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# Commensurate MgO-CaO alloys for GaN and AlGaN gate oxides



Elizabeth A. Paisley

Sandia National Laboratories

Albuquerque, NM

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# And…

Sandia National Laboratories:

- Jon Ihlefeld, Michael Brumbach, Andrew Allerman, Stanley Atcitty, Robert Kaplar, Albert Baca

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- Jon-Paul Maria, Christopher Shelton, James LeBeau, Edward Sachet, Douglas Irving, Benjamin Gaddy, Ramon Collazo, Zlatko Sitar

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- Mark Losego

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- Michael Biegalski, Chris Rouleau, Hans Christen

HexaTech, Inc.:

- Seiji Mita, Spalding Craft

# Why do we want gate dielectrics?

- **Remaining challenges to GaN and AlGaN power electronics:**
  - Gate leakage
  - Normally-off operation
  - Current collapse

The right gate dielectric can overcome these obstacles

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- **<u>Remaining challenges to GaN and AlGaN power electronics:</u>**
  - Gate leakage
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*All of these require forming oxide/semiconductor interfaces that are "perfect"*

The right gate dielectric can overcome these obstacles

# An ideal gate oxide should:

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2. Be chemically/thermally stable in contact with GaN and AlGaN

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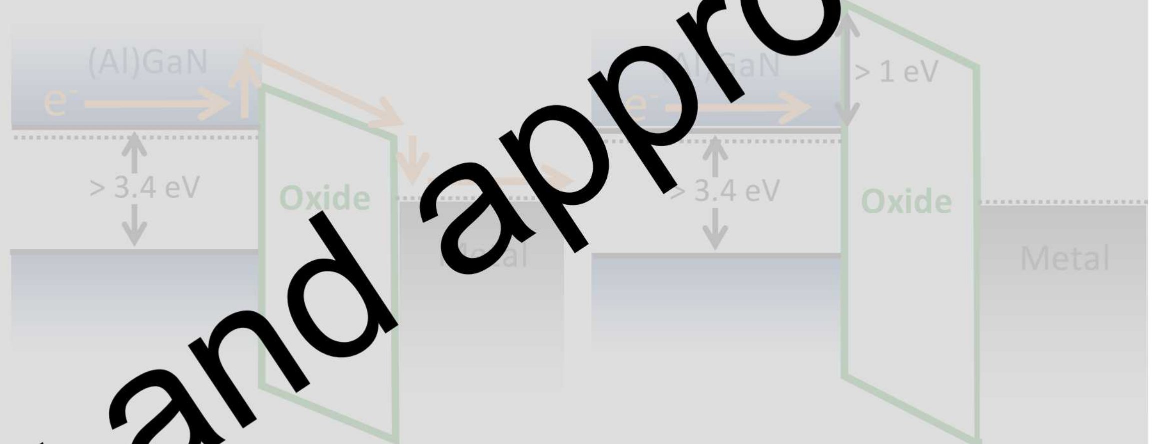



# Gate oxide development

- **Why not use $Ga_2O_3$?**
  - Small band gap: 4.8 eV
    - Valence band offset to GaN: 0.5 eV
    - Conduction band offset to GaN: 1 eV

- **Other commonly investigated gate oxides:**
  - $SiO_2$: low permittivity (~3.9), high interface state density measured
  - $SiN_x$: small valence band offset on GaN, high interface state density measured
  - High *k* ($HfO_2$, $Dy_2O_3$, $Gd_2O_3$): small band offsets measured

- ***Can we engineer an oxide to work better?***
  - *Find suitable band offsets*
  - *Use epitaxy to form well controlled interfaces*

# Gate oxide development

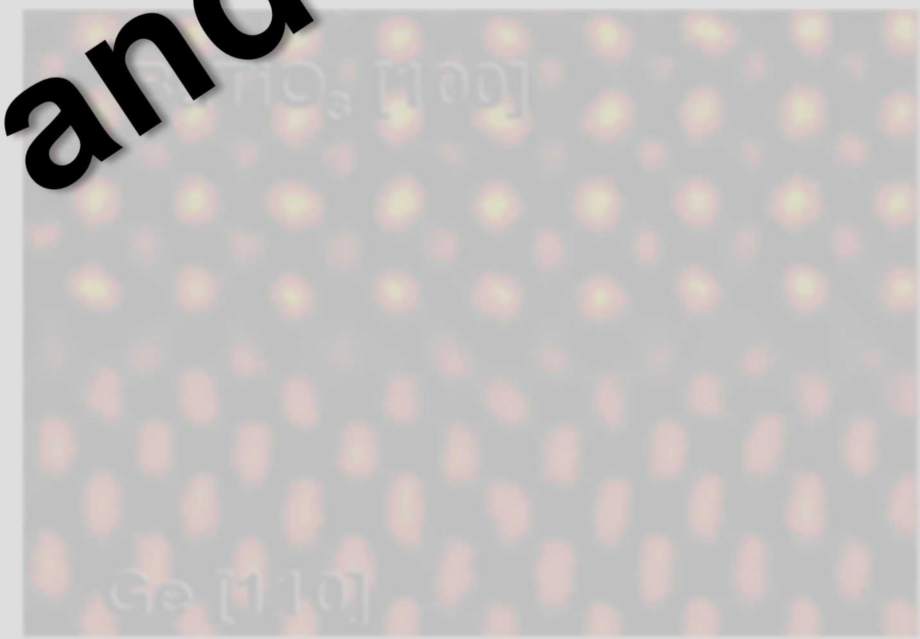
REPORT

## Physical Structure and Inversion Charge at a Semiconductor Interface with a Crystalline Oxide

R. A. McKee, F. J. Walker, M. F. Chisholm

\+ Author Affiliations

*Science* 20 Jul 2001:
Vol. 293, Issue 5529, pp. 468-471
DOI: 10.1126/science.293.5529.468



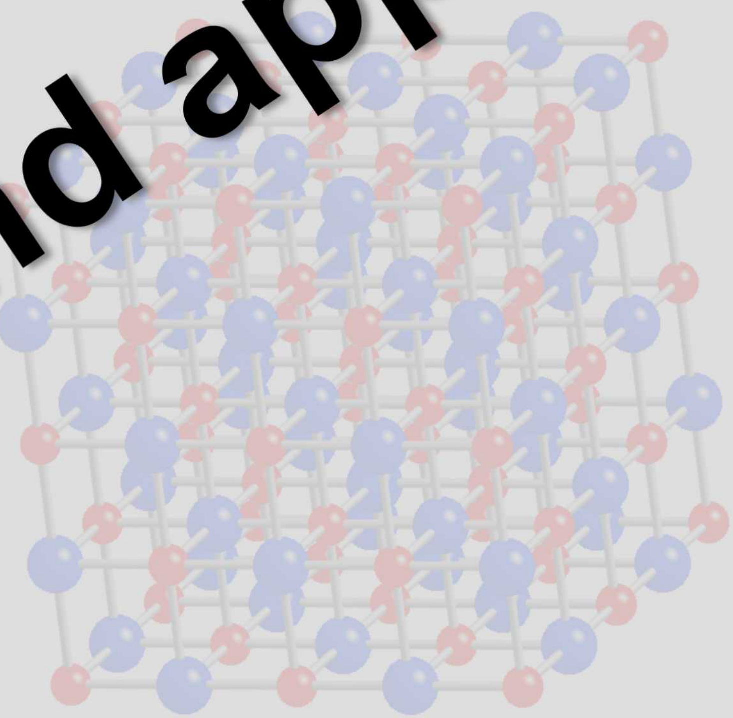
# We propose…MgO-CaO/AlGaN



**Wurtzite**

(Gallium Nitride)

