Bandstructure Effects in Nano Devices With NEMO from Basic Physics to Real Devices and to Global Impact on nanoHUB.org

Gerhard Klimeck
Purdue University

Activities on http://nanoHUB.org in 172 countries

- New Registrations
- Simulation Users
- Tutorial / Lecture Users

nanoHUB.org: 17,000+ / 1.4million Users Annually

nanoHUB.org usage 2013-02-01 00:00:00

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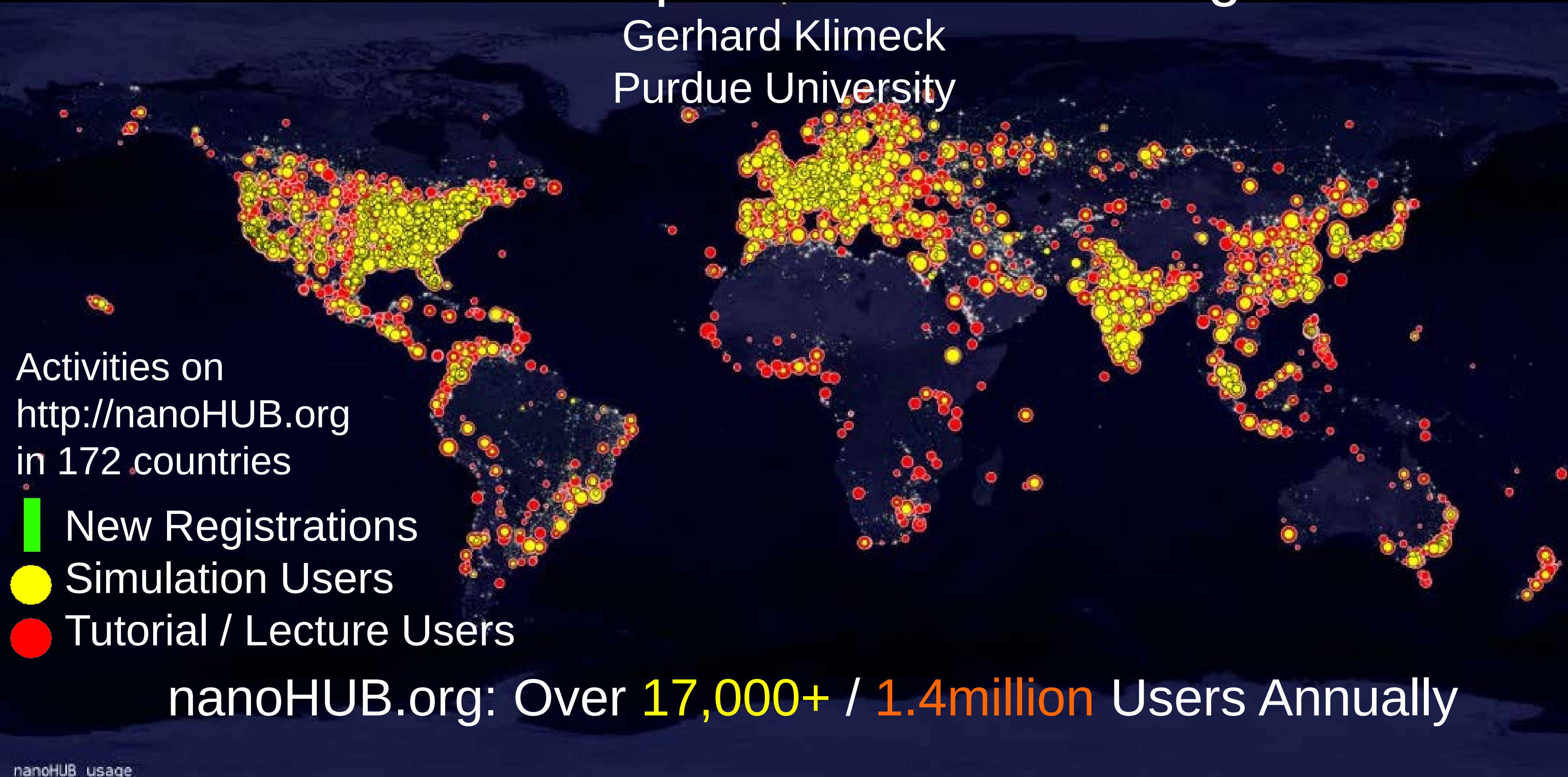

