CHARACTERIZATION OF THE OXIDE-SEMICONDUCTOR INTERFACE IN *4H*-SIC/SIO_2 STRUCTURES USING TEM AND XPS*

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Outline

- Motivation behind analytical microscopy of SiC microelectronics
  - Impacts of NO post-annealing
- TEM-EELS from a collection of SiC/SiO_2 interfaces
  - Previous findings related to the transition layer
  - HRTEM, hyperspectral imaging, machine learning techniques for signal deconvolution
  - Significant changes in interface character after NO-anneal
- Correlation with XPS results
  - What differences are observed with an NO-anneal?
- Conclusions: What's next?

Motivation and background

- SiC: Very promising for high temperature, high power, and high radiation environments
  - Limited by poor channel carrier mobility and reliability
  - Typical device μ_{FE}: 4H-SiC before NO anneal: $< 10\ \frac{\mathrm{cm}^2}{\mathrm{V{\cdot}s}}$; after NO anneal: ~ $45\ \frac{\mathrm{cm}^2}{\mathrm{V{\cdot}s}}$; bulk value: ~ $1{,}000\ \frac{\mathrm{cm}^2}{\mathrm{V{\cdot}s}}$
  - Electrically active defects at the SiC/SiO_2 interface inhibit devices during channel inversion
  - Other defects significantly affect the reliability and stability of devices over time
- What is the true nature of the interface, and how do our processing techniques really affect it?
  - EELS experiments suggest distinct transition region[1,2]
  - Other results (XPS, MEIS, etc.) suggest more abrupt transition [3 – 4]
  - What is NO post oxidation annealing really changing about the interface structurally and chemically?

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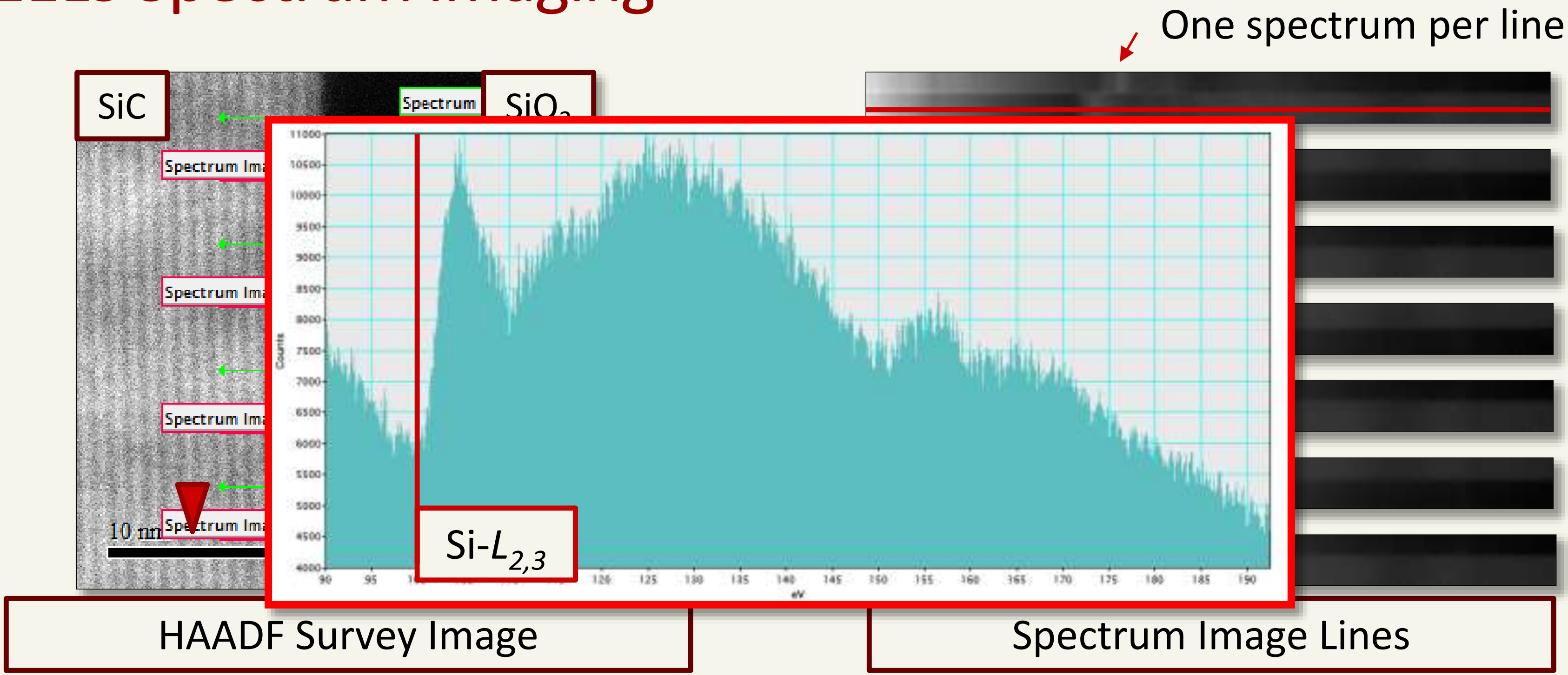
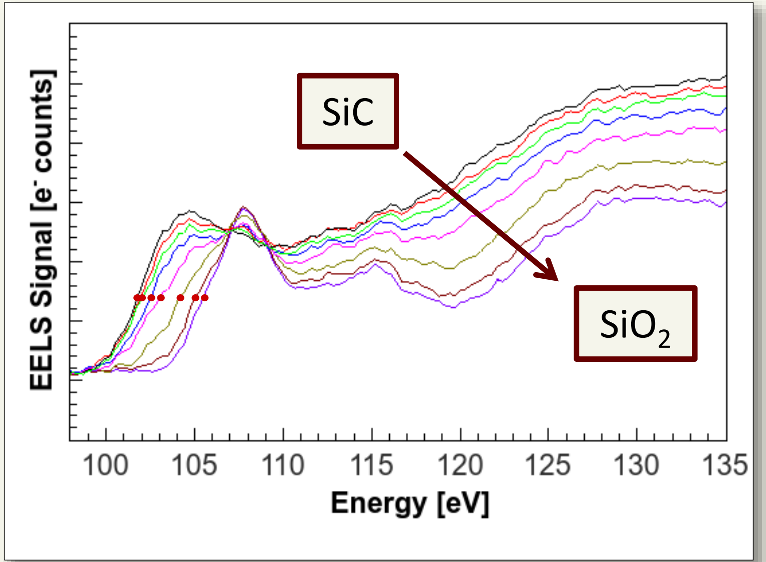
1 J. Taillon, L. Salamanca-Riba, *et al.*, J. Appl. Phys. 113, 044517 (2013).
2 Chang, K. C. *et al.* J. Appl. Phys. 97, 104920 (2005).
3 H. Watanabe, *et al.*, Appl. Phys. Lett., 99(2), 021907 (2011).
4 X. Zhu, *et al.*, Appl. Phys. Lett., 97(7), 071908 (2010).