**Rocksalt**



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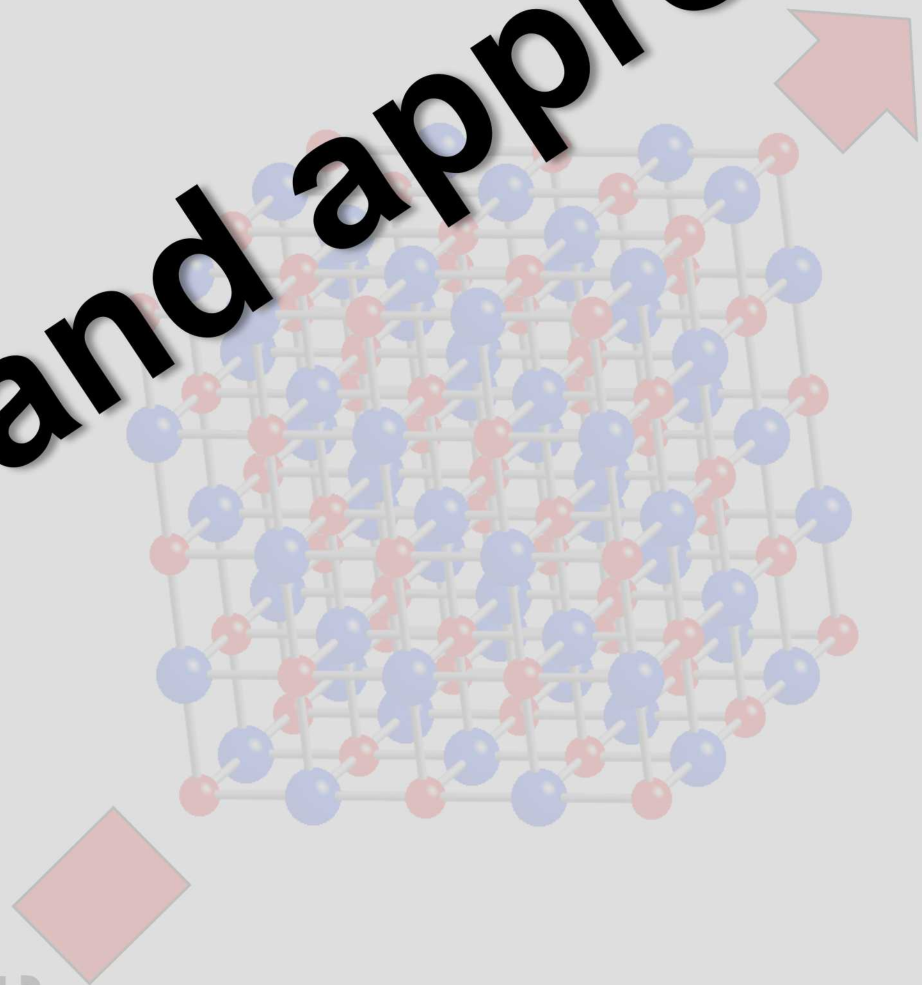
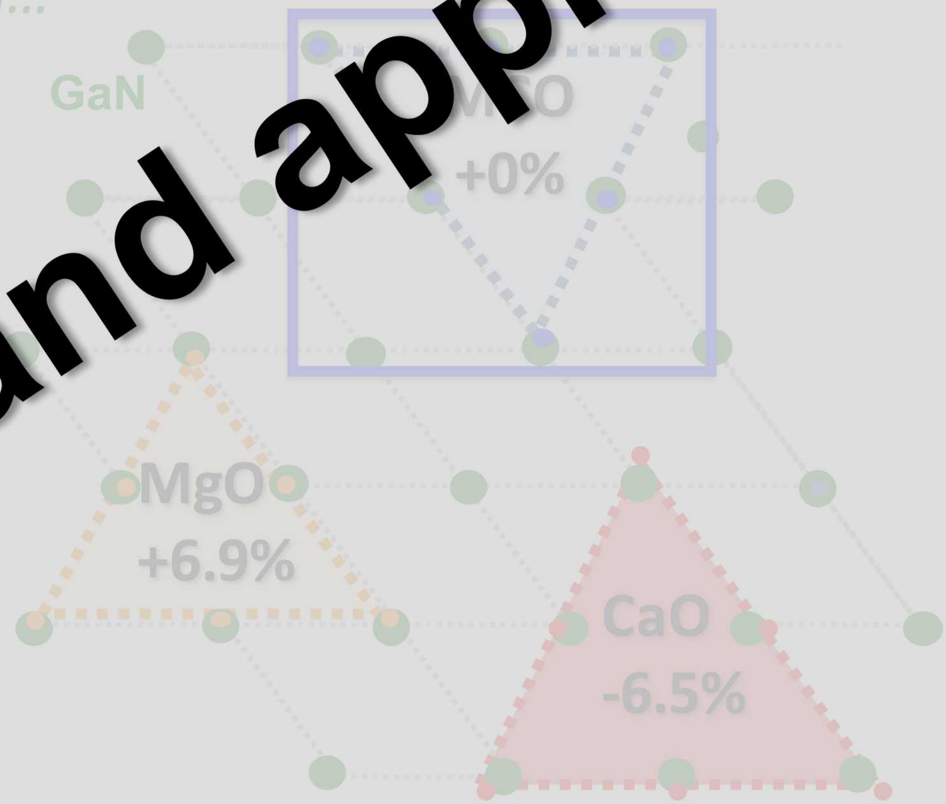


