REVEALING HIDDEN INTERFACIAL STATES IN NO PASSIVATED 4H-SiC/SiO₂ STRUCTURES USING TEM-EELS AND XPS*

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Motivation and background

- SiC: Very promising for high temperature, high power, and high radiation environments
  - NO post oxidation anneal (POA) drastically improves performance
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• What is the true nature of the interface, and how do our processing techniques really affect it?
  • Some work indicates a distinct transition region (EELS)$^{1,2}$
  • Others suggest abrupt transition (XPS, MEIS, etc.)$^{3−4}$

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TEM-EELS EXPERIMENTS
Electron Energy Loss Spectroscopy (EELS)

- E-beam has many interactions with specimen:

- EELS is measurement of the energy lost when an electron interacts with the sample:

EELS Spectrum Imaging

HAADF Survey Image

SiC

SiO$_2$

10 nm
EELS Spectrum Imaging

HAADF Survey Image

SiC

SiO$_2$

EELS Spectrum Image

Simultaneous HAADF Signal

SiC

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EELS Spectrum Imaging

One spectrum per pixel

SiC

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10 nm

EELS Spectrum Image

Intensity

Energy loss (eV)

Si-L EELS edge
NO-anneal effects (previous results)

- Measured $w_{TL}$ with chemical shift
- $w_{TL}$ correlates inverse-linearly with $\mu_{FE}$
- NO-anneal removes/passivates mobility-limiting defects
  - Compositionally and electronically


*Samples fabricated from 2010 SiC stock*
Newer work - Orientation effects

- Investigating effects of substrate orientation:
  - Newer SiC stock (2014)
  - [0001] Si-face, with and without miscut
  - [1120] a-face
  - Each with and without NO
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NEW ANALYSIS TECHNIQUE

Hyperspectral signal decomposition – machine learning

- Si-$L_{2,3}$
- C-$K$
- O-$K$
Decomposition analysis

- EELS spectrum imaging as “big data”
  - Machine learning improves sensitivity; highlights most important features
  - Unsupervised learning promotes bias-free analysis
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• Non-negative matrix factorization (NMF)

Olivetti Faces Dataset

NMF Components
Interface components at NO-annealed interfaces

SiC/SiO$_2$ EELS Spectrum Image

- Simple sum improves S/N, but cannot detect faint or overlapping signals
Decomposition analysis – Si $L_{2,3}$

- No significant variation between orientations
  - $a$-face data shown
Decomposition analysis – Si $L_{2,3}$

- No significant variation between orientations
  - $a$-face data shown
- NO anneal gives rise to interfacial state with doublet peak
Si-L\textsubscript{2,3} Interface Component – N Bonding

- \text{Si}_3\text{N}_4\text{ theory and experiment (Skiff et al.)}
  - Doublet peak at same energy as our peak
- Effect of N-bonding
  - Si-C-N-O bonding configurations?
  - Evidence of N-bonding at interface
  - DFT modeling will reveal further details

Decomposition analysis – C K edge

- **α-face without NO**
- **α-face miscut with NO**

- No significant variation between orientations
  - α-face data shown
Decomposition analysis – C K edge

- No significant variation between orientations
  - \(a\)-face data shown
- NO anneal gives rise to interfacial state with pre-peak intensity attributable to \(sp^2\) from N-bonding

**O K edge analysis**

<table>
<thead>
<tr>
<th>Si-face 4° miscut (Si-NO-4)</th>
<th>Si-face no miscut (Si-NO-0)</th>
<th>a-face no miscut (a-NO-0)</th>
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**Decomposition Results**

- All samples have an O-K pre-peak feature, but a-face is strongest and localized near the interface.
- Intensity at lower energy indicates acceptor levels near edge of band gap, providing insight into the origins of improved mobility.

XPS DEPTH PROFILING
XPS Interfacial analysis – Si-2p

- Can we correlate the EELS?

- XPS is surface-sensitive binding energy measurement

- Measured oxidized and NO-POA samples etched near to the interface

“Raw” Si-2p
XPS Interfacial analysis – Si-2p

• Can we correlate the EELS?

• XPS is surface-sensitive binding energy measurement

• Measured oxidized and NO-POA samples etched near to the interface

Peak-fitted Si-2p
XPS Interfacial analysis – Si-2p

• Can we correlate the EELS?

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SiC signal

2hr NO anneal
**XPS Interfacial analysis – Si-2p**

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![Graph showing SiO₂ signal](image-url)
XPS Interfacial analysis – Si-2p

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- Measured oxidized and NO-POA samples etched near to the interface
Angle resolved XPS - interface width

AR-XPS Si-2p data (NO annealed)

\[ d_{\text{interface}} = 1.69 \text{ nm} \]

\[
\frac{I_{\text{int}}}{I_{\text{bulk}}} = \frac{c_{\text{int}}}{c_{\text{bulk}}} \left[ \exp \left( \frac{d_{\text{int}}}{\lambda \cos \theta} \right) - 1 \right]
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## Angle resolved XPS - interface width

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- Similar values to EELS measurements
- Definitely not “abrupt”
Summary

• The shift of the Si-L$_{2,3}$ edge is a good indicator of the width of the transition region in 4H SiC/SiO$_2$.
  • Newer devices do not follow previously observed trend
  • Measuring interface width does not reveal what is happening inside
• Decomposition of EELS signals reveal a chemically/electrically distinct interface state in all NO-annealed samples
  • Likely significant impacts on mobility and performance
  • Spatial distribution matches measurements of $w_{\text{TL}}$
• XPS corroborates EELS findings of Si$_3$N$_4$-like N bonding at the interface, with similar spatial extent
  • Transition region with approximately 1.5-2.0 nm

Future work

• Theoretical modeling of DOS for explanation
• Exploration of lattice strain in different substrate orientations (CBED, Geometric Phase Analysis)
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THANK YOU

Questions/comments/discussion?
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