

# III-nitride surface chemistry influence on band offsets of gate oxides on GaN

Elizabeth A. Paisley<sup>1</sup>, Michael Brumbach<sup>1</sup>, Christopher T. Shelton<sup>2</sup>, Christina M. Rost<sup>2</sup>, Michael P. King<sup>1</sup>, Robert Kaplar<sup>1</sup>, Stanley Atcitty<sup>1</sup>, Jon-Paul Maria<sup>2</sup>, and Jon F. Ihlefeld<sup>1</sup>

<sup>1</sup> Sandia National Laboratories

<sup>2</sup> North Carolina State University



Exceptional service in the national interest

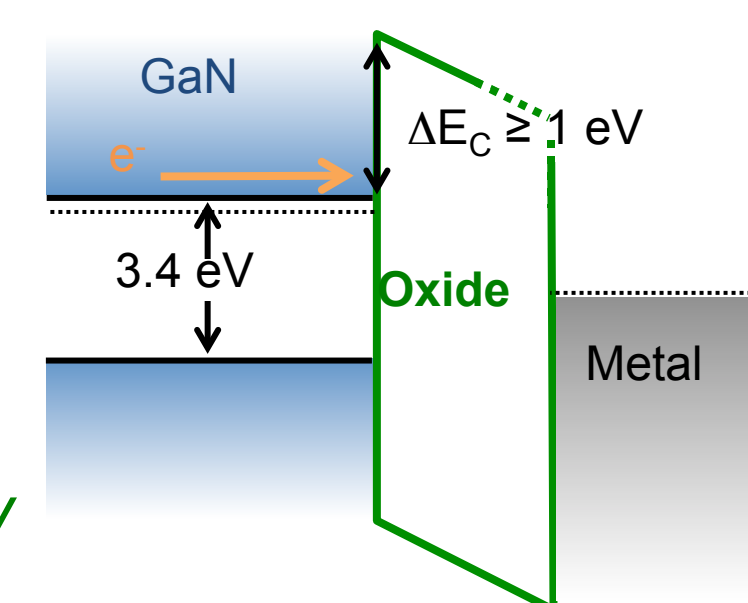
## MOTIVATION:

- Gate oxides offer the possibility of providing normally off GaN/AlGaIn HEMT operation with simultaneous gate leakage suppression.
  - But, the oxide|nitride band offset must be sufficient and accurate band offset information is critical.

### Band offsets give us expectations for:

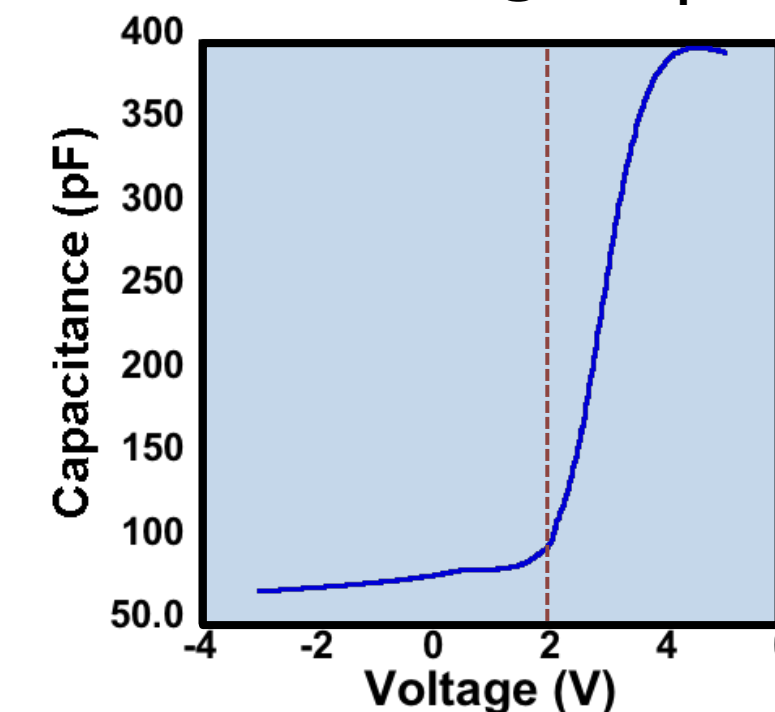
#### 1. Can we suppress gate leakage?

