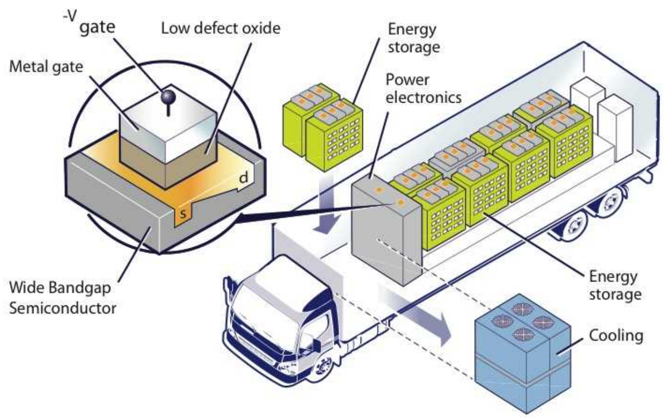
Power Electronics for Electrical Grid



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

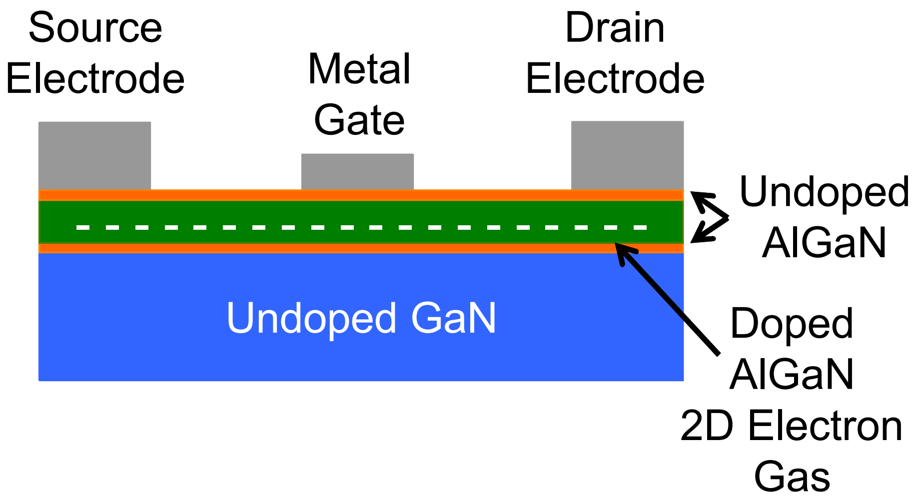
- Power electronics are necessary for energy modulation and introduction of storage on the electrical grid
- Leading technology today is Si-based IGBTs
  - Si-based devices are limited in operating temperature and electric field
- Costs and low mobility associated with SiC technology makes GaN devices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

