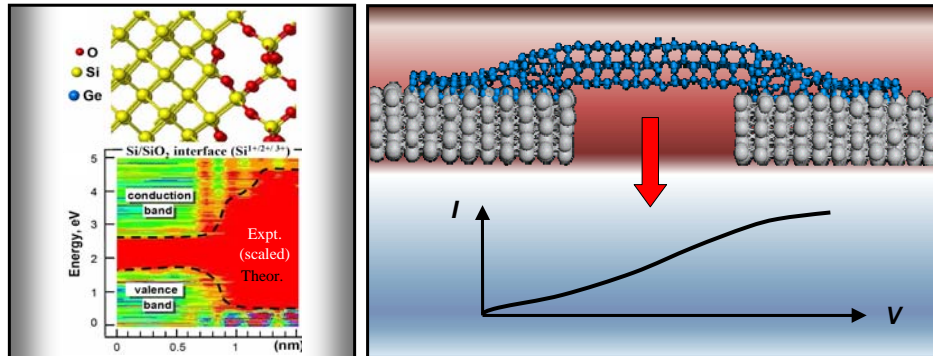




Ab-Initio Assisted Process and Device Simulation for Nanoelectronic Devices



Wolfgang Windl

Materials Science and Engineering
The Ohio State University, Columbus, OH, USA

← Computational Materials Science and Engineering →



Acknowledgments

- Tao Liang, Dipanjan Sen, Karthik Ravichandran, Weiqi Luo (OSU)
- Peter Pichler, Christian Steen, Alberto Martinez-Limia (Fraunhofer IISB)
- Benjamin Liu, Leonardo Fonseca, Roland Stumpf (Motorola)
- Gerd Duscher, Nathan Stoddard, Sergei Lopatin (NCSU)

Funding:

- Fraunhofer-Bessel Fellowship, Fraunhofer Society and Humboldt Foundation
- SRC, NSF-EU, NASA-Glenn
- Ohio Supercomputer Center