For n-type GaN, we want the conduction band offset,  $\Delta E_C \geq 1$  eV



#### 2. Can the oxide threshold voltage, $V_T$ , enable a normally off operation?

For n-type GaN, we want  $V_T \geq 2$  V.



- Many aspects of the interface can significantly change the oxide|nitride band offset. However, these effects are not well understood for oxides on GaN.

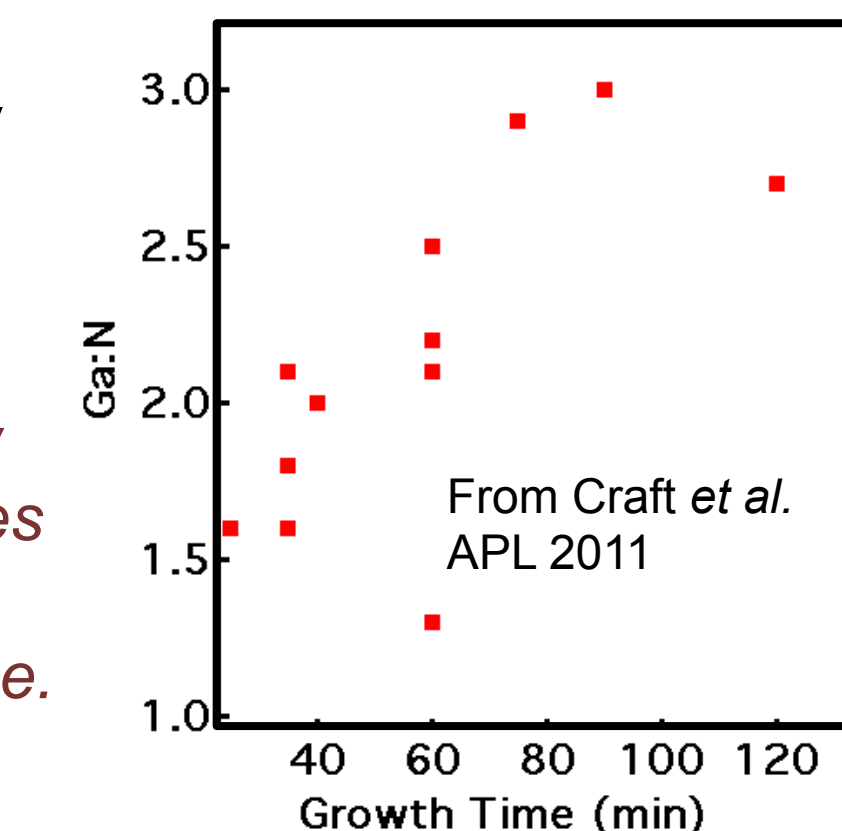
### Properties that can affect the band offsets of the oxide|nitride interface:

- Surface chemistry** of the GaN surface: substrate cleaning and GaN growth procedure.
- Dislocation density** of the GaN template: GaN growth procedure.
- Interface state density ( $D_{it}$ )** of the oxide|nitride interface: oxide growth procedure and substrate cleaning.

## A. SURFACE CHEMISTRY:

- GaN growth and substrate cleaning can influence the final surface chemistry of the GaN substrate.

Craft et al. show measured changes in Ga:N ratio v. reactor growth time.



