TCAD Process/Device Modeling Challenges and Opportunities for the Next Decade

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- Portland Technology Development
- Portland Quality and Reliability Engineering
- K. Goodson, W. Tsai, W. Windl

Presentation Scope/Goals

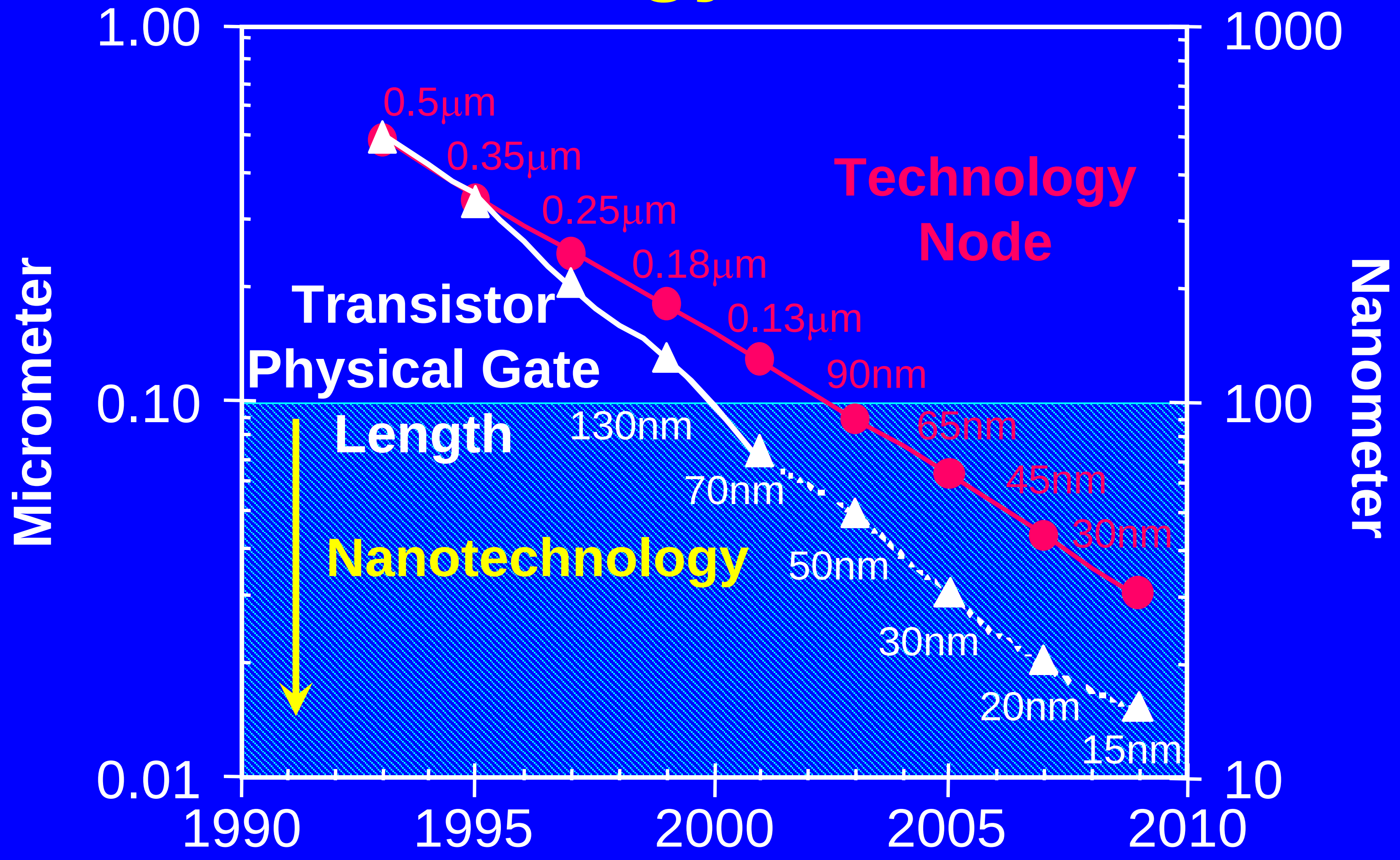
- Industrial perspective
- Front-end process/device modeling
- Logic technology development focus

- How has TCAD contributed to technology development?
- What TCAD capabilities does industry need through the next decade?

Outline

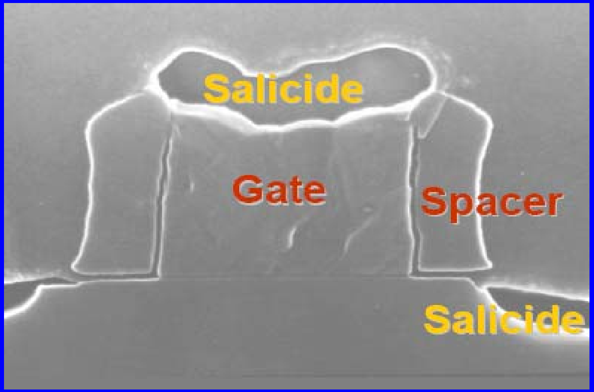
- Introduction
  - Technology scaling
  - Changing demands on TCAD
- Critical Modeling Needs
  - Computational Materials Science
  - Atomistic Modeling of Device Operation
  - Multiscale Hierarchical Modeling
- Conclusions

Nanotechnology in Production



- Product die will exceed 1.7 billion transistors in 2005
- Physical gate length ~15nm before the end of this decade