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

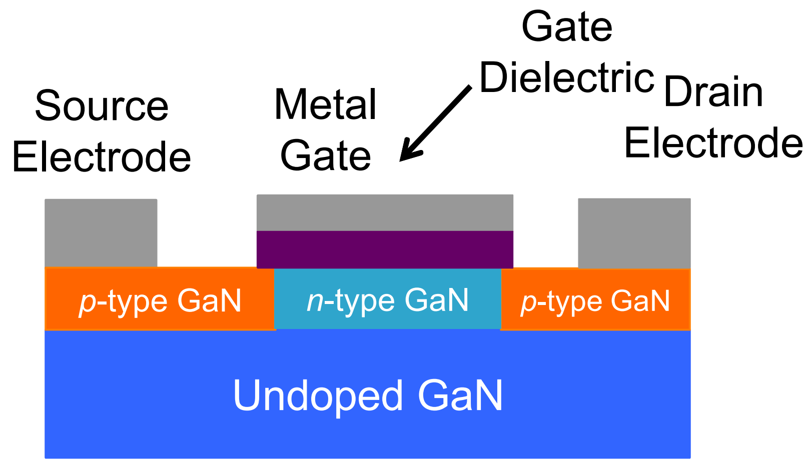
GaN Devices

- "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 would be advantageous

HEMT

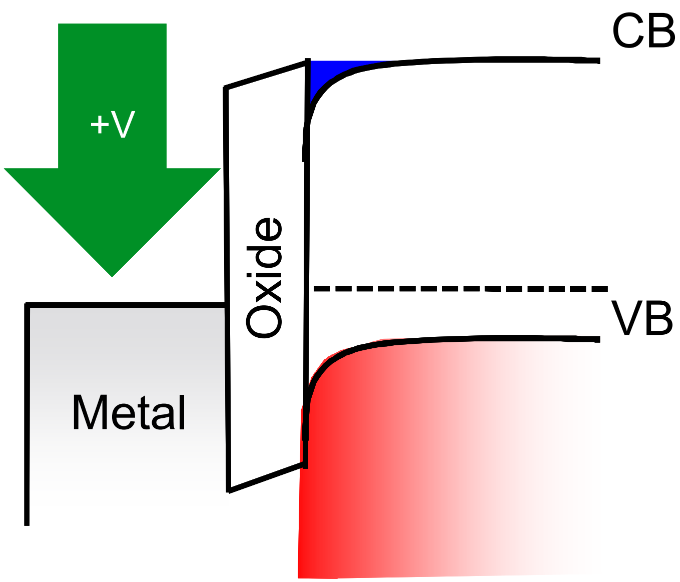


MOSFET



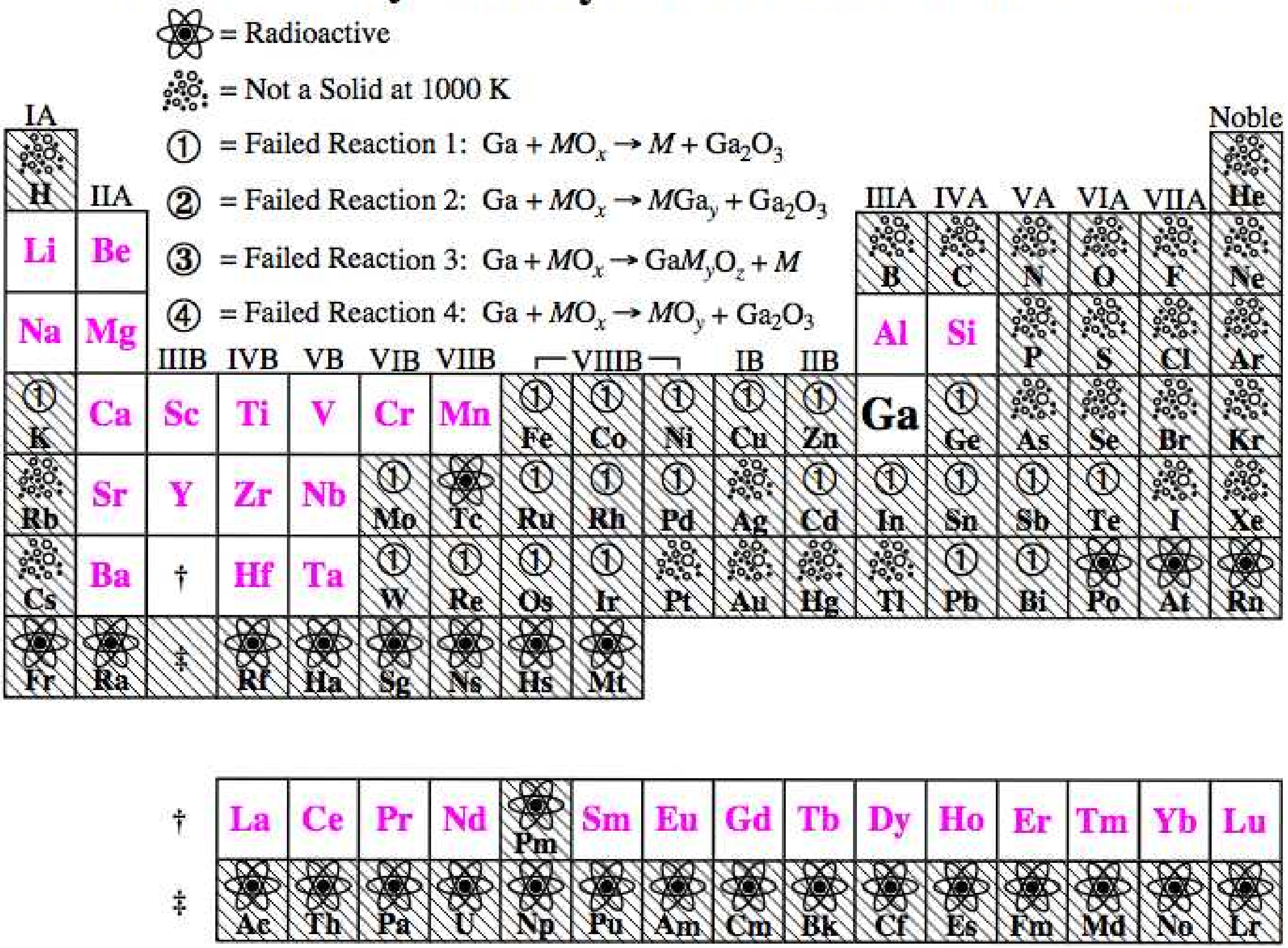
GaN Devices

- 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

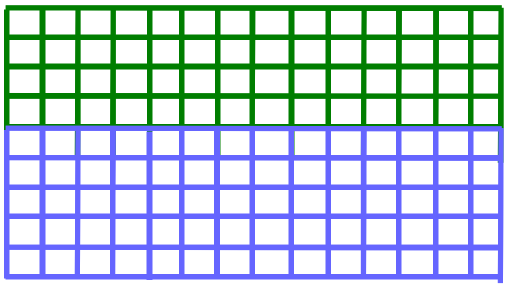


Insufficient Thermodynamic Data to Complete Calculations

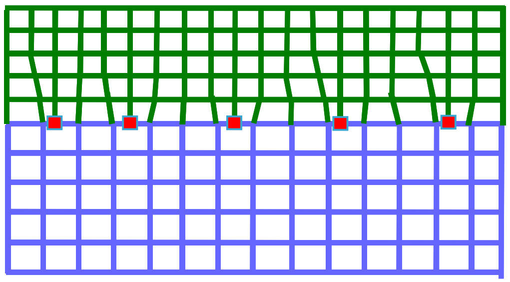
Experimentally Demonstrated

Lanthanide Oxides: Candidate Materials

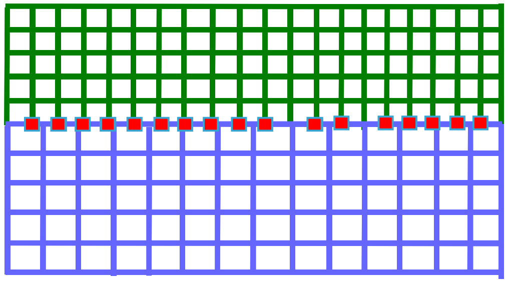
0% Strain
Coherent Interface
Satisfied Bonds