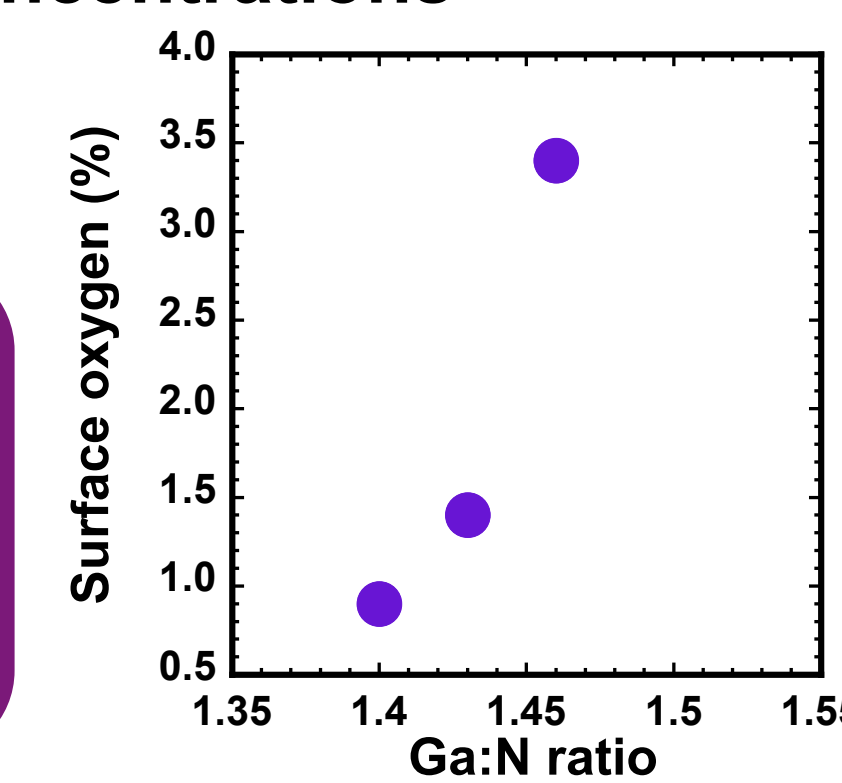
- A similar type effect is expected for GaN substrates from different vendors or substrates with different cleaning procedures.
- Three wide-ranging GaN substrates are cleaned with the identical procedure: acetone, methanol, and 5:95 HF:DI water.

Substrate Source	Growth Method	Polarity	Si doping ( $\text{cm}^{-3}$ )	Thickness ( $\mu\text{m}$ )
NCSU	MOCVD	Ga-polar	UID	1.2
Lumilog	HVPE	Ga-polar	$1.9 \times 10^{18}$	3.5
MTI	HVPE	Ga-polar	UID	5.0

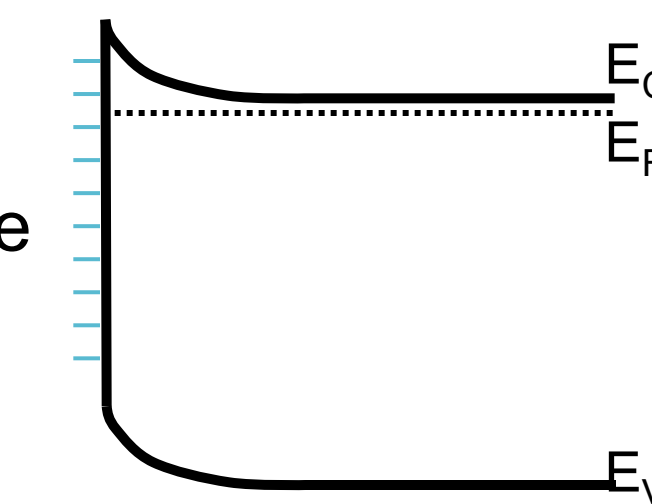
## A. SURFACE CHEMISTRY:

- GaN surface chemistry, Ga:N ratio and oxygen surface concentrations were measured using XPS:

Surface oxygen content increases for higher Ga surface stoichiometries.

