



atomera

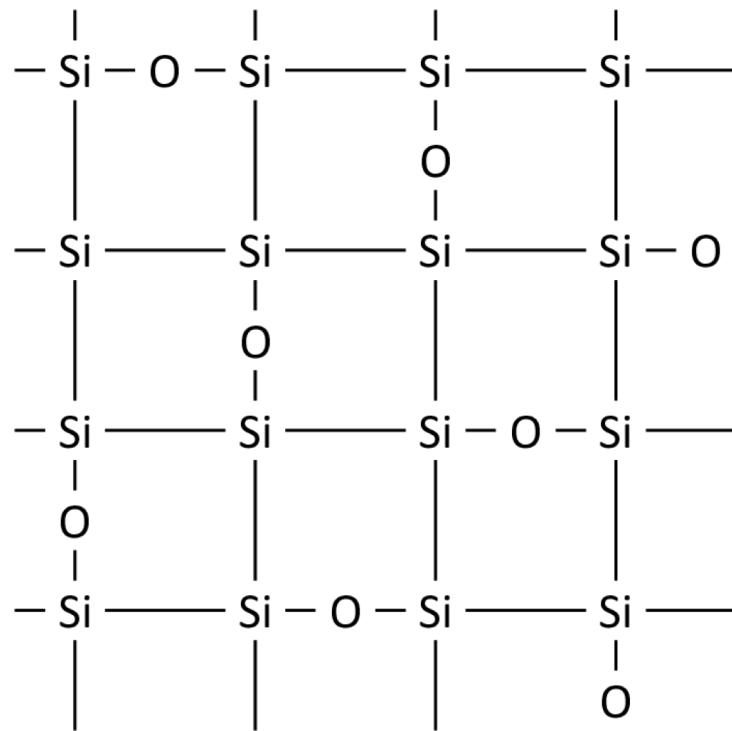
MST[®] Process Modeling with Sentaurus TCAD

Daniel Connelly

Atomera Inc

MST Structure

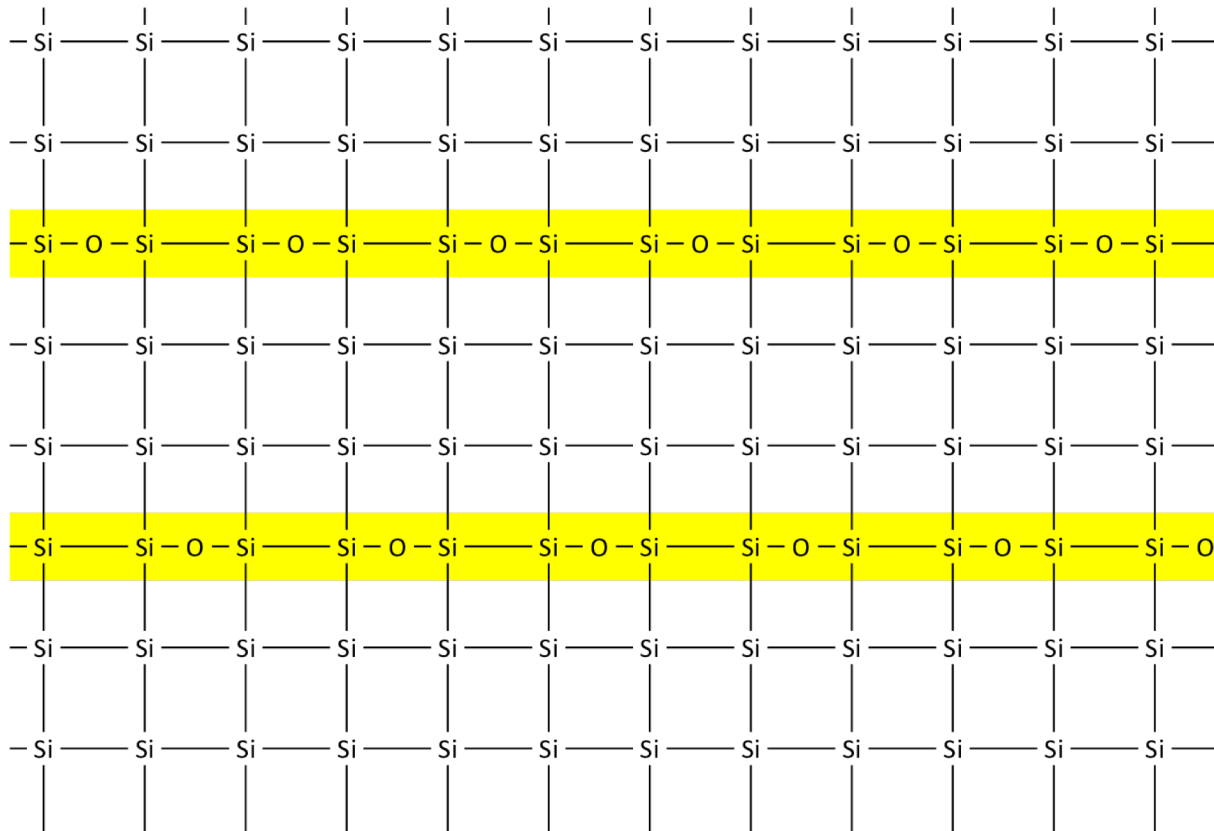
MST Layer Planar Schematic



cartoon sketch: OI plane

- **MST Oxygen Insertion (OI) plane** shown
- **Planar insertion of oxygen** into Si lattice.
- **metastable:** O emitted during thermal cycles.

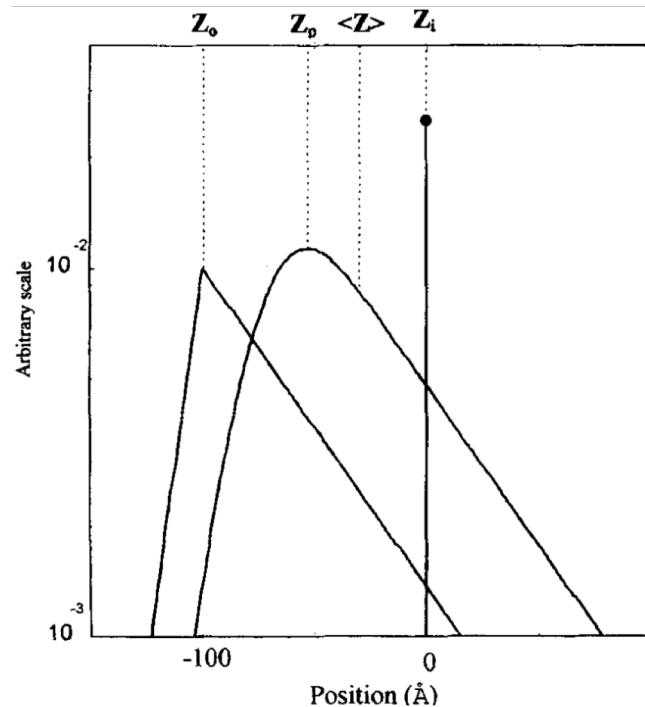
MST Vertical Layer Structure



- multiple oxygen inserted layers
- Si between OI layers
- different than SiO_2 .