# We propose…MgO-CaO/GaN

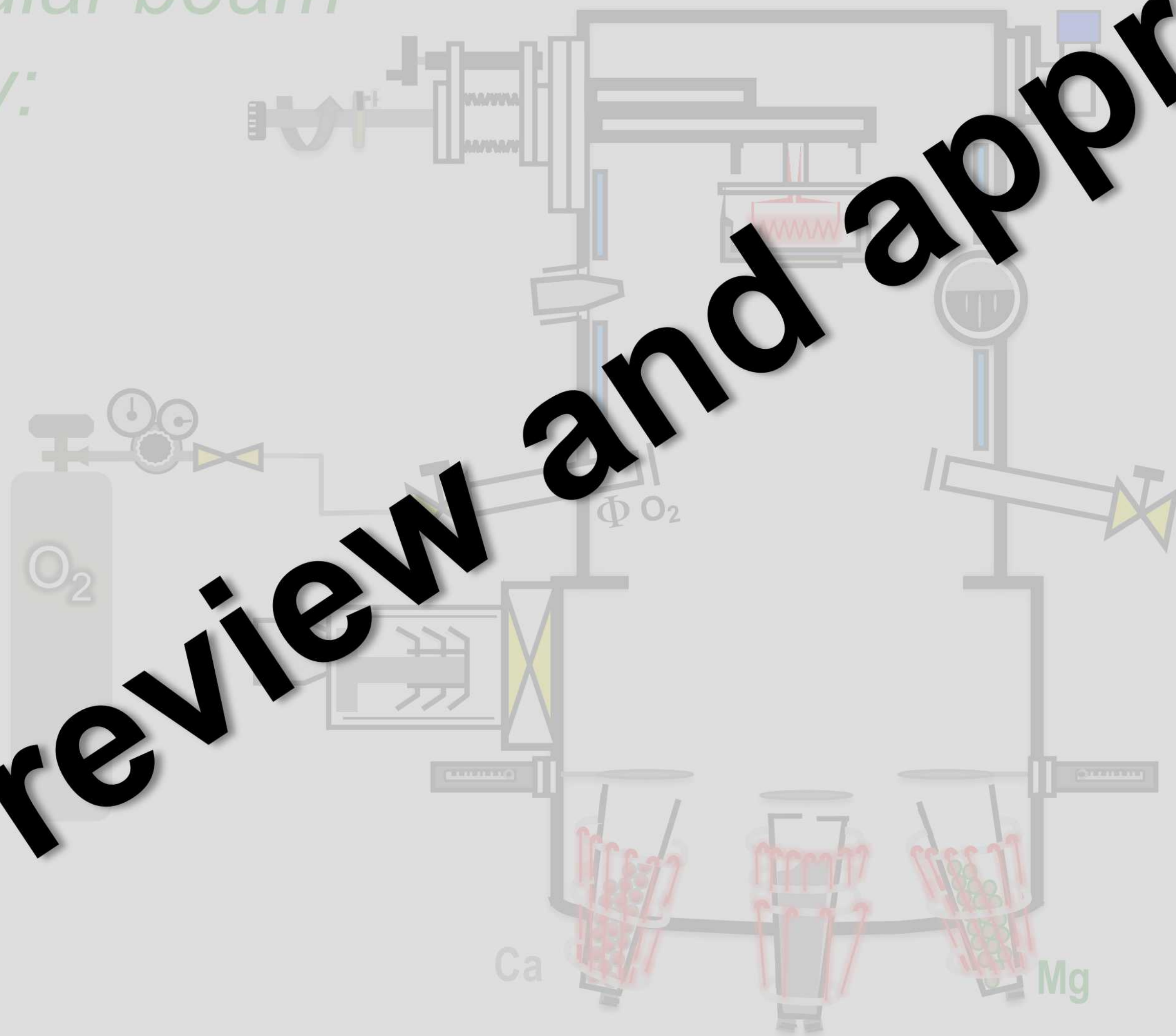

*We can lattice-match to GaN through AlN…*




- MCO|GaN: $Mg_{0.52}Ca_{0.48}O$
- MCO|[illegible]% AlGaN: $Mg_{0.63}Ca_{0.37}O$

# MCO | AlGaN growth description

*Molecular beam epitaxy:*



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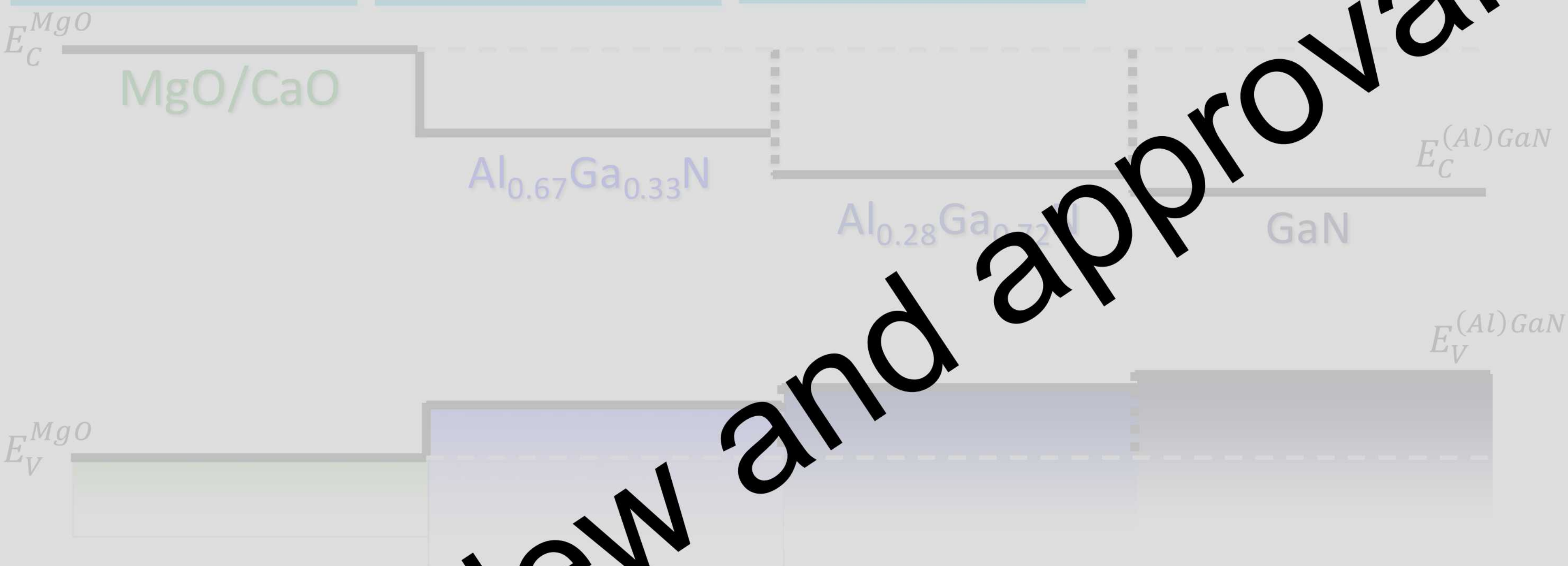
# Band offsets:




- *Experiment:*
  - *Measure MgO/GaN band offsets by XPS:*

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

GaN substrate

Thin MgO on GaN

Thick MgO on GaN

# MgO|Al$_x$Ga$_{1-x}$N band offsets

# Oxide/GaN band offset literature:


Paisley *et al.* APL 2015

Cra[illegible] *et al.* APL 2007

Chen *et al.* APL 2006

Lay *et al.* J. Cryst. Growth 2005

Chang *et al.* Adv. Mater 2009

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Etc…

***We expect < 0.1 eV differences…***

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Etc…

***What role does the substrate surface chemistry play?***

***We expect < 0.1 eV differences…***

# Experiment:

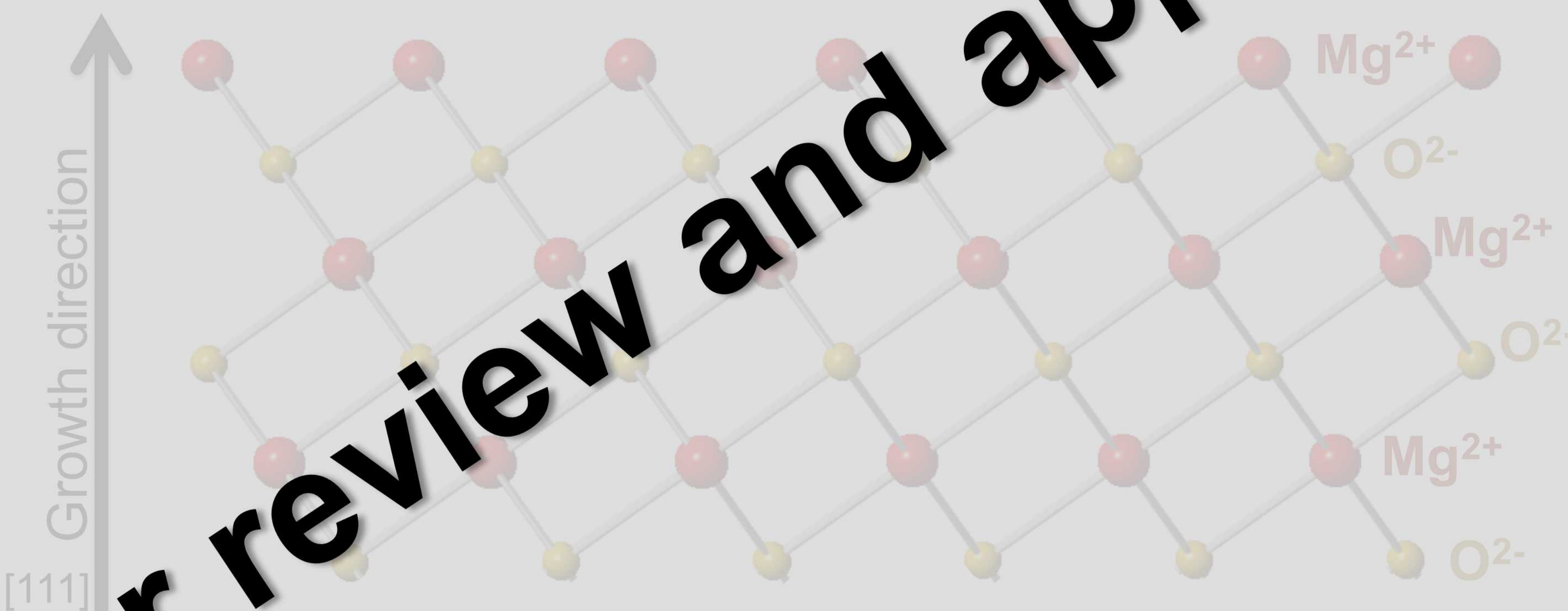
*Test the role of substrate surface chemistry in oxide|nitride band offsets:*

1. **Acquire 5 GaN substrates**: Lumilog, MTI, Sandia, and two from NCSU
2. **Clean substrates identically**: acetone, methanol, UV-$O_3$, and HF
3. **Grow epitaxial MgO identically**
4. **Measure band offsets with XPS**: XPS by M. Brumbach, SNL

# Band offsets with oxygen:

# Surface chemistry of GaN:

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



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


*We expect abrupt MgO|GaN interfaces.*

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# Ambient temperature stability

# An ideal gate oxide should:

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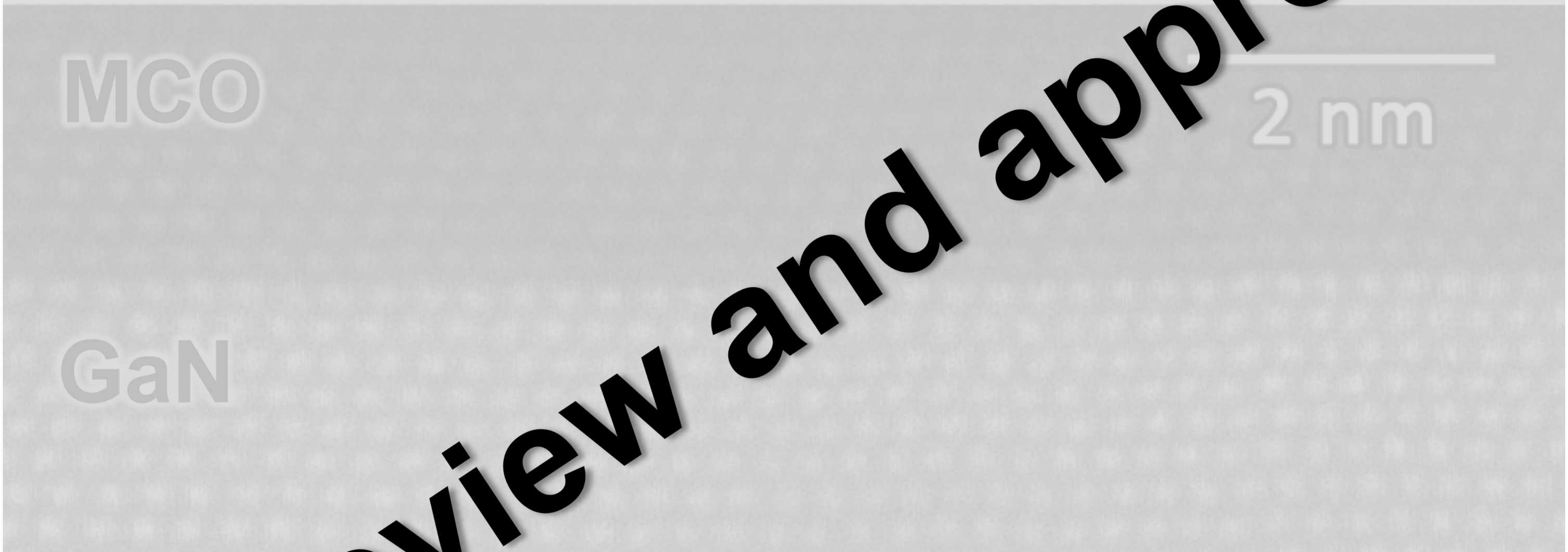
3. **Reduce conduction pathways and interface states**