~< 10% Strain
Pseudomorphic
With Dislocations



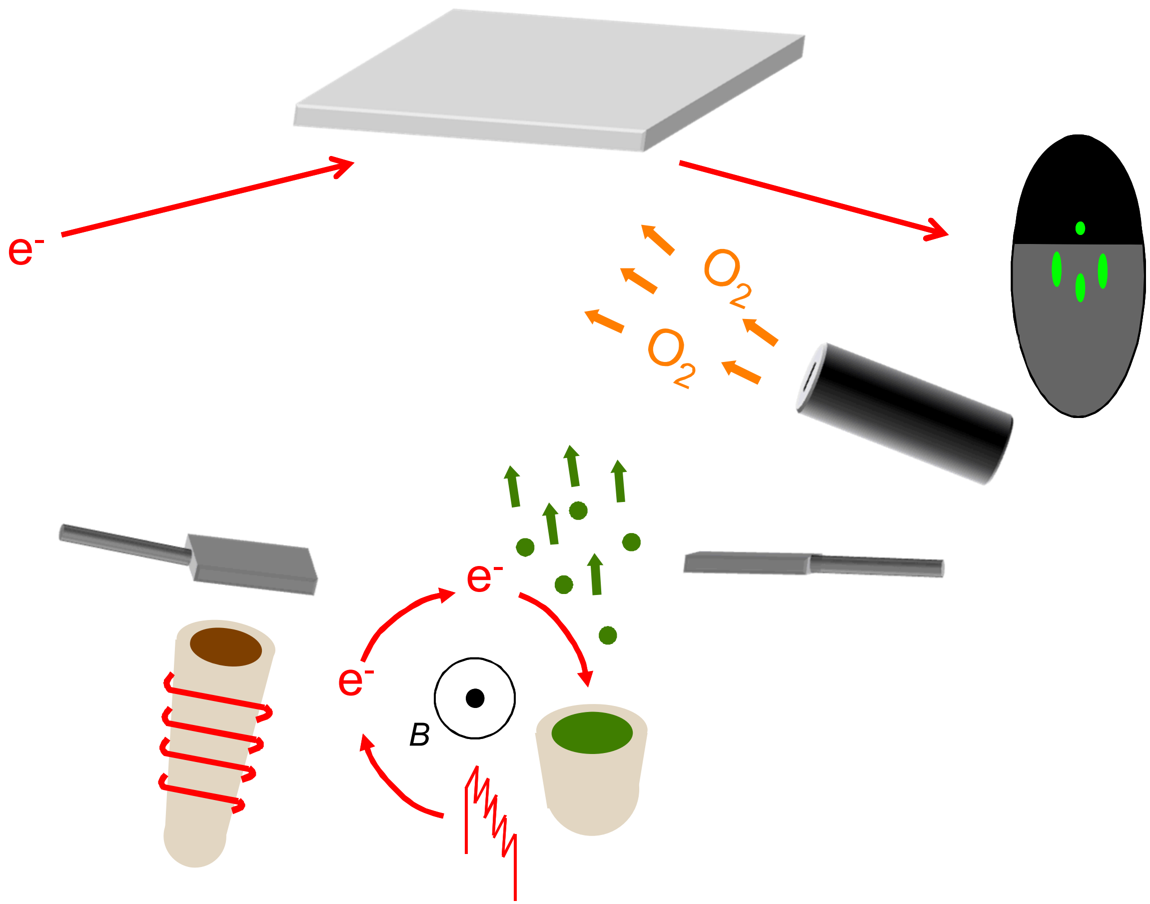
~>10% Strain
Incoherent
With Dislocations



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

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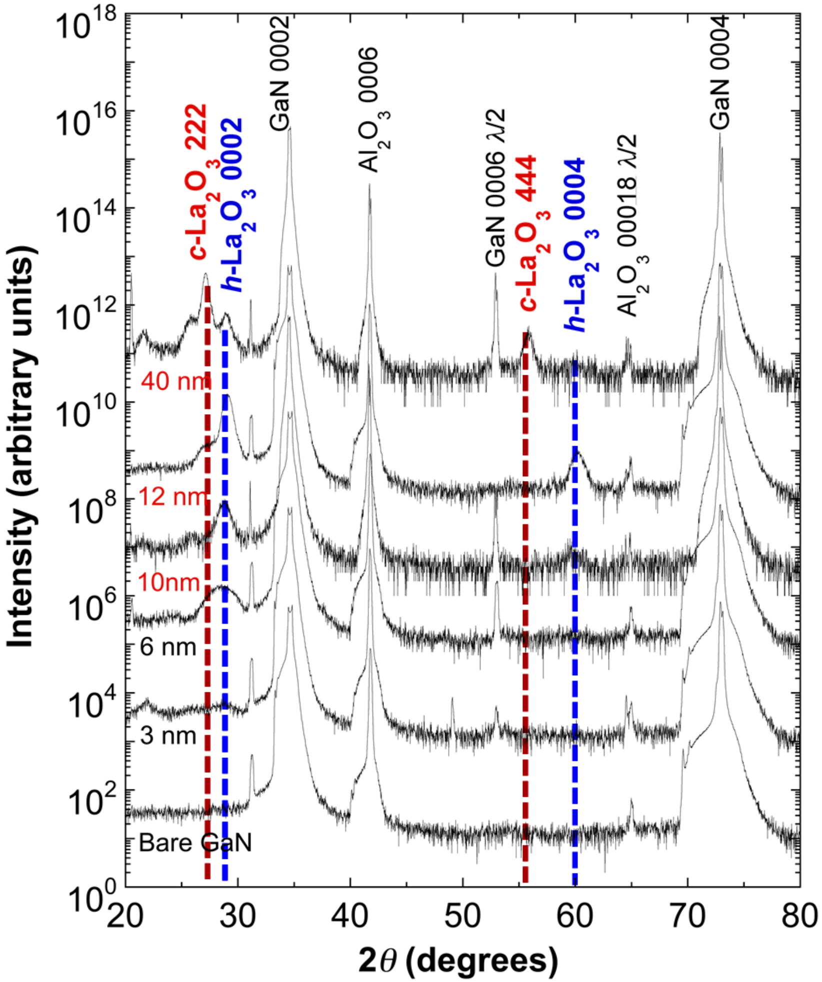
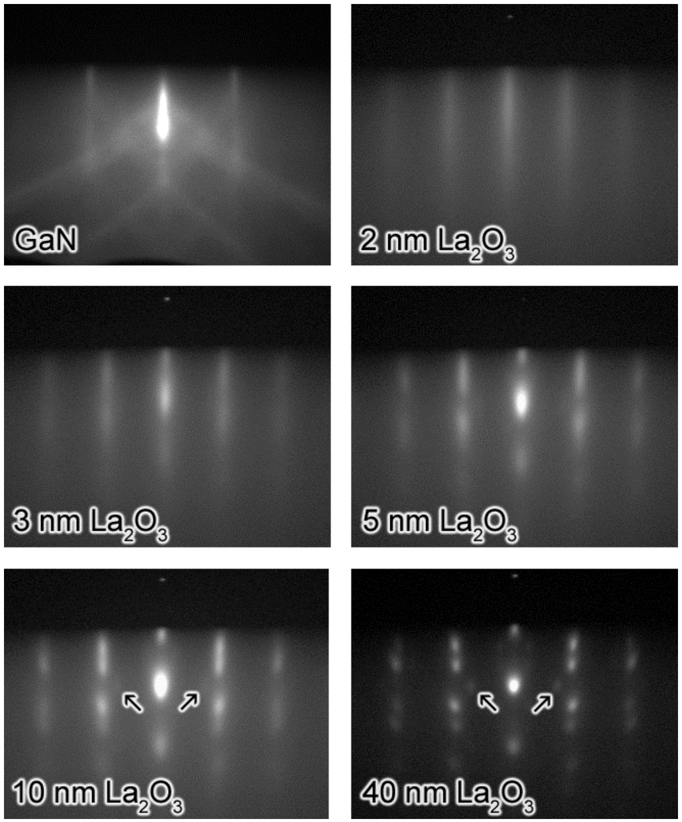
X-ray Diffraction