TEM-EELS EXPERIMENTS

EELS Spectrum Imaging



Si-$L_{2,3}$ chemical shift

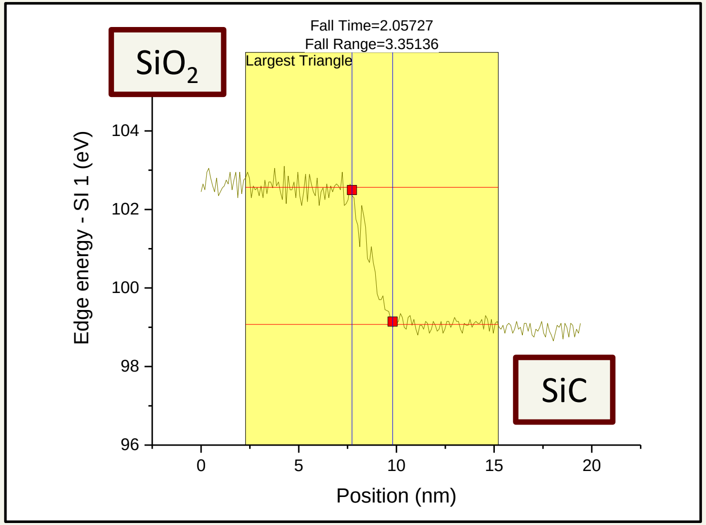


- EELS fine structure (ELNES) reflects local unoccupied density of states
  - Semiconductor → insulator
  - Edge onset → minimum energy needed to excite core shell e^-
  - Band gap widens, core levels depressed relative to E_F[1]
    - Charge transfer from Si → C/O
    - Onset shifts to higher energy

[1] D. Muller, Ultramicroscopy **78**, 163 (1999).

Si-$L_{2,3}$ chemical shift – measuring w_{TL}

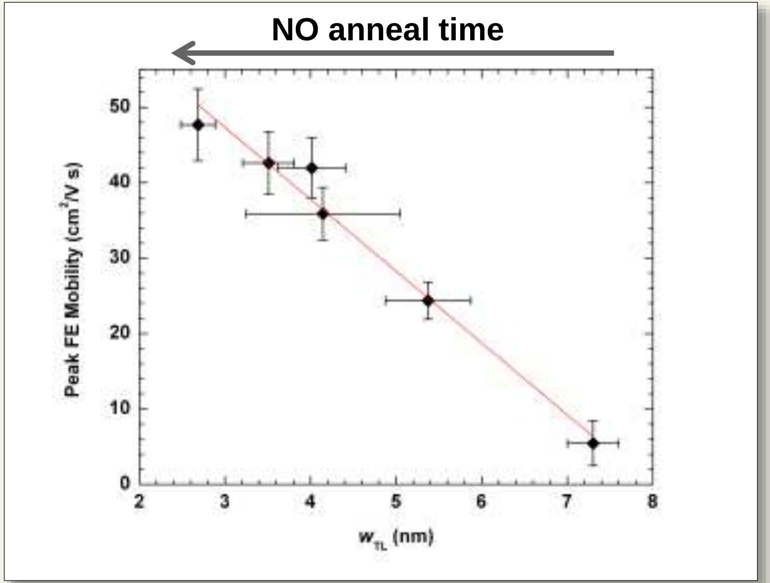
- Track inflection point of edge onset across interface[1]
- Gradual and monotonic shift
  - Si bonding changes gradually and uniformly across the interface
- Measured using rise/fall time calculations typical in signal processing



[1] D. Muller, P. Batson, and J. Silcox, Physical Review B **58**, 11970 (1998).