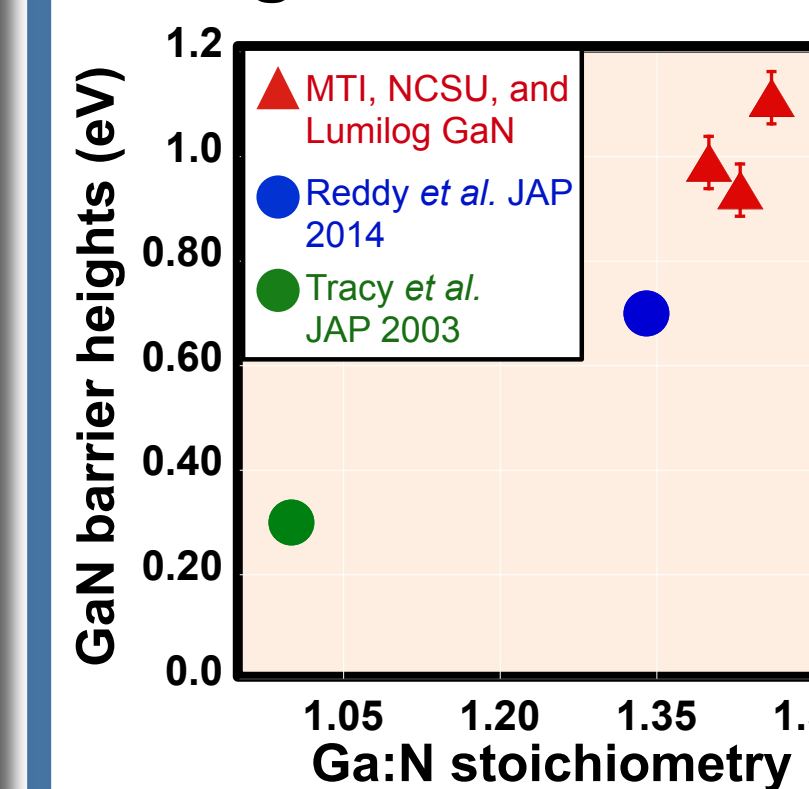


- An increase in native oxide forms more negative surface charge causing upward band bending of the GaN surface.



- We test this by measuring the GaN barrier height of each substrate by XPS.

- Influence of Ga:N ratio on GaN barrier heights:



As Ga:N ratio increases, band bending at the CNL increases.

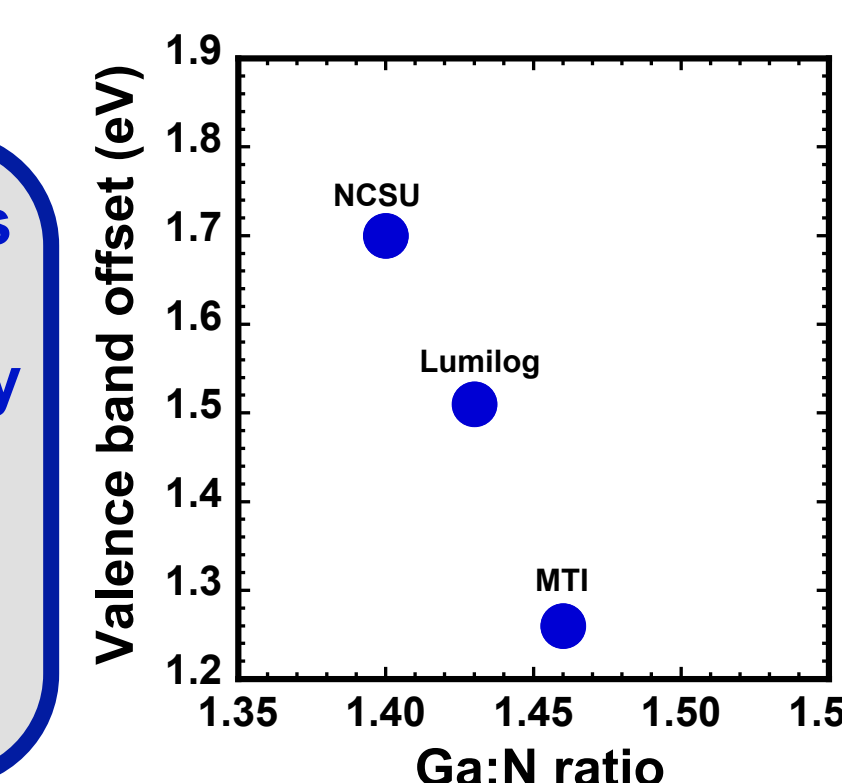
- This implies Ga:N ratio will affect Schottky barrier heights to metal contacts and band offsets to gate oxides.