# MgO-CaO on GaN


*MCO allows us to rid the interface of dislocations due to lattice-mismatch*

# HRTEM of 5 nm of $Mg_{0.52}Ca_{0.48}O$ on GaN




- Interfaces that are free of:
  - ✓ Dislocations
  - ✓ Roughness

Paisley *et al.*, J. Appl. Phys. 115, 2014

# But, if we zoom out a bit…

*We would like smooth, abrupt interfaces…*


**Problem:** rough, faceted morphology is likely to enable unwanted conduction pathways

# Primary Challenge

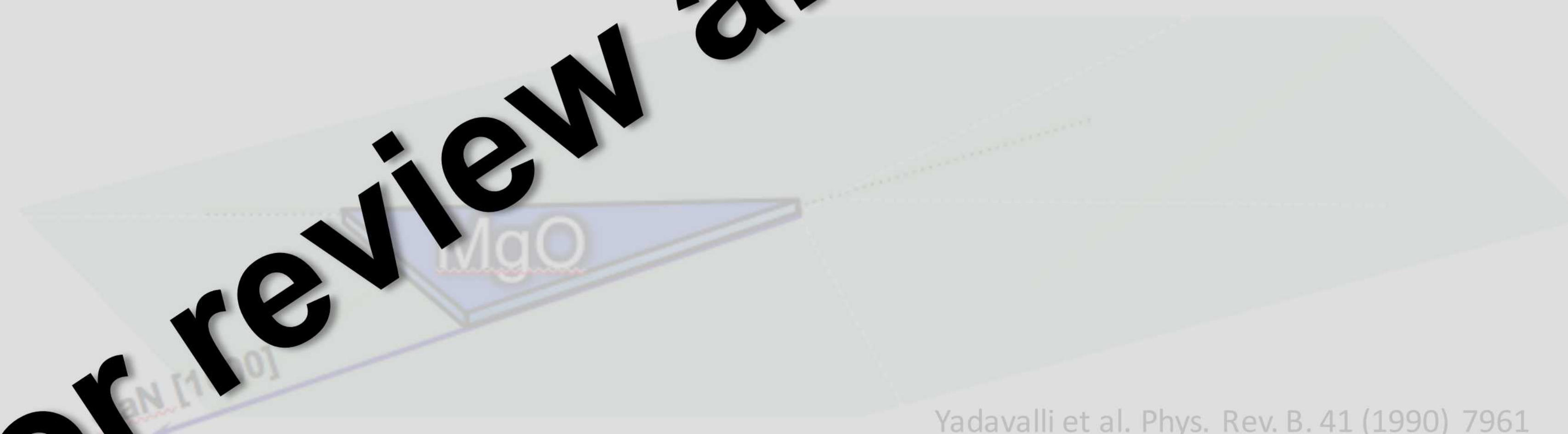
- *Some crystals have bad habits…*

- We want a cubic oxide on a hexagonal (0001) nitride
    - <111> MCO : <0001> GaN

- MgO and CaO both have a close-packed, FCC sublattice:
    - (111) face is not the lowest energy face → faceting

# Surface energy minimization

- Faceting occurs as a mechanism to reduce the system free energy
- (001) is the lowest surface energy facet




Yadavalli et al. Phys. Rev. B. 41 (1990) 7961
Mei et al. Chin. Phys. Lett. 21 (2004) 410
Sugawara et al. Surf. Sci. 558 (2004) 211
Li et al. Phil. Mag. A 65 (1992) 403…

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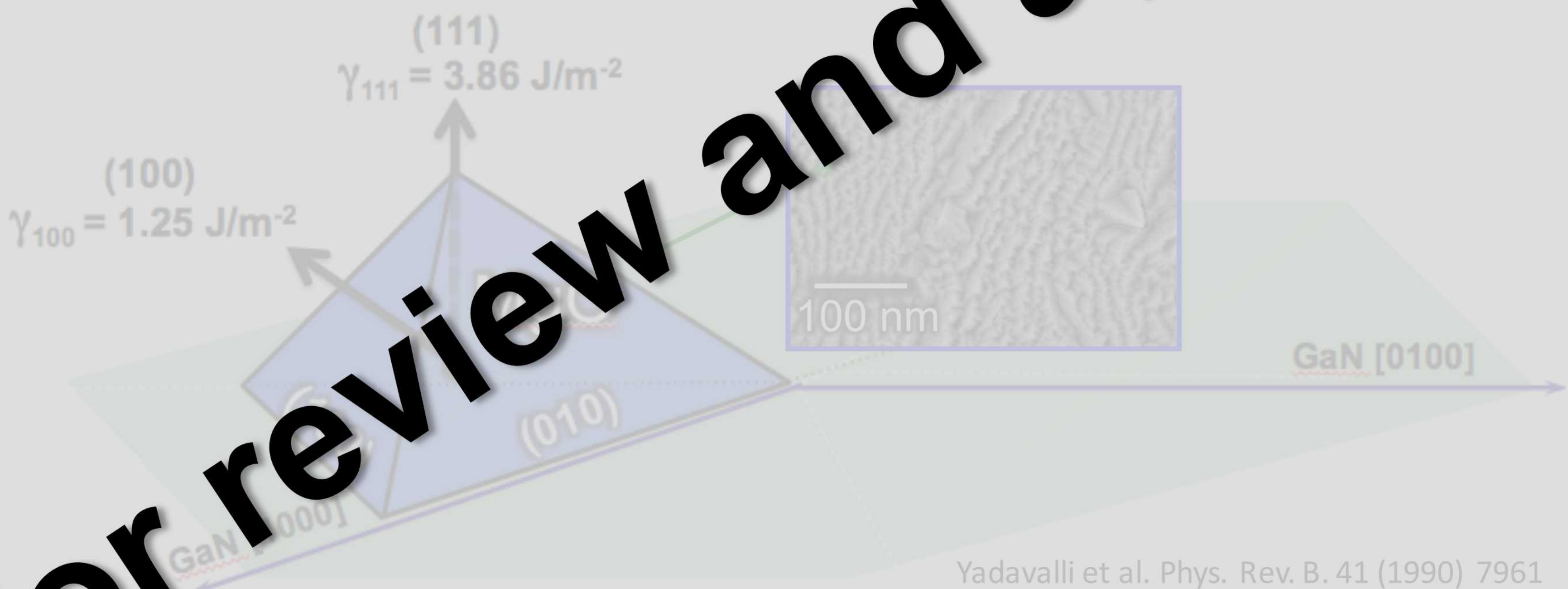



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# Options for stabilization?

Hacquart et al., Chem. Phys. Lett., 439 (2007) 91:

MgO "smoke"