NO-anneal results (previous results)

- w_{TL} correlates inverse-linearly μ_{FE}
  - Also correlates with decreased trap density: John Rozen, *et al*. IEEE Trans. Elec. Dev. (2011).
- NO-anneal removes/passivates mobility-limiting defects
  - Compositionally and electronically
- **Conclusions:**
  - w_{TL} decreases with increasing NO anneal time
    - New chemical shift of Si-$L_{2,3}$ edge onset was most reliable method
    - No excess C on either side of interface



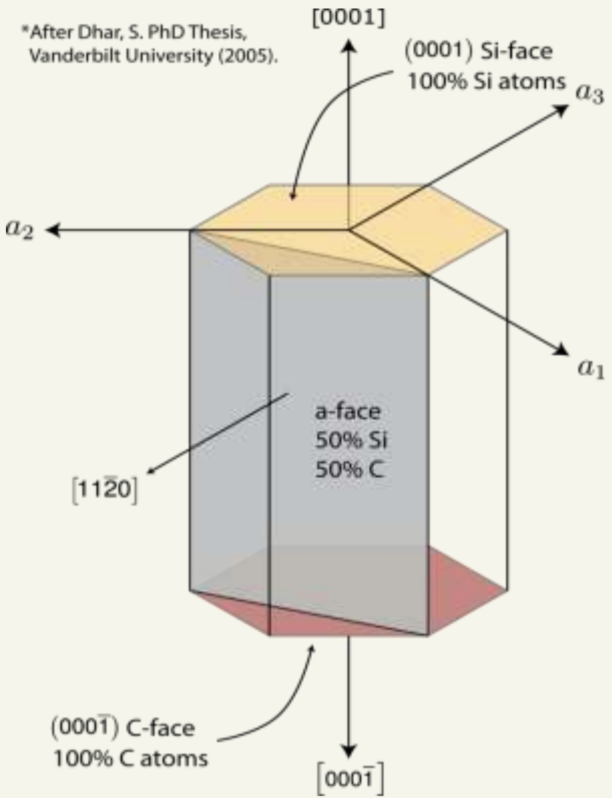
J. Taillon, L. Salamanca-Riba, *et al.*, *J. Appl. Phys.* **113**, 044517 (2013).

Samples investigated – TEM/EELS

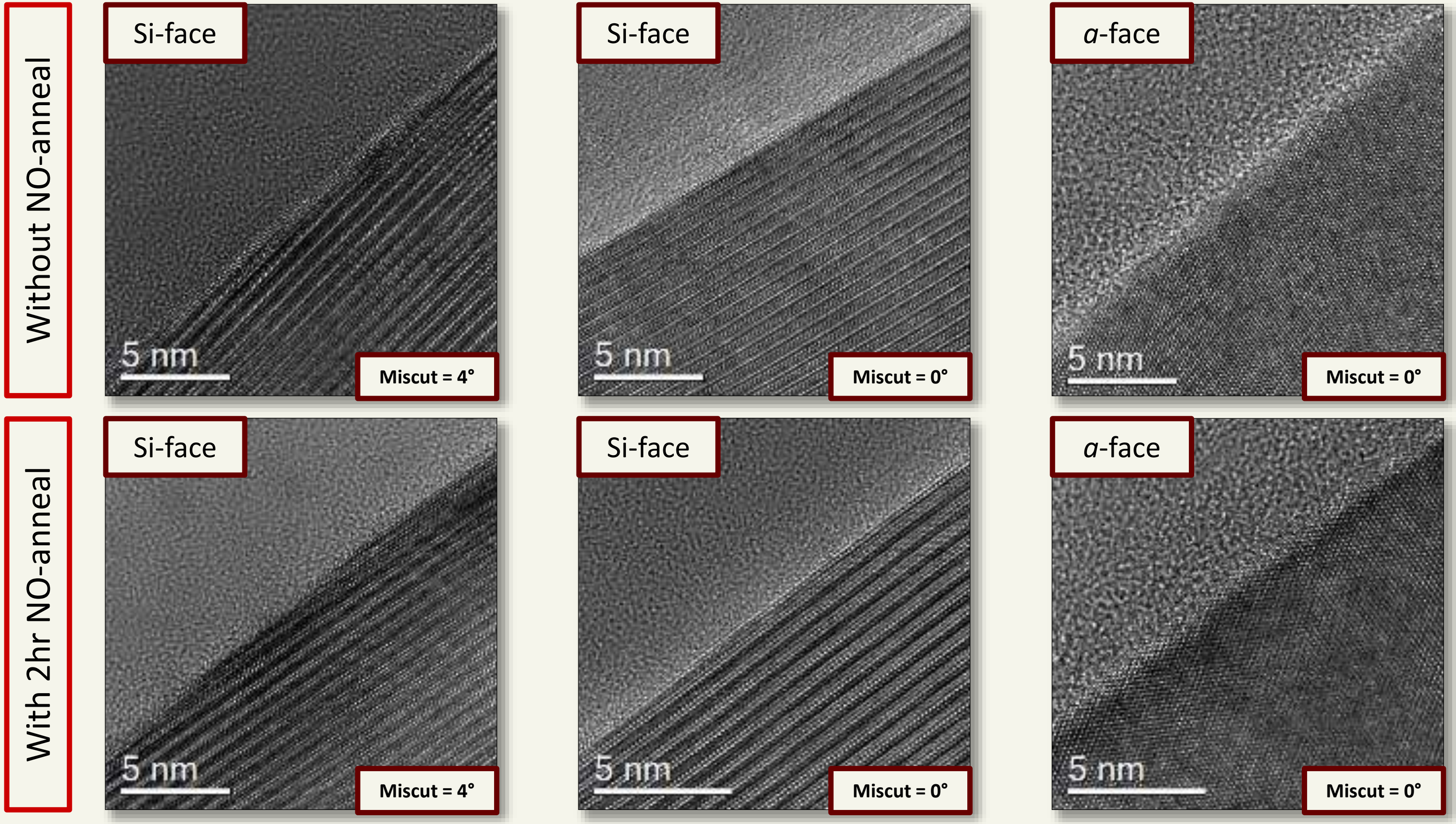
- 2 x 3 matrix aimed at comparing substrate orientation (and miscut) with processing conditions:
  - NO POA is for 2hr, all SiC substrates are n-type, SiO_2 ~60 nm thick