SIMS Modeling

- **comparing simulation to experiment:** experiment uses SIMS, so simulation should also be “SIMSified”
- **Sentaurus** : no model for SIMS
- **Gautier** : described linear model for SIMS artifact
- **post-processing:** convolutions implemented with S-Visual



SURFACE AND INTERFACE ANALYSIS, VOL. 24, 733-745 (1996)

Deconvolution of SIMS Depth Profiles of Boron in Silicon

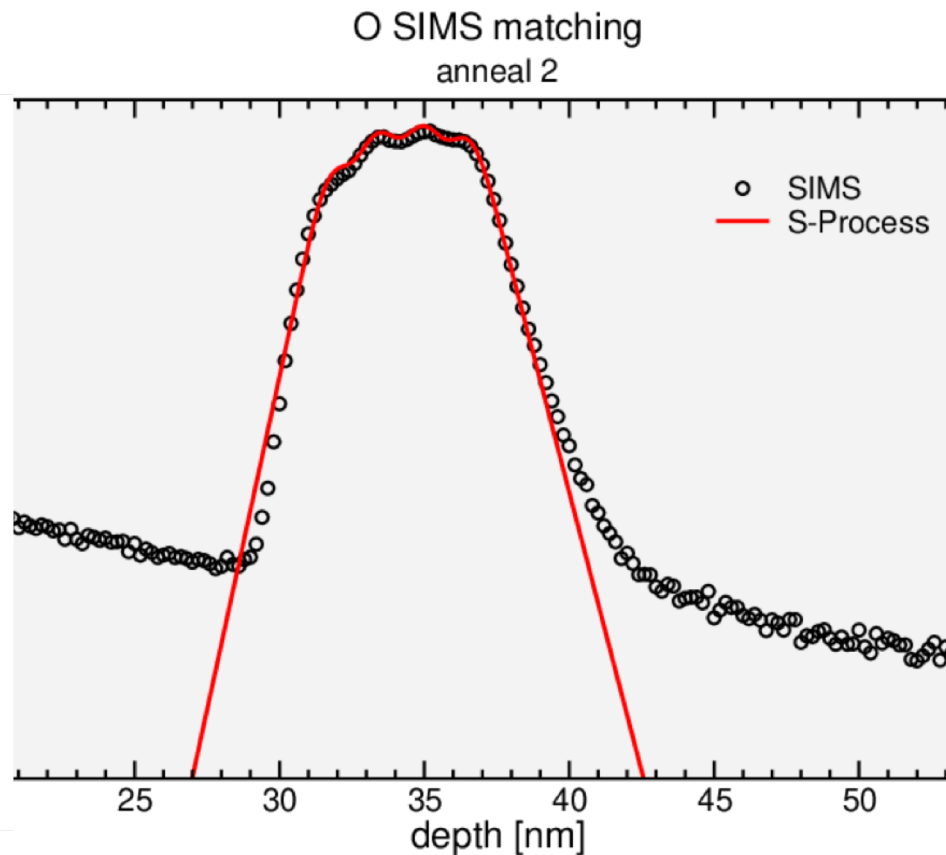
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- Gautier (1996): represent SIMS effect as convolutions
- Convolution 1: normal Gaussian with standard deviation σ , peak $(2\pi\sigma^2)^{-1/2}$
- Convolution 2: unit two-sided exponential with λ_1 , λ_2 , peak $(\lambda_1 + \lambda_2)^{-1}$

Oxygen SIMS modeling

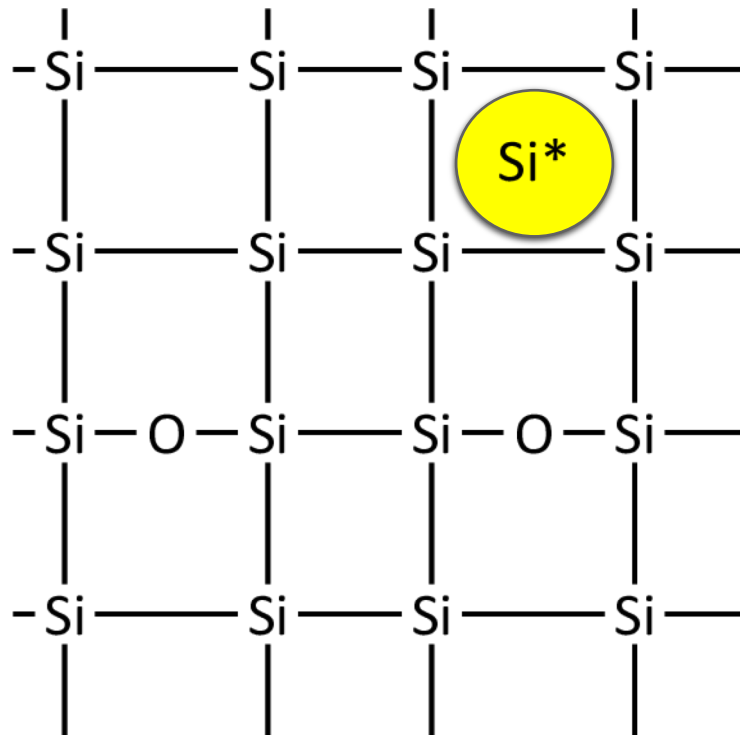


Wed Jan 16 11:07:54 2019

- **SIMS**: combination of free and interface oxygen
- **model**: trapped oxygen @ interface, plus free oxygen
- **Gautier convolution kernel** matches experimental peak.
- **free oxygen** to match remaining profile

Process Mechanisms

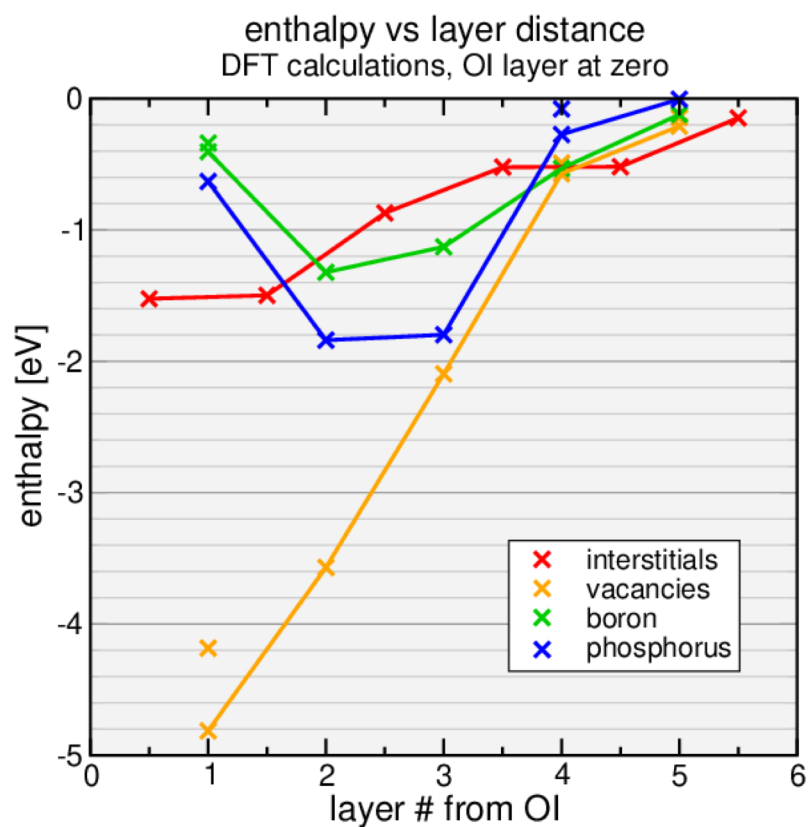
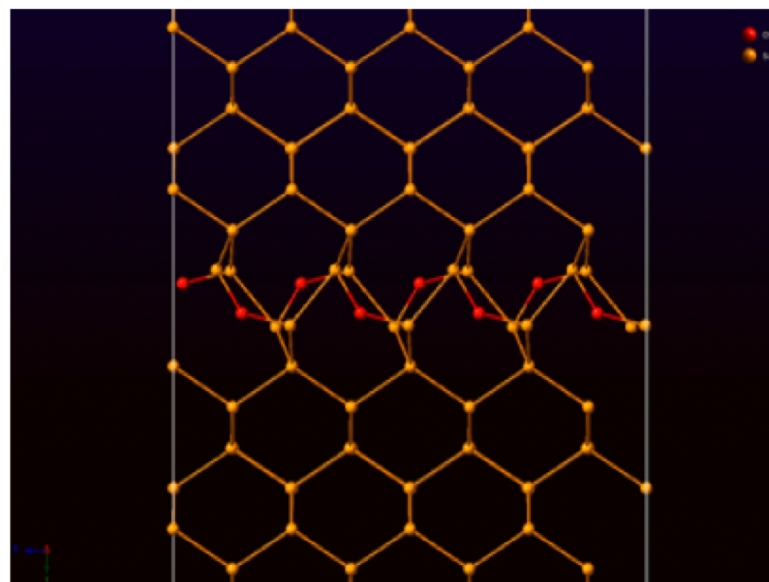
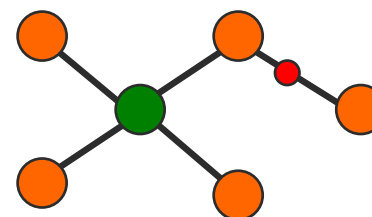
Interstitial Trapping