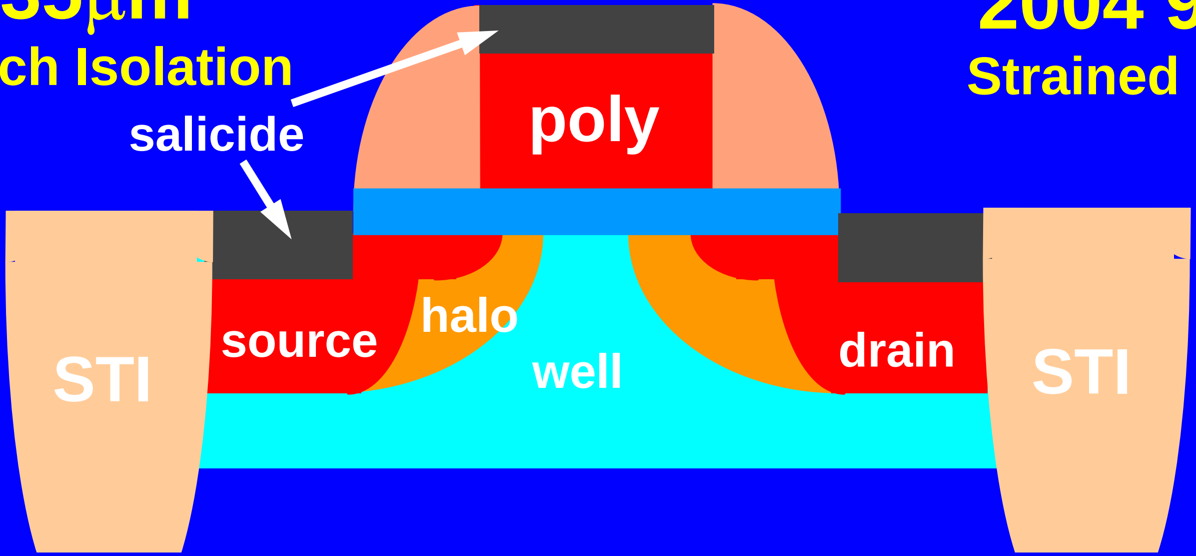
Transistor Scaling – Past Decade



Gate oxide scaling
Dopant engineering

1994 0.35μm
Shallow Trench Isolation

2004 90nm
Strained Silicon



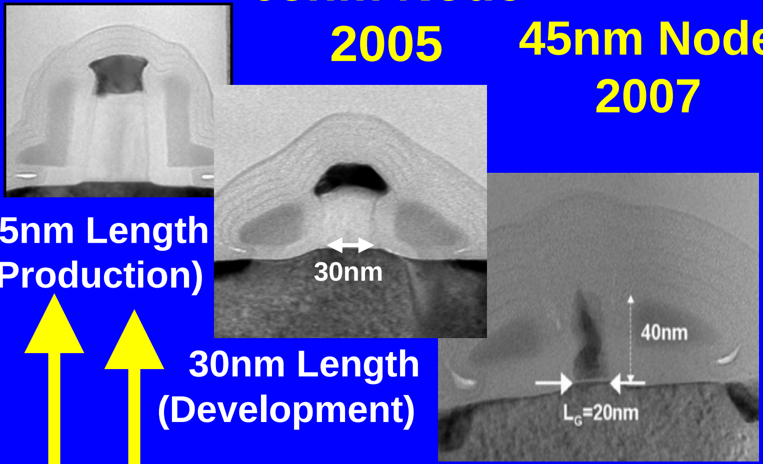
- Continuum models used for the vast majority of TCAD process/device applications

Transistor Scaling – Next Decade

90nm Node
2003

65nm Node
2005

45nm Node
2007

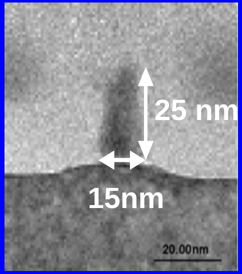


45nm Length
(Production)

30nm Length
(Development)

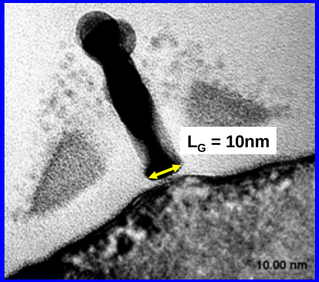
20nm Length
(Development)

32nm Node
2009



15nm Length
(Research)

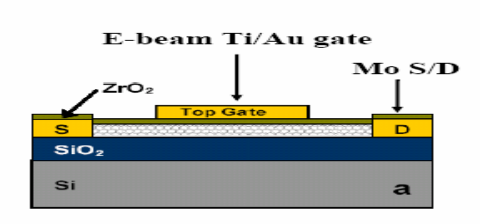
22nm Node
2011

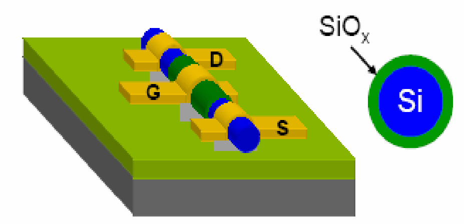


10nm Length
(Research)

2013-2019

Nanowire/
Nanotube

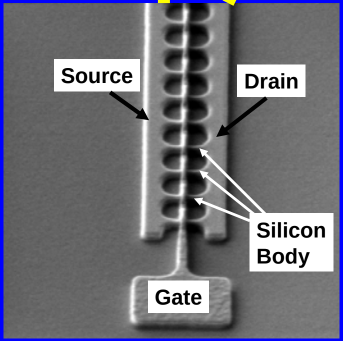




Uniaxial Strain

SiGe S/D

High-K/ Metal-Gate



Tri-Gate Architecture

Nanotechnology Eras

Evolutionary CMOS

Traditional scaling up to the 22nm node

High-k/metal gate, strained Si/SiGe, fully depleted UTB SOI, double gate MOS, trigate MOS, new silicides, FUSI, …

Revolutionary CMOS

Extending charge-based technology to its ultimate limits; 22nm node and beyond

New channel materials, ballistic transport, barrier engineering e.g. Ge FETs, III-V on Si, nanowire FETs, carbon nanotube FETs, …

Exotic Technologies

Novel technologies beyond charge-based devices; beyond the roadmap

Spin logic, phase logic, molecular devices, photonics, …

Process/Device TCAD Industry Needs

Evolutionary CMOS → **Materials**

Extend traditional TCAD capabilities to next generations of devices, providing accurate models to enable technology optimization despite rapid introduction of new materials and structures

Revolutionary CMOS → **Devices**

Physical device models and analysis to enable detailed evaluation of intrinsic device performance and impact of parasitics; strong connection to fabrication processes/materials; enable selection and adoption of beyond-silicon devices

Exotic Technologies → **Systems**

Models for initial assessment of device and technology choices to enable exploration of radically new systems / architectures

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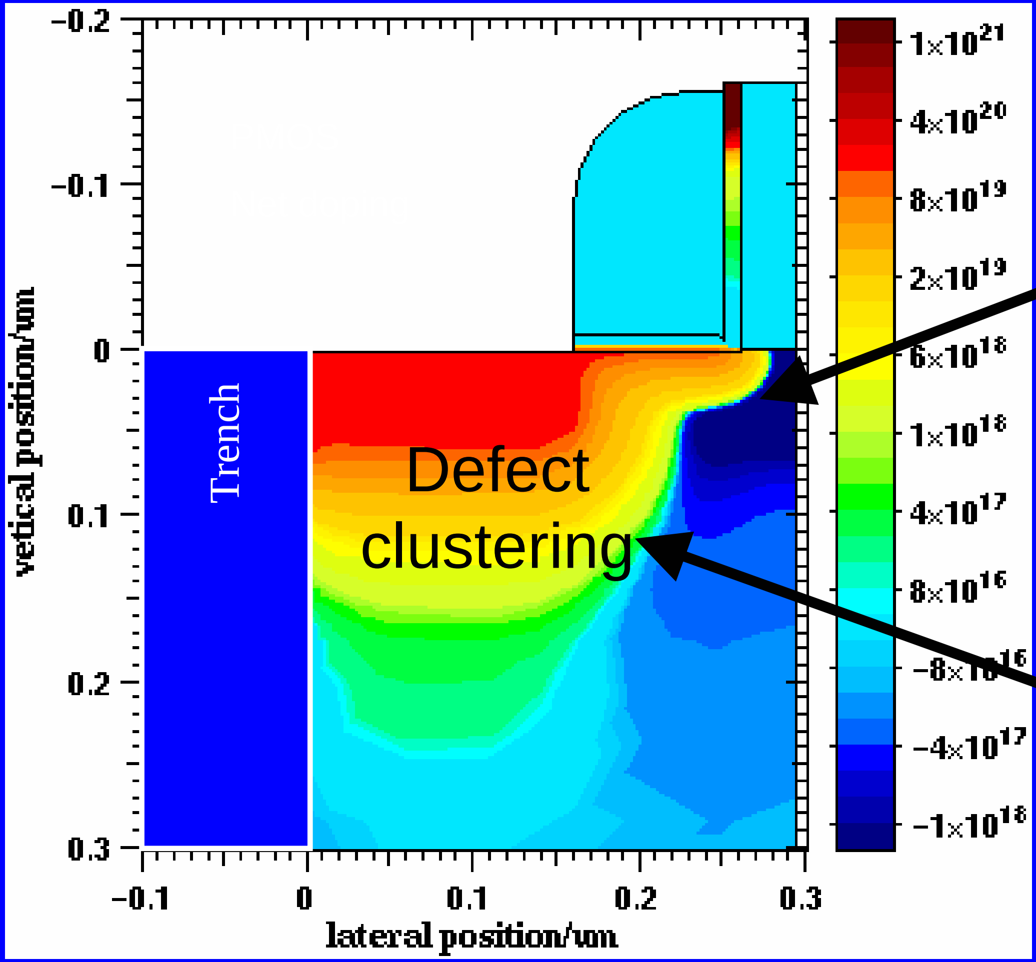
Computational Materials Science