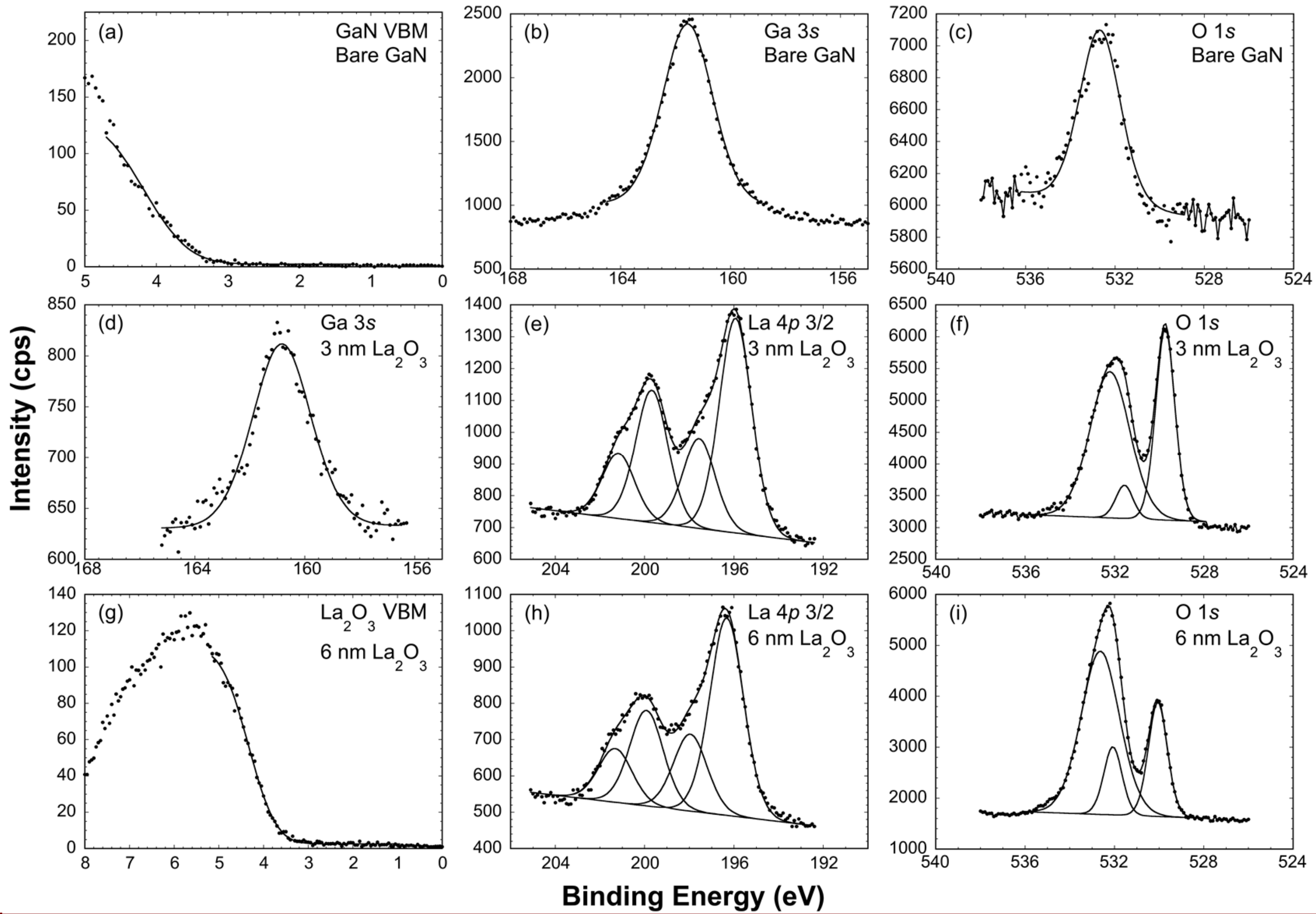
RHEED



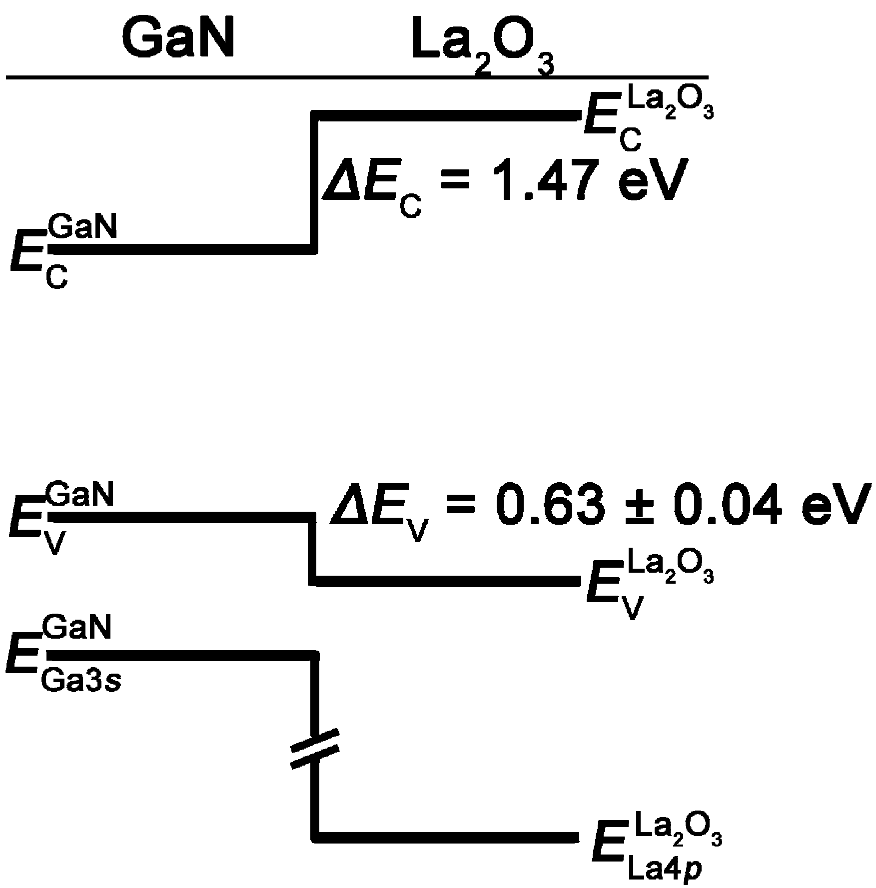
- Hexagonal growth observed for thicknesses of ≤ 6nm
- Transitions to rough cubic phase for thicknesses > 6nm