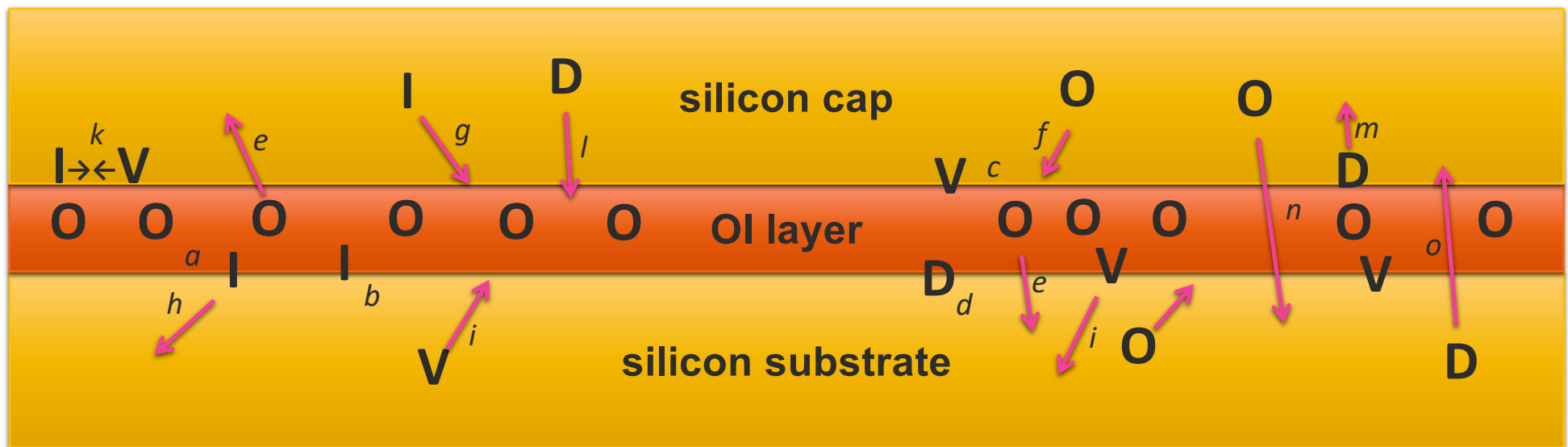
cartoon sketch: vertical

- **perpendicular** to OI plane.
- **lattice distortion** out-of-plane
- **Local tensile strain:** gaps for Si interstitials.
- **Local compressive strain:** stress relieve by Si vacancies.
- **Result:** point “trapped” by OI layers, then “recombine”.

Trapping: Density Functional Theory

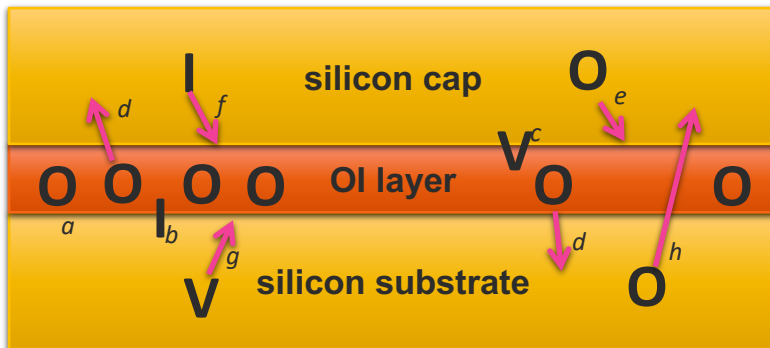


Process Mechanisms



- | | | |
|--------------------------|---------------------------|-----------------------|
| (a) trapped oxygen | (f) oxygen capture | (k) V-I recombination |
| (b) trapped interstitial | (g) interstitial capture | (l) dopant trapping |
| (c) trapped vacancy | (h) interstitial emission | (m) dopant emission |
| (d) trapped dopant | (i) vacancy capture | (n) oxygen diffusion |
| (e) oxygen emission | (j) vacancy emission | (o) dopant diffusion |

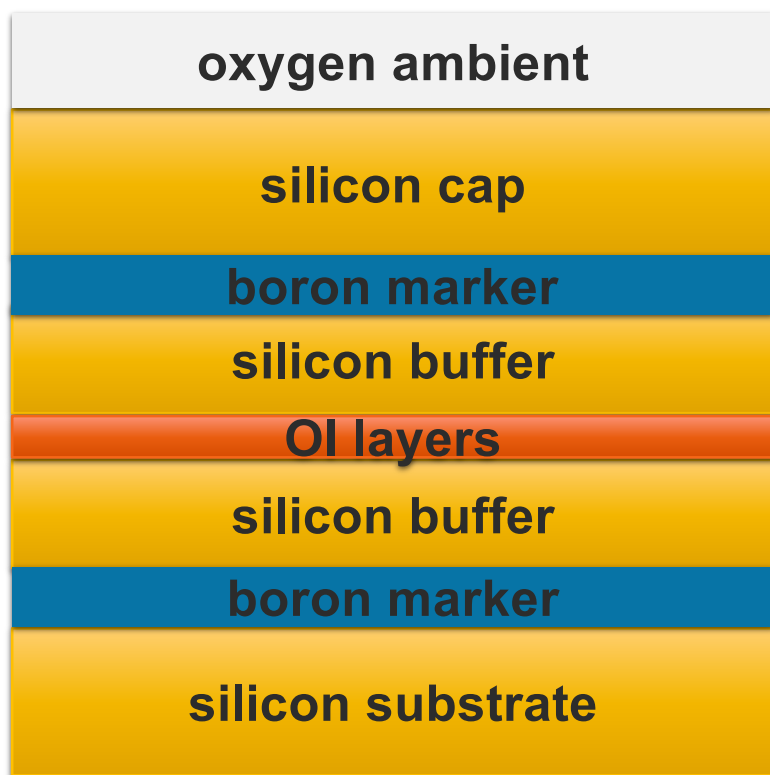
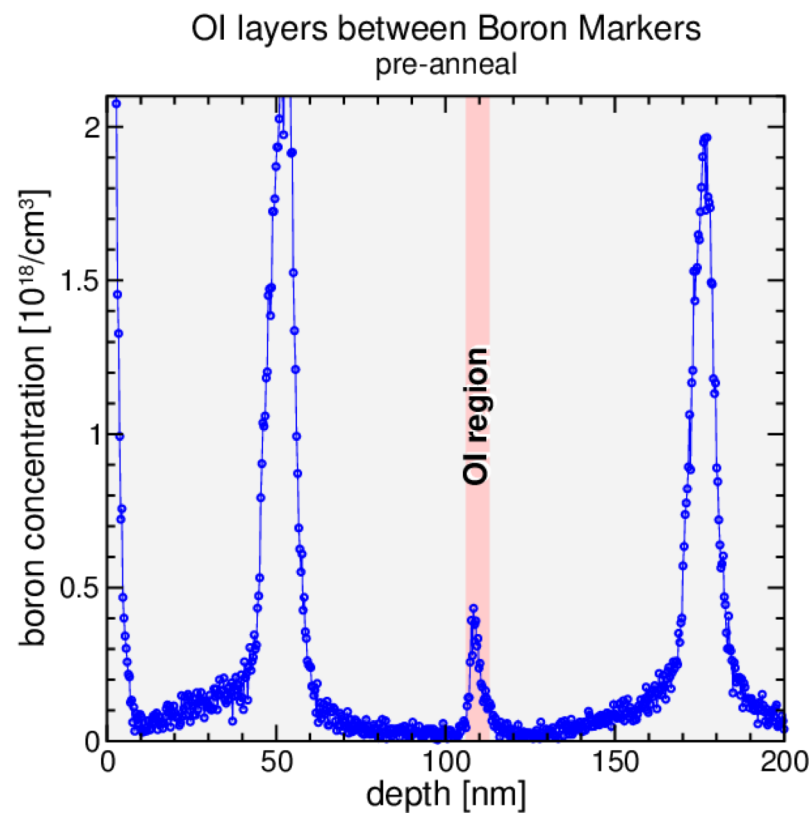
linear kinetic equations