Sample Labels:	**Only oxidized**	**NO Post-annealed**
Si-face on-axis	Si-O_2-0	Si-N-0
Si-face miscut (4°)	Si-O_2-4	Si-N-4
a-face on-axis	a-O_2-0	a-N-0

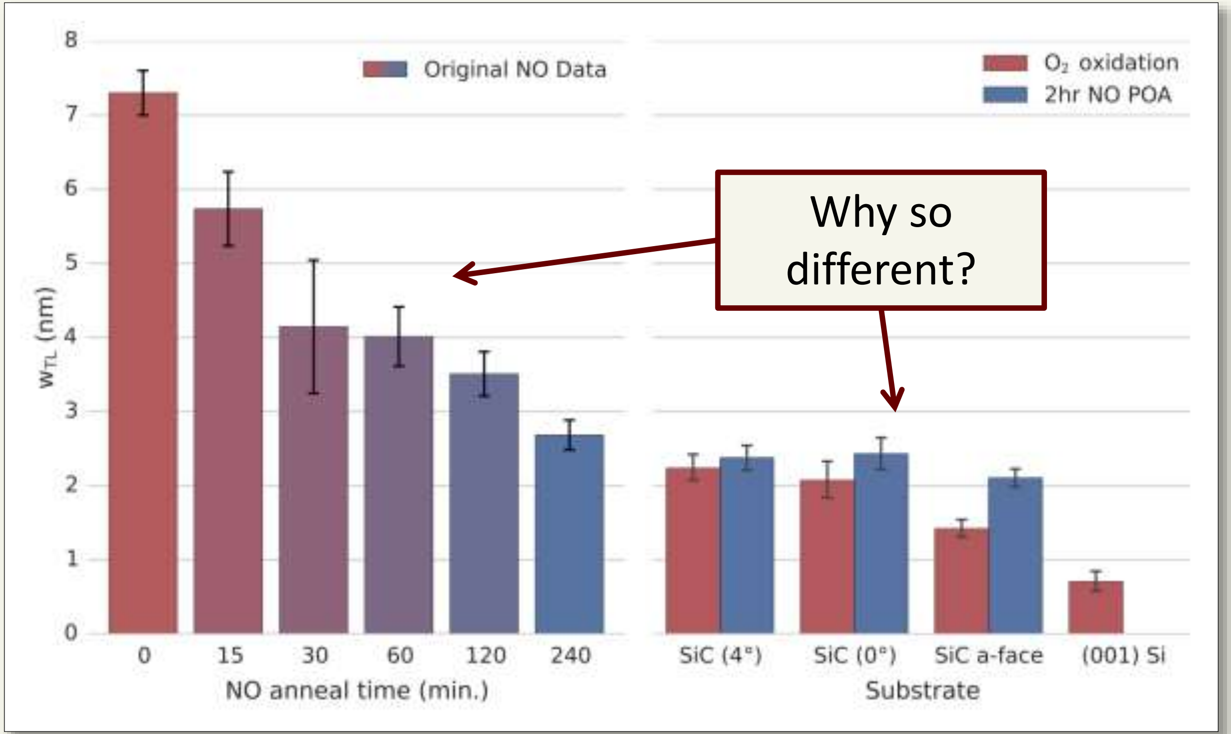
*After Dhar, S. PhD Thesis, Vanderbilt University (2005).