Example: dopant-defect diffusion

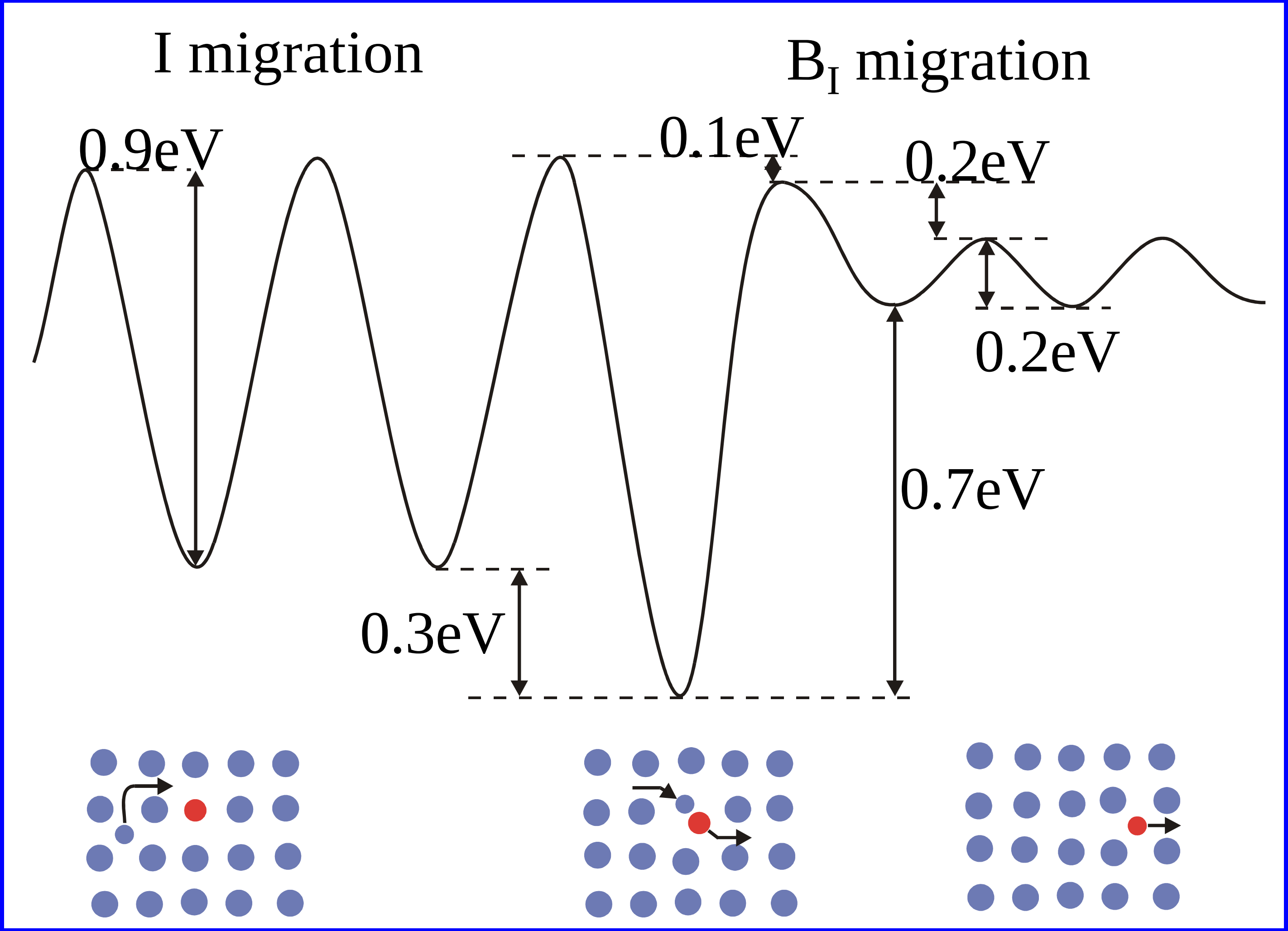


Diffusion in
tip and halo is
influenced
by S/D damage

S/D dopants and
damage encroach

Continuum reaction-diffusion models provide a powerful and efficient capability that can incorporate atomistic dopant-defect energetics

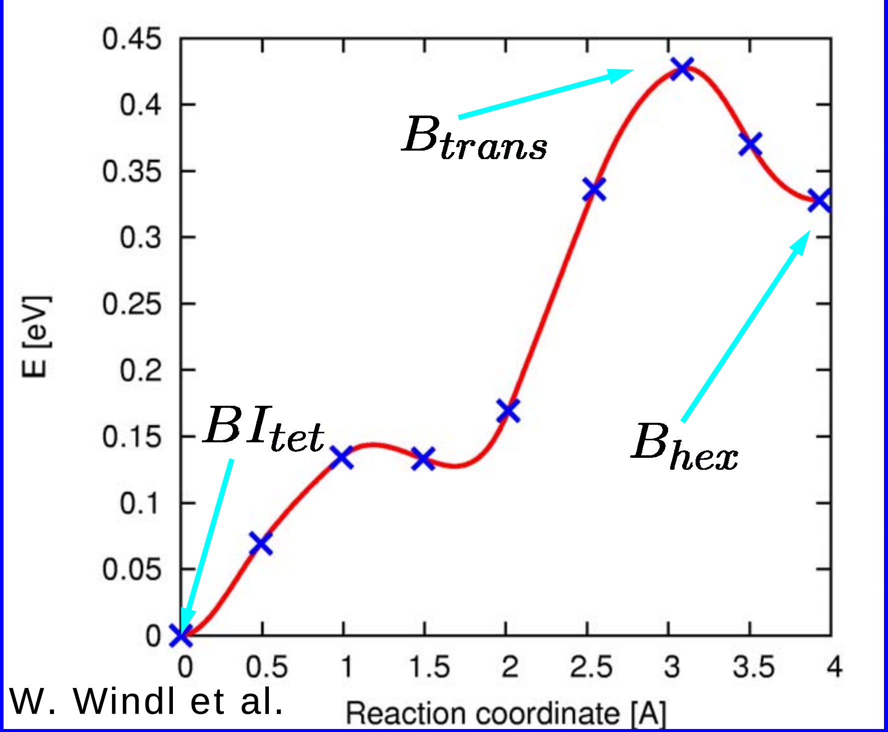
Boron-Interstitial diffusion



Jing Zhu, LLNL 1996

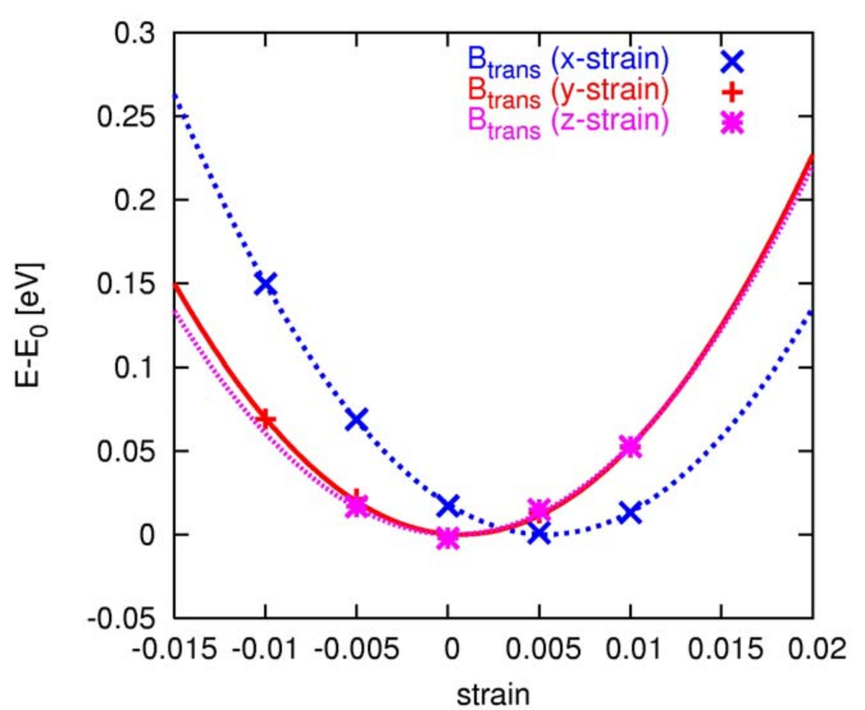
Boron Diffusivity under Stress

Transition (NEB):