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

XPS Determination of Band Offsets



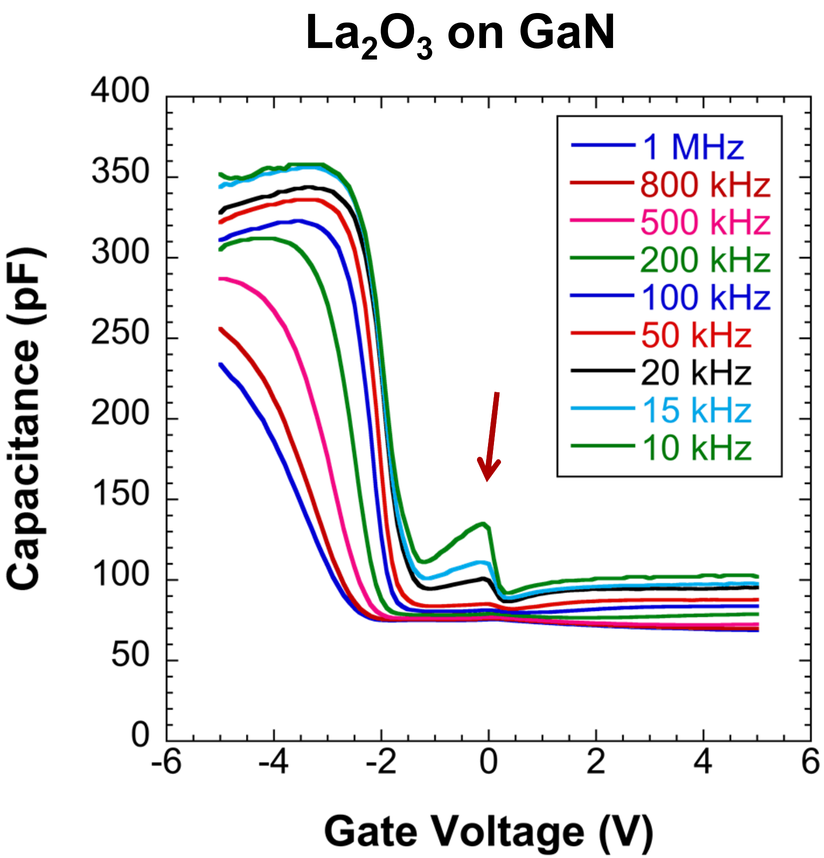
La_2O_3/GaN Band Alignments



- 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)

La_2O_3/GaN Electrical Characterization



- 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

Gd_2O_3 as Gate Dielectric

ADVANCED MATERIALS www.advmat.de

COMMUNICATION

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

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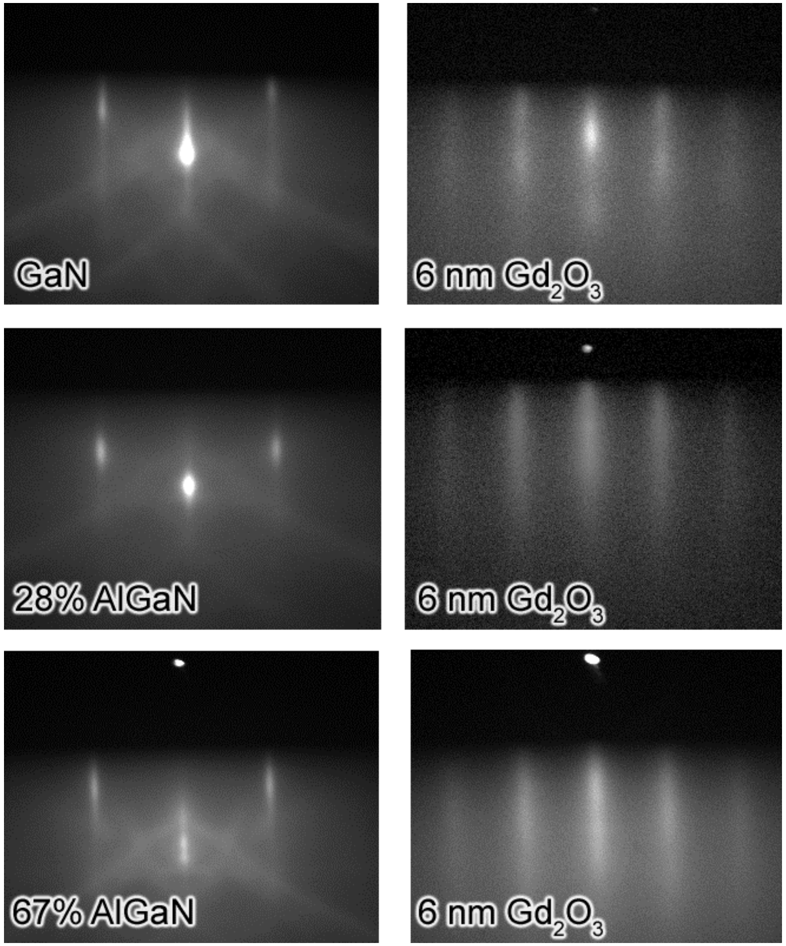
(Received June 23, 2001; accepted August 4, 2001)

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)

Gd_2O_3 on AlGaN Growth

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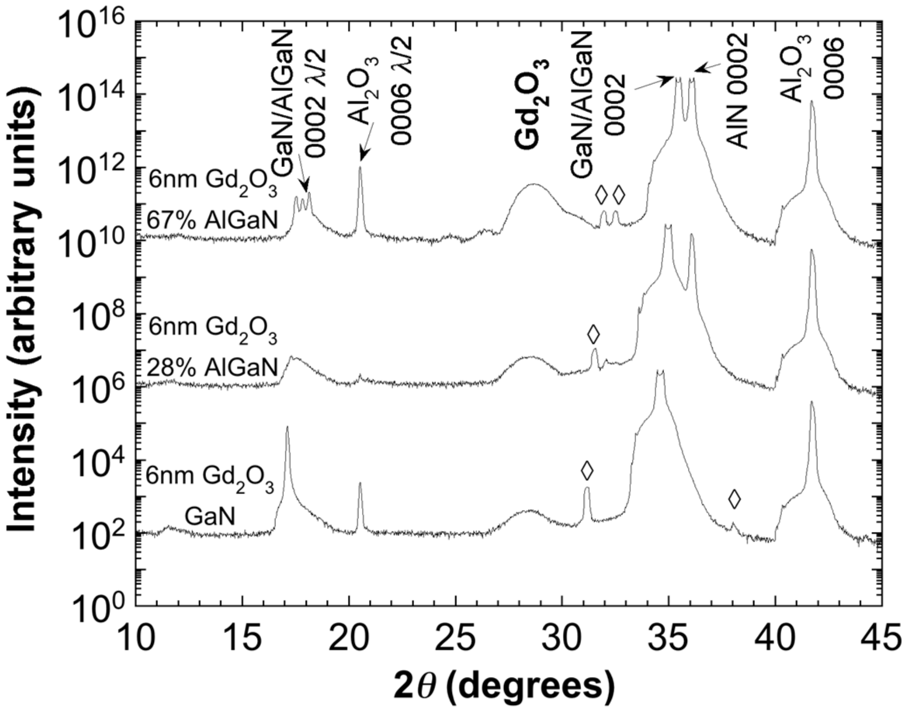

