Gate Dielectric Metrology Using Advanced TEM Techniques

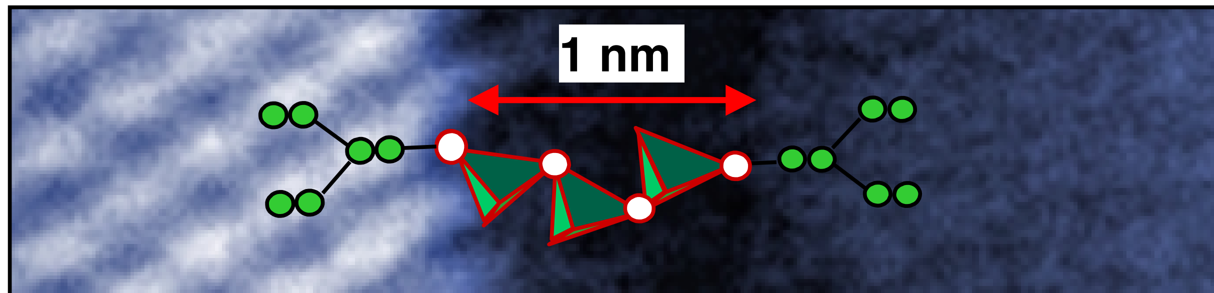
David Muller,

Frieder Baumann, Tom Sorsch, Steve Moccio
Joe Rosamalia, Kenneth Evans-Lutterodt,
Greg Timp

Bell Labs, Lucent Technologies

Jeff Neaton,

Physics Dept, Cornell University



silicon **SiO_2** **polysilicon**

Nature, **399**, 758 (1999), *Phys. Rev. Lett.* (Aug 3)

Lucent Technologies
Bell Labs Innovations

When do we stop?

Reliability: ~~25~~ ~~22~~ ~~18~~ 16 Å

processing and yield issue

Tunneling : 15 Å

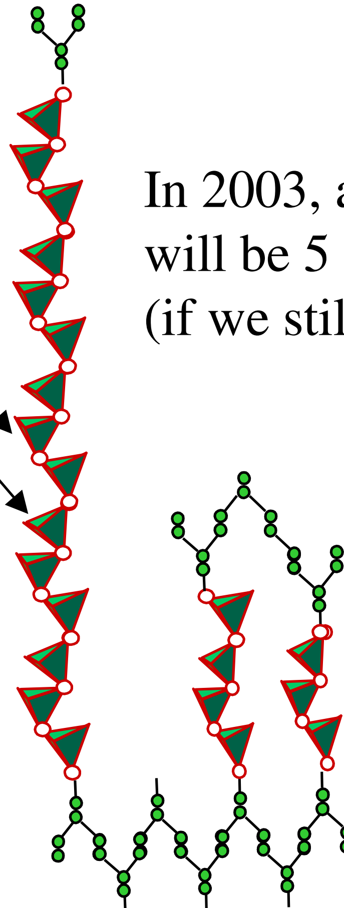
Design Issue: chosen for 1A/cm² leakage
I_{on}/I_{off} >> 1 at 12 Å

Bonding:

Fundamental Issue- how many atoms
- do we need to get bulk-like properties?
- Is the interface electronically abrupt?
- Can we control roughness?

In 1997, a gate oxide was 15 silicon atoms thick.

.
.
.



In 2003, a gate oxide will be 5 silicon atoms thick (if we still use SiO_2),

and at least 2 of those 5 atoms will be at the interfaces.

DC Performance / Gate Leakage Current Density

(I_{off} < 2 μA/μm)

Decreasing Thickness

GATE CURRENT (A/cm²)

10^2, 10^0, 10^{-2}, 10^{-4}

t_{ox} ~ 1.5nm

pMOSFET
40 < Lg < 51nm

nMOSFET
• 43 < Lg < 52nm

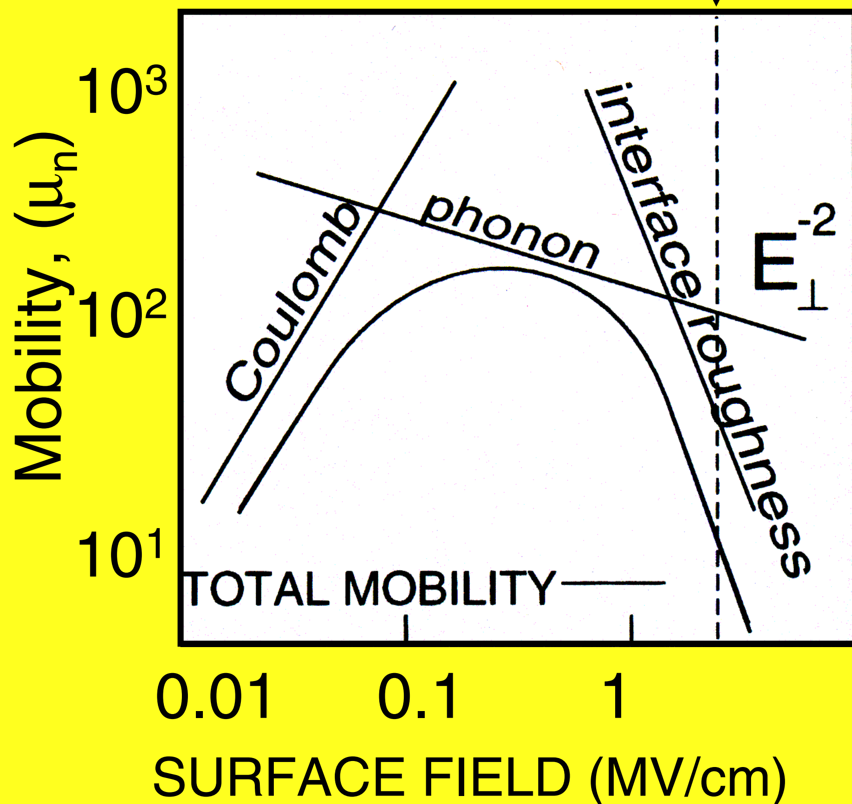
0.75 -0.50 -0.25 0 0.5 1.0 1.5

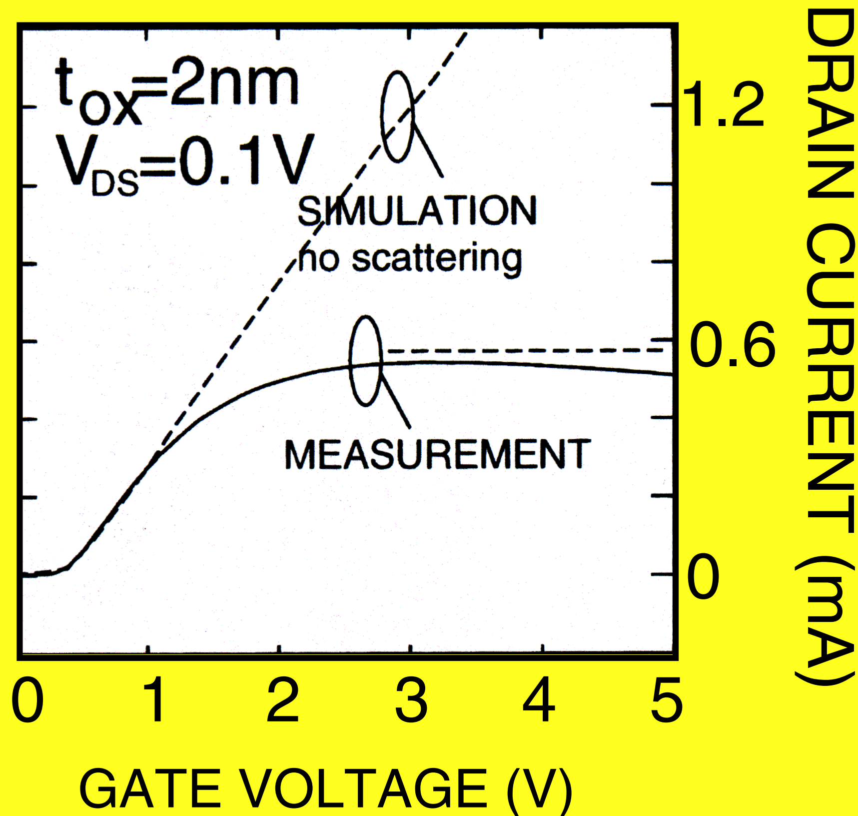
DRAIN CURRENT (mA/μm)

While gate current deteriorates,
drive current does not improve for t_{ox} < 1.3 nm

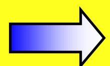
Interface Roughness Scattering in MOSFET