← Computational Materials Science and Engineering →



Semiconductor Devices – MOSFET

Metal Oxide Semiconductor Field Effect Transistor

0 V_G $-V_D$

Insulator (SiO_2) Gate (Me) Spacer

Source P Channel N Drain P

Si

$-V_G$ $-V_D$

Gate I_D

Source P Drain P

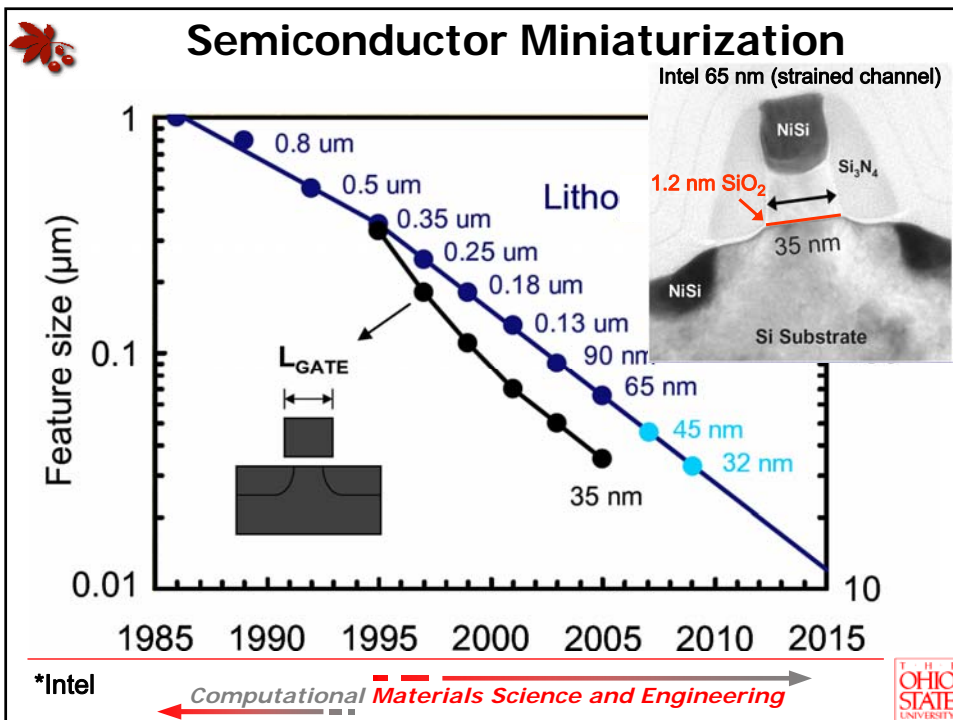
Si

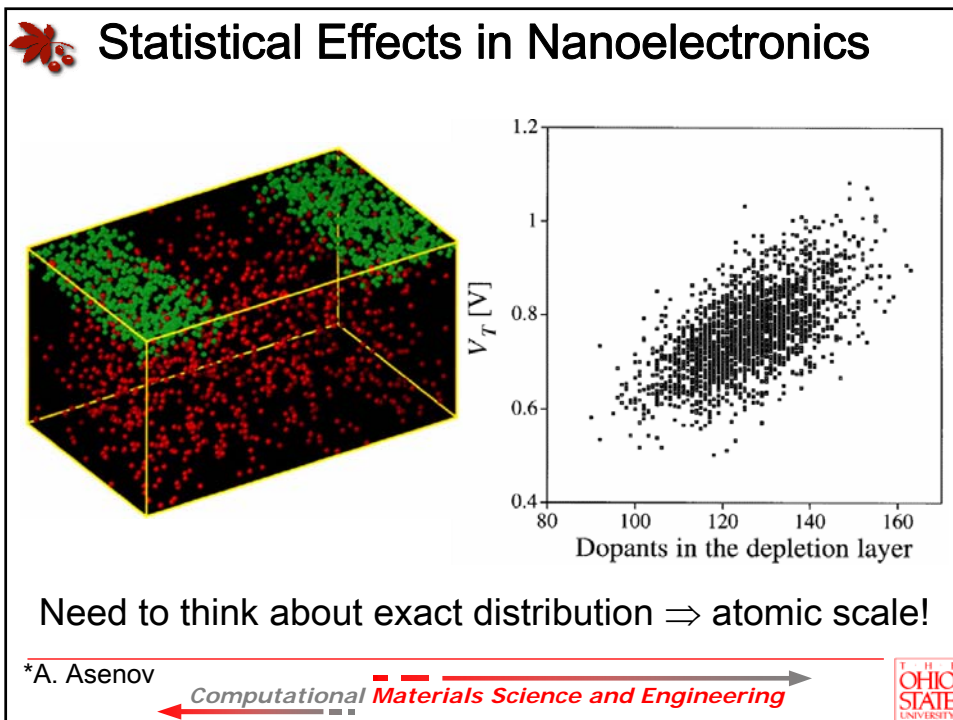
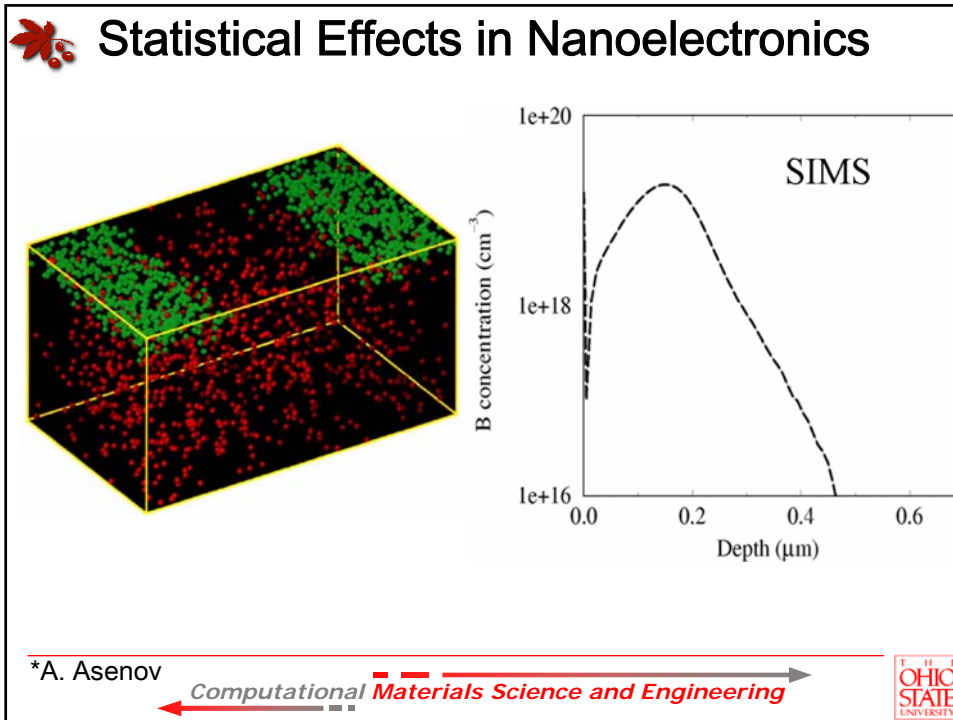
Doping:
 N: e⁻, e.g. As (Donor) P: holes, e.g. B (Acceptor)

- Analog: Amplification
- Digital: Logic gates

Computational

Materials Science and Engineering







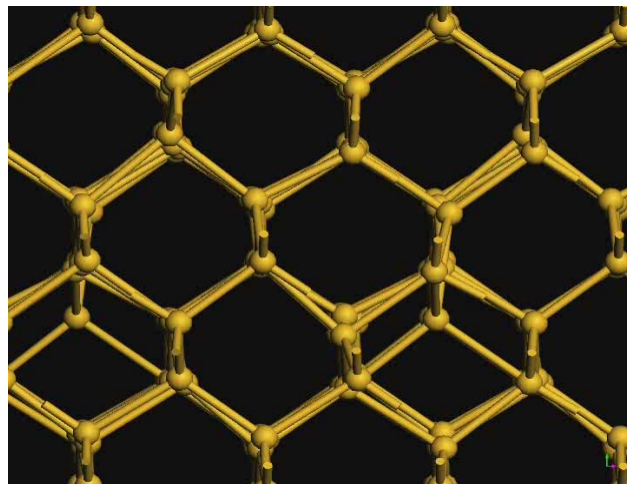
Role of Ab-Initio Methods on Nanoscale

1. Improving traditional process modeling to include nanoscale (atomic-scale) effects
2. Nanoscale characterization
= *Combination* of experiment & ab-initio calculations
3. Atomic-level process + transport modeling
= structure-property relationship

← Computational Materials Science and Engineering →



Ab-Initio MD: Si-Interstitial



1200 K
GGA
65 atoms

← Computational Materials Science and Engineering →



“Moore’s MD Law”

- Direct simulation of kinetics: Molecular Dynamics
- Infrequent event system: often times > ms between events
- Problem:
 - MD often does not get to relevant time scales

Accessible simulated time*

* 1-week simulation of 1000-atom metal system, EAM potential

Transition State Theory (TST)

TST escape rate = **equilibrium flux** through **dividing surface** at $x = q$

$$r_{A \rightarrow B}^{TST} = \langle \delta(x - q) | \dot{x} \rangle \quad (\text{exact flux})$$

$r_{A \rightarrow B}^{HTST} = \nu_0 \exp(-\Delta E / k_B T)$

(harmonic approx.)

- classically exact rate if no recrossings or correlated events
- no dynamics required
- excellent approximation for materials diffusion
- can also exploit TST formalism to develop methods that do not require knowing in advance where the dividing surface is

How To Find Saddle Points

- **“Easy”**: Can guess final state & diffusion path (e.g. vacancy diffusion)

$\Delta E \sim 0.4 \text{ eV}$

Energy

ΔE

- Reliable search for diffusion path: **“Nudged elastic band method”** (Jónsson *et al.*). Used in this work.
- Less reliable search for diffusion path: **“By hand”**, **“drag”** methods etc. Extensive use in the past.