W. Windl et al.

Transition state energy:

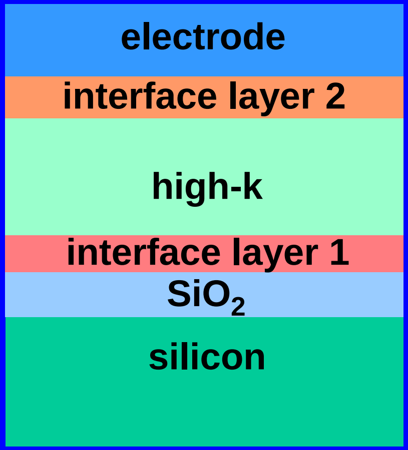


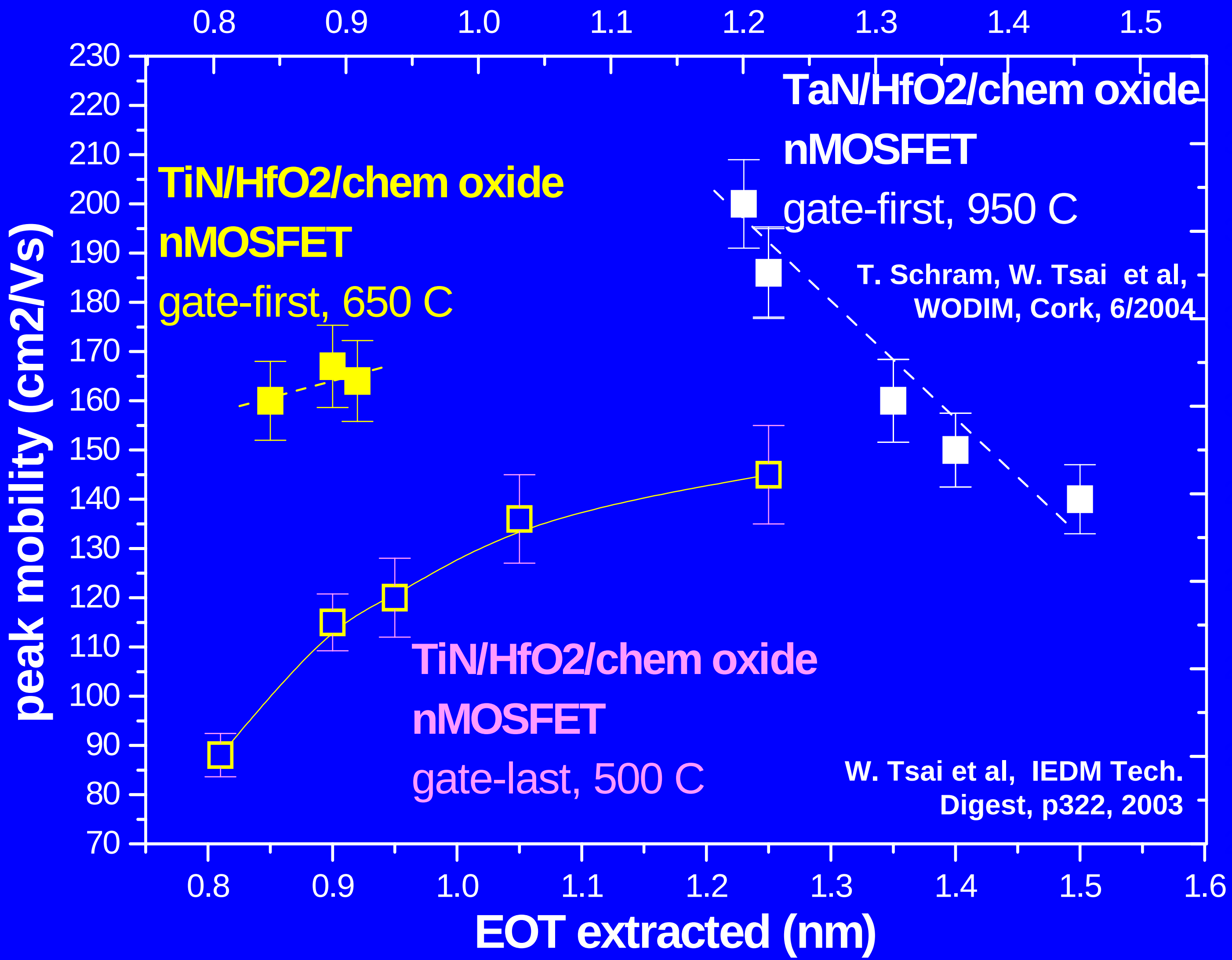
M. Diebel, SISPAD 2003

Hop direction: $\vec{d} = \frac{a}{8}(3,1,1)$

$\Rightarrow$ **anisotropic diffusivity**

Interfaces Critical in Scaled Devices



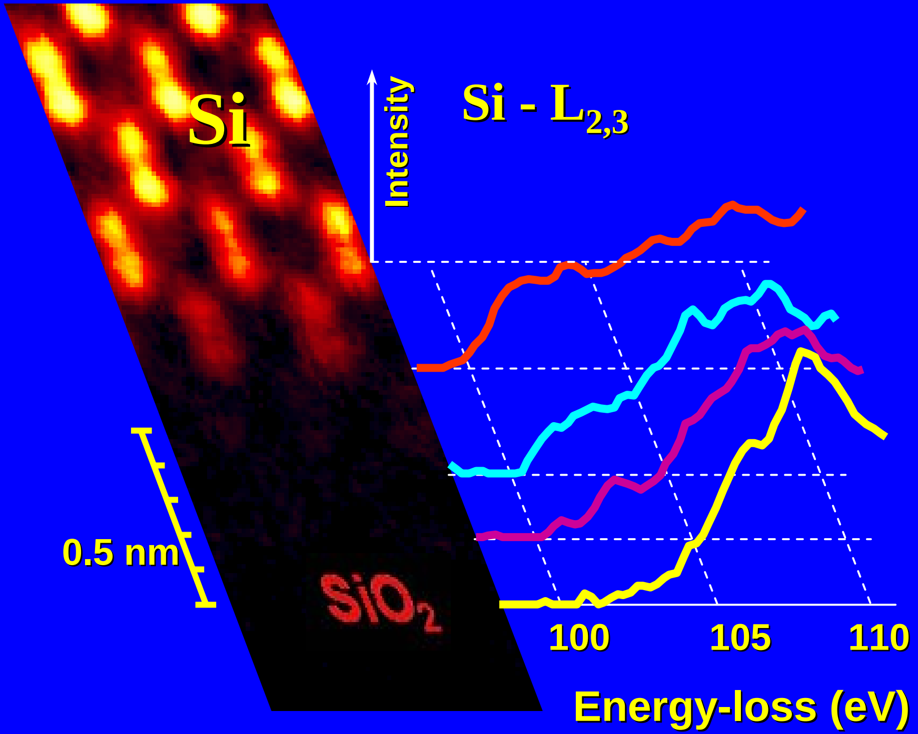


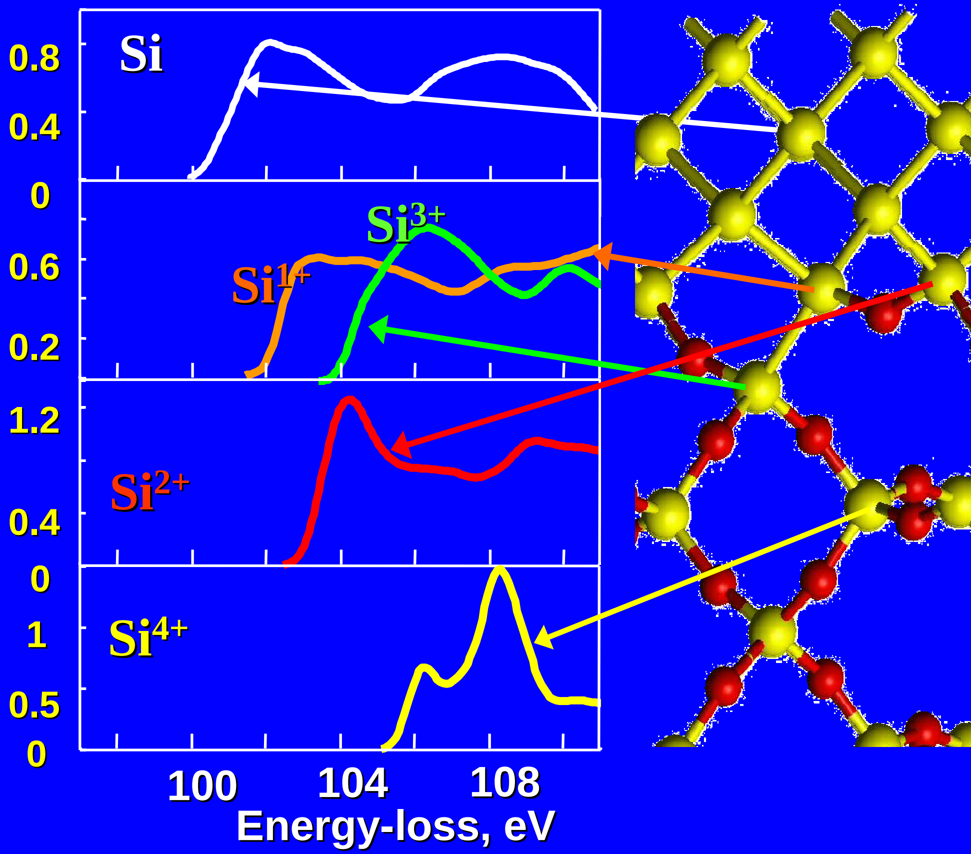
T. Schram, W. Tsai et al, WODIM, Cork, 6/2004

W. Tsai et al, IEDM Tech. Digest, p322, 2003

Electron mobility for scaled high-k as a function of process flow

DFT Calculation of Interface Structure





Experiment

Model

Interface structure understanding

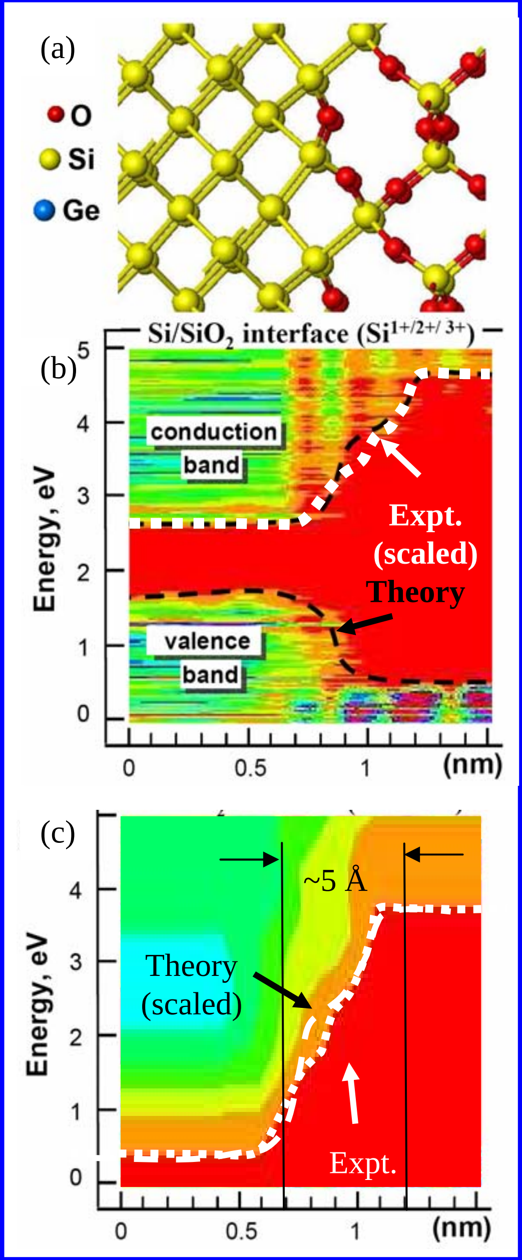
Application: Si/SiO_2 vs. Ge/SiO_2

Structure
(from EELS fit)