50 nm



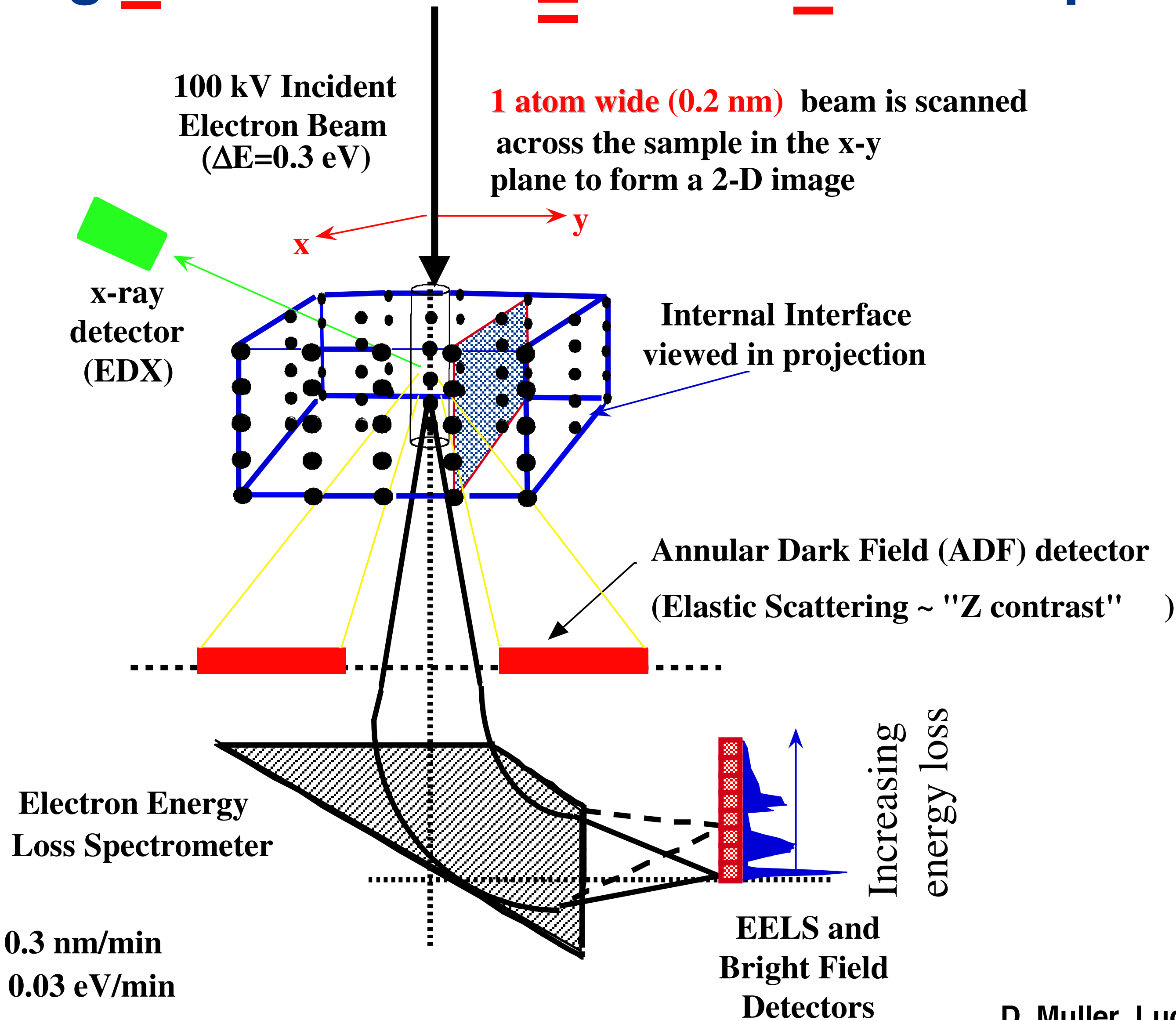


Surface scattering predominates for $E_\perp$>0.5 MV/cm

 Need to reduce roughness (even for High *k*)

G. Timp, J. Bude & a cast of thousands, IEDM 1999

Spatially Resolved Electron Energy Loss Spectroscopy in a Field Emission Scanning Transmission Electron Microscope

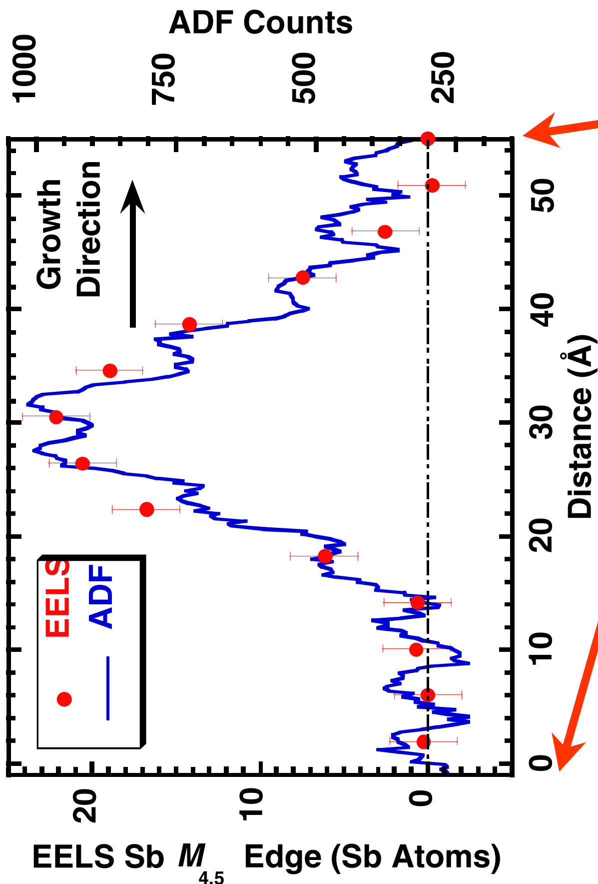


Spatial Drift < 0.3 nm/min
Energy Drift < 0.03 eV/min

D. Muller, Lucent Technologies

2D-Dopant Profiling in Silicon:

Imaging Sb Atoms in a δ-doped layer



Growth Direction

10 Å

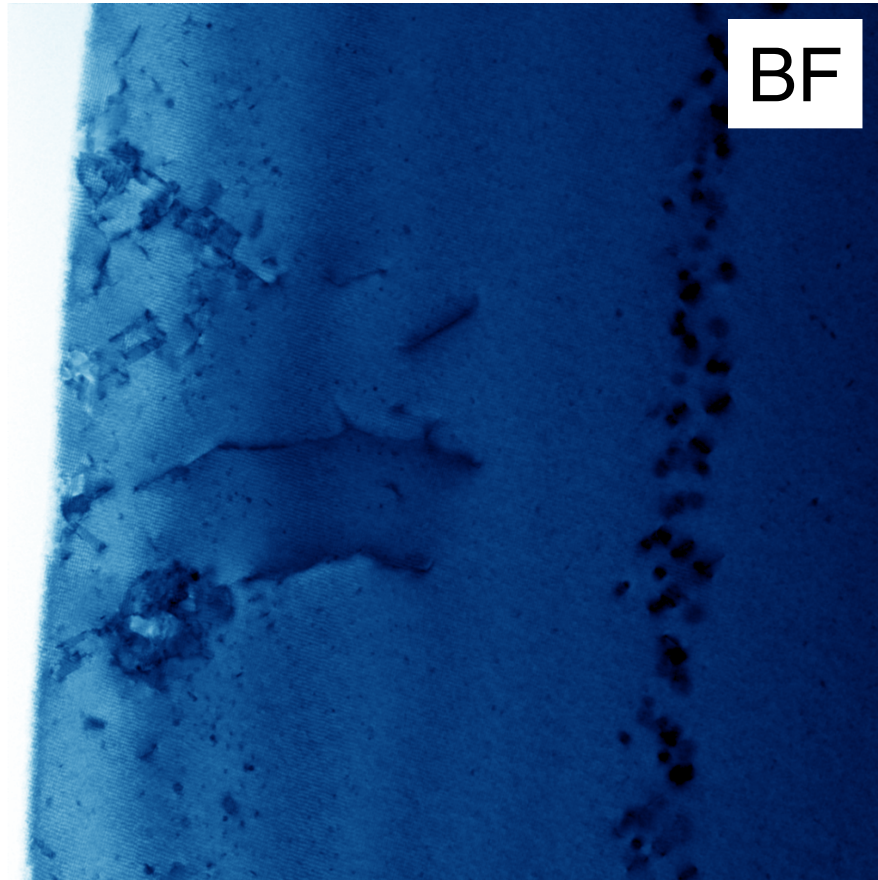
Detection Limit is ±2 atoms by EELS, ± 0.5 atoms by ADF