HRTEM of Si-face and *a*-face with and without NO annealing



w_{TL} measurements

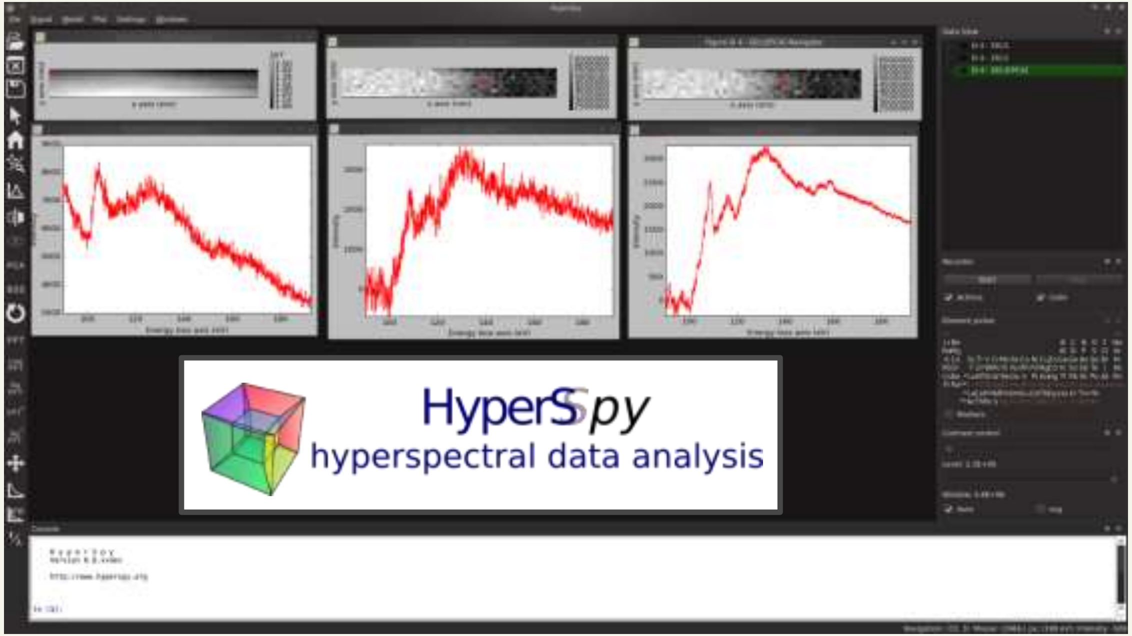


- Results from STEM EELS transition layer measurements show that w_{TL} values are similar
- w_{TL} in NO-annealed samples for these devices are actually slightly larger than the non-annealed
- a-face interfaces are the smallest, which does correspond with their higher mobilities (in NO)
  - 40 cm^2/V s for Si-face
  - 85 cm^2/V s for a-face

HyperSpy for analytical microscopy

http://hyperspy.org

DOI 10.5281/zenodo.16850



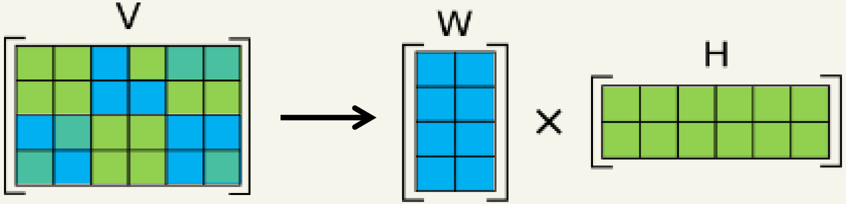
- **Open source** hyperspectral analysis package for Python
  - GUI and/or web notebook (traceability!)

- Data-agnostic, but…
  - Specialized routines for EDS and EELS

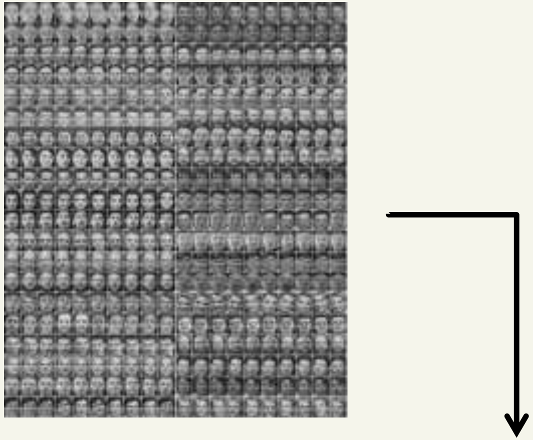
- Easy access to PCA, ICA, and signal modeling

Decomposition analysis

- Machine learning for hyperspectral decomposition
  - How to tease out convoluted and complex signals
  - Use redundancy of information in spatial dimensions to learn more about differences in the signal dimension(s)
- Non-negative matrix factorization
  - Finding simpler descriptive basis vectors of overall data; one component per "source"