- A similar effect of surface stoichiometry is then expected for band offsets between GaN and gate oxides.

- We test this by measuring the valence band offset of MgO to each GaN substrate by XPS.

- Influence of Ga:N ratio on band offsets to MgO:

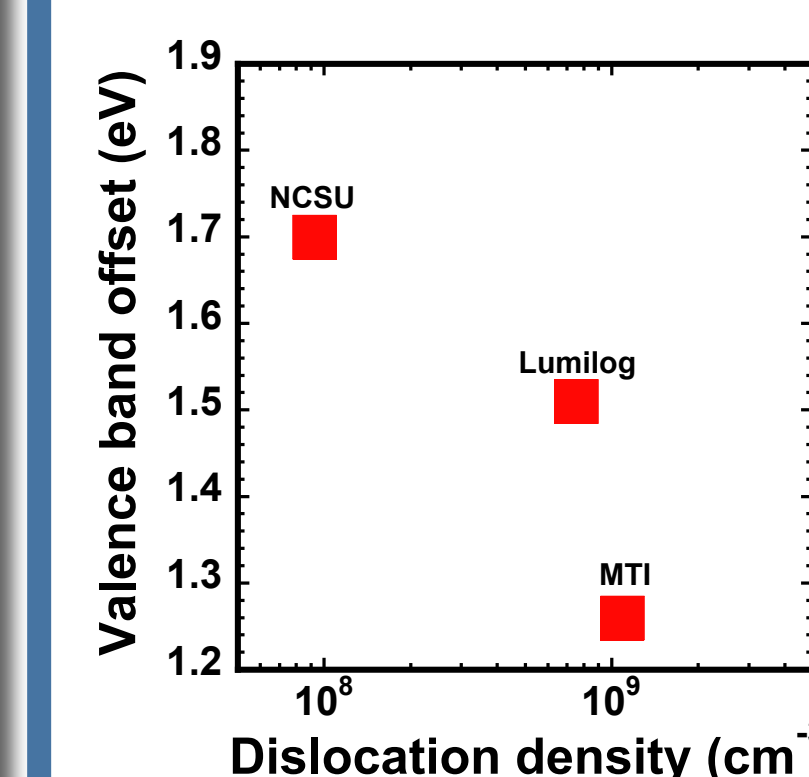
Valence band offsets of the MgO|GaN interface decrease by  $\sim 0.44$  eV for small changes in GaN surface stoichiometry.



## B. DISLOCATION DENSITY:

- Dislocation densities of the GaN substrates were measured using HR-XRD.

- Dislocation densities range from  $7.5 \times 10^7 - 1.1 \times 10^9 \text{ cm}^{-2}$ .



- A similar effect to surface stoichiometry is seen for substrate dislocation density.

- Valence band offsets to the gate oxide decrease with increasing GaN dislocation density.

## C. INTERFACE STATE DENSITY:

- Changes in the GaN surface alter the surface screening charge of the polar substrate.

- However, it is likely that the resultant change in band offset to the gate oxide is only observable if the interface state density is low.