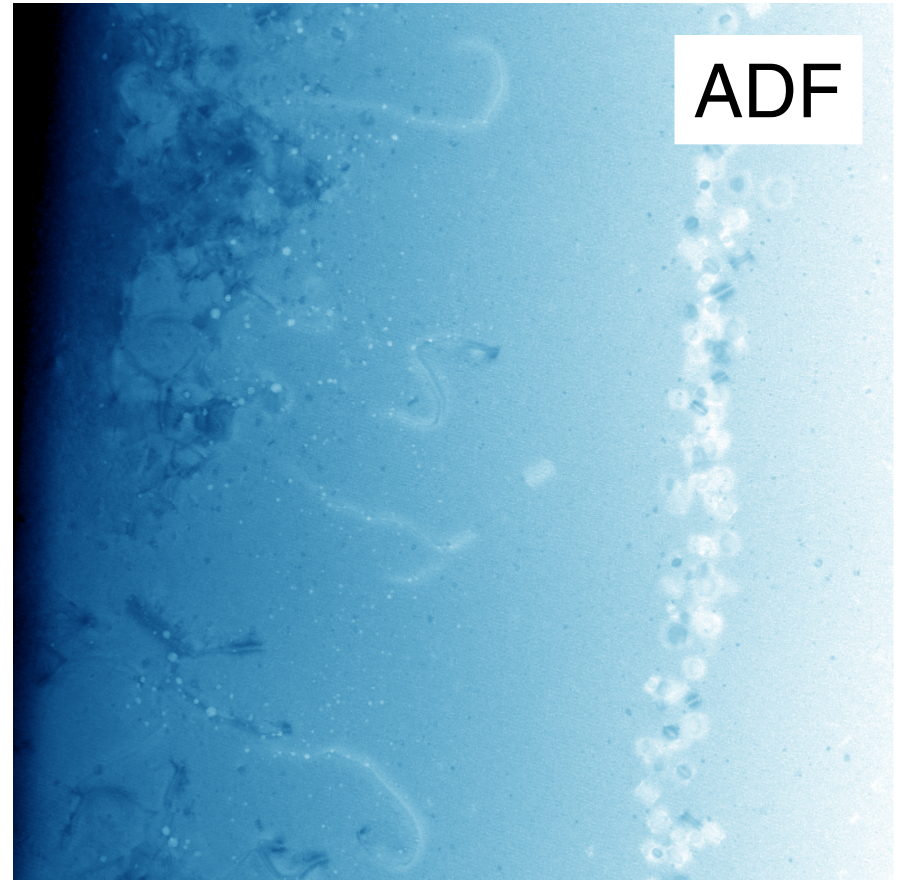
David Muller, Paul Citrin, Hans Gossman, R. Vanfleet, *Phys. Rev. Lett.* 1999

Lucent Technologies
Bell Labs Innovations

ADF is Not Always "Z-Contrast"

(Hf Implants in Si)



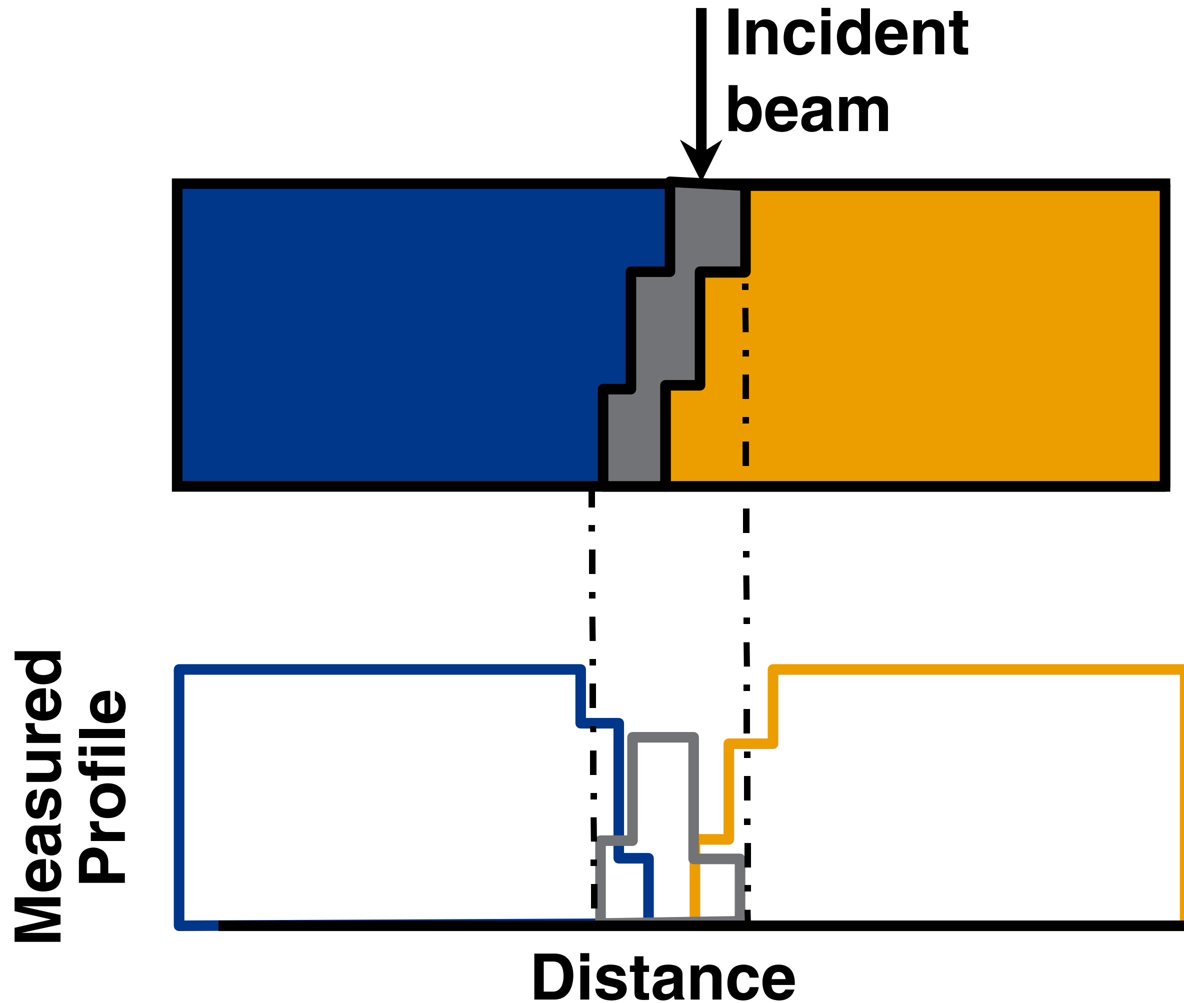


BF: Thickness+diffraction contrast

ADF: strain contrast from dechanneling in thick samples

D. Muller, Lucent Technologies

A Problem with Roughness: The interface is viewed in projection

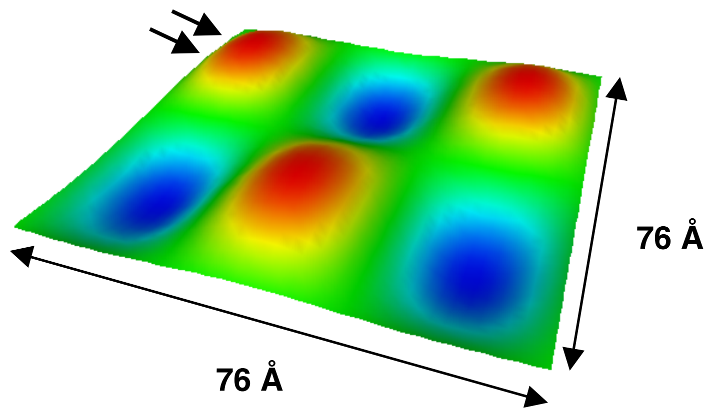


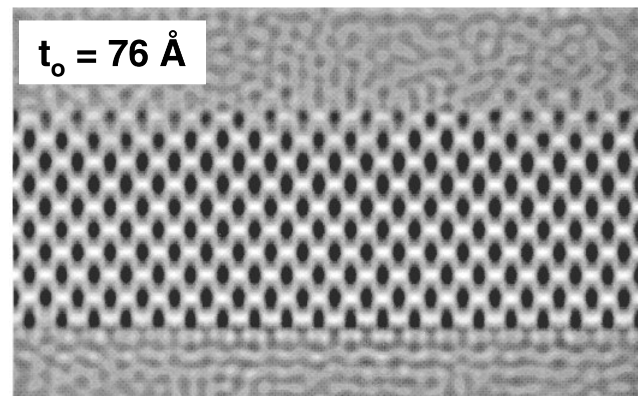
Roughness increases the apparent width of the interfacial region