- **“Difficult”**: Final state unknown (e.g. I_1 cluster decay) \Rightarrow MD, dimer

Bridging the Length Scales: Ab-Initio to Continuum

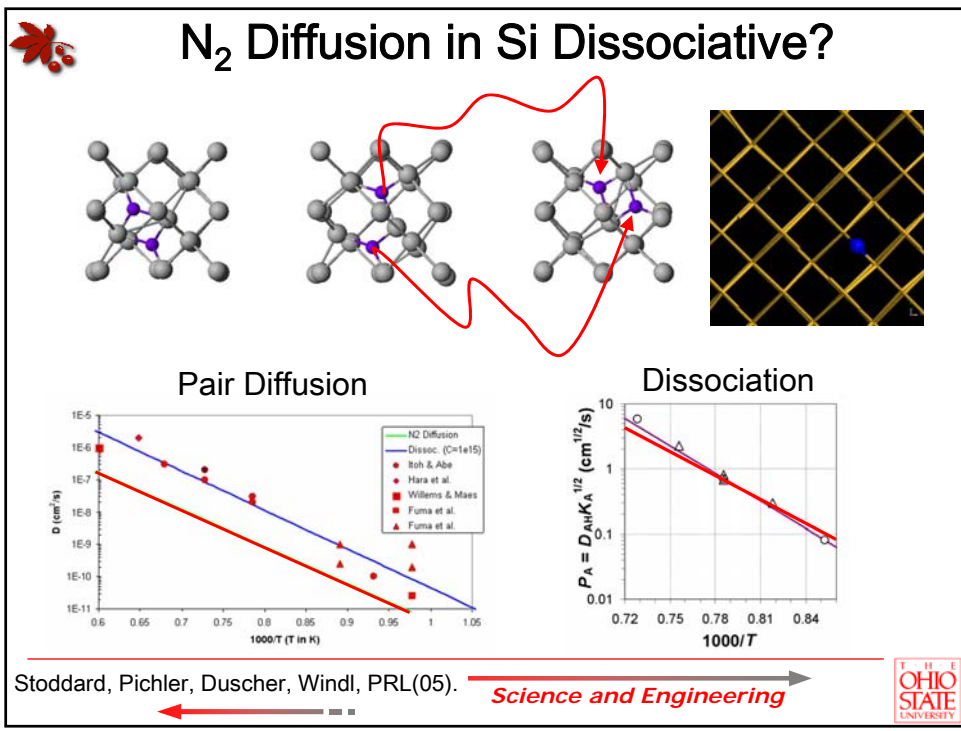
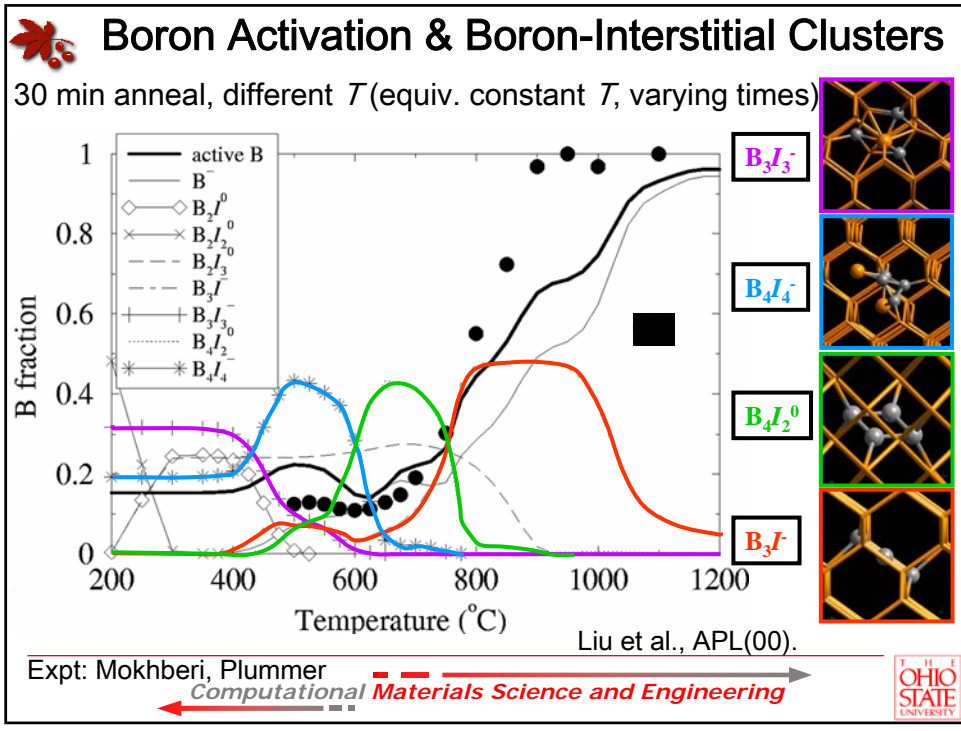
$$\frac{dC_I}{dt} = \nabla \cdot (D_I \nabla C_I) - 2K_{I_2}^f C_I^2 + 2K_{I_2}^r C_{I_2} + \dots$$