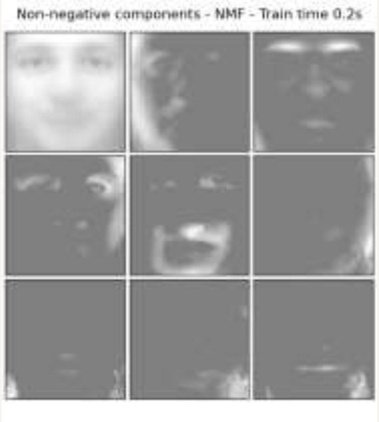


Adapted from: https://upload.wikimedia.org/wikipedia/commons/f/f9/NMF.png

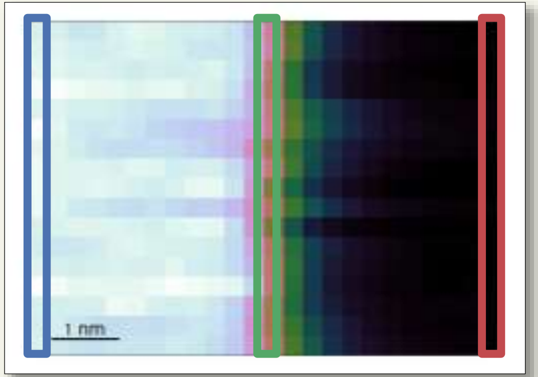


Example applied to Olivetti faces

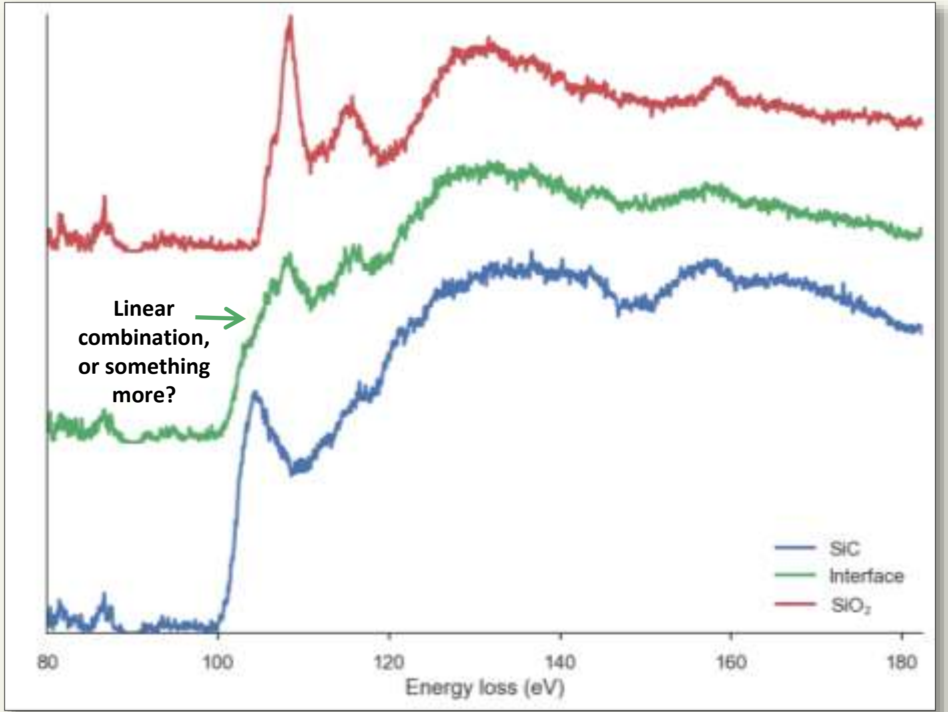
What features are found most often in the training set?