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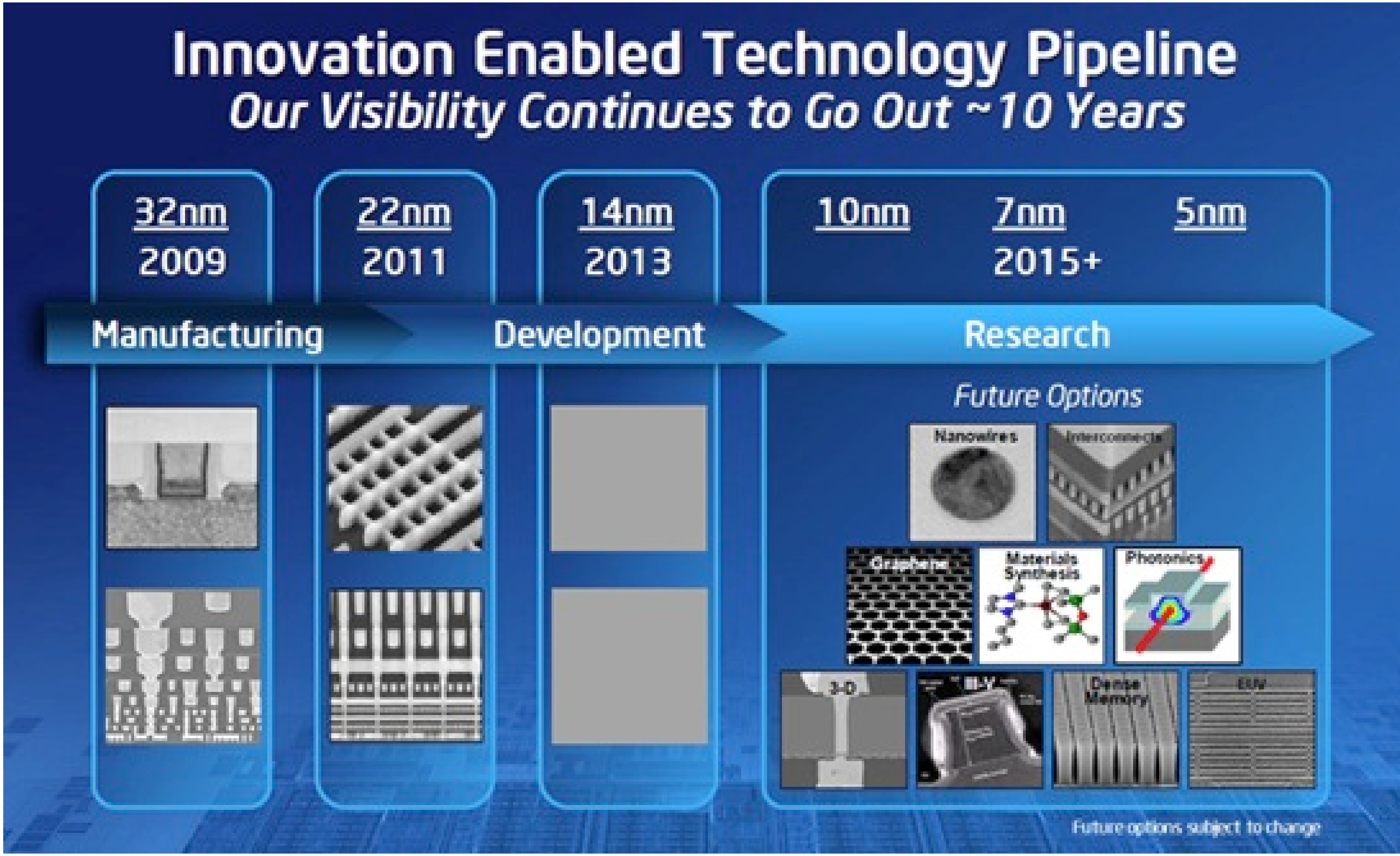
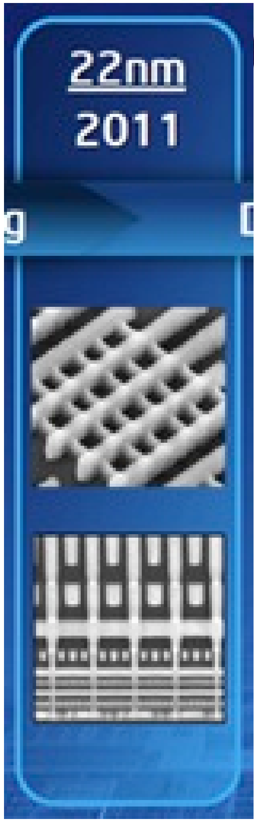
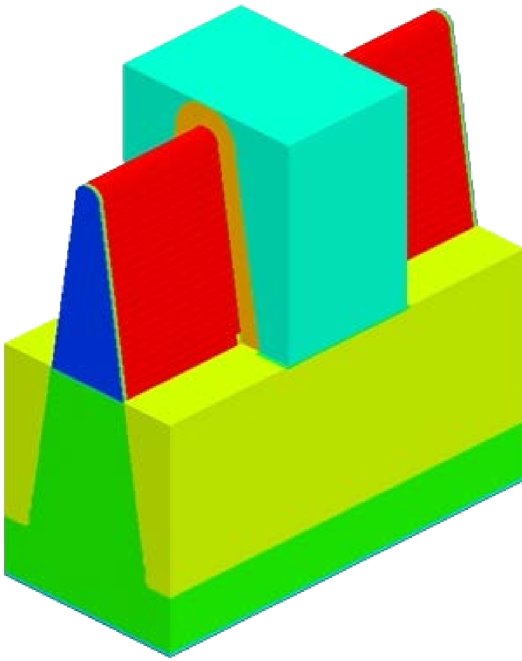
nanoHUB usage