D. Muller, Lucent Technologies

Imaging Interface Roughness in Projection

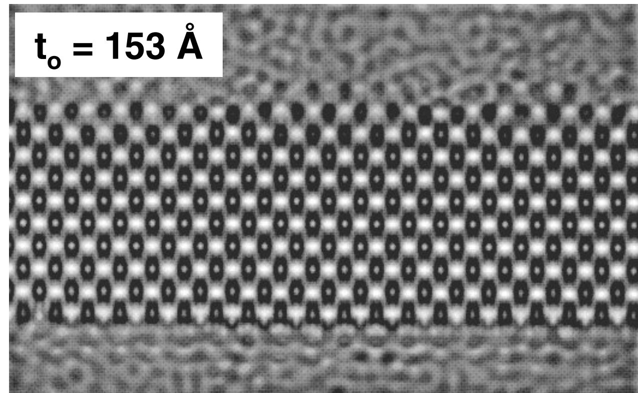
CTEM or BF-STEM





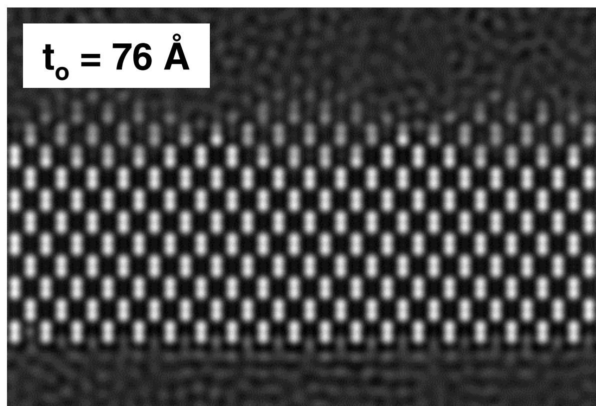
Rough interface

Smooth interface

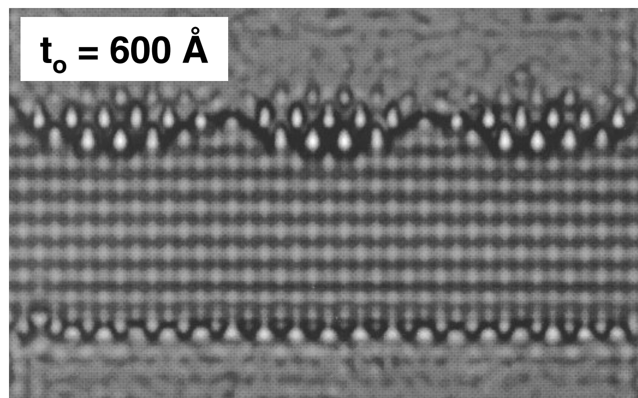


Rough interface

Smooth interface



ADF-STEM

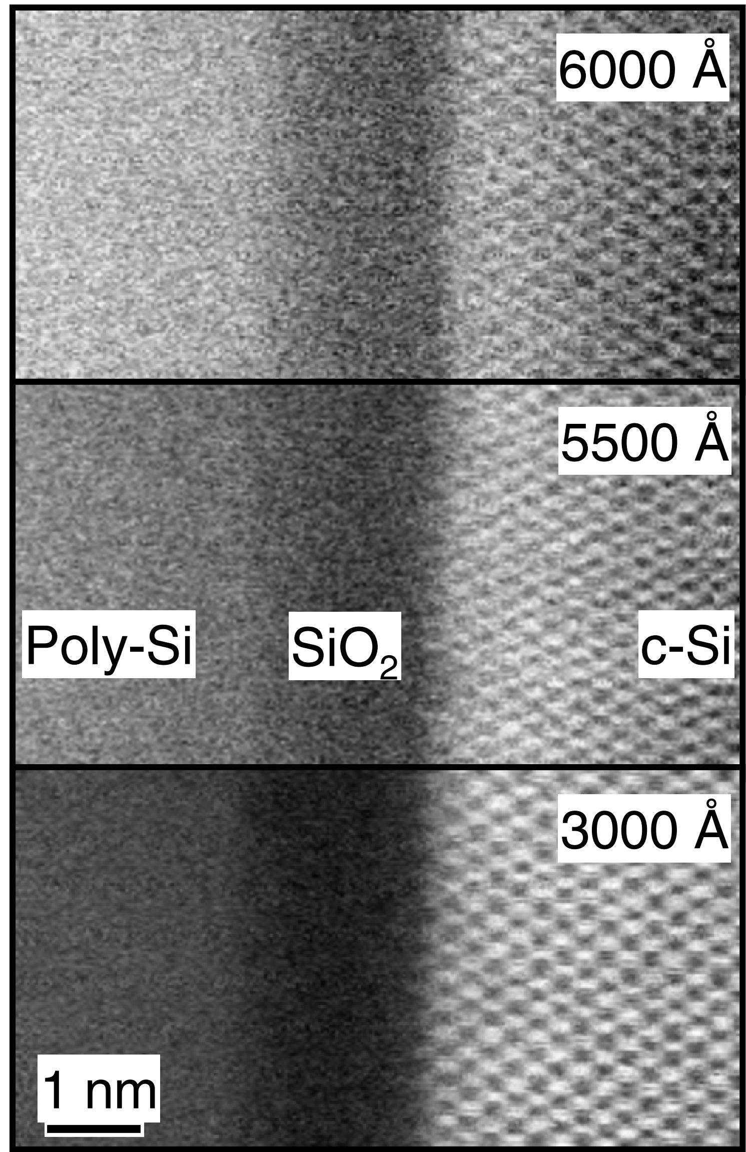


Rough interface

Smooth interface

(F. H. Baumann et al., MRS Spring 2000, Akatsu and Ohdomari, App. Surf. Sci. **41** 357 (1888))

Imaging Thick Cross-Sections



Gate Oxide Thickness: 20 Å

- ADF Images decay gracefully with increasing thickness
- Apparent Oxide Thickness is unchanged with thickness
- Apparent Interface Roughness increases from 1.6 to 2.7 Å rms
- “white band” develops (depends on thickness and ADF angles)

Measuring Projected Roughness

Lucent Technologies
Bell Labs Innovations

(180 nm Gate Length Transistor)

Distance (Å)

120
100
80
60
40

Expt
Fit

ADF Intensity

Expt
Fit

ADF Derivative

Poly-Si
SiO_2
c-Si
15 Å

ADF Image

Gate Oxide Thickness: 15.3 Å, Si/SiO_2 Roughness σ<1.56 Å

Imaging atomic scale Roughness

Lucent Technologies
Bell Labs Innovations

(Filtered ADF-STEM Images of 1 nm Gate Oxides)

a-Silicon
Gate Oxide
1 nm
Silicon

Standard Clean
5.4 Å Peak-Peak Roughness
2.3 Å rms roughness (ADF)
2.2 Å rms roughness (xray)
(1.1 Å rms by AFM)

New Surface Preparation
1.8 Å Peak-Peak Roughness
1.25 Å rms roughness (ADF)
1.1 Å rms roughness (ADF)
0.5 Å rms by AFM

David Muller, Tom Sorsch (Silicon Research) 1998

Spatially Resolved Electron Energy Loss Spectroscopy in a Field Emission Scanning Transmission Electron Microscope

Lucent Technologies

Bell Labs Innovations

100 kV Incident Electron Beam (ΔE=0.3 eV)

1 atom wide (0.2 nm) beam is scanned across the sample in the x-y plane to form a 2-D image

x

y

x-ray detector (EDX)

Internal Interface viewed in projection

Annular Dark Field (ADF) detector

(Elastic Scattering ~ "Z contrast")

Electron Energy Loss Spectrometer

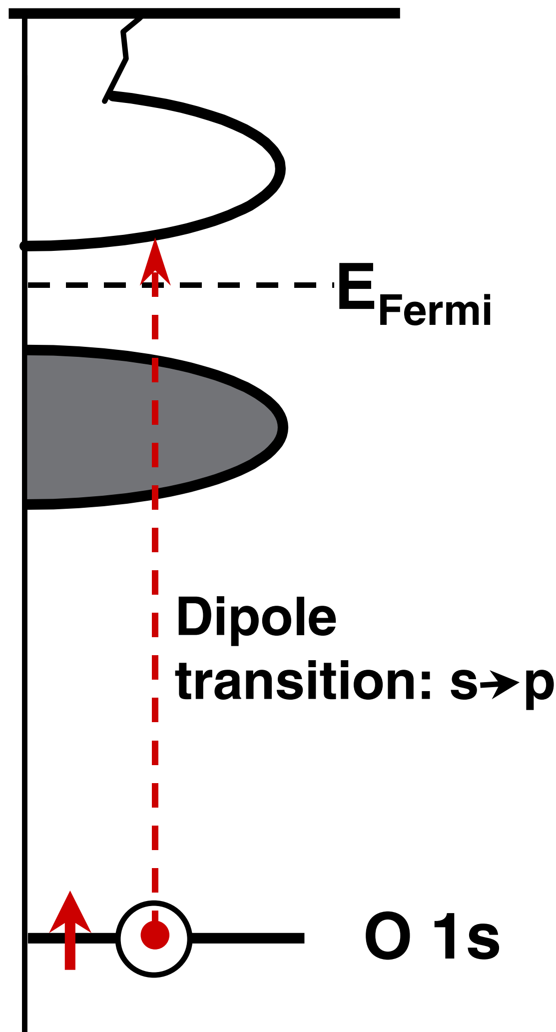
Increasing energy loss

EELS and Bright Field Detectors

Spatial Drift < 0.3 nm/min

Energy Drift < 0.03 eV/min

Core-Level Electron Energy Loss Spectroscopy



EELS measures a local density of states partitioned by

- site - as the probe is localized,
- element - the core level binding energy is unique
- angular momentum (s,p,d states separately)

Probes the conduction band and so provides local electronic information

O-K edge measures the empty O p-DOS which is sensitive to O-O 2nd neighbors (XPS is mostly nearest neighbors)

→ EELS (and electrical) interface is wider than XPS (chemical)

David Muller, 1998

Imaging the Si/SiO_2 Interface on an atomic scale requires a sharp interface

ADF O-K

ADF Counts

1500
1400
1300
1200
1100
1000
900
800
700

O-K Edge Counts

800
600
400
200
0

5 10 15 20 25 30

Distance (Å)

David Muller, Tom Sorsch (Silicon Research) 1998

Lucent Technologies
Bell Labs Innovations

Oxygen Bonding at the Si/SiO_2 Interface

Lucent Technologies
Bell Labs Innovations

O-K Edge Counts (arb. units)