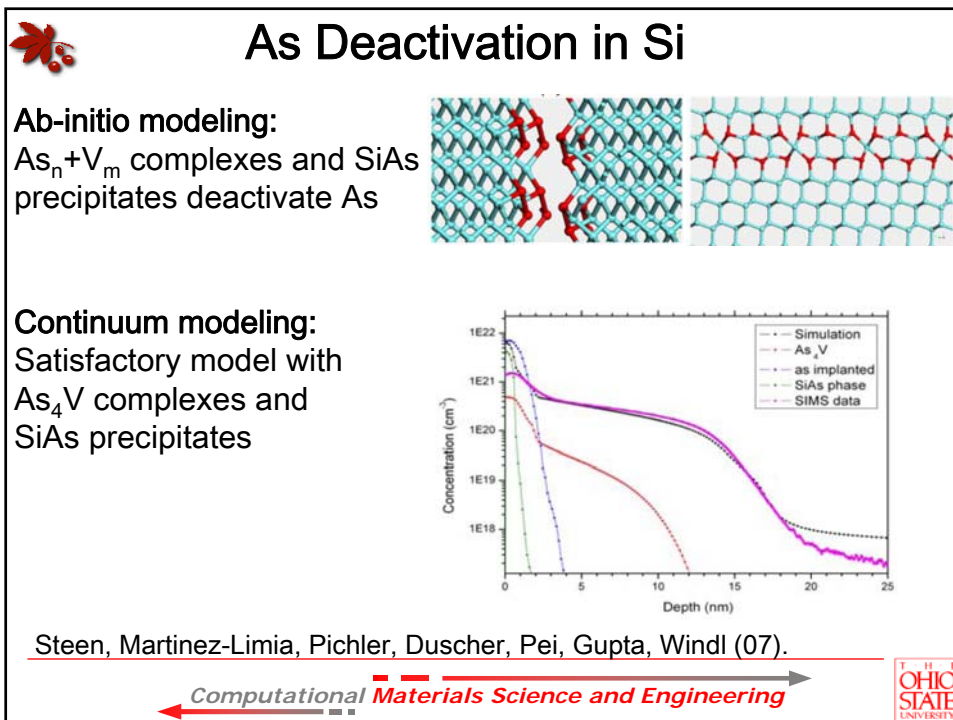
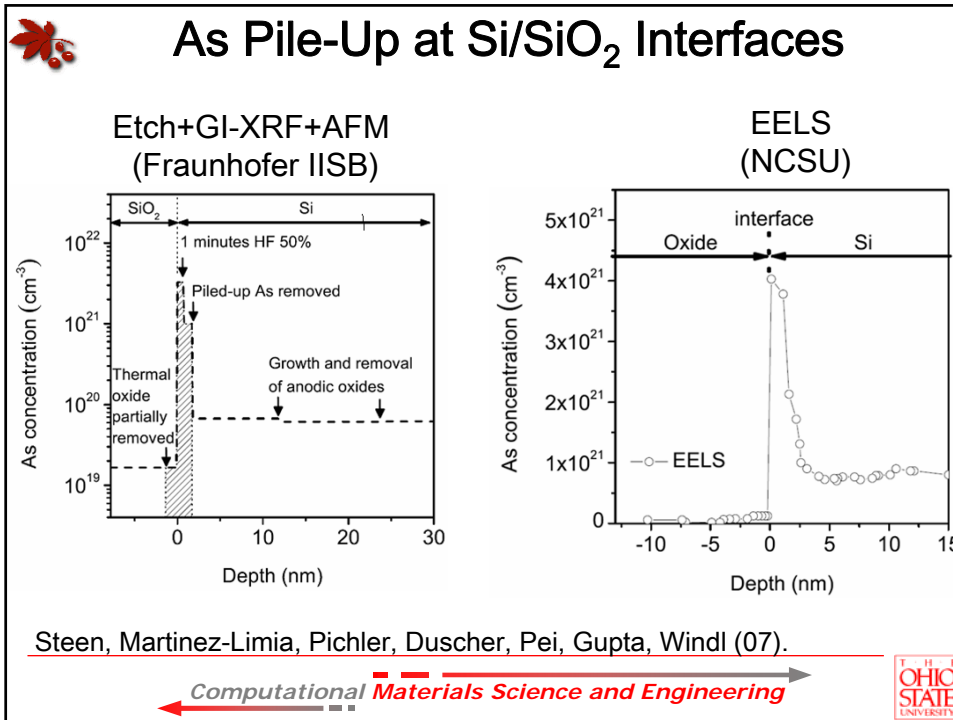
$$D_I = D_I^0 \exp(-E_a / kT)$$

$$K_{I_2}^r \propto D_I a_{I_2} \exp(-E_b^{I_2} / kT)$$

Need to calculate:

- Diffusion prefactors [Stoddard *et al.*, PRL (05)]
- Migration barriers [Windl *et al.*, PRL (99)]
- Binding energies [Liu *et al.*, APL (00)]
- Capture radii [Beardmore *et al.*, Proc. ICCN (02)]