MgO octahedra

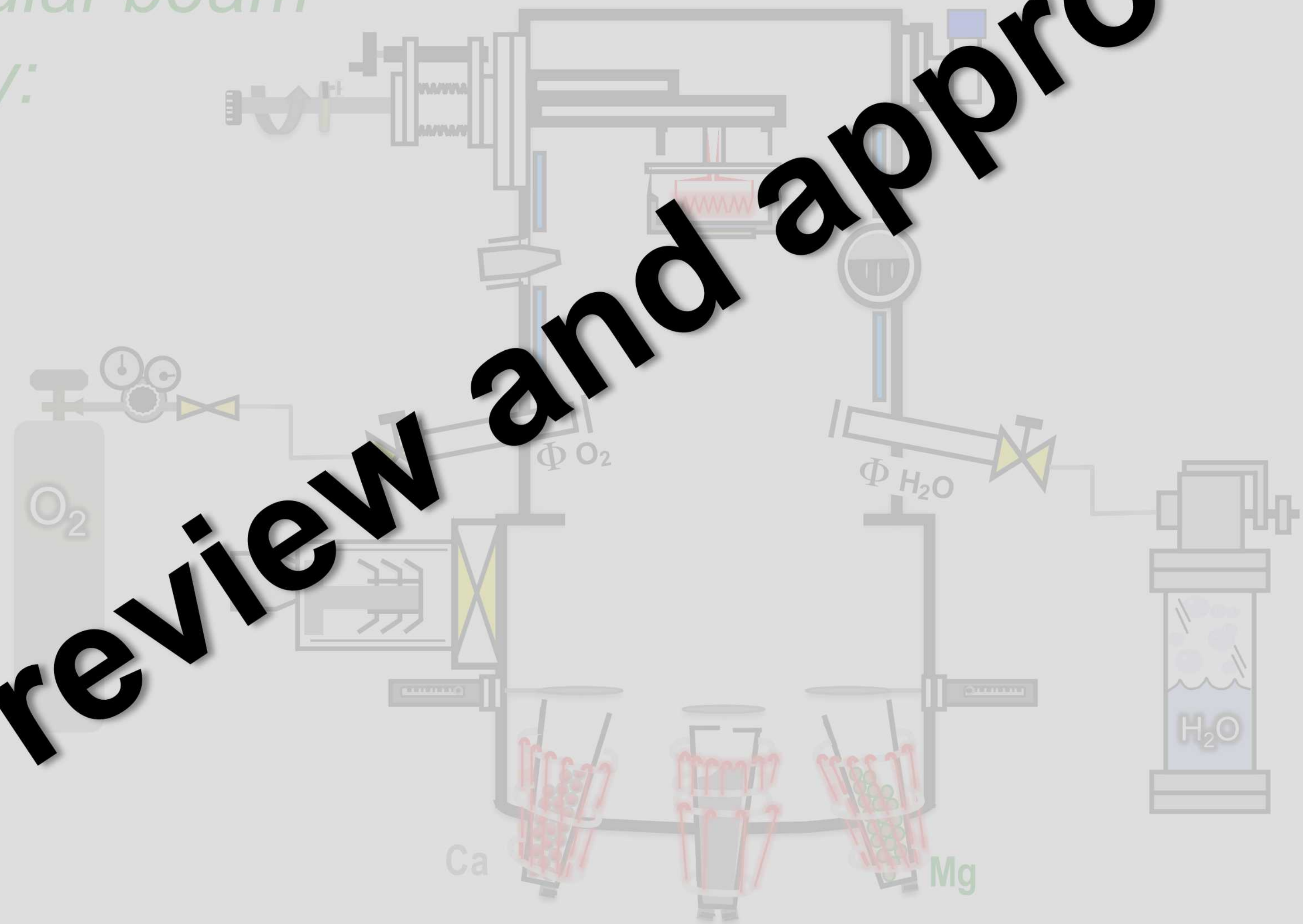

Refson et al., PRL 15 (1995): stabilize (111)-rocksalt oxide surface by OH-termination

- (111)-$OH^-$ = - 20 kJ/mol
- (100)-$OH^-$ = + 130 kJ/mol

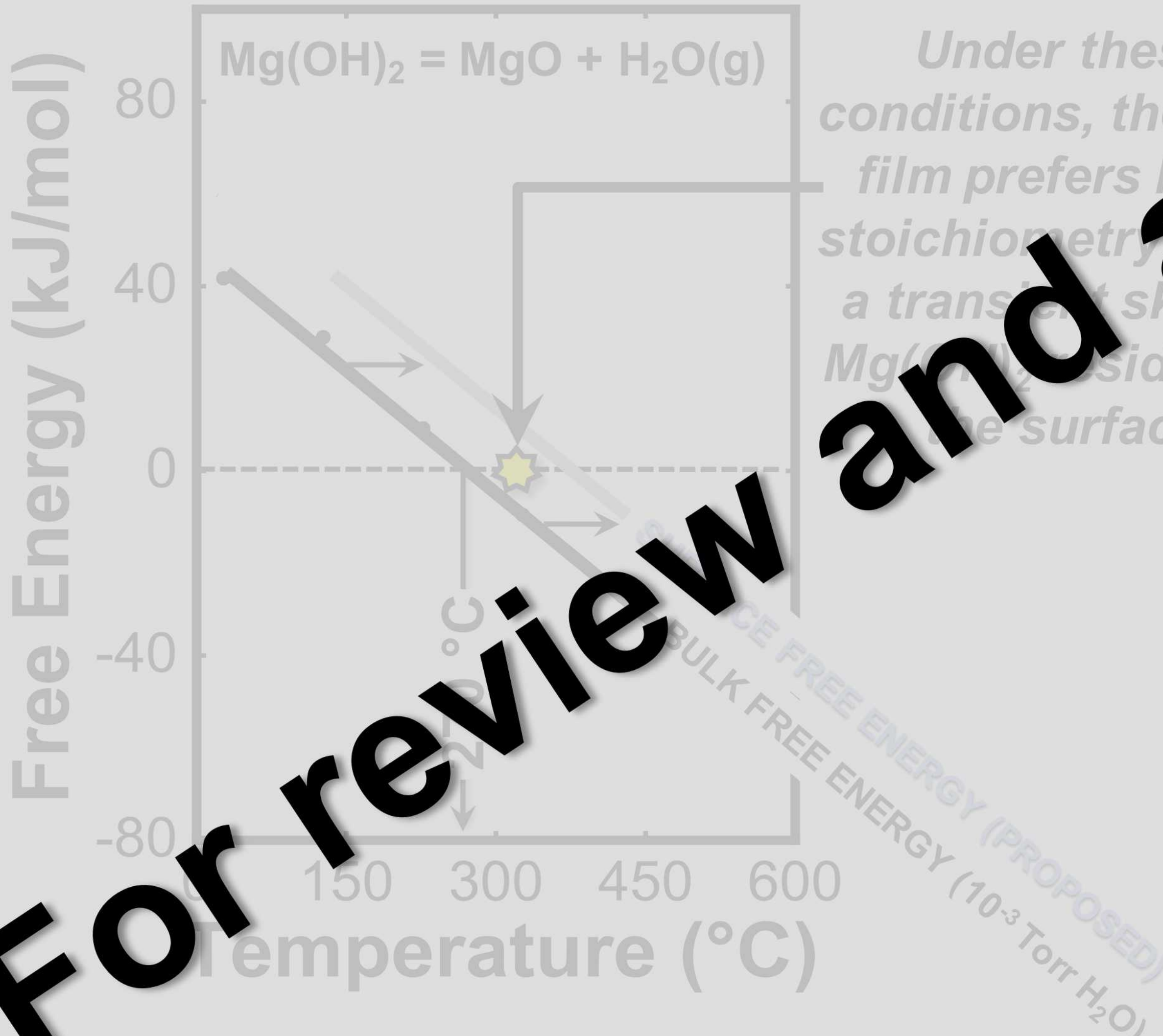
Can we extend this bulk process in to our PVD growth?