200
150
100
50
0

520 530 540 550 560 570

Energy Loss (eV)

a
b

Interfacial Oxide
Bulk a-SiO_2

The edge onset is 3 eV lower at the interface

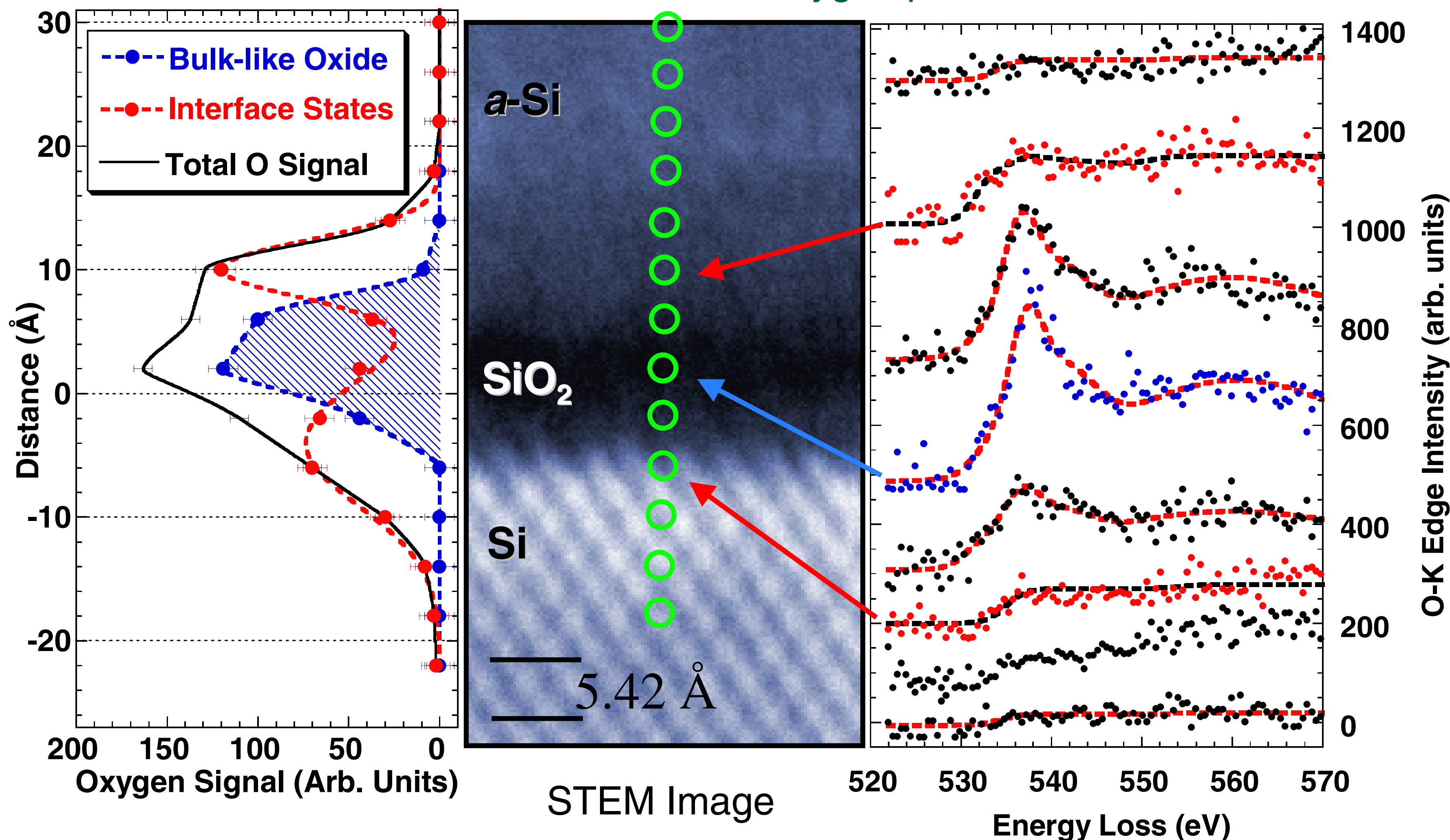
David Muller, 1998

Oxygen Bonding from EELS (Chemistry on an Atomic Scale)

Nominal 1.1 nm SiO_2:

0.8 - 1 nm Bulk SiO_2

1.6 nm wide oxygen profile



Lucent Technologies
Bell Labs Innovations

Oxygen Profile

"10 Å" Gate Oxide :

- 60±5% Interfacial Oxide
- Bulk-Like FWHM: 8.5 Å
- Total Oxygen FWHM: 16 Å

"18 Å" Gate Oxide :

- 35±5% Interfacial Oxide
- Bulk-Like FWHM: 16 Å
- Total Oxygen FWHM: 21 Å

Oxygen Signal (Arb. Units)
Bulk-like Oxide
Sub-Oxide
Total O Signal
Bulk-like Oxide
Interfacial Oxide
Total O Signal
Distance (Å)

David Muller, 1998

Oxygen Profile before and after annealing

Lucent Technologies
Bell Labs Innovations

Oxygen Signal (Arb. Units)
200
150
100
50
0

Bulk-like Oxide
Interfacial Oxide
Total O Signal

Oxygen Signal (Arb. Units)
160
120
80
40
0

Total O Signal
Bulk-Like Oxide
Interfacial Oxide

-24 -16 -8 0 8 16 24
Distance (Å)

Before Annealing:

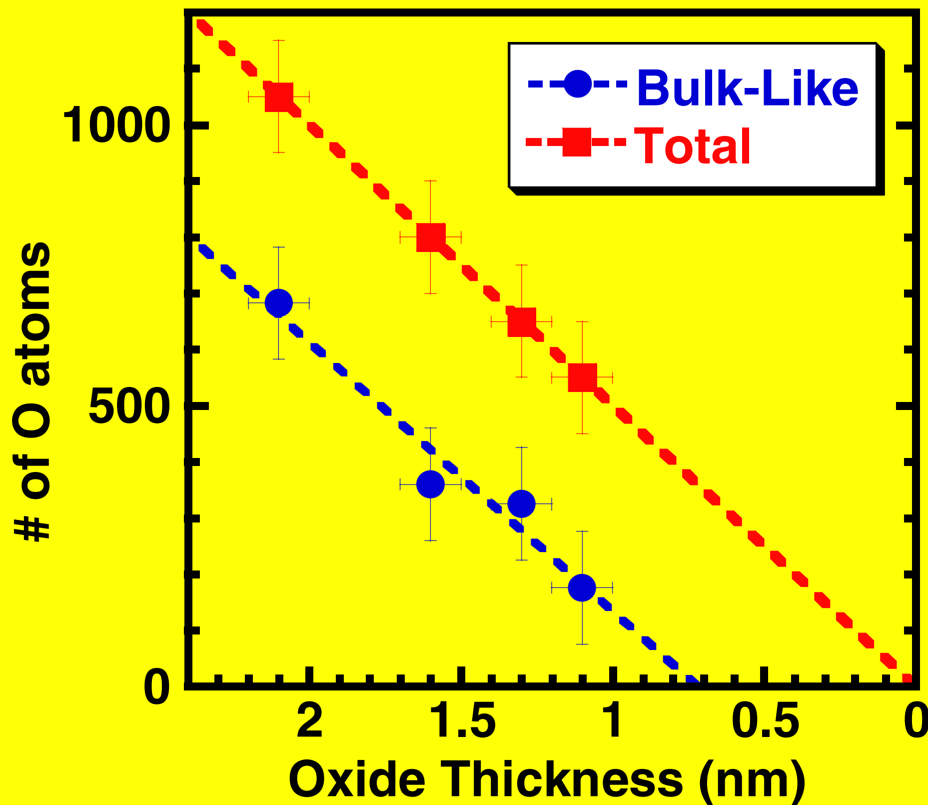
- 60±5% Interfacial Oxide
- Bulk-Like FWHM: 8.5 Å
- Total Oxygen FWHM: 16 Å
- Upper interface is smoother than the lower.

After Annealing:

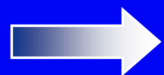
- 50±5% Interfacial Oxide
- Bulk-Like FWHM: 8.5 Å
- Total Oxygen FWHM: 13 Å
- Lower interface unchanged
- Upper interface is now as rough as the lower.

David Muller, 1998

The End of the Roadmap for SiO_2



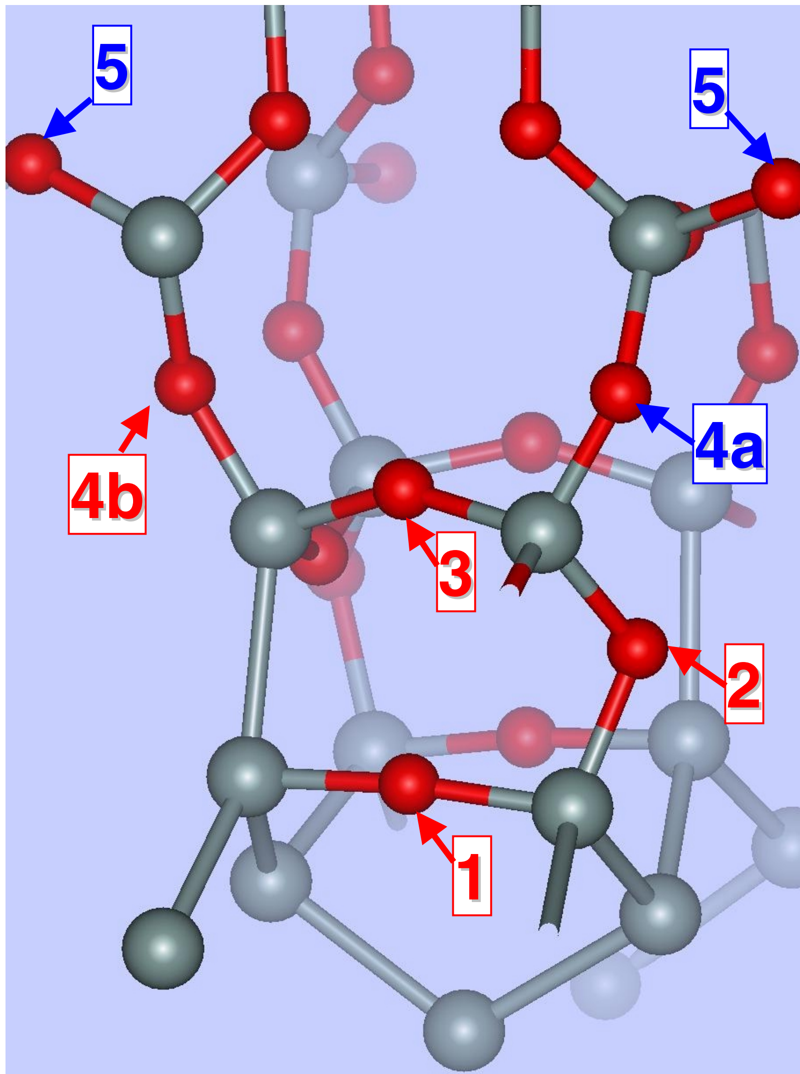
The Interface width is fixed



There will be no more Bulk-like bonding when the Oxide is less than 0.7 nm.