Intel Roadmap

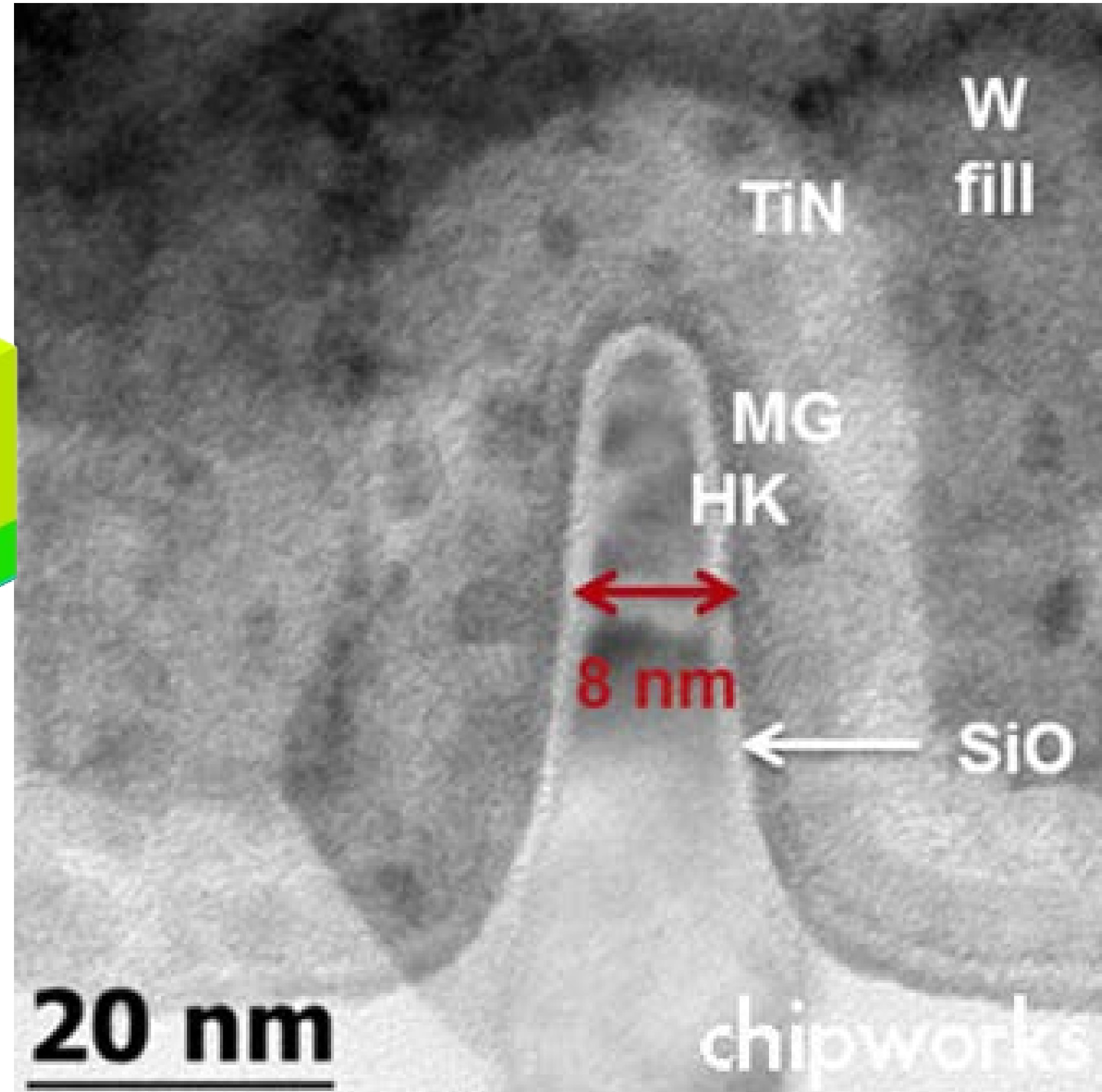


Today: non-planar 3D devices Better gate control!





Intel 22nm finFET



http://www.goldstandardsimulations.com/index.php/news/blog_search/simulation-analysis-of-the-intel-22nm-finfet/
http://www.chipworks.com/media/wpmu/uploads/blogs.dir/2/files/2012/08/Intel22nmPMOSfin.jpg