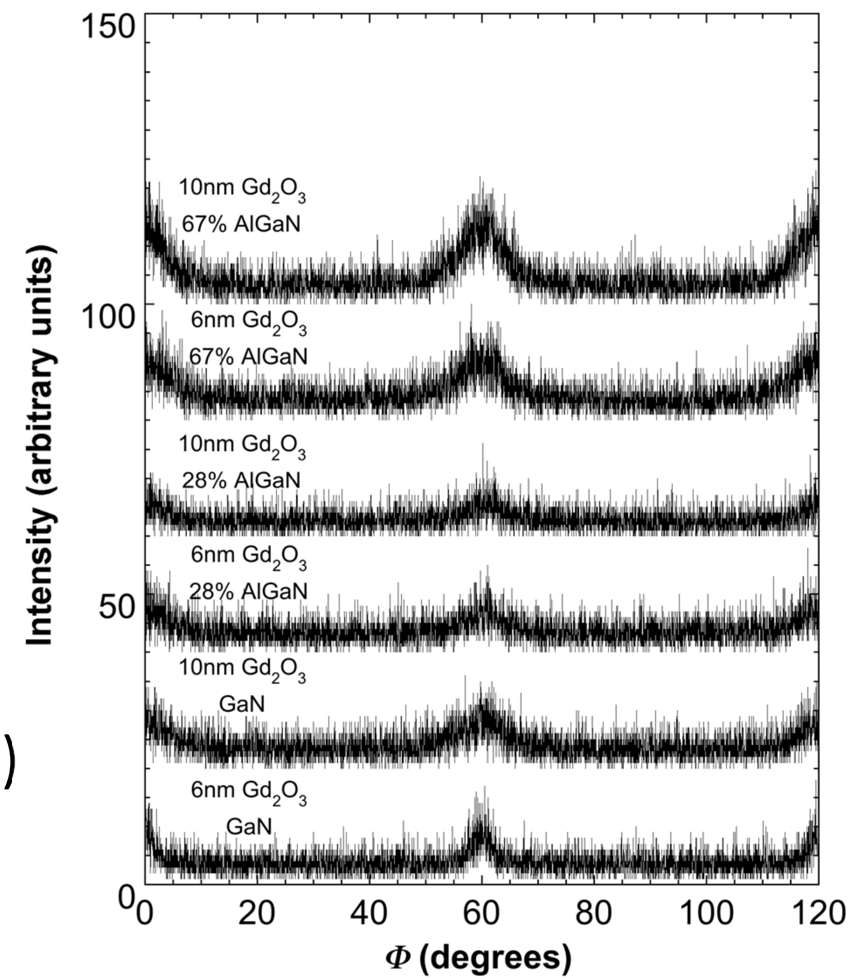

400 reflection of cubic Gd_2O_3
($2\theta = 33.2°$, $\Psi = 54.7°$)