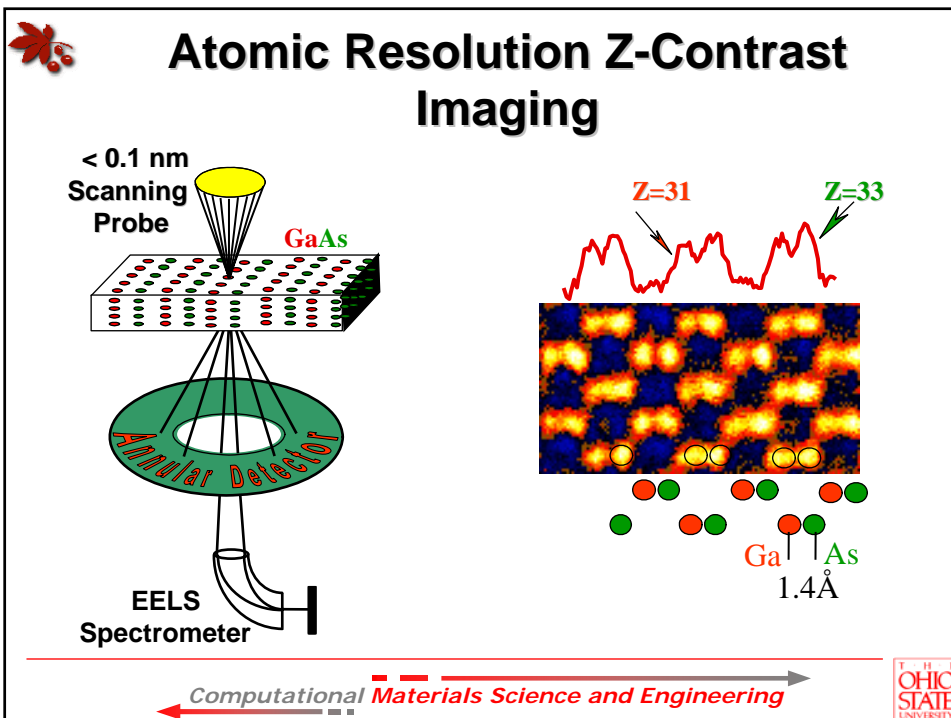


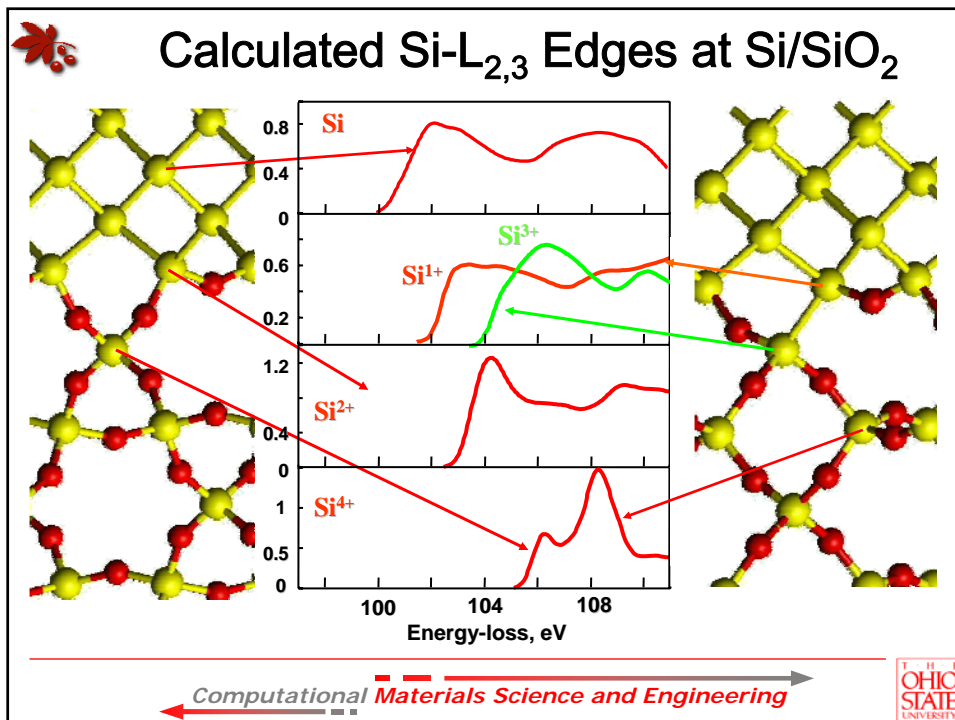
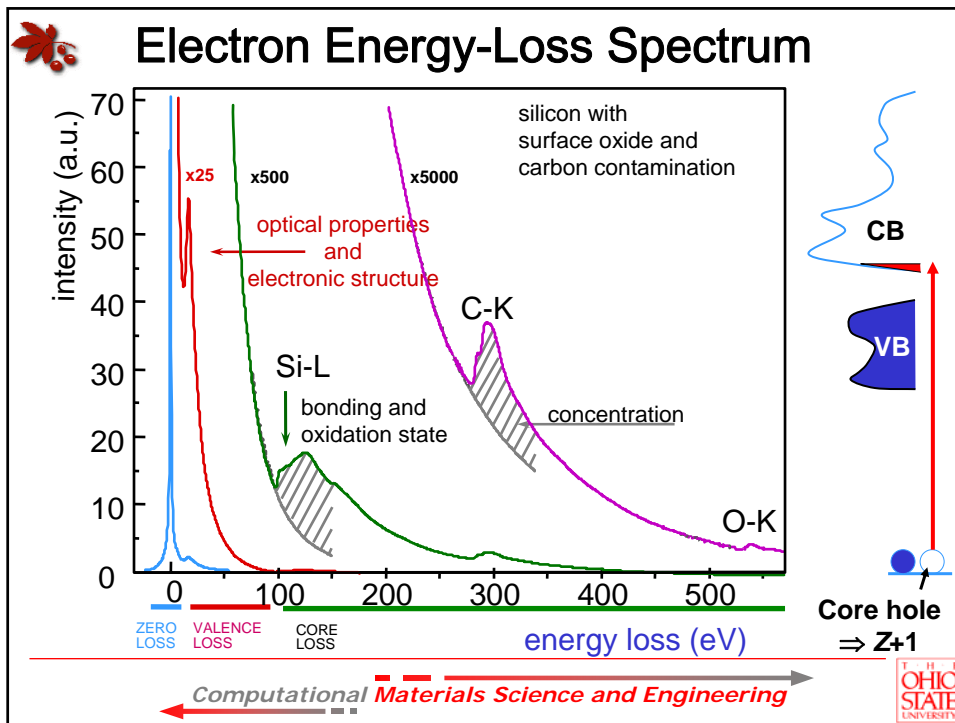


2. The Nanoscale Characterization Problem

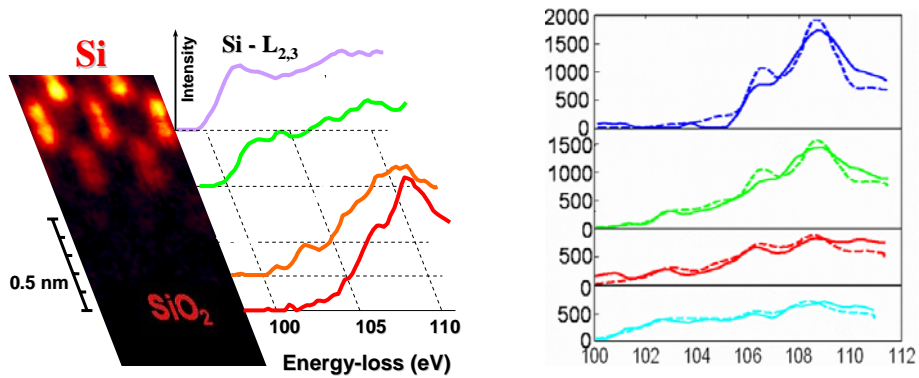
- Traditional characterization techniques, e.g.:
 - SIMS (*average* dopant distribution)
 - TEM (interface quality; *atomic-column* information)
- Missing: “Single-atom” information
 - Exact interface (contact) structure (previous; next)
 - Atom-by-atom dopant distribution (strong V_T shifts)
- Our approach: atomic-scale characterization (TEM) **plus** modeling