David Muller, 1999

A Model Si/SiO_2 Interface



O *p*-projected DOS

Density of States (arb. units)

0, 20, 40, 60, 80

Energy (eV)

0, 2, 4, 6, 8, 10, 12

Si Cond Band

SiO_2 Cond Band

5 — 6 O-nn

4a — 6 O-nn

4b — 5 O-nn

3 — 5 O-nn

2 — 4 O-nn

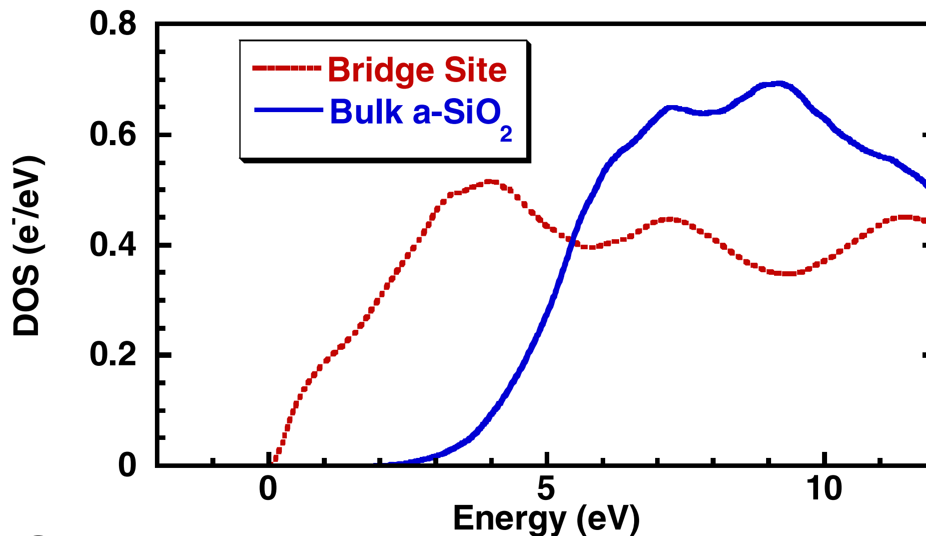
1 — 1 O-nn

More O-O 2nd Nearest Neighbors

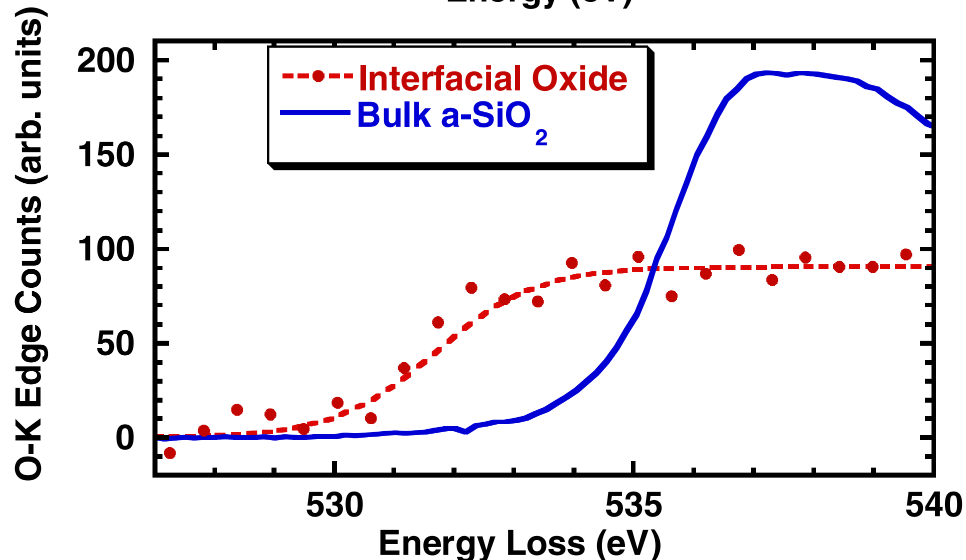
(Model-3 of A. Pasquarello, M. S. Hybertson, R. Car, PRB)

Oxygen Bonding at the Si/SiO_2 Interface

Lucent Technologies
Bell Labs Innovations



Theory



Experiment

The edge onset is 3 eV lower at the interface

David Muller, 1998

Comparison of the Measured Oxygen-K Edge with *ab-initio* Calculations

Calculated O p-DOS
Measured O-K Edge

DOS (e^-/eV)
0.12
0.09
0.06
0.03
0

0
10
20
30
40
Energy (eV)

No strong core-hole effects on the oxygen-K Edge

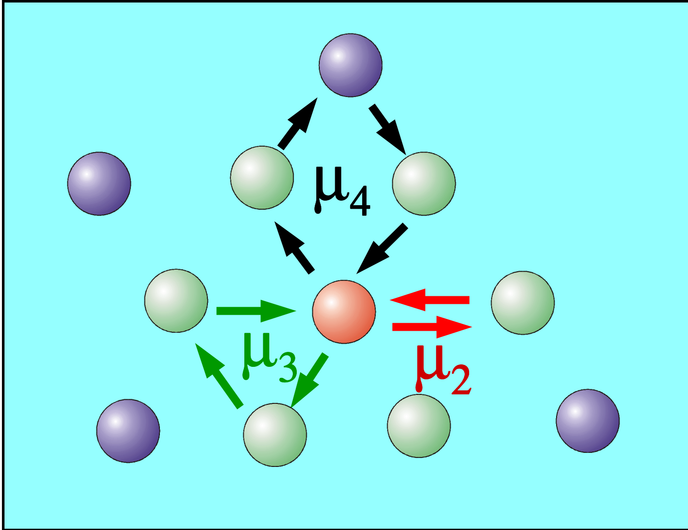
(not true for the Si L edge)

Jeff Neaton & David Muller, 1999

Lucent Technologies
Bell Labs Innovations

Cyrot-Lackmann's Moments Theorem:

The shape of the local DOS depends on the local atomic arrangement:



2nd Moment: $\mu_2 = \sum \beta^2 = z\,\beta^2$

(Variance)

⇒ Bandwidth, $W = \sqrt{\mu_2} = \sqrt{z}\,|\beta|$

⇒ W depends only on neighbors

3rd Moment: $\mu_3 = \sum \sum$

(Skewness)

$\mu_3>0$ $\mu_3<0$

4th Moment: $\mu_4 = \sum \sum \sum$

(Kurtosis)

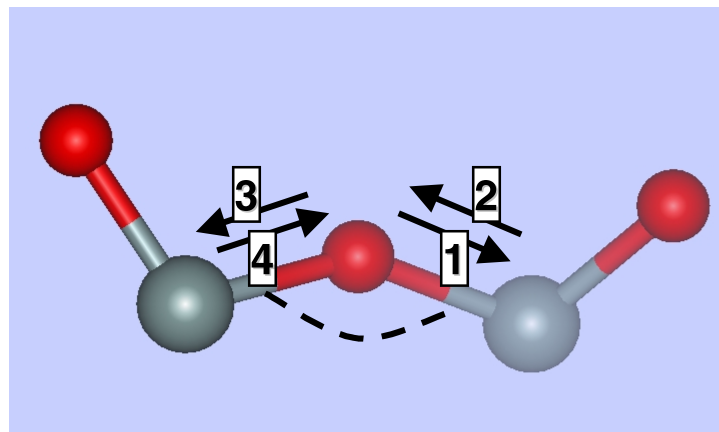
$\gamma_4 = \mu_4 / (\mu_2)^2$

$\gamma_4<2$ $\gamma_4>2$

Fourth Moments in SiO_2

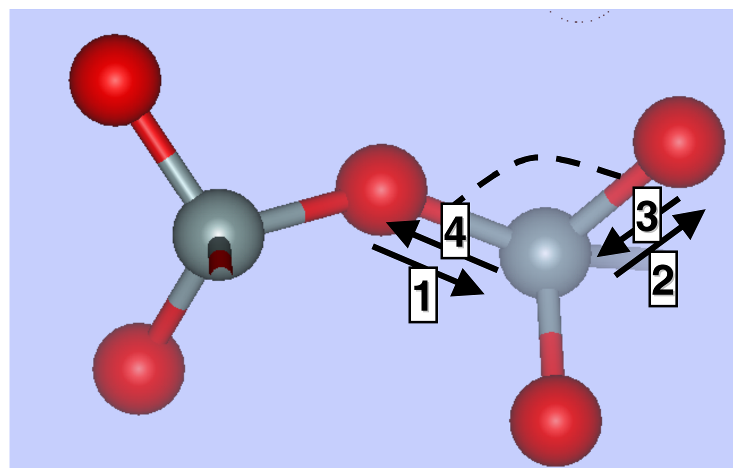
Lucent Technologies
Bell Labs Innovations