Interface components at NO-annealed interfaces

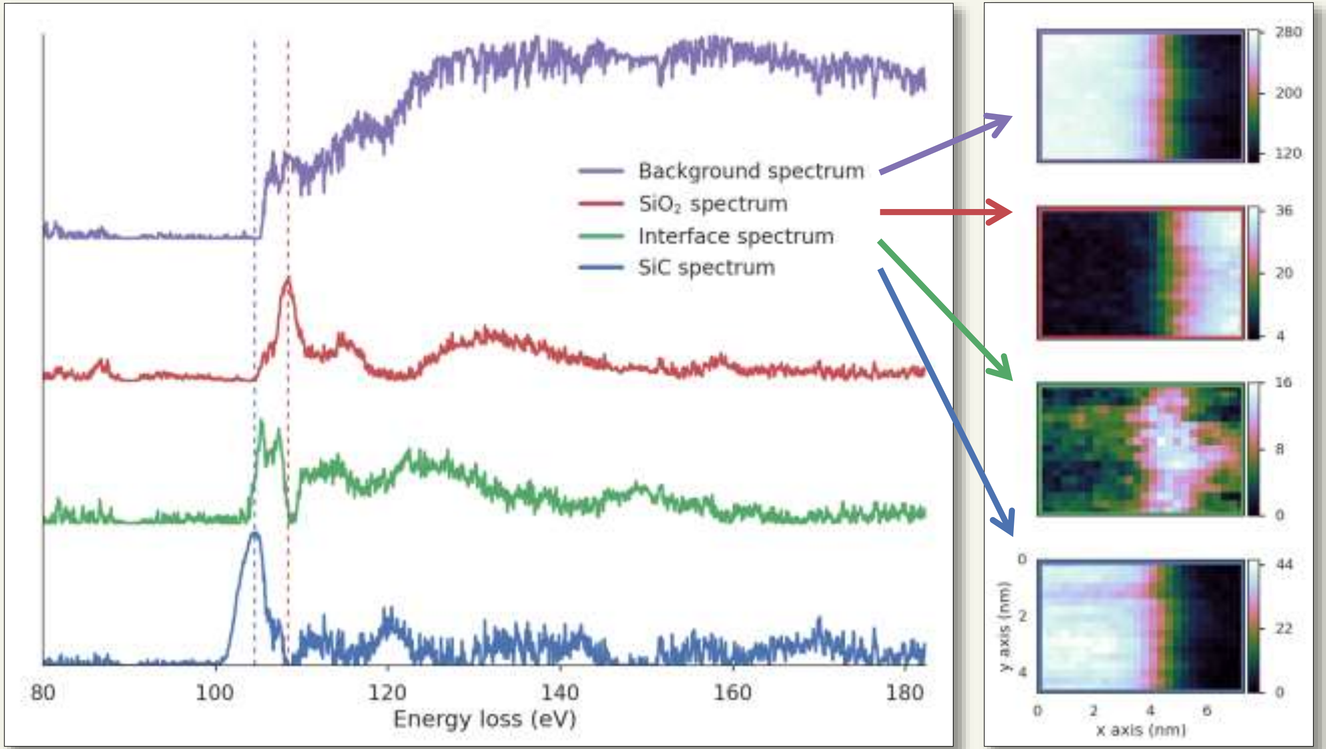


- Simple sum improves S/N, but cannot detect faint or overlapping signals

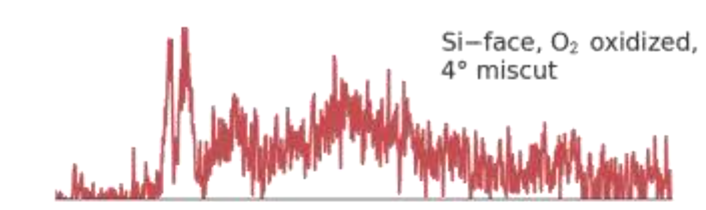
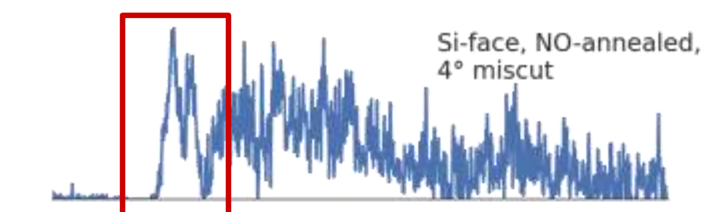
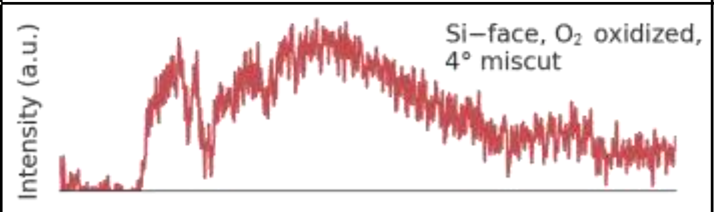
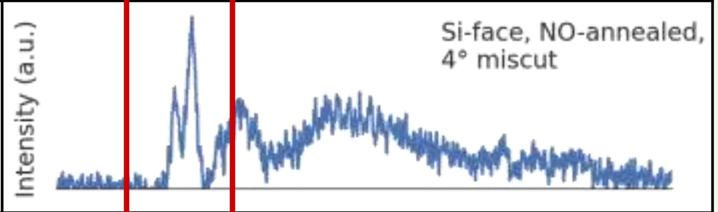
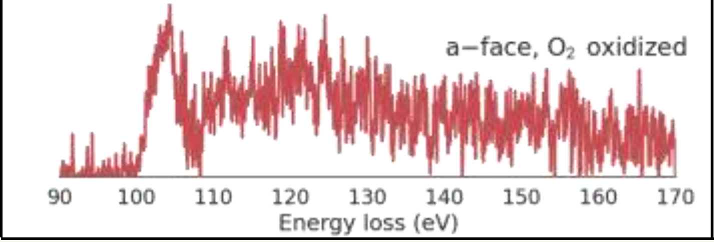
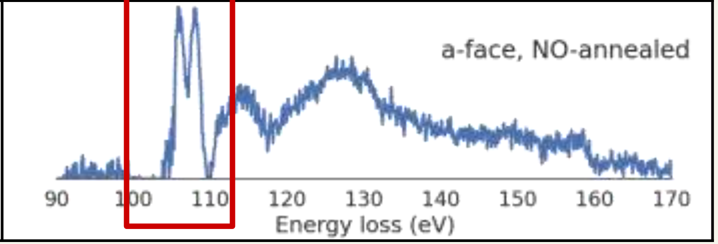


Interface components at NO-annealed interfaces

- Signal decomposition (NMF) is much more powerful
  - Significant detection of unique orthogonal component at interface
- New component that is distinct from SiO_2 and SiC was observed
  - Non-linear combination of signals!

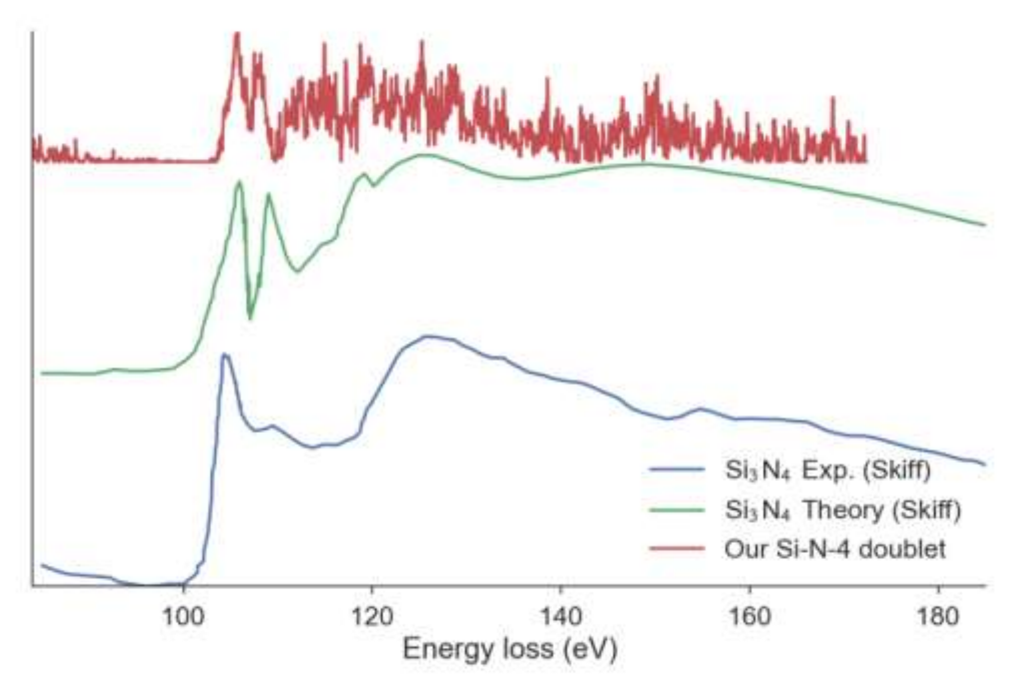


Decomposed Si-$L_{2,3}$ comparison of interface components

Face / Treatment	O_2 oxidation	O_2 oxidation + NO POA
Si-face 4° miscut (Si-X-4)		
Si-face no miscut (Si-X-0)		
a-face no miscut (a-X-0)		

What does it mean?