# *Modified* MCO | GaN growth description

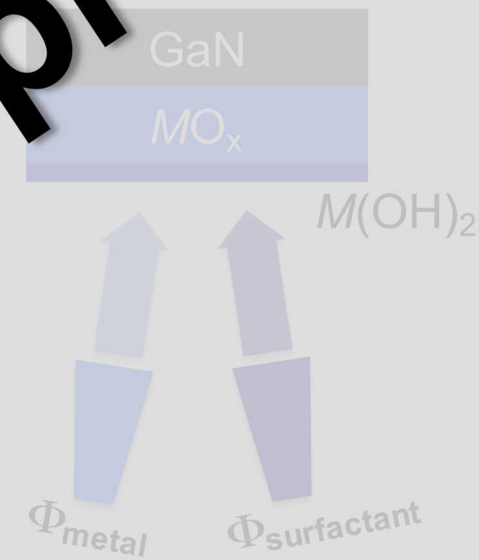
*Molecular beam epitaxy:*



# Water-surfactant MgO growth

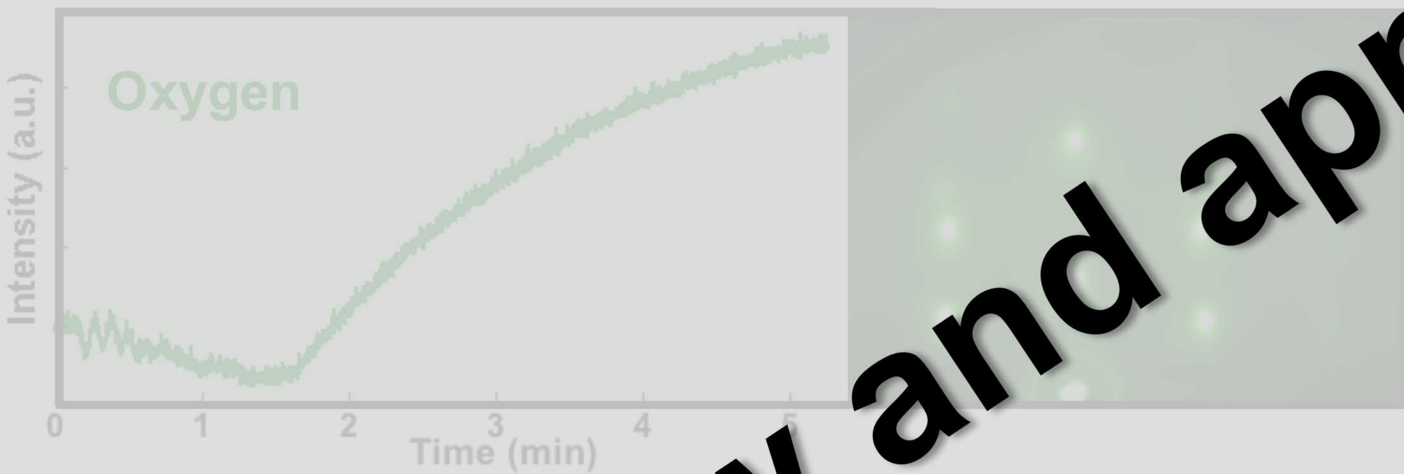



***Under these conditions, the bulk film prefers MgO stoichiometry, but a transient skin of $Mg(OH)_2$ resides on the surface***




Grow at a temperature higher than $T_{sub}$: 270 °C and monitor with RHEED

# Water-surfactant MCO growth







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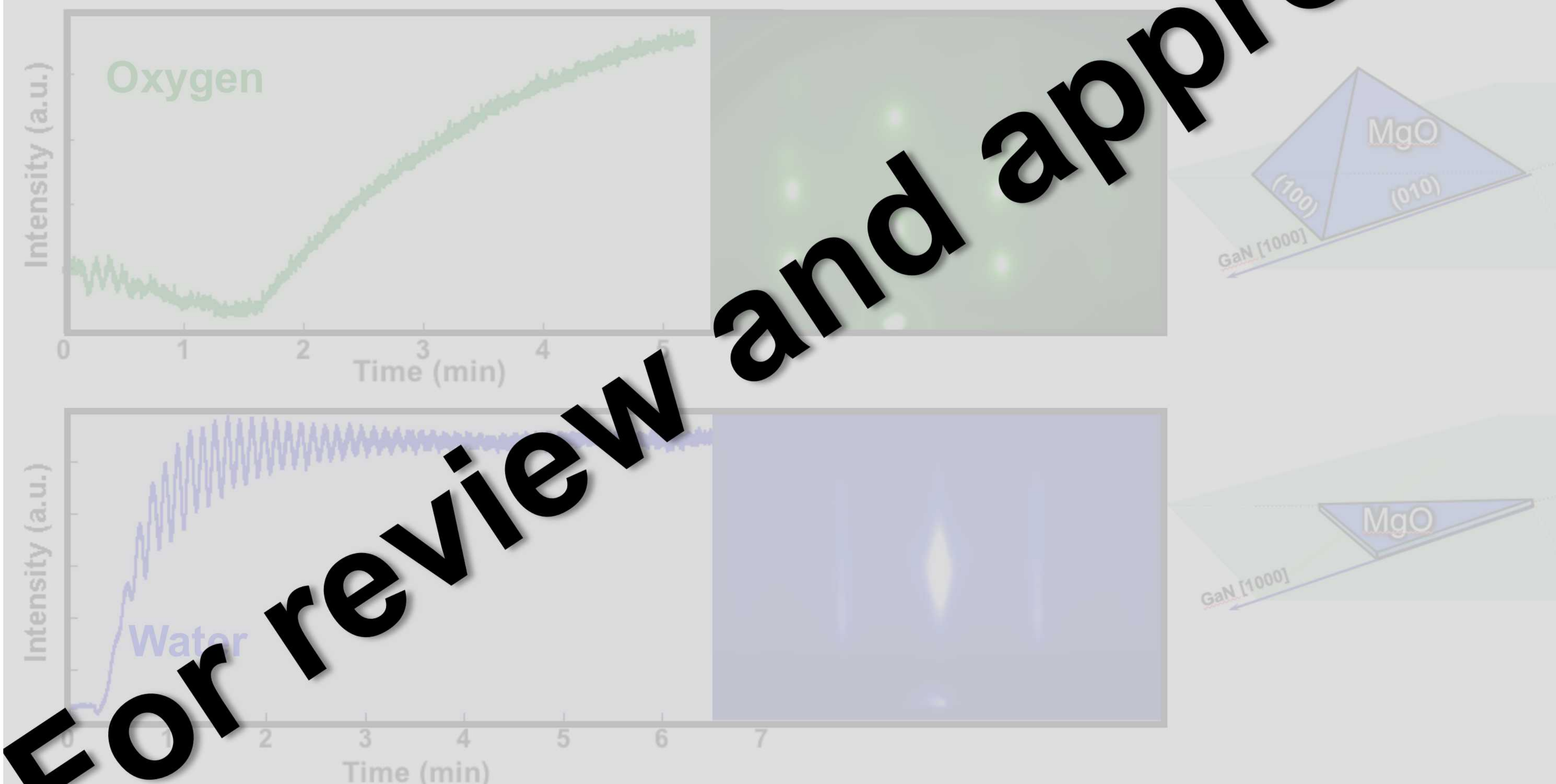

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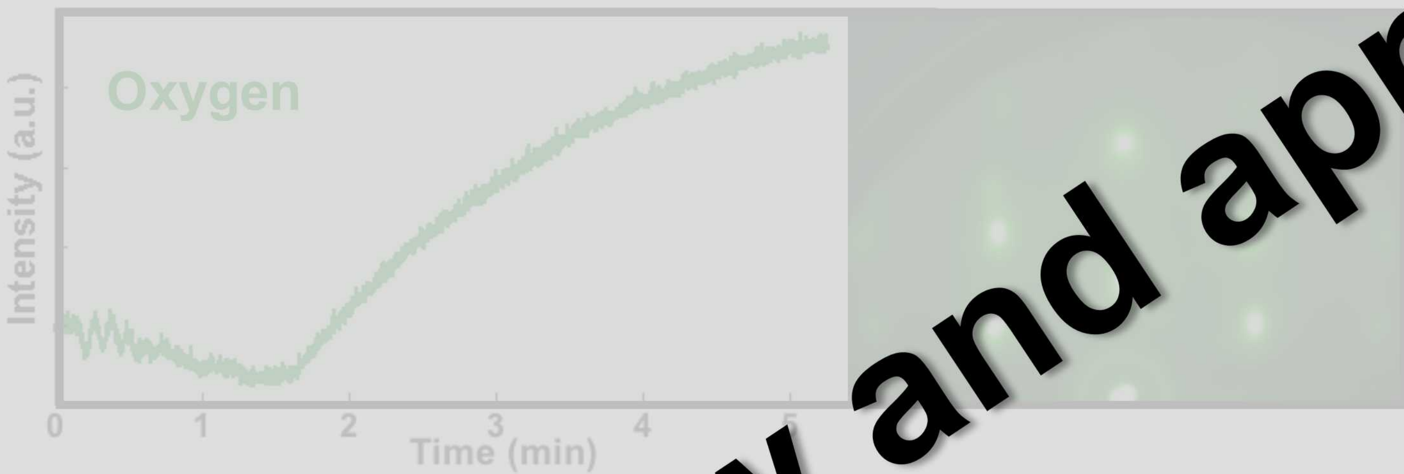