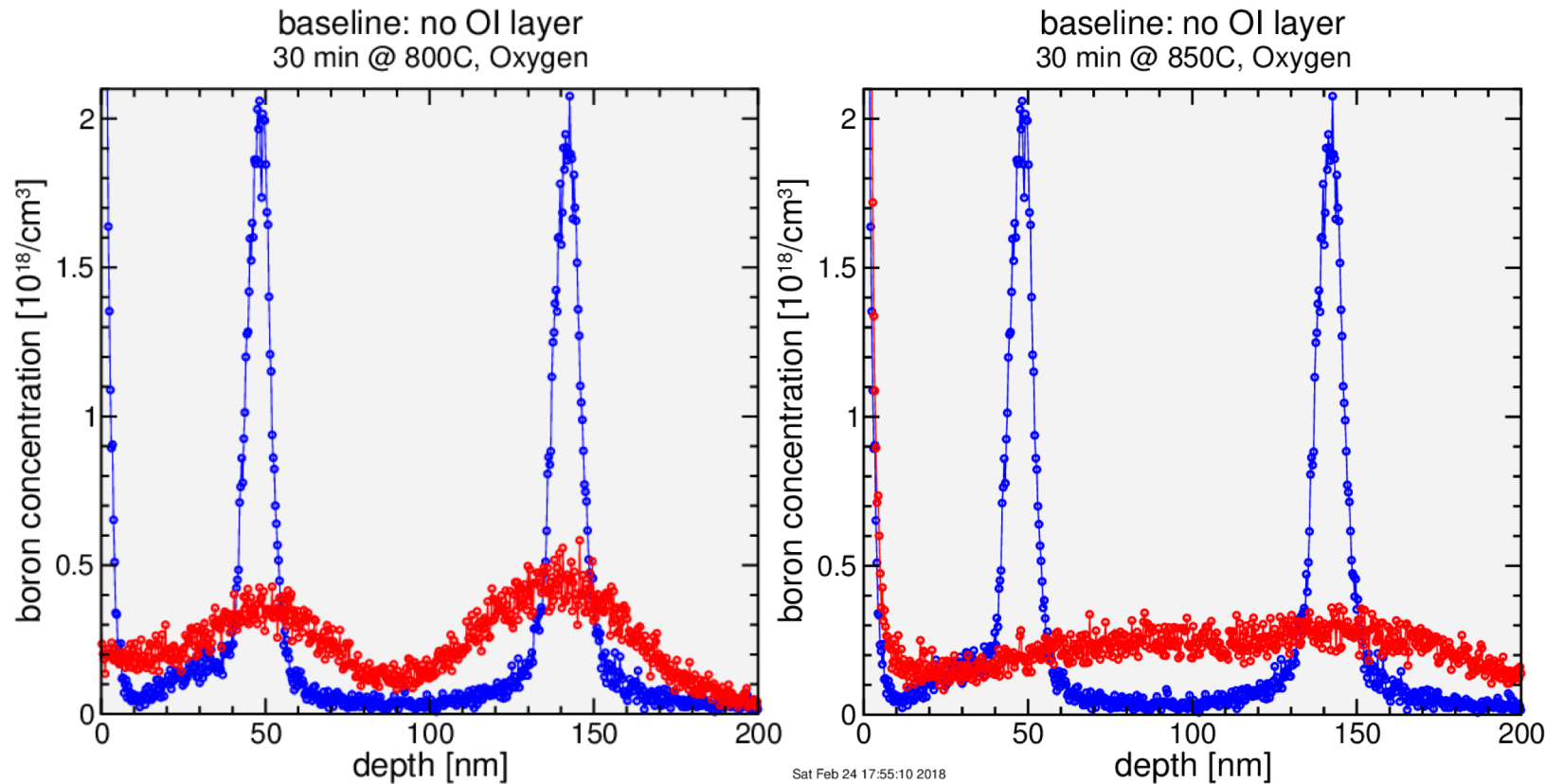
- **Interstitial trapping (f)**, from each side:
Trapping rate = $k_{\text{trapI}} O_{\text{trap}} I_{\text{free}}$
- **Vacancy trapping (g)**, from each side:
Trapping rate = $k_{\text{trapV}} O_{\text{trap}} V_{\text{free}}$
- **Oxygen trapping (e)**, from each side:
Trapping rate = $k_{\text{trapO}} O_{\text{trap}} O_{\text{free}}$
- **Oxygen emission (d)**, to each side:
Emission rate = $k_{\text{emitO}} O_{\text{trap}} / 2$
- **activation energy**: oxygen same,
point defects zero
- **oxygen diffusion** retarded proportional to OI oxygen
 $\Delta O_{\text{free}} = k_{\text{diffO}} O_{\text{trap}} D_{\text{O}} \nabla O_{\text{free}}$

Model Calibration

MST Boron Marker Experiments



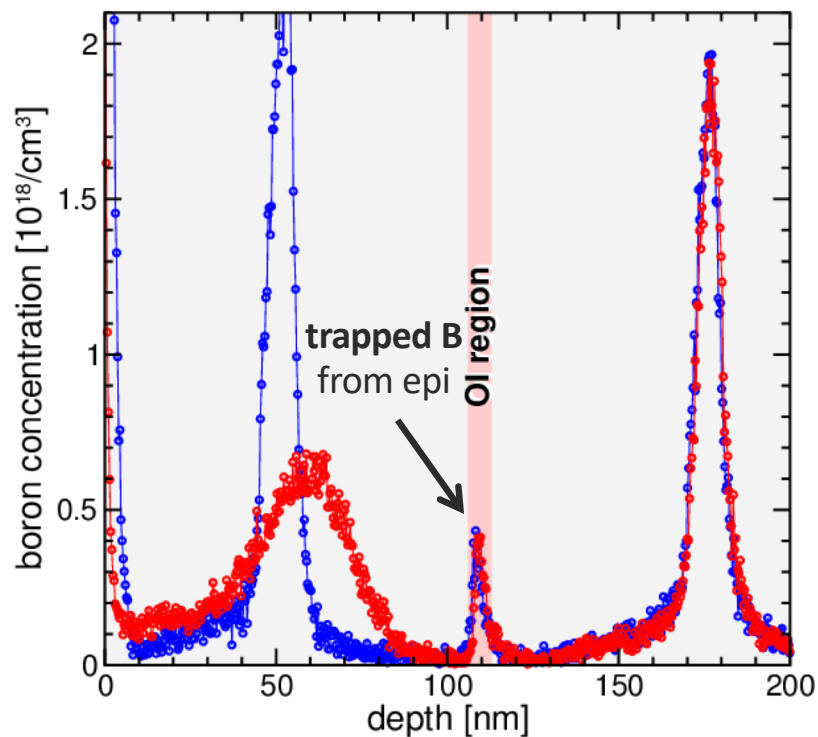
Control no MST/ OI: Boron Oxygen-Enhanced-Diffusion



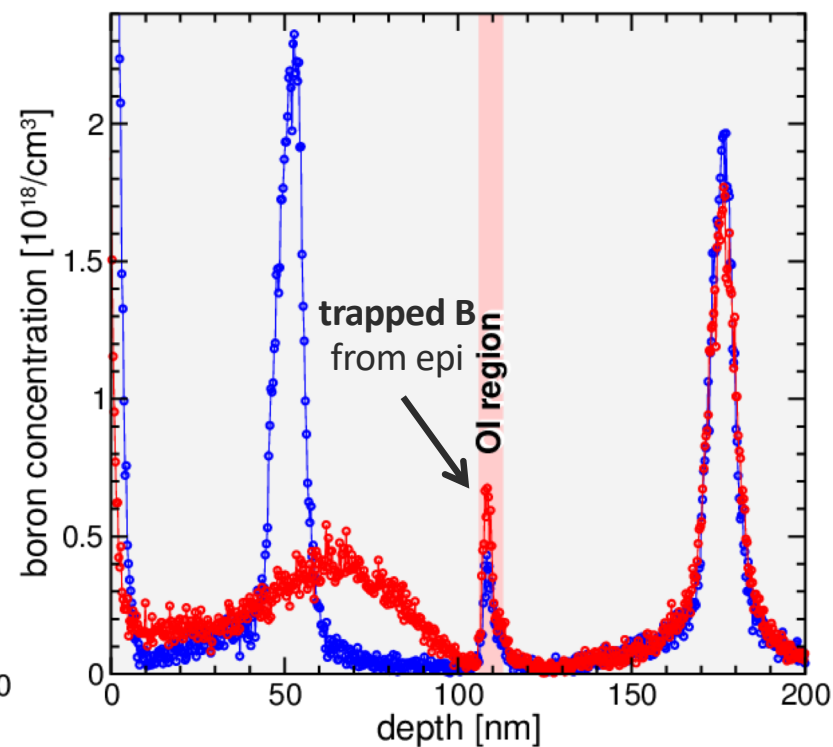
- **both peaks diffuse:**
interstitials reach both markers.
- **850C anneal:**
peaks merge.