Computational **Materials Science and Engineering**





Combining Theory and Experiment



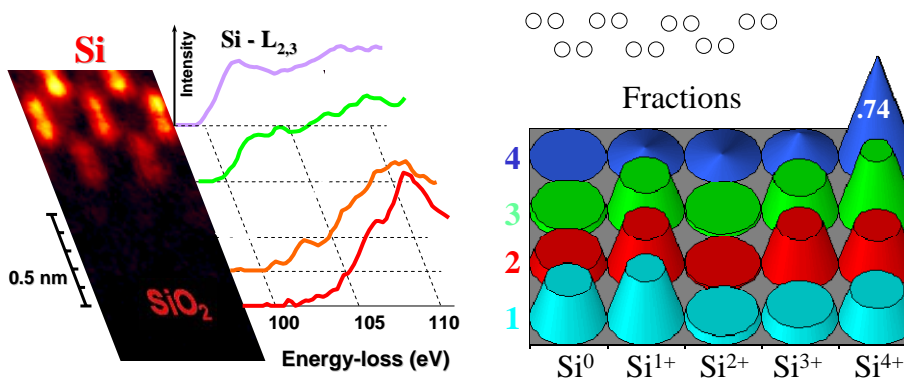
- Linear combination of different single-atom spectra
- Fit to EELS spectra line scans
- ⇒ “Measure” amorphous interface structure

← Computational Materials Science and Engineering →



Combining Theory and Experiment

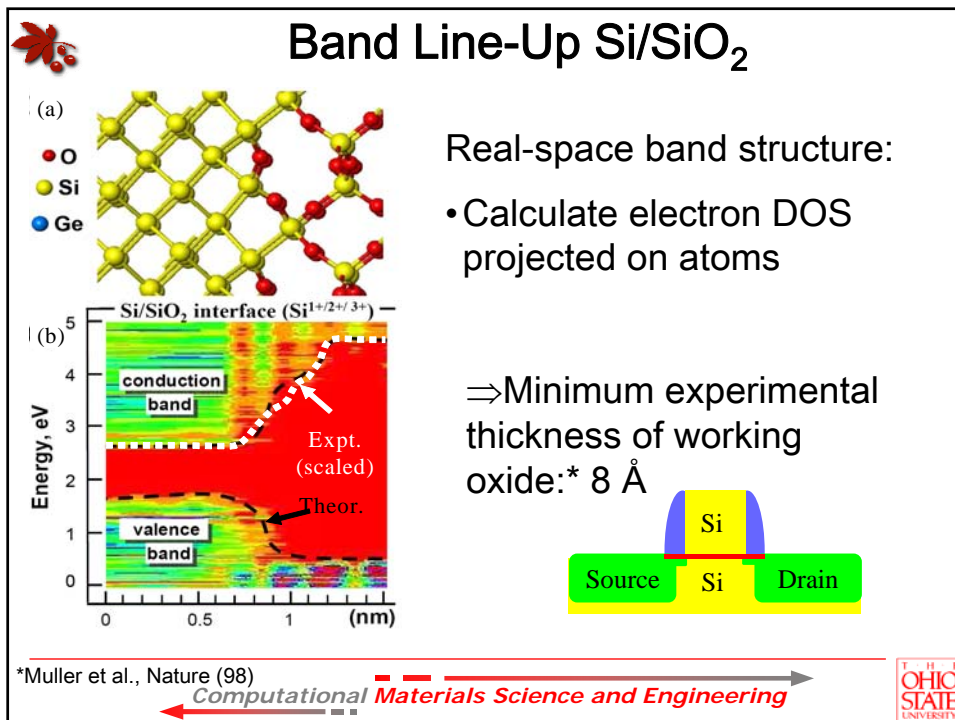
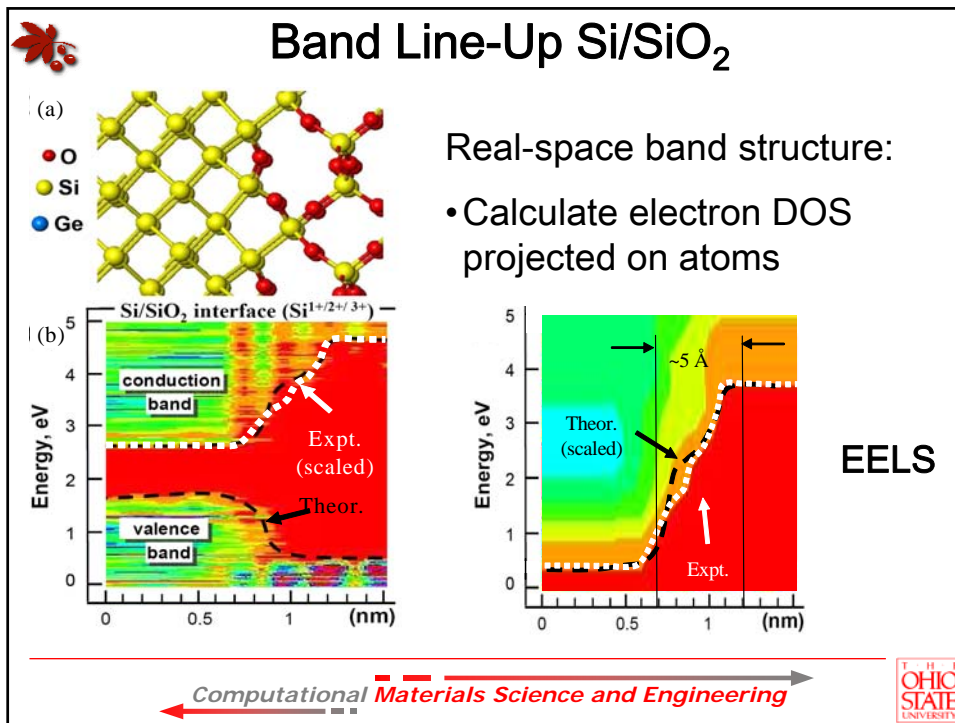
Calculation of EELS Spectra from Band Structure