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

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

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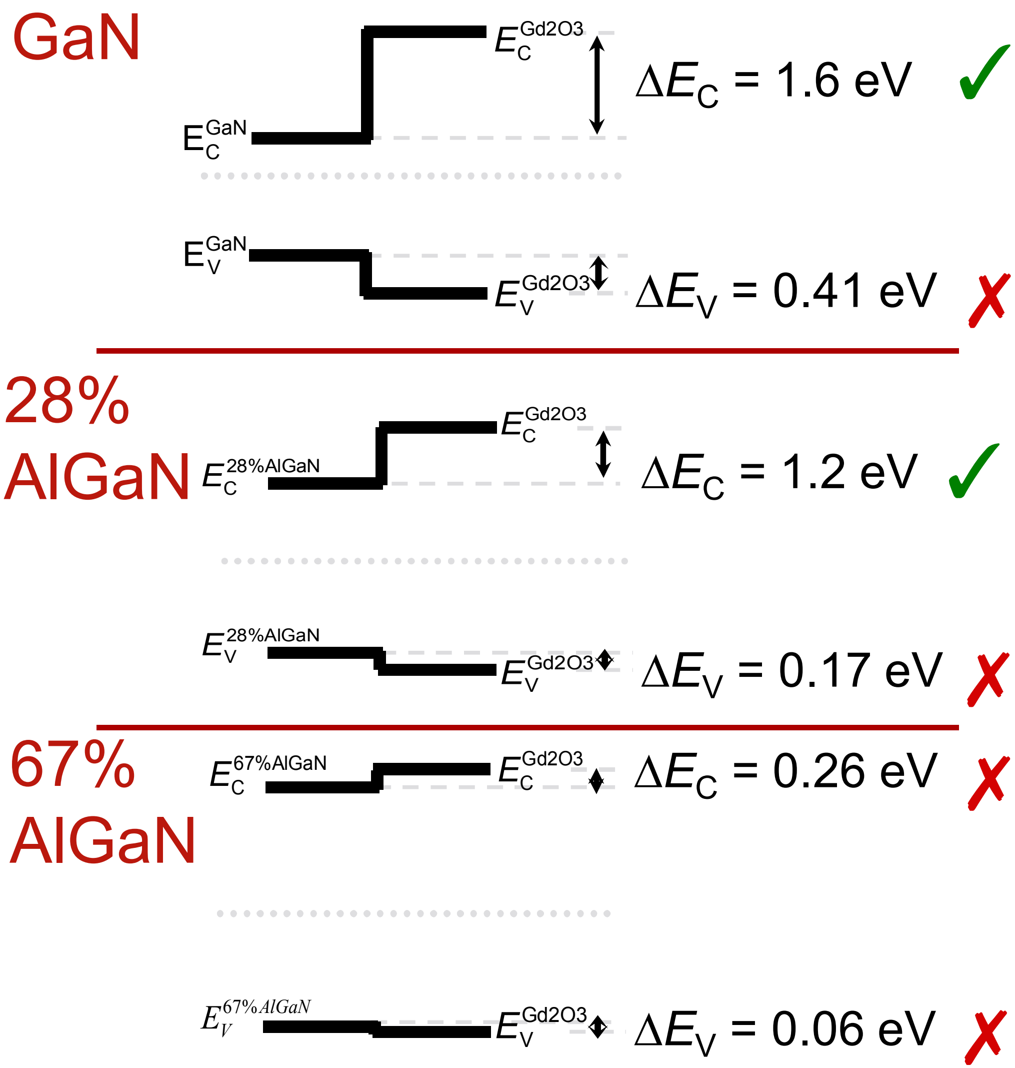
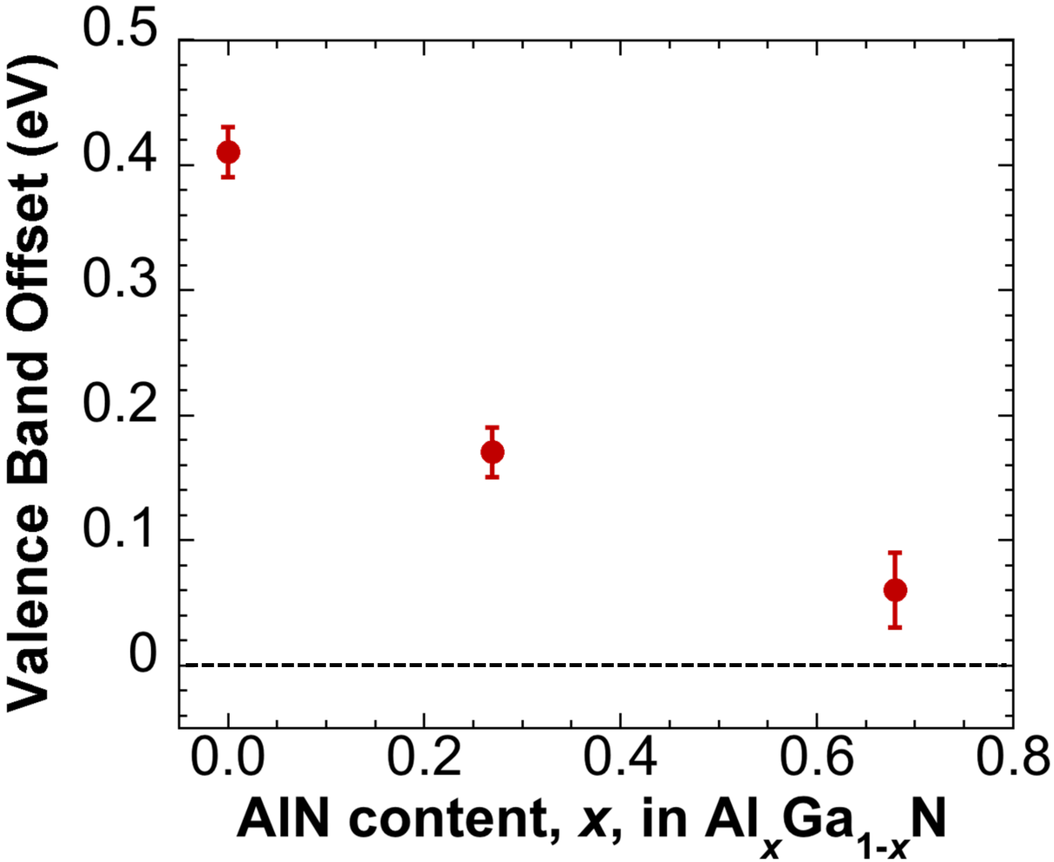


- Band offsets are semiconductor bandgap dependent
- All valence band offsets are < 0.5 eV
- ***Lanthanides will not work for UWBG devices***

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 will not work for UWBG devices***

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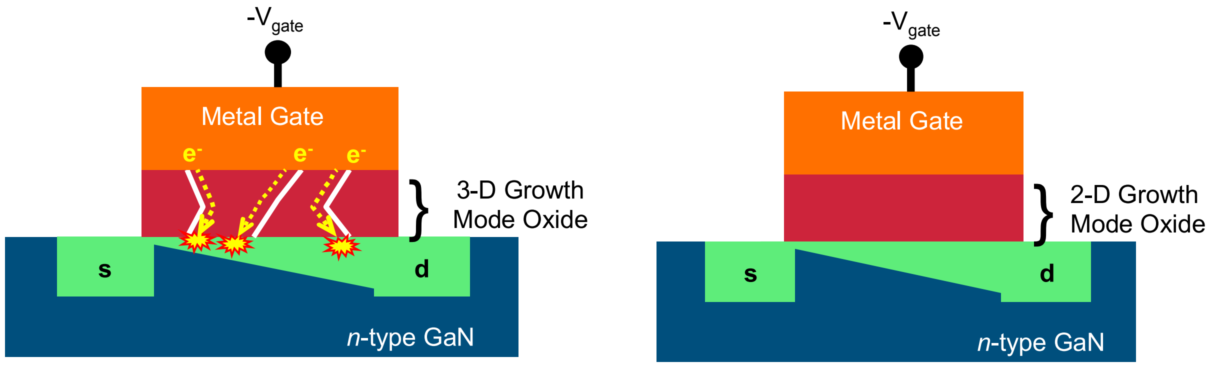
Summary

- Enhancement mode GaN semiconductor devices are desirable for electric grid power management applications
- One candidate embodiment to achieve a nominally off device is a MOSFET structure
- 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 make lanthanide oxides poor choices for GaN and AlGaN gate dielectric applications***

Oxide/GaN Growth and Structural Issues



- Rough growth results in grain boundaries that act as defect sources for gate leakage ➔ poor performance
- Smooth growth should have fewer threading defects ➔ greater reliability and performance
- ***Amorphous oxides (e.g. SiO_2) do not work well for WBG gates owing to poor interface control***