With MST OI layers: OED suppression

OI layers between Boron Markers
30 min @ 800C, Oxygen

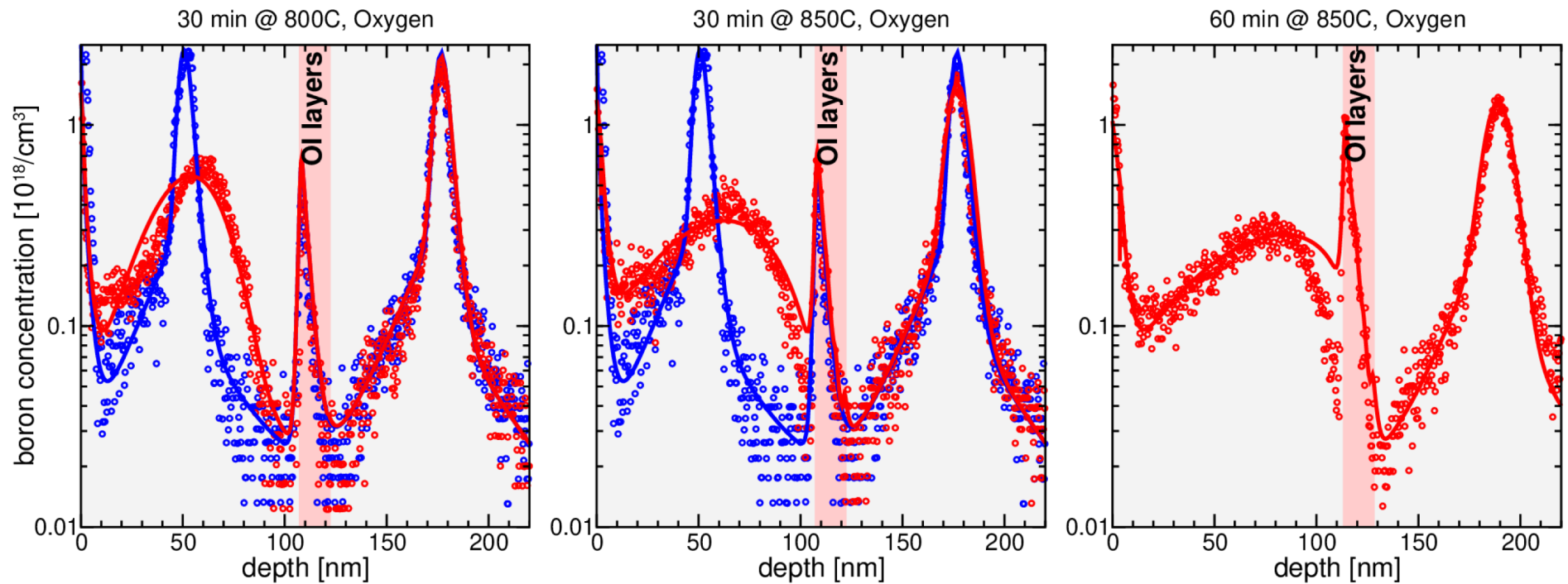


OI layers between Boron Markers
30 min @ 850C, Oxygen



- **Surface peak:** oxidation-enhanced diffusion (OED).
- **Buried peak:** very little diffusion.
- **Central peak:** boron was unintentionally trapped in OI during deposition.