- Si_3N_4 theory and experiment (Skiff et al.)
  - Calculated ΔE between doublet peaks 3.4 eV compared to our 2.08 eV
- Not SiO_2 or SiC
  - Those were also identified, and peak positions do not match
- Effect of N-bonding
  - Si-C-N-O bonding configurations?
  - Likely that this is evidence of N-bonding at interface
  - DFT modeling will reveal further details

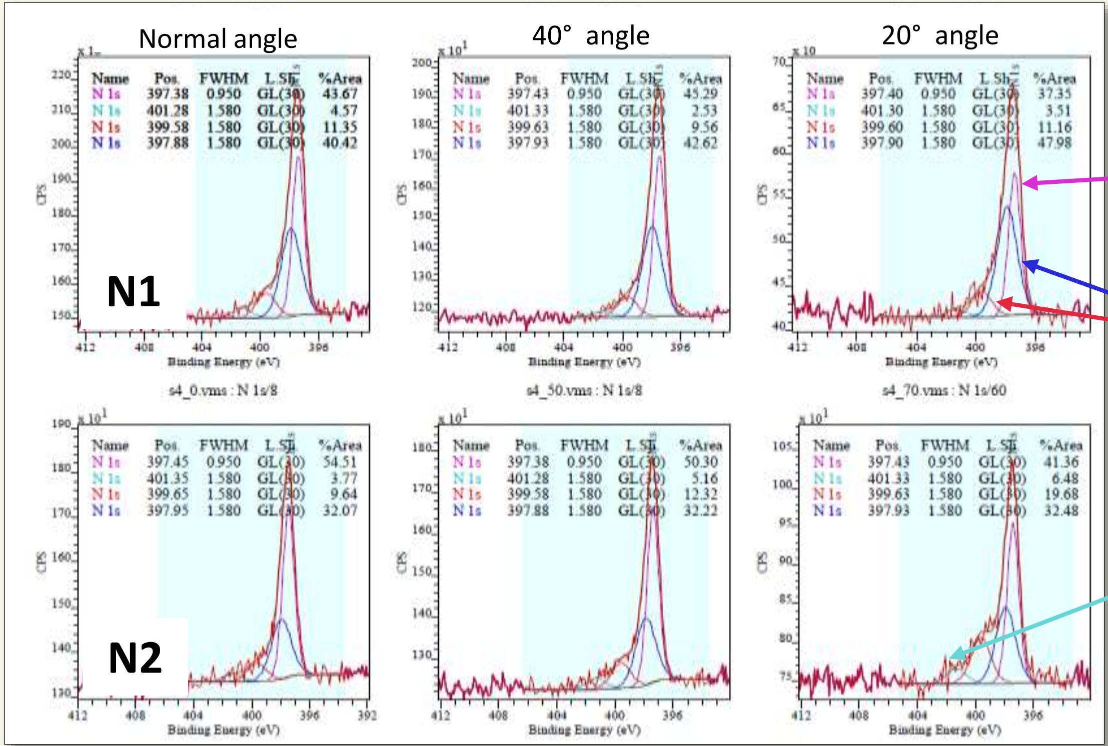


Skiff, W. M., *et al.*, *J. Appl. Phys.* **62,** 2439–2449 (1987).

XPS DEPTH PROFILING

A. JAMES CLARK SCHOOL OF ENGINEERING

XPS N 1*s*



- 4 components found in constrained fit:
  - Primary peak is consistent with silicon nitride-like bonding
  - Other peaks likely to be successively more oxygen bonding and/or carbon bonding
  - Additional component at higher energy compared to previous results[1]

[1]Y. Xu, L. C. Feldman, *et al.*, J. Appl. Phys., 115(3), 033502 (2014).

XPS N 1*s*

Elemental composition (peak area integration)					
	Measurement	C 1s %	N 1s %	O 1s %	Si 2p %
Completely etched	**N1 - normal**	40.95	1.67	9.56	47.82
	N1 – 40°	41.43	2.66	16.44	39.47
	N1 – 20°	41.20	2.73	20.59	35.49
2 – 4 nm oxide layers	**N2 – normal**	29.92	1.01	21.80	47.28
	N2 – 40°	33.59	1.37	29.46	35.58
	N2 – 20°	36.28	1.45	33.57	28.70

- N content decreases when thick oxide is present, and is still present after all original oxide is etched off
- N is localized in SiC near interface (in agreement with recent findings from Rutgers[1])

- Results are consistent with TL observed by EELS
  - Further corroboration of N-bonding hypothesis of what is being observed at the interface

[1]Y. Xu, L. C. Feldman, *et al.*, J. Appl. Phys., 115(3), 033502 (2014).

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 Si-$L_{2,3}$ EELS edge reveals a chemically/electrically distinct interface state
  - Likely significant impacts on mobility and performance
  - Spatial distribution matches measurements of w_{TL}
- a-face samples have narrower transition region than Si-face.
- XPS indicates Si_3N_4-like N bonding at the interface, with N incorporated primarily at interface

Future work

- Further analysis of EELS signals (O-*K*, C-*K* edges and low-loss region) at the interface
- Theoretical modeling of DOS for explanation
- Exploration of lattice strain in different substrate orientations

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HyperSpy hyperspectral data analysis
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HyperSpy developers:

- Francisco de la Peña
- Pierre Burdet
- Tomas Ostasevicius
- Vidar Tonaas Fauske
- And many others…

THANK YOU

Questions/comments:

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