Oxide Electronic Properties: Importance of Band Gap

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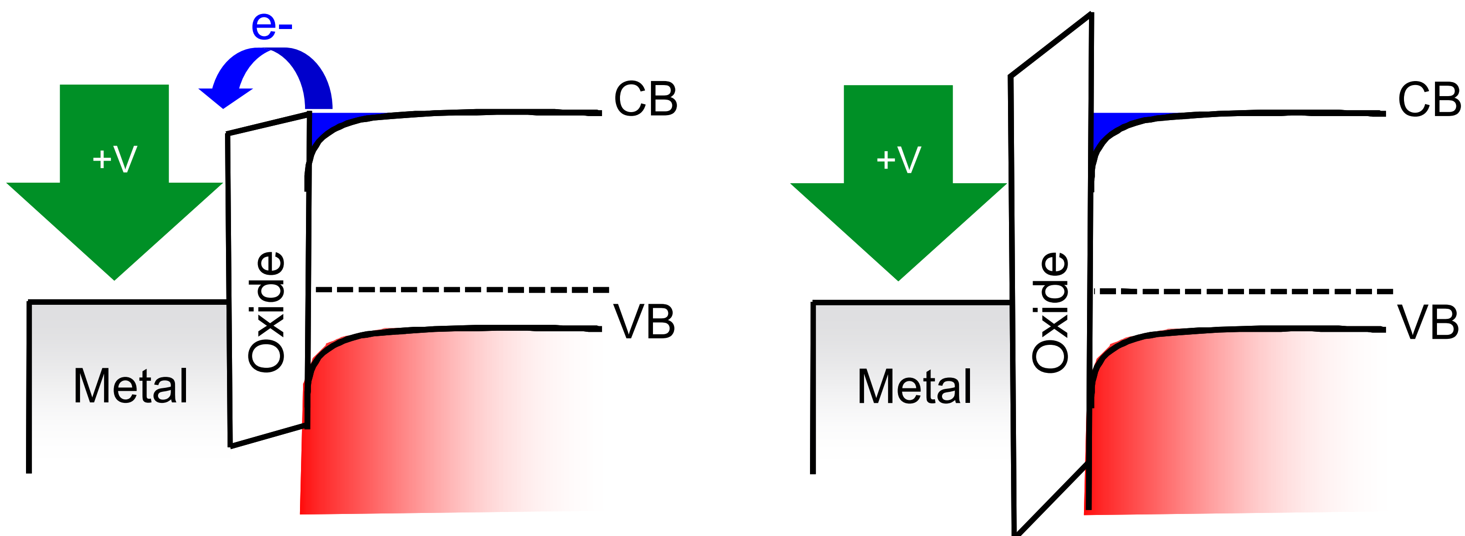
E_g^{GaN}=3.4 eV

Ln_2O_3	La	Nd	Sm	Gd	Dy	Ho	Er	Tm	Yb	Lu
E_g	5.5	4.7	5.0	5.4	4.9	5.3	5.3	5.4	4.9	5.5
κ	20-30	10	11	12	12	12	14		13	9

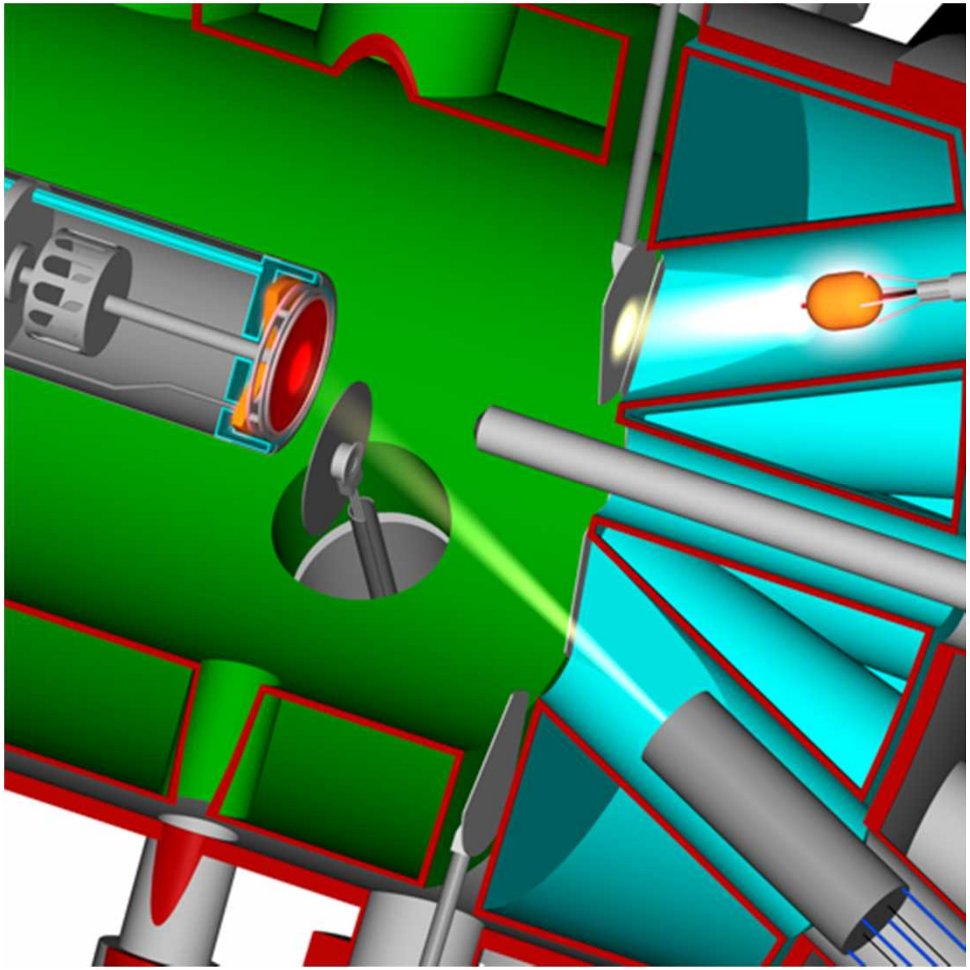


Low Bandgap
Low Band Offsets
Low Efficiency

Large Bandgap
Potentially Large Band Offsets

Data from: J-P. Maria in *High Dielectric Constant Materials* (2005).

Oxide/Nitride Growth



Reactive MBE

- Metallic sources
- e-beam evaporation
- Oxidizing atmosphere
- *in situ* RHEED

ALD

- Organometallic sources
- Oxidizing atmosphere
- Low temperature processing

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