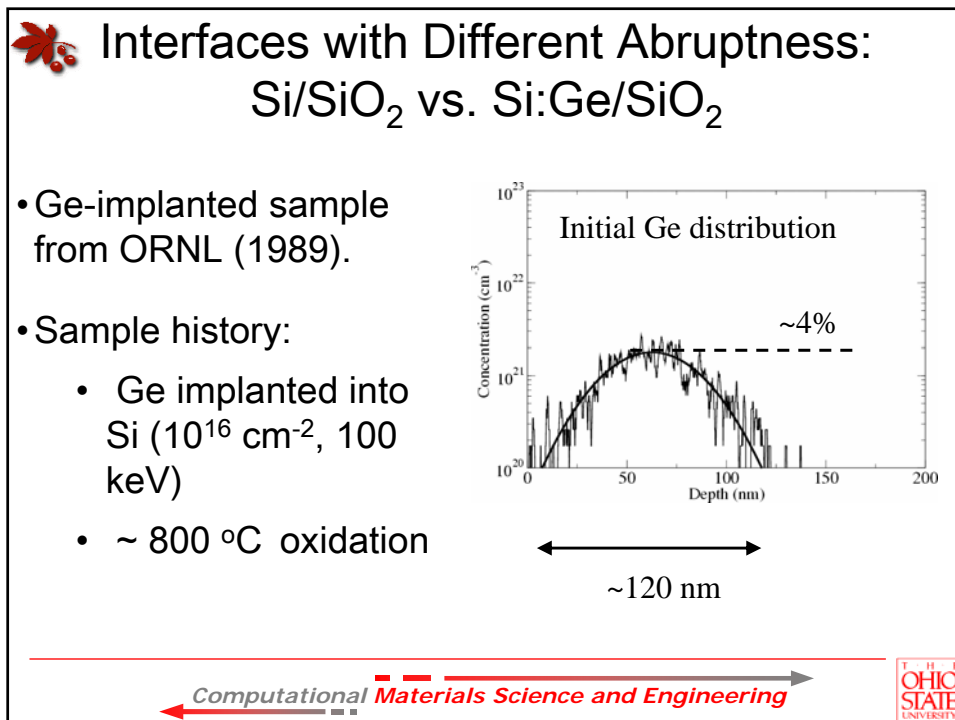
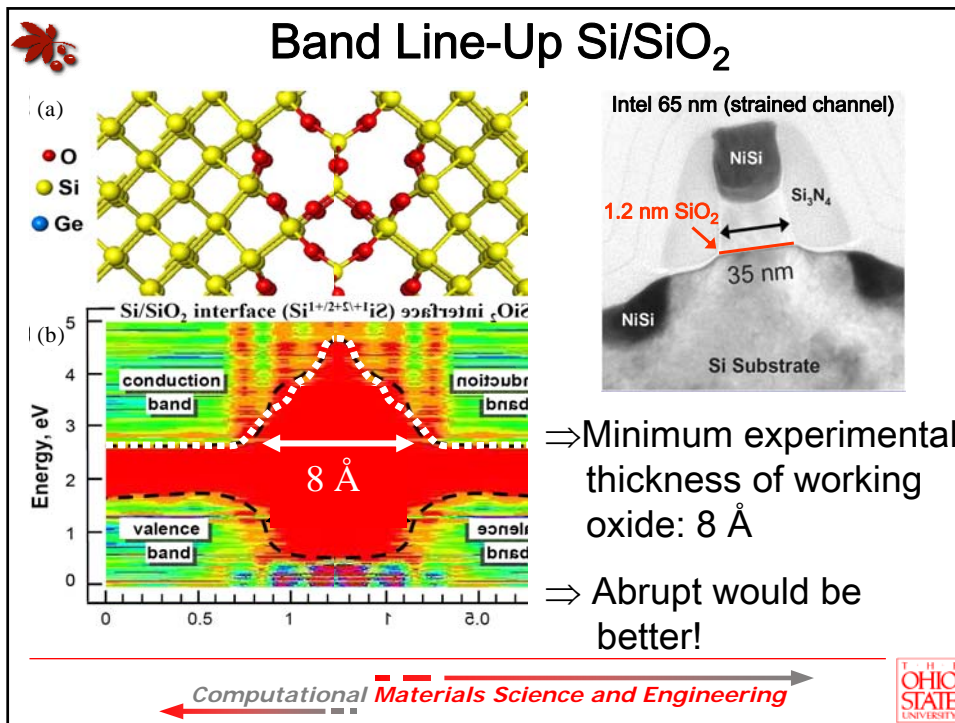


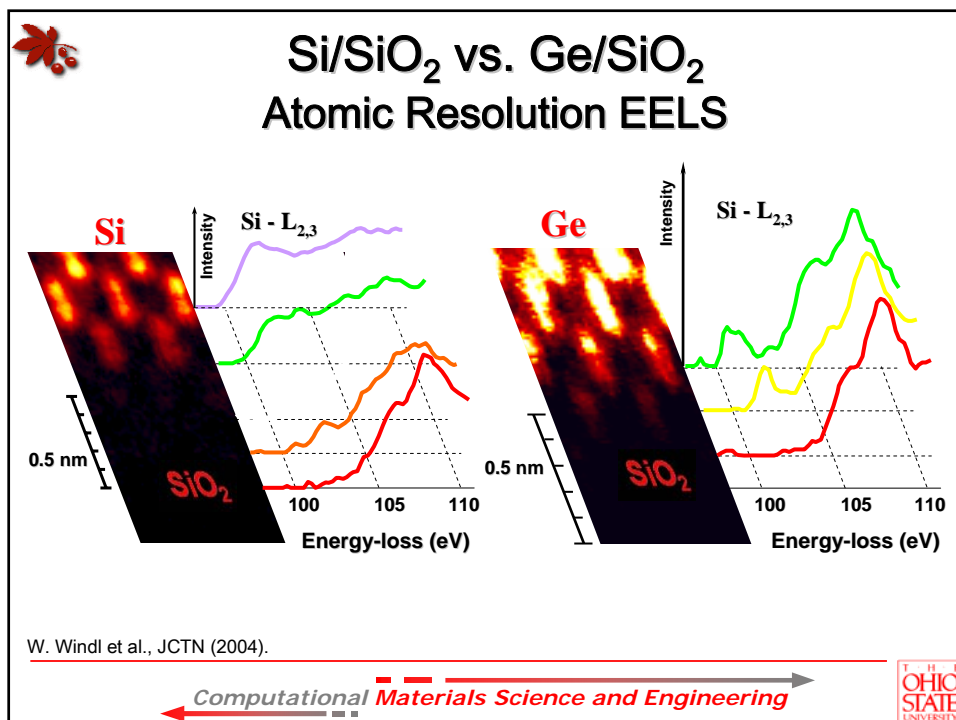
⇒ “Measure” atomic structure of amorphous materials.