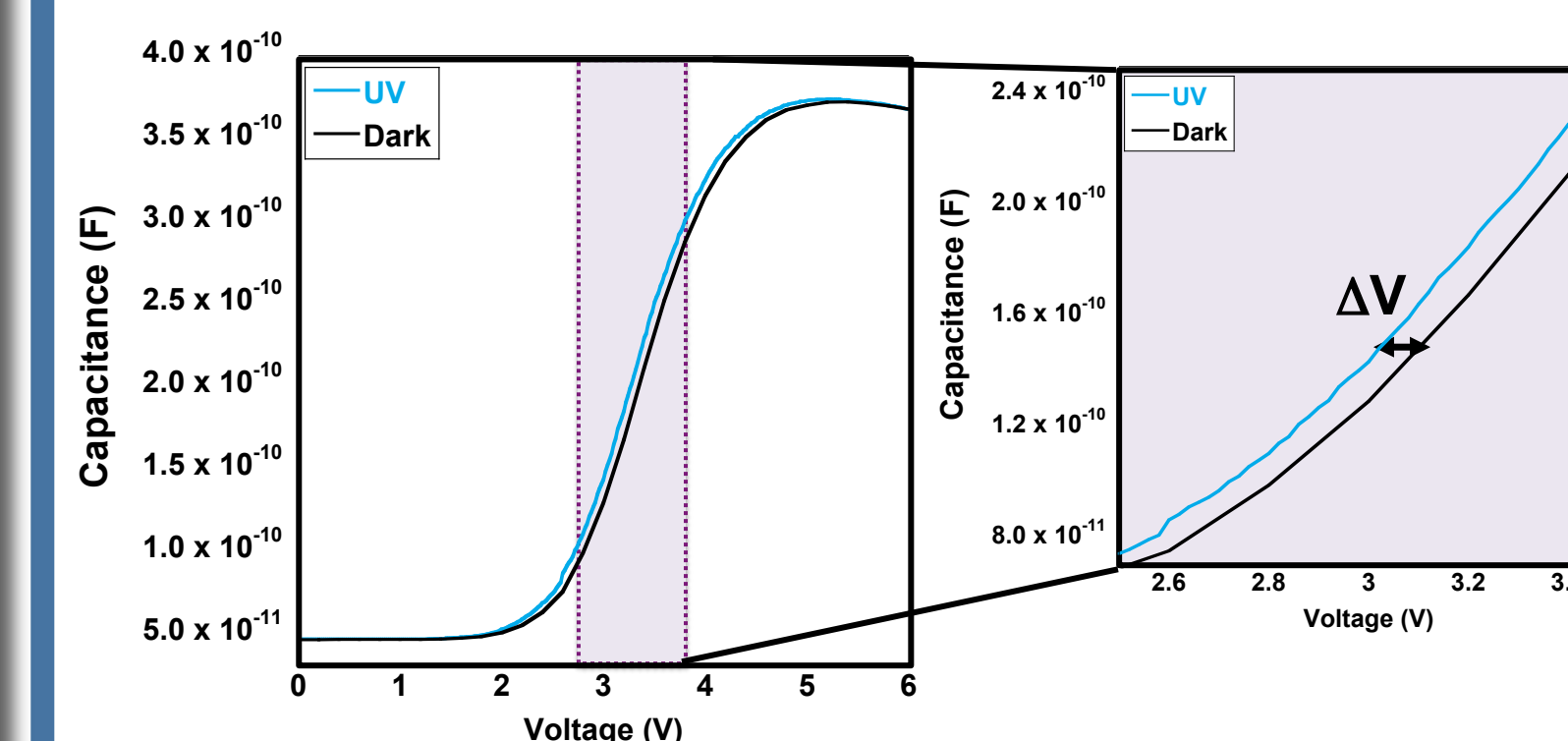
- We test this by measuring the interface state density ( $D_{it}$ ) of the MgO|GaN interface.