Spatially
resolved
DOS

EELS
(plus CB edge
from DOS)

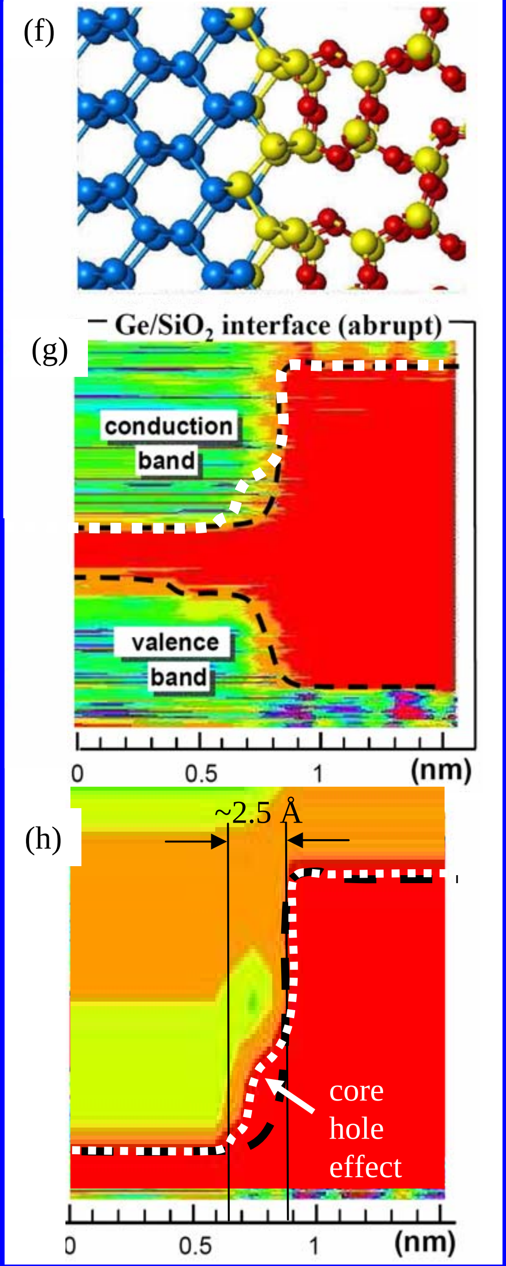
W. Windl, Ohio
State University



Si/SiO_2 ←

Ge/SiO_2 →

Find Ge/SiO_2 interface is atomically sharp with “text book” band line-up



Computational Materials Science

Where we need to be:

- Atomistic models for process effects extensible to new materials/interfaces
- Accurate enough to enable process optimization
- Handles bandgap/charge effects and large configuration spaces of real structures
- Strongly linked to process fabrication chemistry

- Value extends beyond front-end modeling needs to device and fabrication

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Atomistic Modeling of Device Operation