← Computational Materials Science and Engineering →

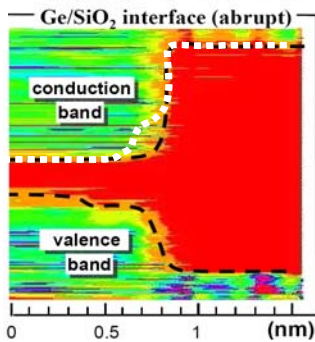
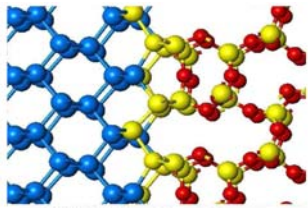








Oxidation of Si:Ge: "Ultimate" Device?



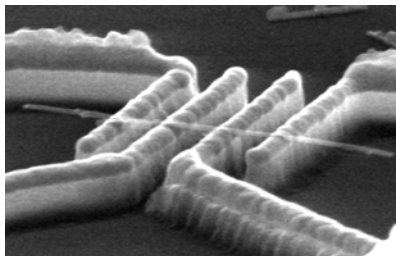
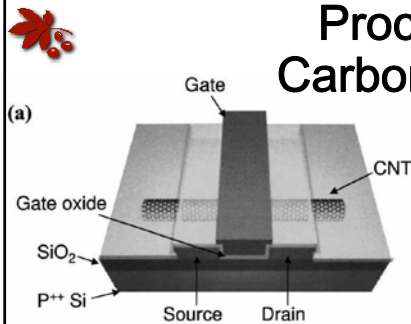
High-T oxidation of Si:Ge:

- Repulsive Ge-O interaction results in atomically sharp interface.
- Additionally, Ge channel (high mobility)
- Additionally, oxidation of Ge

← Computational Materials Science and Engineering →

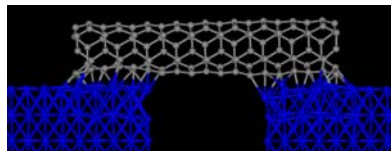


Process Simulation for Carbon Nanotube Devices



Possibilities:

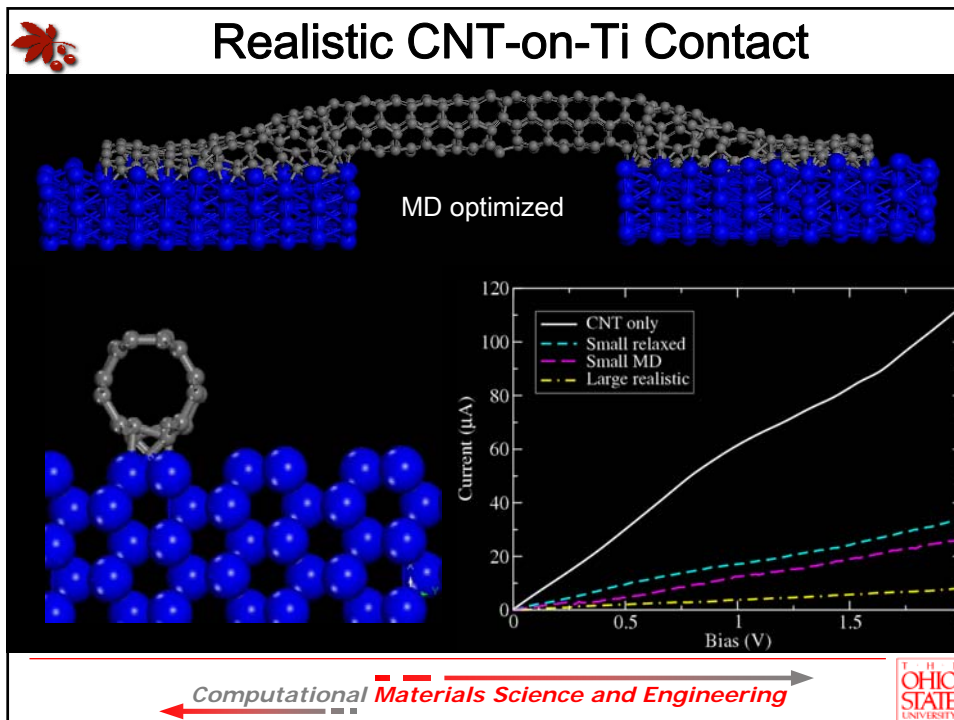
- Carbon nanotubes (CNTs) as channels in field effect transistors
- Ballistic electron transport in perfect SWNTs.



Wind *et al.*, JVST B, 2002.

← Computational Materials Science and Engineering →





Conclusions

- Ab-initio calculation of kinetic parameters for higher-level process modeling (TCAD, KMC) well understood.
 - Parameters for annealing of B, N, As in Si
- Characterization plus ab-initio modeling may solve the characterization problems for nanoelectronic devices
- “Process simulation” for molecular devices crucial
 - Only possibility: (Accelerated) MD techniques

← Computational Materials Science and Engineering →

THE OHIO STATE UNIVERSITY