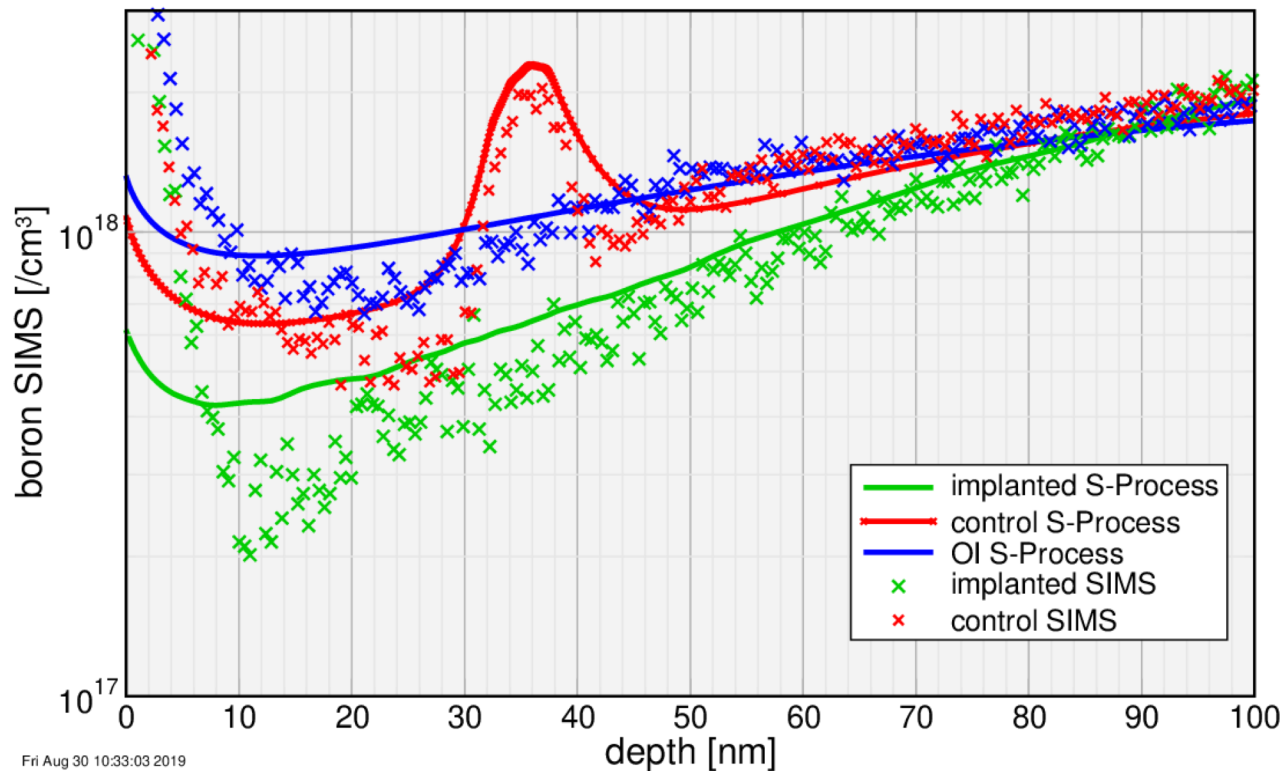
MST OI layer modeling



Modeling Boron Implantation Experiment

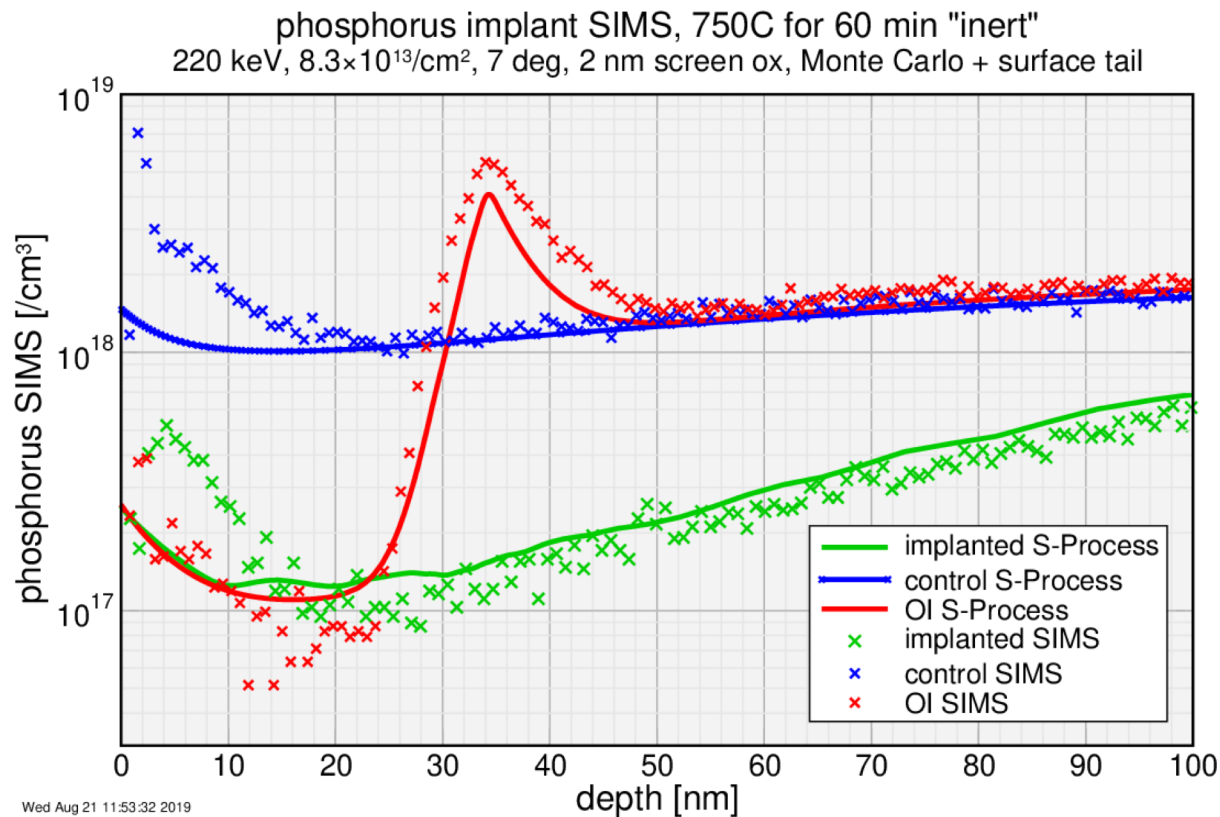


boron implant SIMS, 950C for 10 min "inert"
120 keV, $8.3 \times 10^{13}/\text{cm}^2$, 7 deg, 2 nm screen ox, Monte Carlo + surface tail



- epitaxy followed by implant then anneal
- interstitial trapping reduced relative to marker experiment
- demonstrates boron trapping in addition to interstitial trapping
- insensitive to vacancy trapping

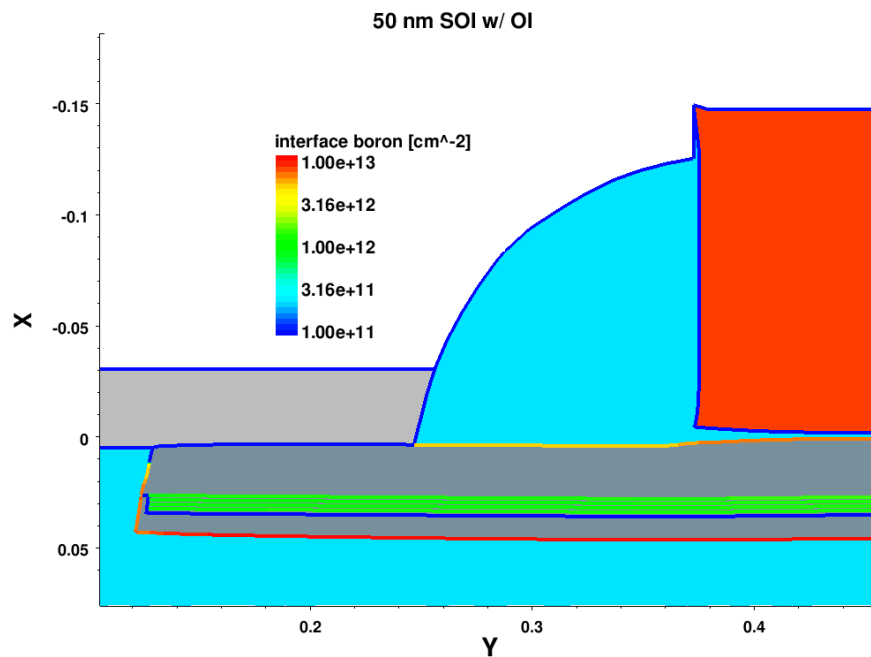
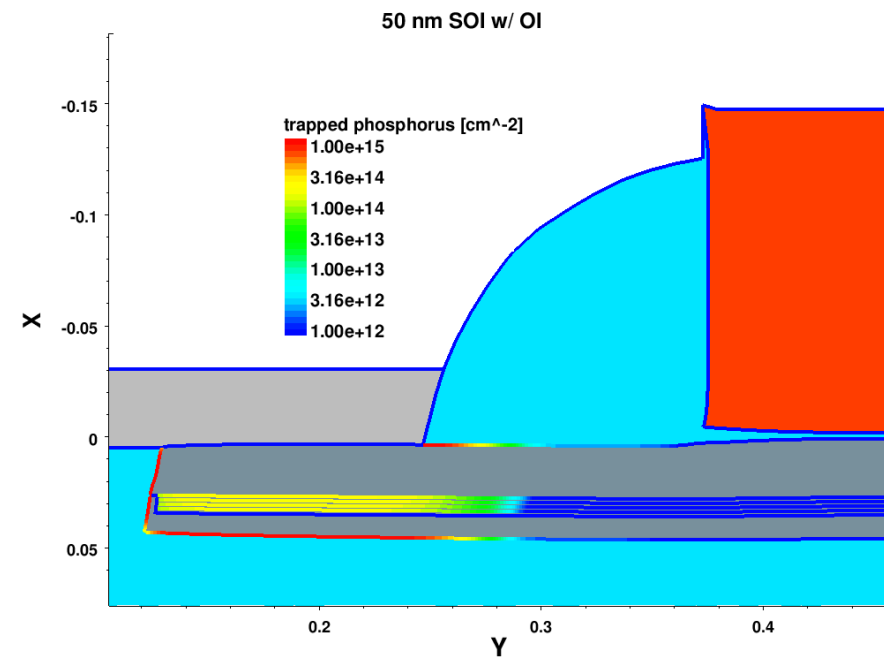
Modeling Phosphorus Implantation Experiment



- epitaxy followed by implant then anneal
- interstitial trapping reduced relative to marker experiment
- demonstrates boron trapping in addition to interstitial trapping
- insensitive to vacancy trapping