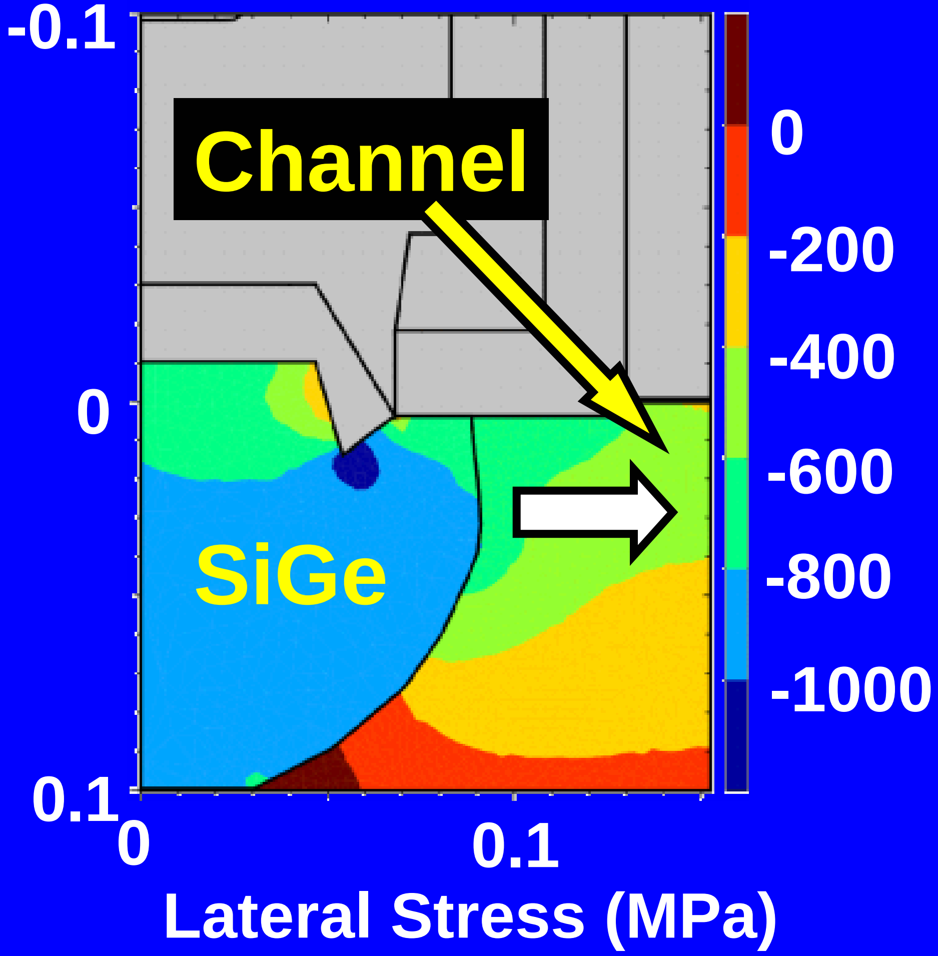
Where we are now:

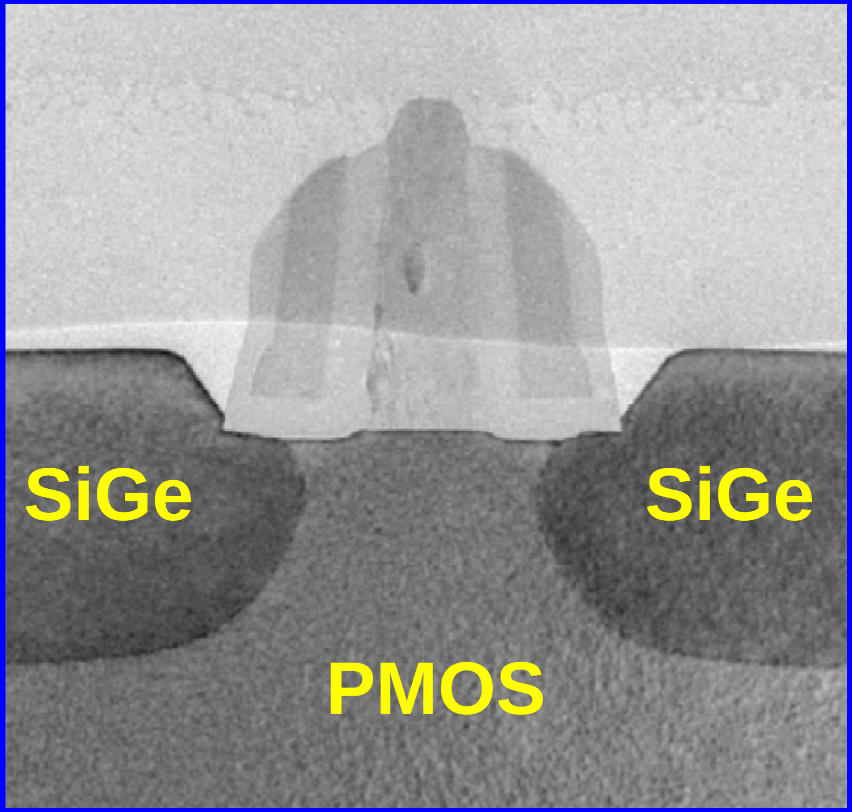
- Drift-diffusion approach has been pushed far into the submicron MOS regime
- Entering new phase of Evolutionary CMOS with expanding materials and structures

↓

- New requirements for atomistic physical modeling in current technology development
- Many needs for detailed evaluation of revolutionary CMOS options