- Photo-assisted capacitance-voltage  $D_{it}$  analysis:

- UV light is used to photo-populate interface states.

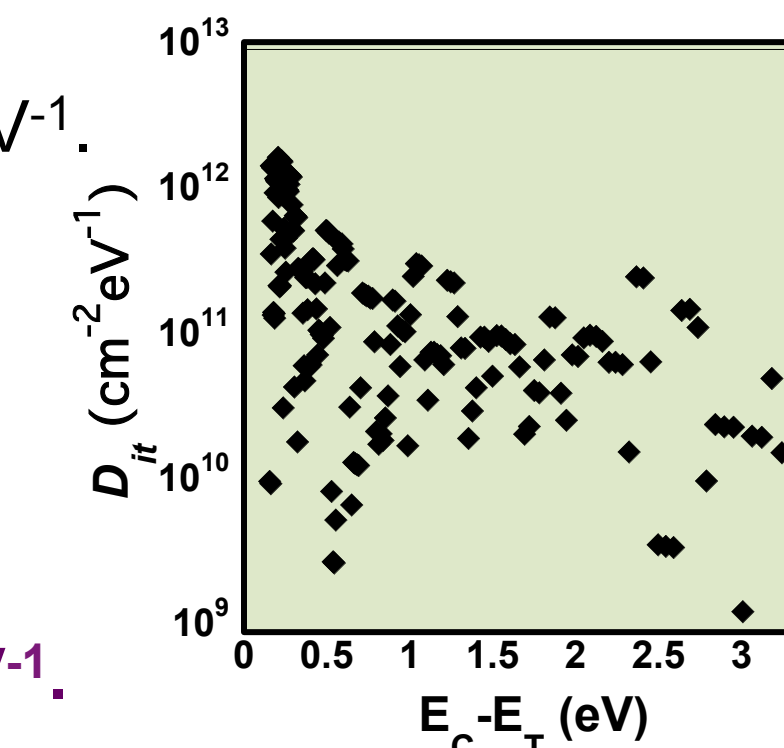
- $\Delta V$  between dark and post UV curves yields information on  $D_{it}$ :

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



- An average  $D_{it}$  across the band gap of GaN is found to be  $\sim 9.3 \times 10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$ .

- At 0.23 eV from the conduction band edge,  $D_{it}$  reaches a maximum of  $1.6 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ .



- Comparison with literature  $D_{it}$  values:

Dielectric	GaN $D_{it}$ ( $\text{eV}^{-1} \text{cm}^{-2}$ )
$\text{La}_2\text{O}_3$	$1 \times 10^{12}$
MgO	$9.3 \times 10^{10}$
CaO	$2.2 \times 10^{11}$
$\text{Ga}_2\text{O}_3$	$4.2 \times 10^{11}$
$\text{Si}_3\text{N}_4$	$5 \times 10^{12}$
$\text{Al}_2\text{O}_3$	$5 \times 10^{11} - 3 \times 10^{12}$

Average values for MgO and CaO are low compared to other systems in the literature.

- We hypothesize that the low  $D_{it}$  value of MgO allows observation of changes to the oxide|nitride band offset.

- Current efforts focus on measuring higher  $D_{it}$  materials to see if  $D_{it}$  can screen the surface charge effect of the GaN.

## CONCLUSIONS:

- For high quality oxide|GaN interfaces, the GaN substrate surface chemistry and dislocation density influence band offsets.

- Valence band offsets of MgO on GaN ranging from 1.26 to 1.70 eV were measured for small changes in oxygen content and Ga:N ratio.

- Current efforts focus on extending analysis to  $\text{Al}_2\text{O}_3$  | GaN to confirm the screening factor proposed higher  $D_{it}$  interfaces.

This work was supported, in-part, by the U.S. Department of Energy's Office of Electricity Energy Storage Program managed by Dr. Imre Gyuk.