CMOS application

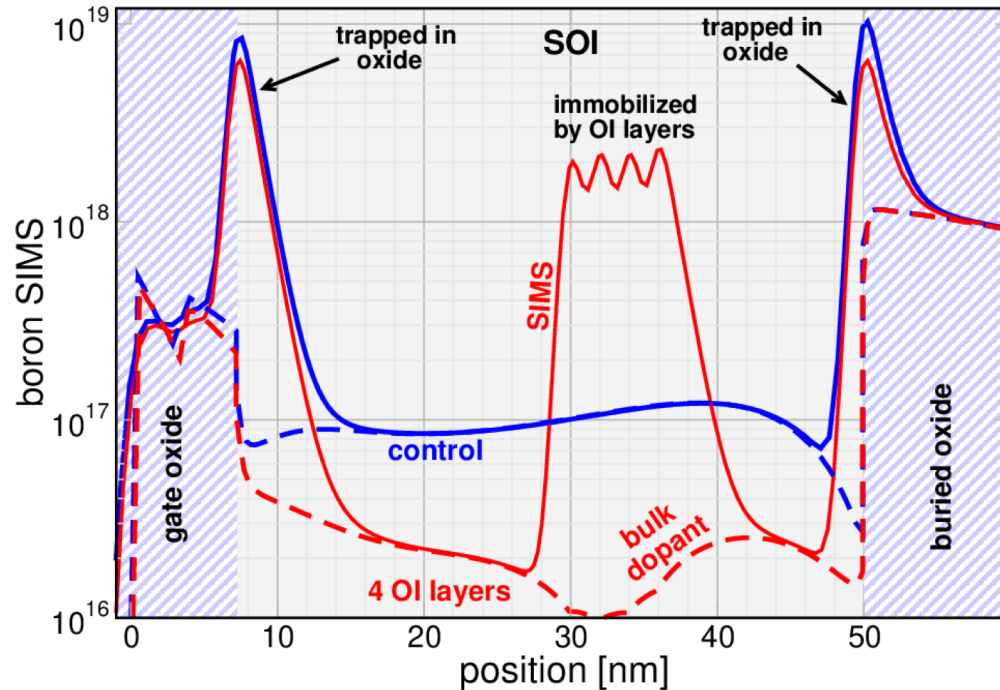
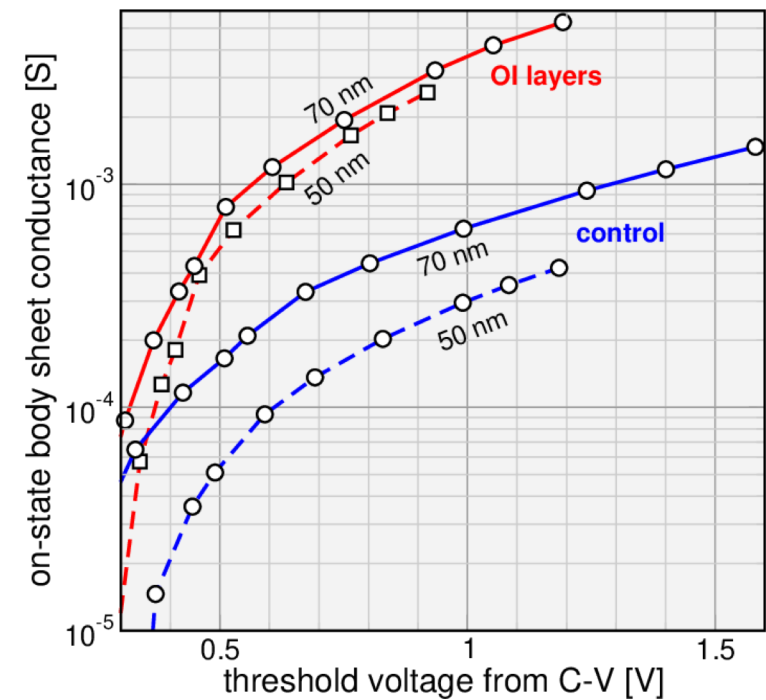
PDSOI application



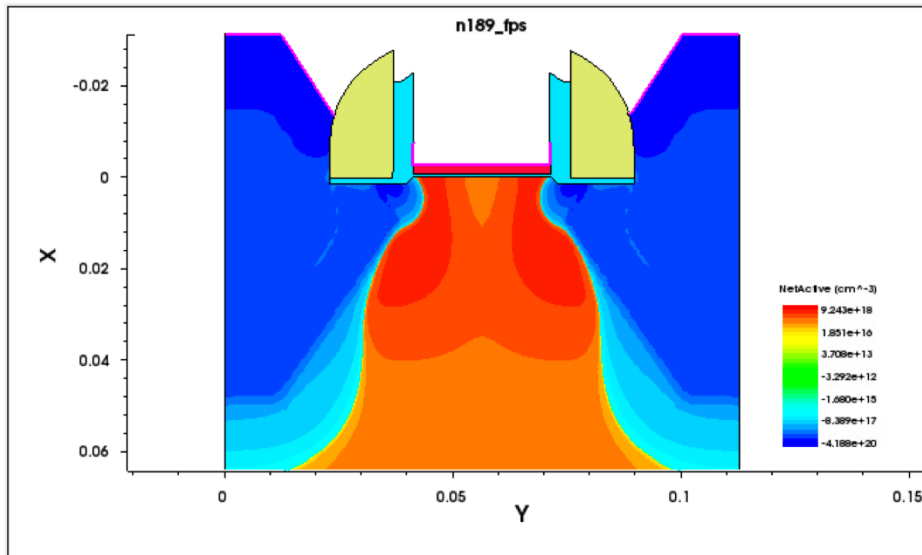
50 nm PDSOI w/ MST OI layers: trapped boron and phosphorus

PDSOI: Long-channel cut

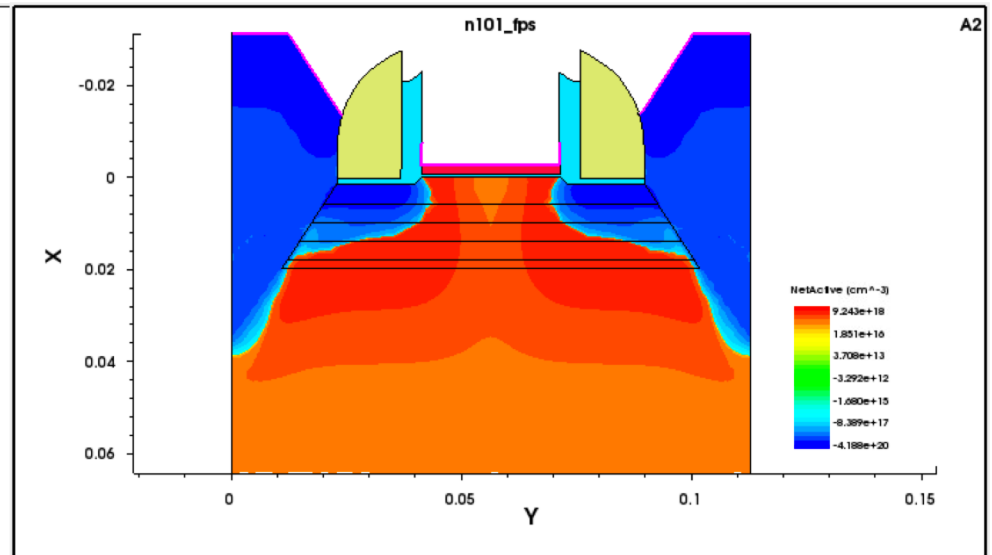
simulated SOI boron profiles
50 nm SOI, 30 nm cap