Nearest Neighbors
and
Si-**O**-Si Bond Angle



Small:
- 2 terms
- Node on O

Second Neighbors
and
O-**Si**-O Bond Angle



Large:
- 6 terms
- No Node on Si

⇒ 4th Moment will scale with the number of O-O 2nd Neighbors

David Muller, 1999

The 4th moment measures the development of the local energy-gap

Lucent Technologies
Bell Labs Innovations

O *p*-DOS

Normalized 4th Moment

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3

0 1 2 3 4 5 6

# of O-O 2nd neighbors

Model 3
Model 4

Smaller bandgap

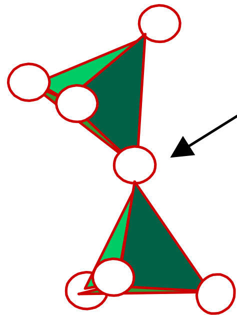
Larger bandgap

Any Si/SiO_2 Interface must have a reduced bandgap
(last O layer has ≤ 3 O-O 2nd neighbors)

Minimum electronic interface width is 2.7 Å

Minimum Thickness for Bulk Energy Gap

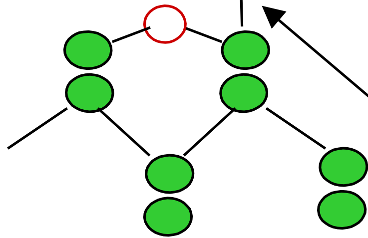
Lucent Technologies
Bell Labs Innovations



For this O atom to have a bulk-like energy gap, it needs 6 O neighbors,

HOWEVER

There is a 50% bond density mismatch with Si, so the last layer of O is 1/2 concentration



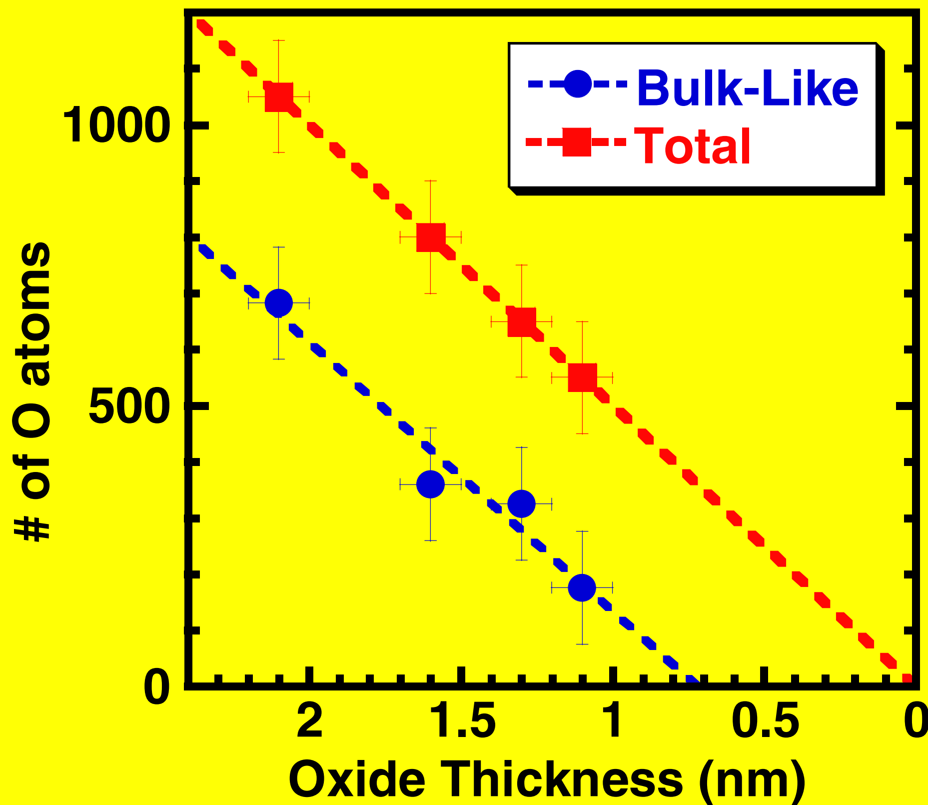
This adds another Si-O bond length (1.6 Å)

Total interface thickness is then ~ Si-O (1.6 Å) + O-O (2.7 Å)

With Si-O-Si angular distortions,

the minimum oxide thickness ≈ 6.9- 8.3 Å

The End of the Roadmap for SiO_2



The Interface width is fixed

→ There will be no more Bulk-like bonding when the Oxide is less than 0.7 nm.

David Muller, 1999

ADF Image of a Alumina Gate Oxide

(Nominally 100 Å of Al_2O_3 on Si)

David Muller, 1998

EELS Profile of the Graded $Al_xSi_yO_z$ Interlayer

(Originally 100 Å of Al_2O_3 on Si)

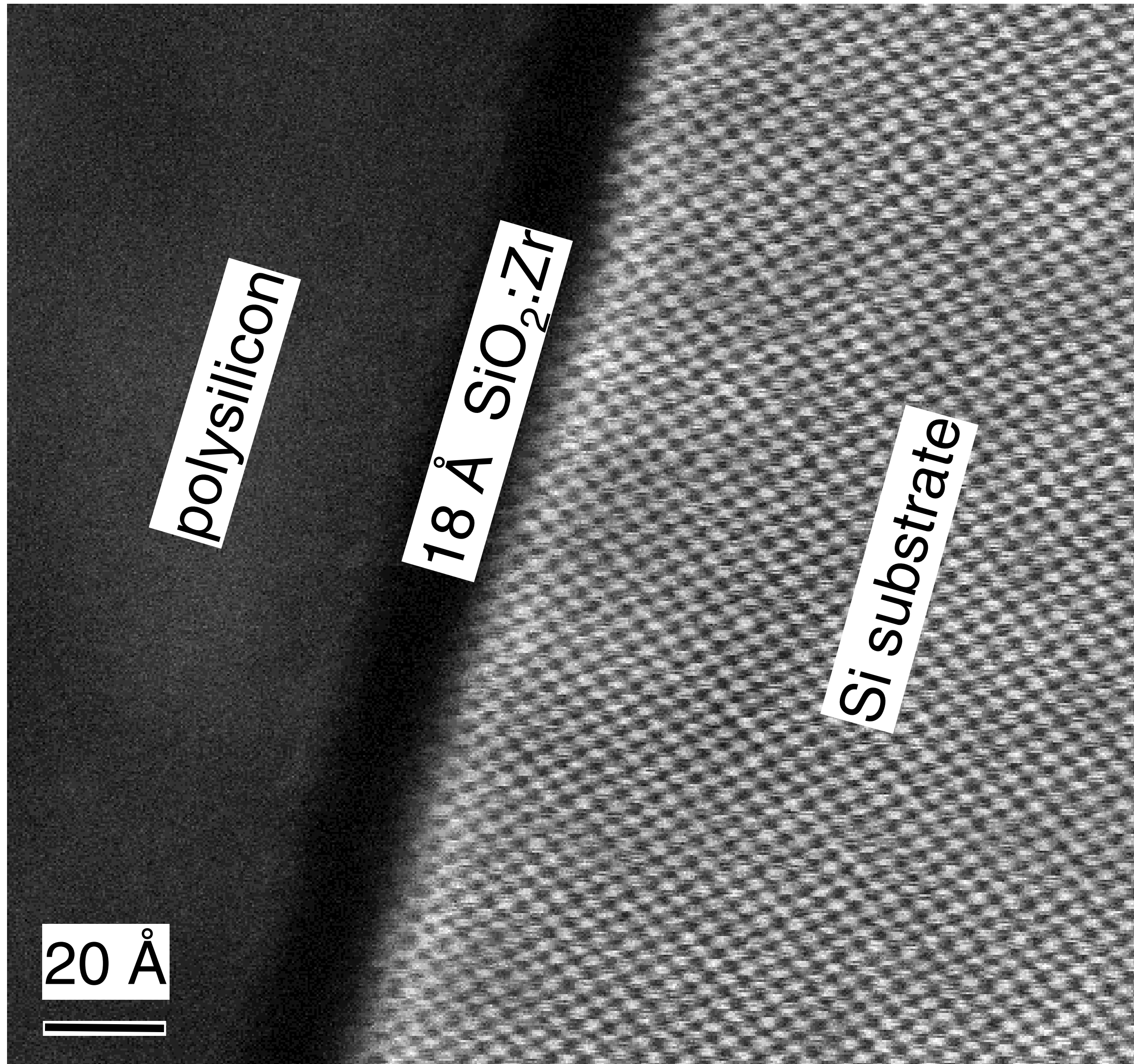
ADF Counts: 1700, 1600, 1500, 1400, 1300, 1200
Distance (nm): 0, 5, 10, 15, 20, 25
Labels: Al_2O_3, Al, Si