Strain Engineered 90nm Technology

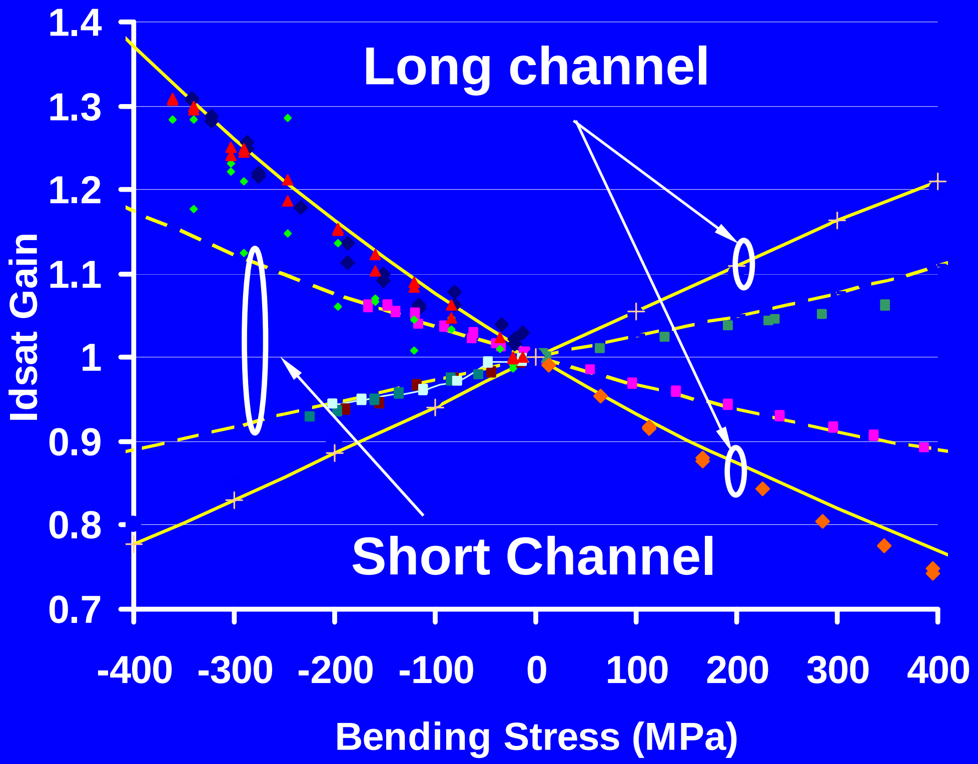




30% IDSAT gain

PMOS Drive Current Gain with Stress

Heavy hole band
50meV isosurface

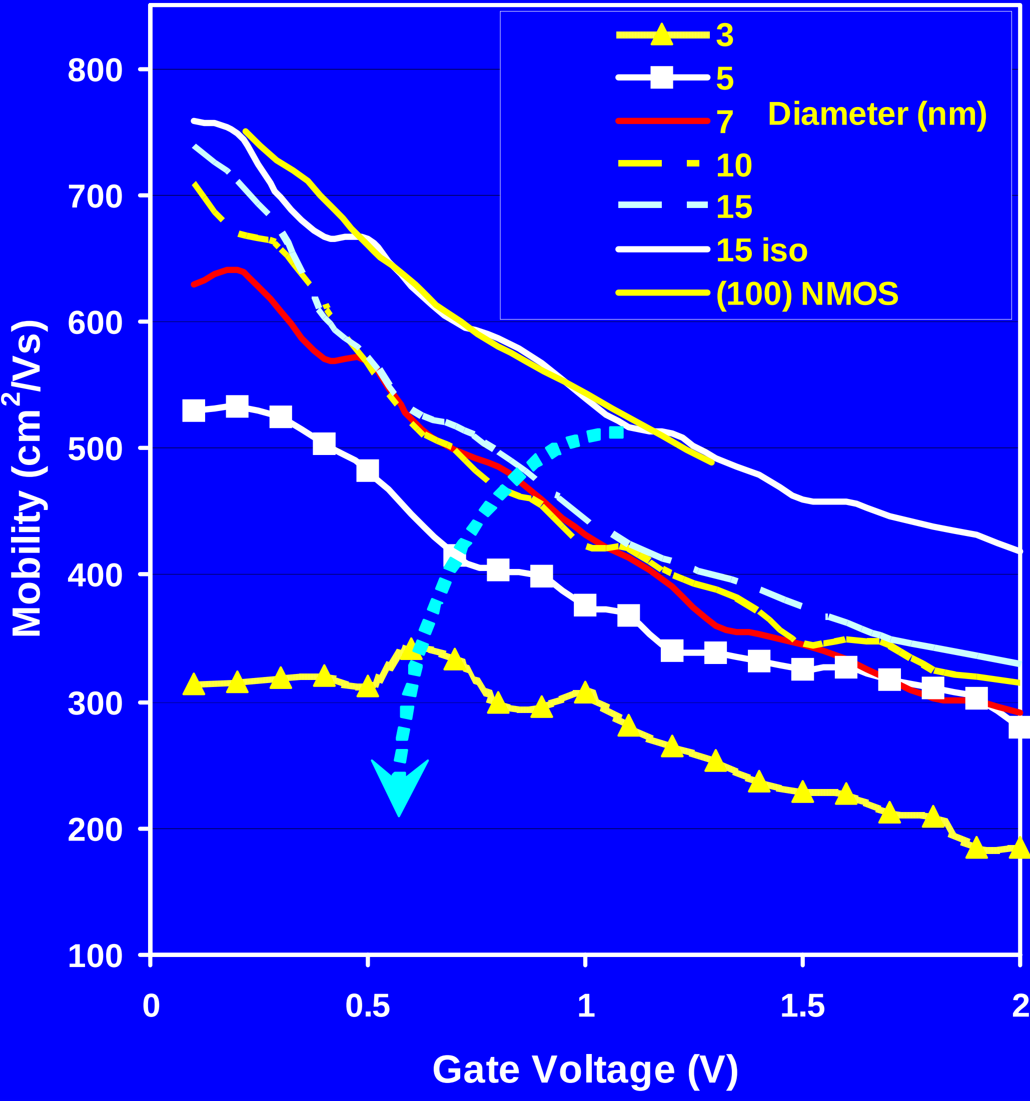


- Bandstructure calculations enable understanding of physical dependencies of PMOS stress response

Phonon Mobility in Nanowires

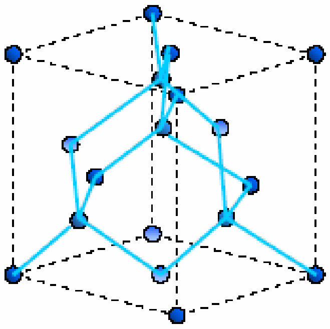
SiO2 cladding

- **Rigorous 1D Mobility calculation in nanowires**
  - **Schrödinger-Poisson solution for wavefunctions**
  - **Scattering/BTE solution**
  - **Compute mobility as a function of diameter**



Self-Consistent Monte Carlo and Quantum/Atomistic Electrothermal Simulation of Nanotransistors

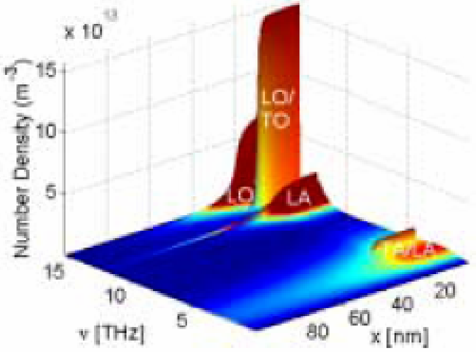
Physics



Molecular Dynamics

- Phonon scattering experiments
- Input to BTE modeling

Devices



Split-Flux Phonon BTE / Monte Carlo

- Predict steady & transient phonon populations
- Link to electron transport

Circuit level CAD

Compact Multi-scale Model

- Temperature response
- Sub-continuum predictability in TCAD

Atomistic Modeling of Device Operation

Where we need to be:

- Continue to drive the development of atomistic models across the range of device options
- Strengthen the link to atomistic models of fabrication and materials properties
- Go beyond point solutions to bring the resulting tools to the maturity needed for industrial application