35 nm CMOS application



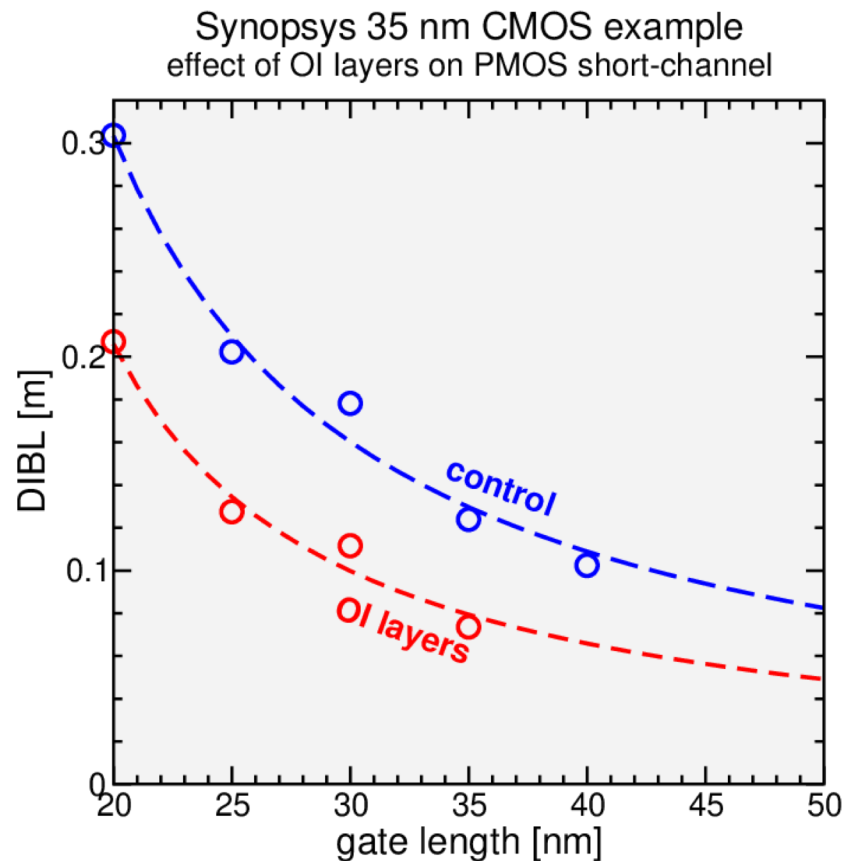
control case



w/ MST OI layers

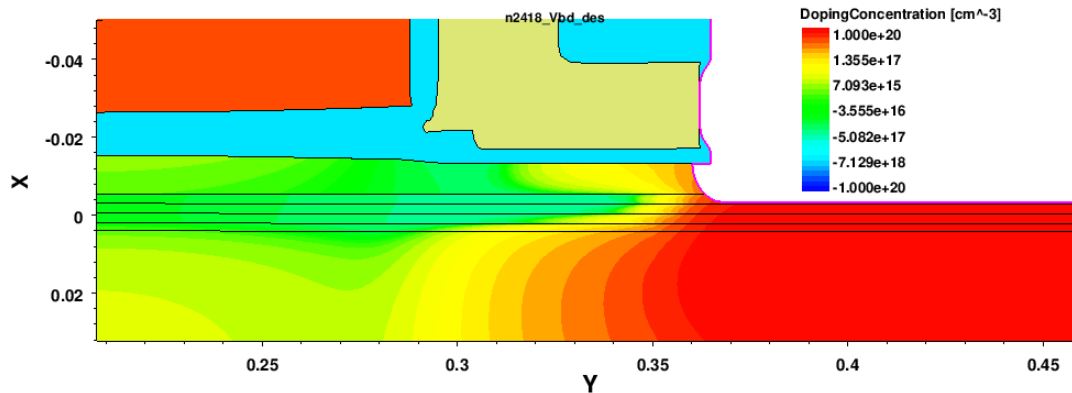
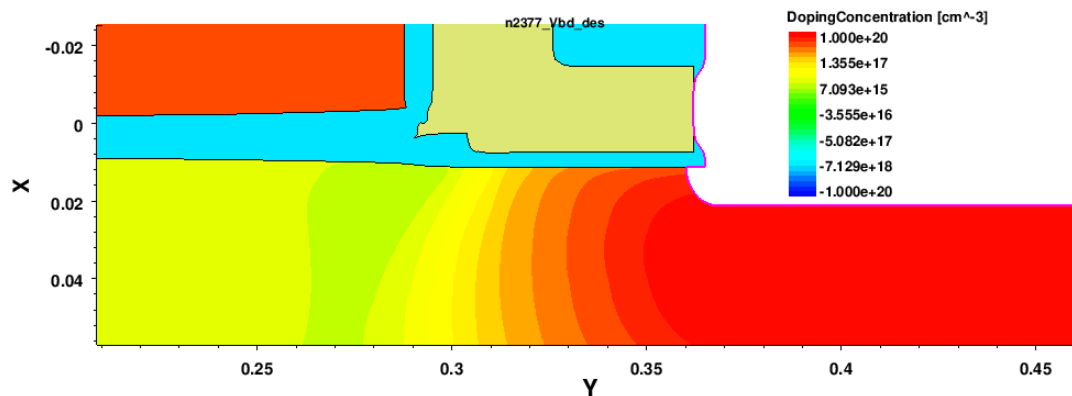
- gate oxidation, polysilicon oxidation changed from deposited to grown
- interstitial injection during polysilicon oxidation 10× (RSCE calibration)

35 nm CMOS: improved PFET short-channel



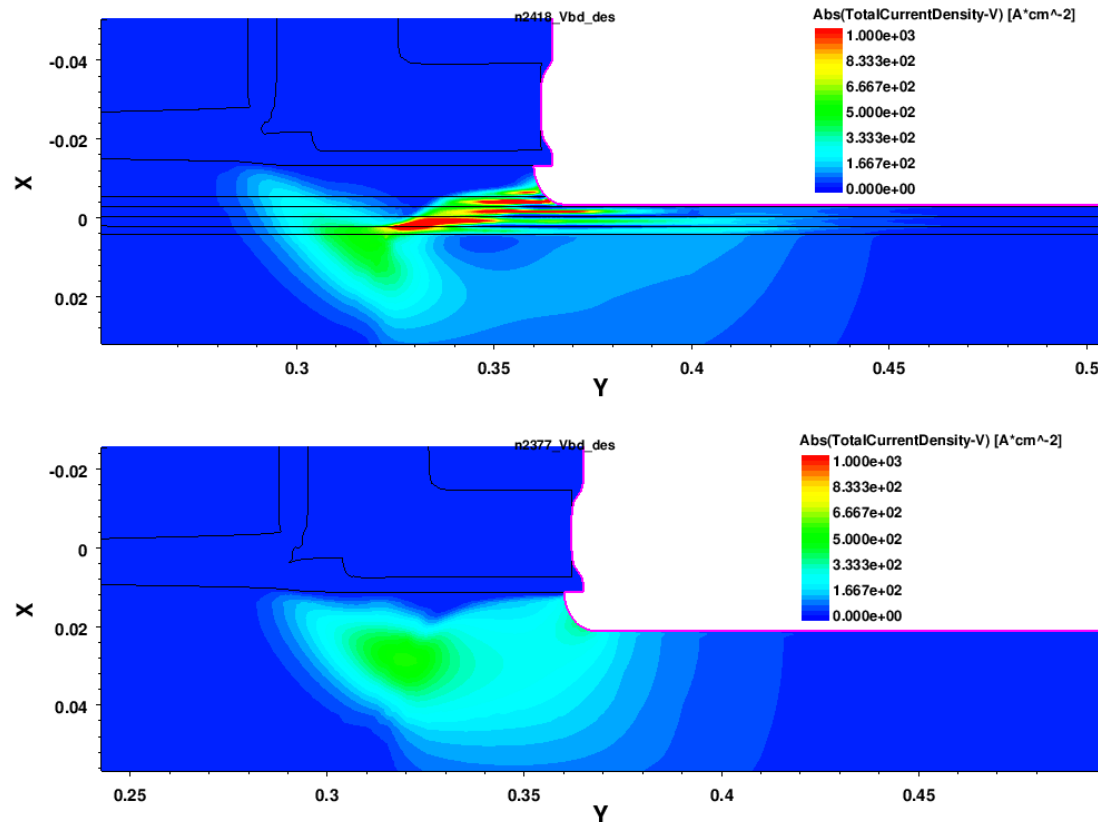
- trapped dopant modeled as surface charge
- S-Device simulation: δ -potential excluded
- reduced DIBL with MST OI layers
- boron diffusion retarded by interstitial trapping

5V NFET Breakdown: current contours



- MST layers move doping from the interface
- trapped dopant in the MST layer is not rendered here.

5V NFET Breakdown: current contours



- linear current scale
- At the breakdown condition (100 nA/ μm), current peak in MST structure is focused at MST layers.
- in control device, current peak is closer to surface.
- result: 1.2 V increase in V_{BDSS}

Summary

Summary



- MST OI layers are sheets of oxygen inserted into Si lattice
- process modeling with S-Process
- trap dopants, directly immobilizing them
- trap point defects, reducing dopant diffusion
- result: steeper surface doping profiles; anchoring of implant dopants
- application example: doping control for improved CMOS scaling