Al K Edge Signal (a.u.): 0, 2, 4, 6, 8, 10
ADF Signal: 0, 500, 1000, 1500, 2000, 2500, 3000, 3500
Distance (nm): 0, 1, 2, 3, 4, 5
Labels: Al_2O_3, Interlayer, Si

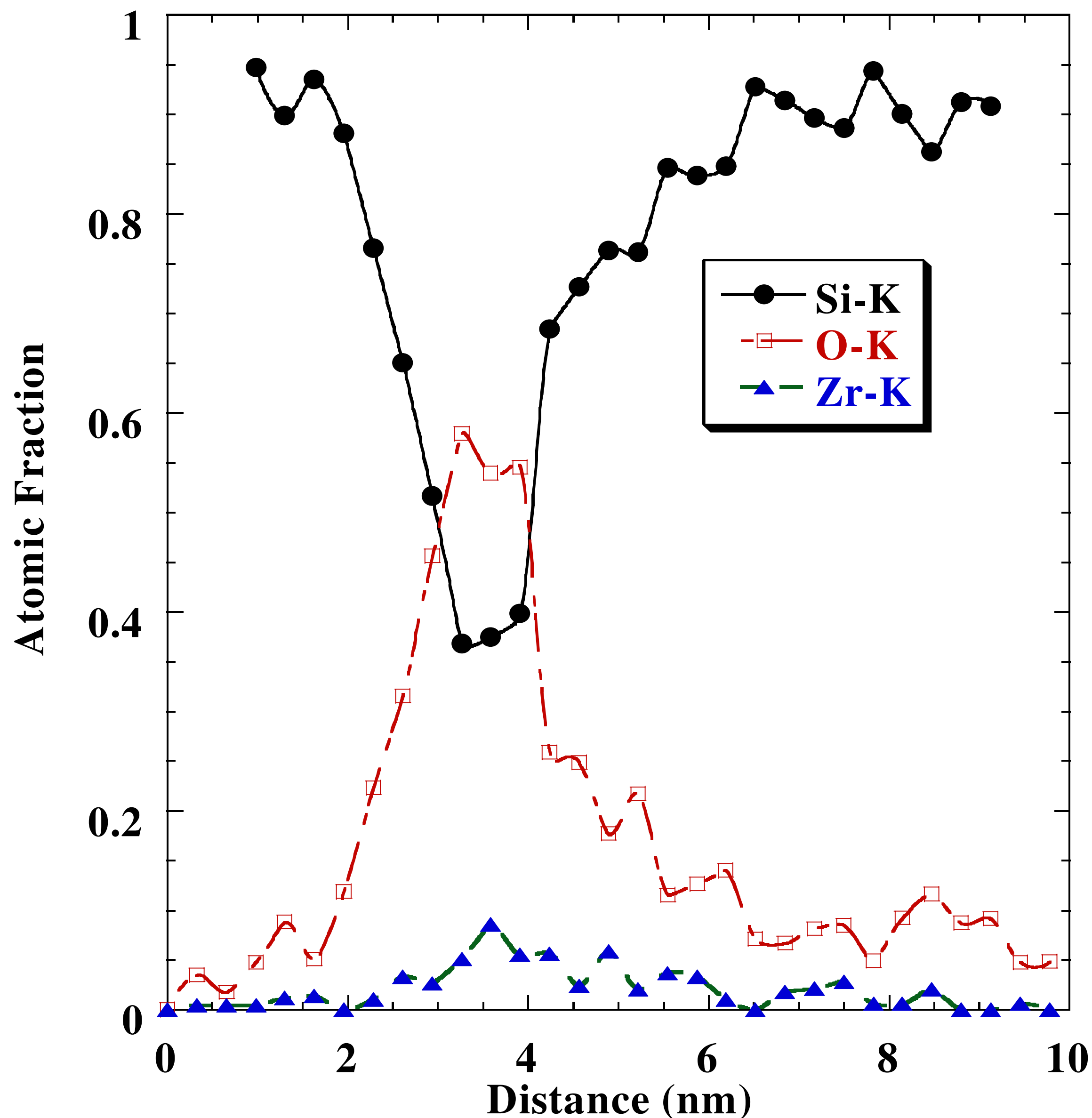
David Muller, 1998

Lucent Technologies
Bell Labs Innovations

ADF Image of the SiO_2:Zr gate Oxide (1100C)

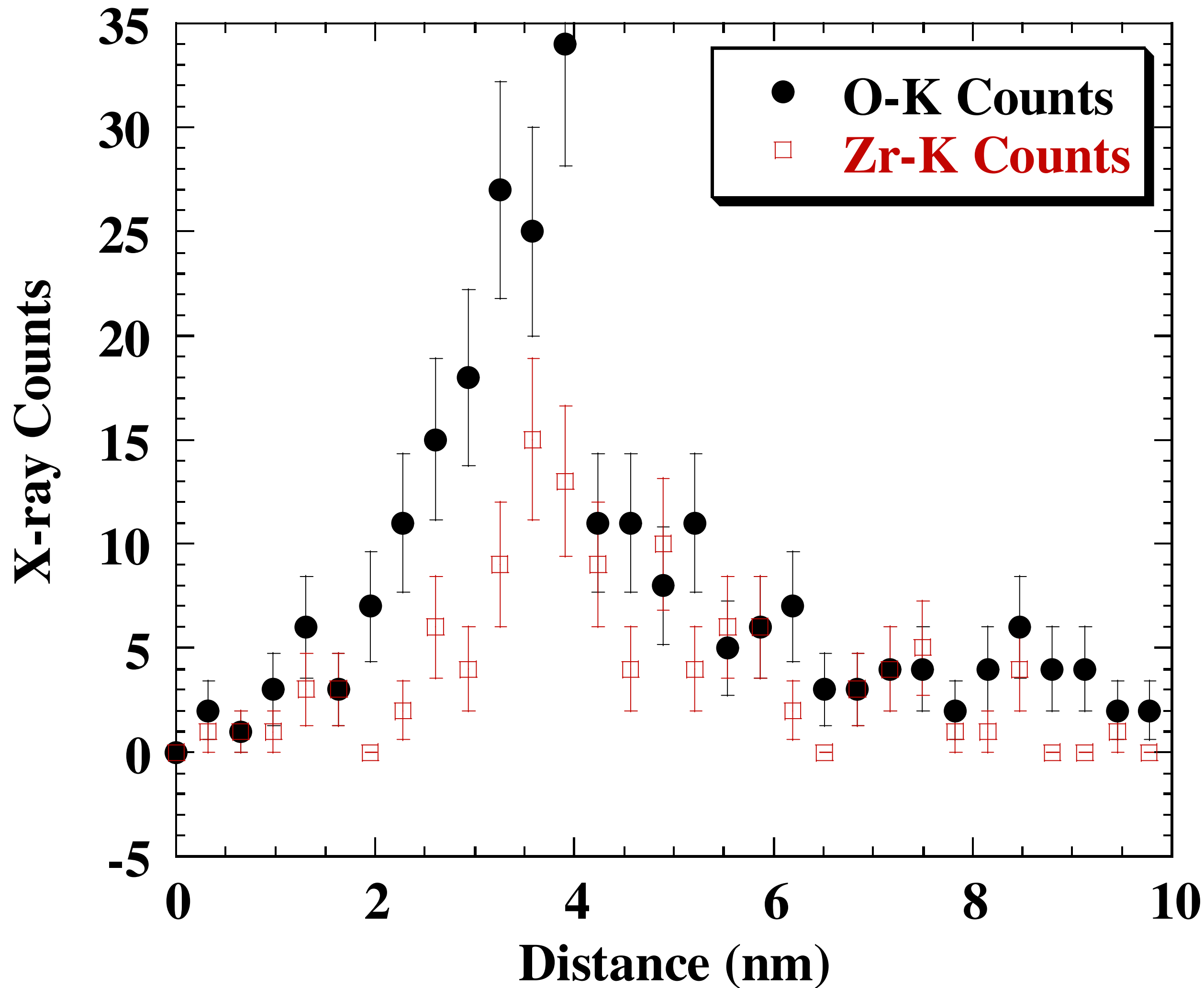


X-ray profile of the SiO_2:Zr gate Oxide



Peak Zr concentration is 8%

X-ray profile of the SiO_2:Zr gate Oxide



There may be 0.5 nm Zr-free region at the lower Si/SiO_2 interface

Oxygen Bonding at the Si/SiO_2:Zr Interface

Lucent Technologies
Bell Labs Innovations

The edge onset is 3 eV lower at the interface (like SiO_2)

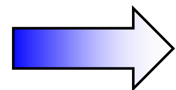
David Muller, 1998

Gate Oxide Metrology Using STEM

- EELS: Chemistry and bonding at atomic resolution
  Thin samples (hard to make&interpret)
- ADF : Chemically sensitive images at TV rates
  Thick cross-sections (easy to prepare&interpret)

Physical Properties we measured (at the atomic scale):

- Correlation between local gap and O-O neighbors.
- There is an intrinsic layer (>3 Å) with a reduced bandgap at all Si/SiO_2 interfaces.


Limits how thin we can grow a gate oxide

- Interface Roughness must be controlled to take advantage of high-k Materials

David Muller, 1999

Lucent Technologies
Bell Labs Innovations