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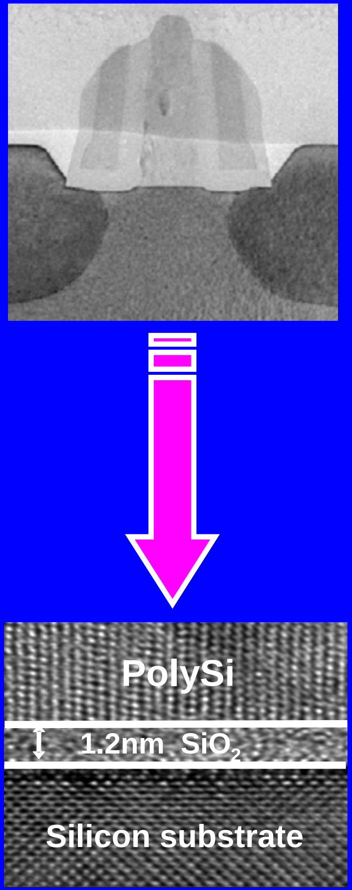
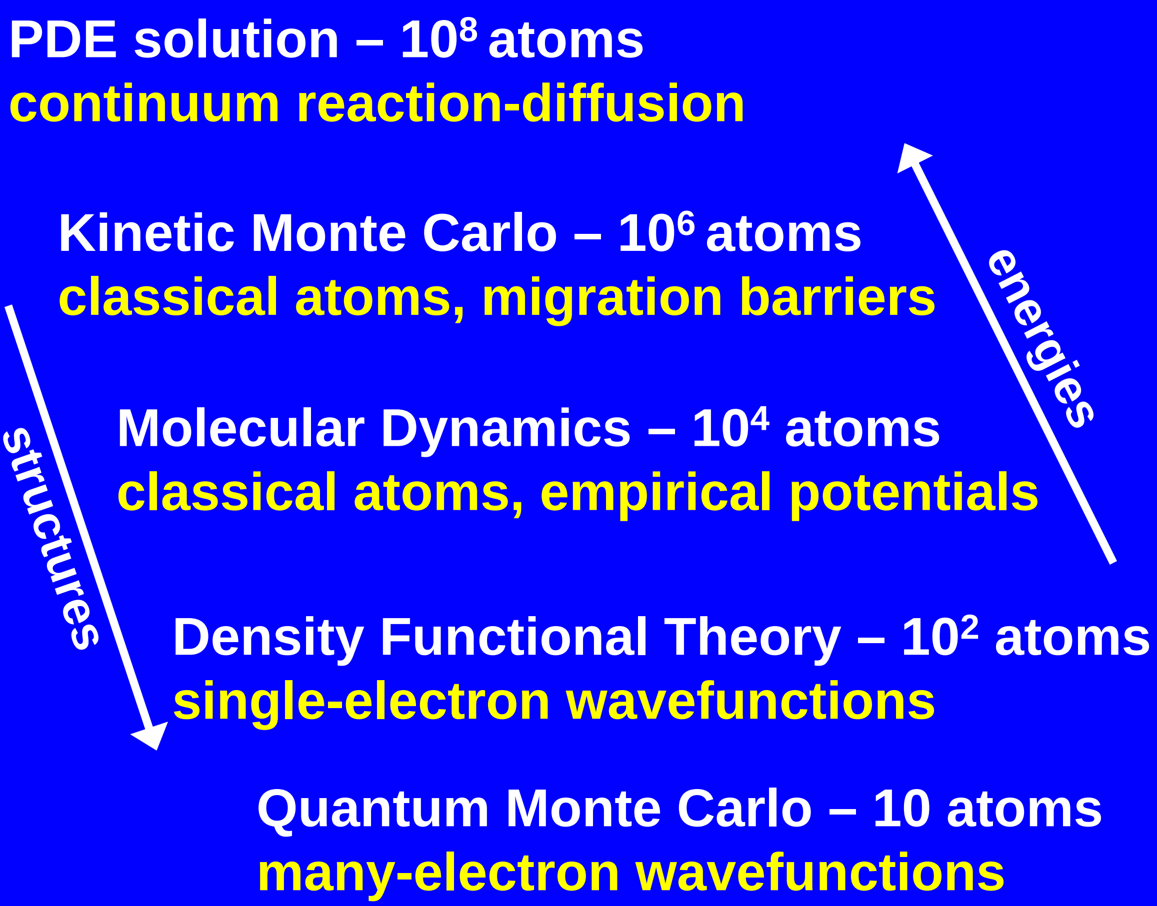
Multi-scale, Multi-phenomena Modeling





PDE solution – 10^8 atoms
continuum reaction-diffusion

Kinetic Monte Carlo – 10^6 atoms
classical atoms, migration barriers

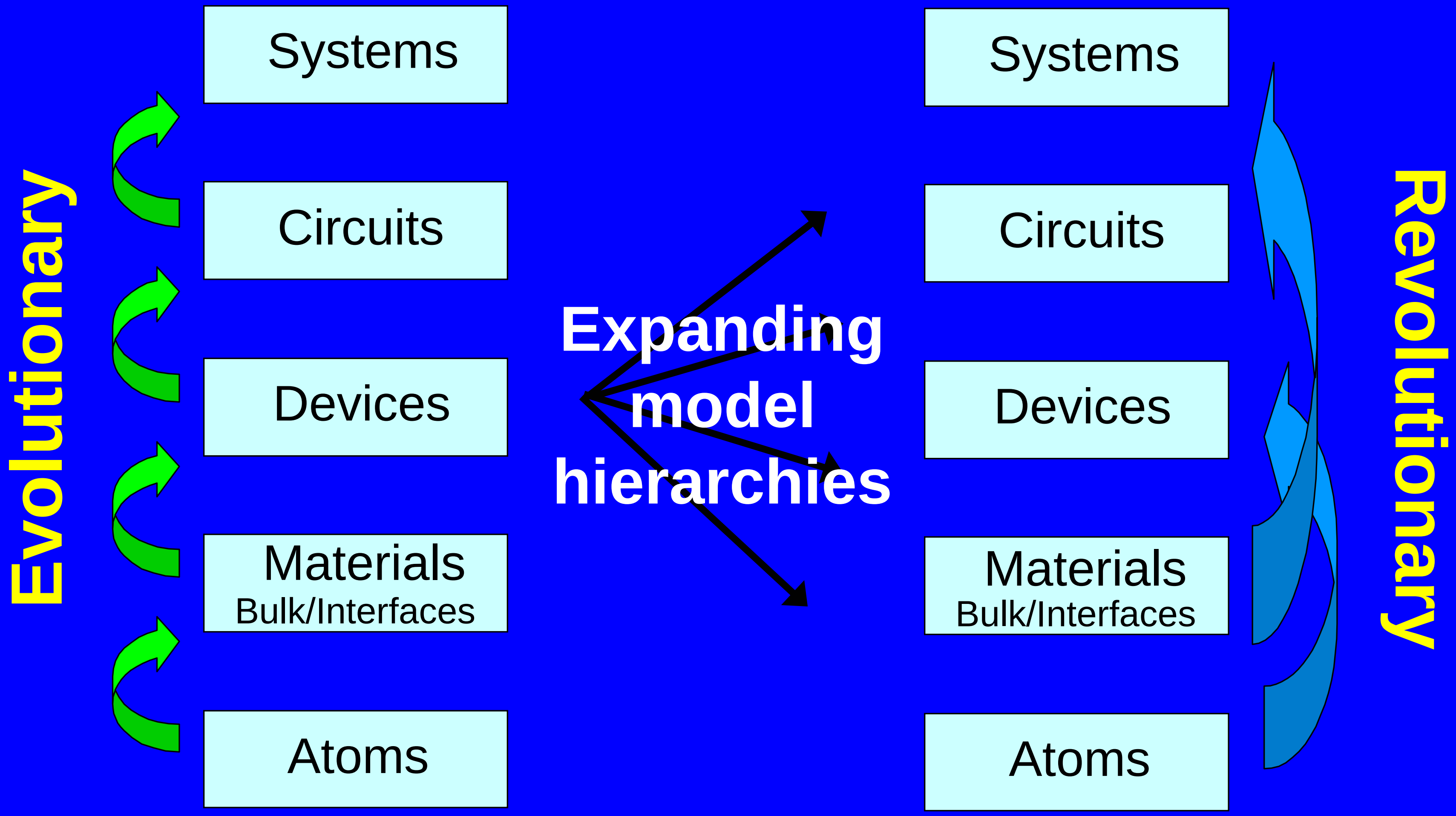
Molecular Dynamics – 10^4 atoms
classical atoms, empirical potentials

Density Functional Theory – 10^2 atoms
single-electron wavefunctions

Quantum Monte Carlo – 10 atoms
many-electron wavefunctions

Hierarchical modeling approaches are well recognized as essential within modeling areas

Hierarchical Modeling Systems



Evolutionary

Systems

Circuits

Devices

Materials
Bulk/Interfaces

Atoms

Expanding model hierarchies

Systems

Circuits

Devices

Materials
Bulk/Interfaces

Atoms

Revolutionary

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Conclusions

- TCAD process and device modeling has a critical role in enabling future technology development
- Evolutionary CMOS
  - Analysis and optimization of new materials and structures
- Revolutionary CMOS
  - Detailed evaluation of the strengths and weaknesses of beyond-silicon devices
- Exotic Technologies
  - Exploration of radically new systems and architectures
- Atomic-scale physical modeling as the foundation of a hierarchical modeling approach is the key to successfully meeting these diverse challenges