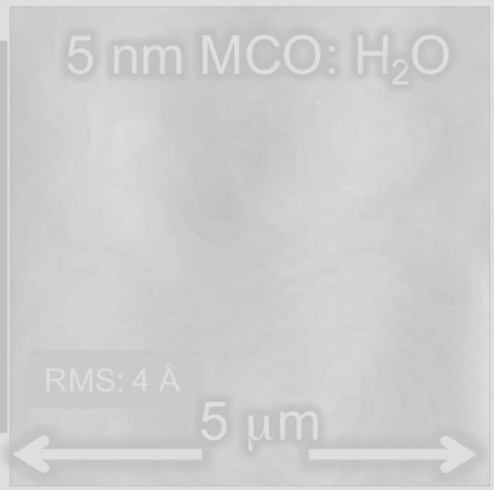




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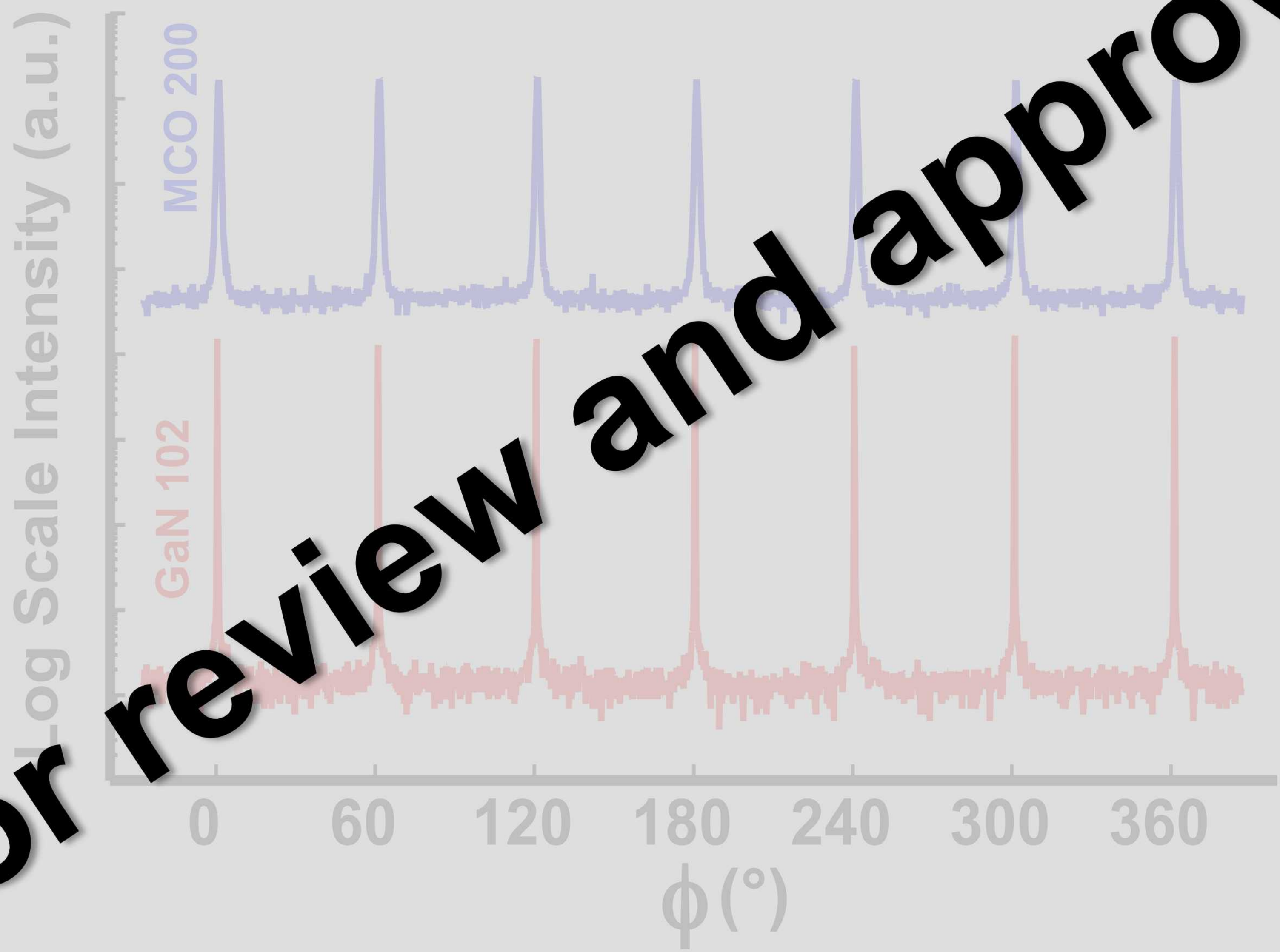

# I-V analysis




Paisley *et al.*, J. Appl. Phys. 115, 2014

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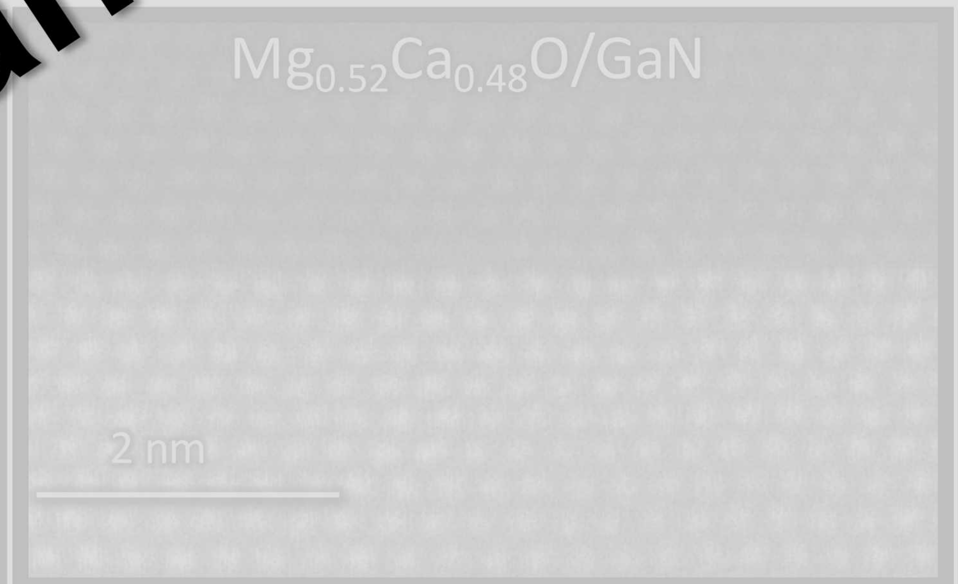
TEM curtesy of David Muller, Cornell University

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# Acknowledgements


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