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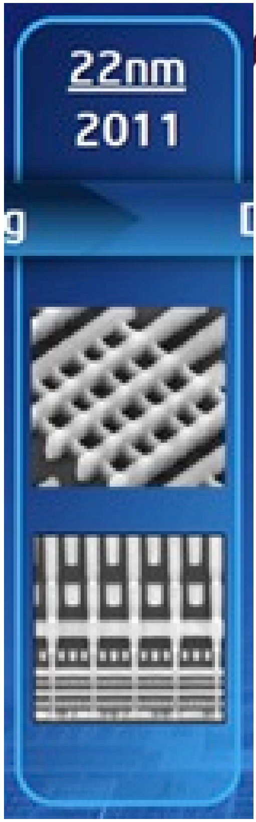
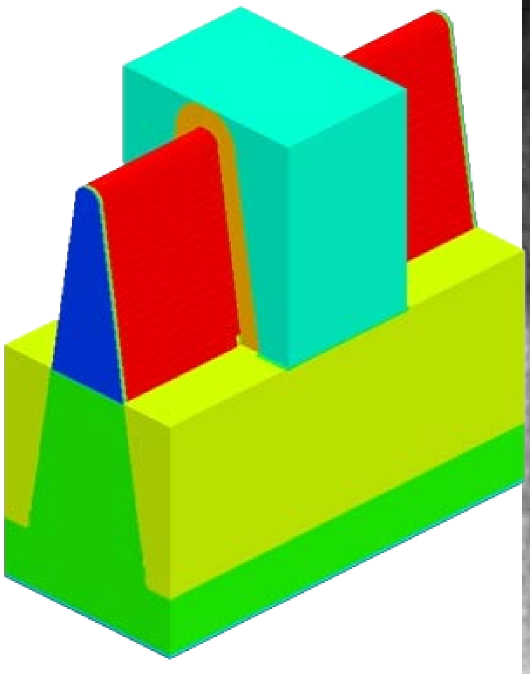
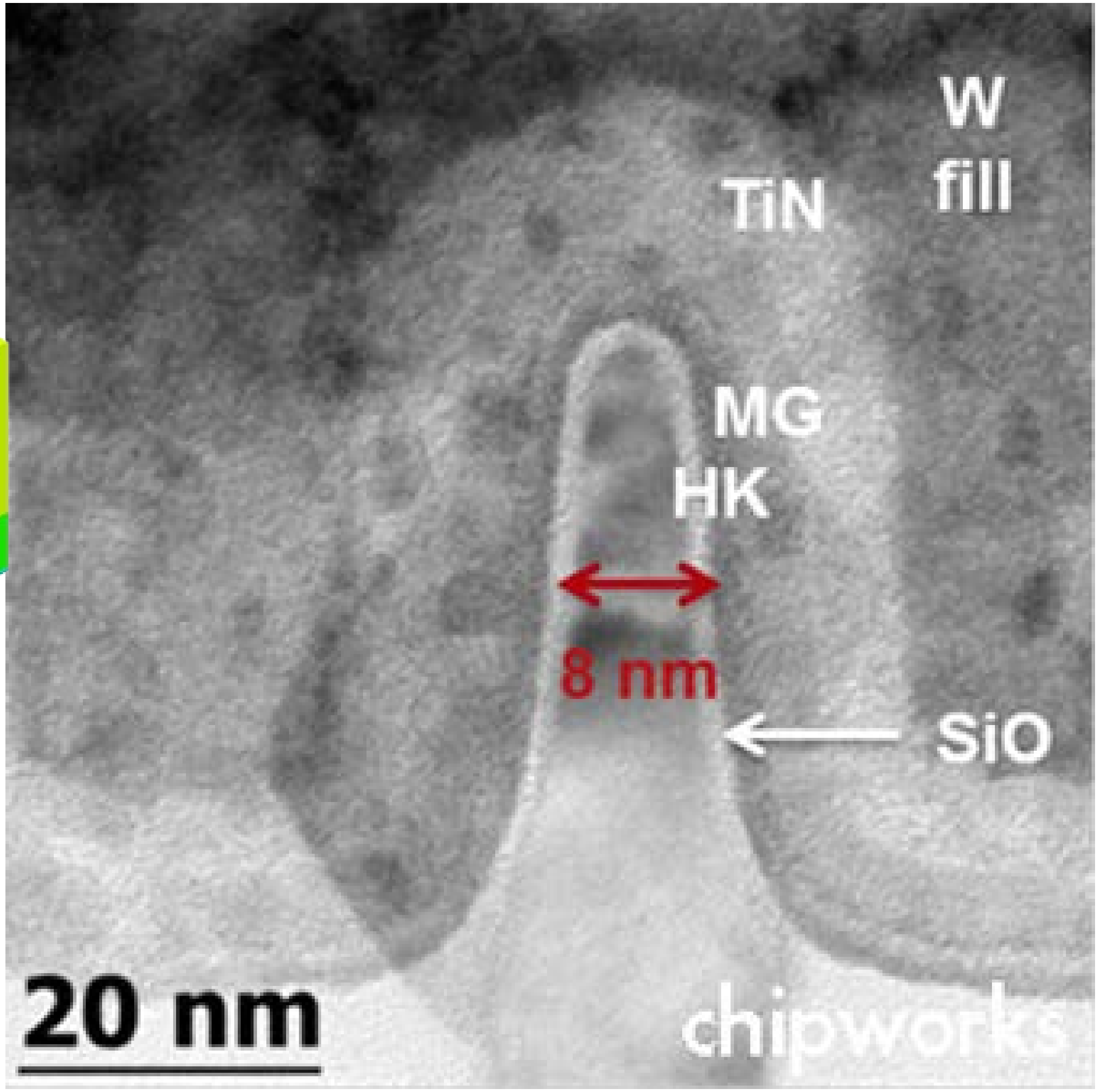




22nm = 176 atoms

8nm = 64 atoms



http://www.goldstandardsimulations.com/index.php/news/blog_search/simulation-analysis-of-the-intel-22nm-finfet/

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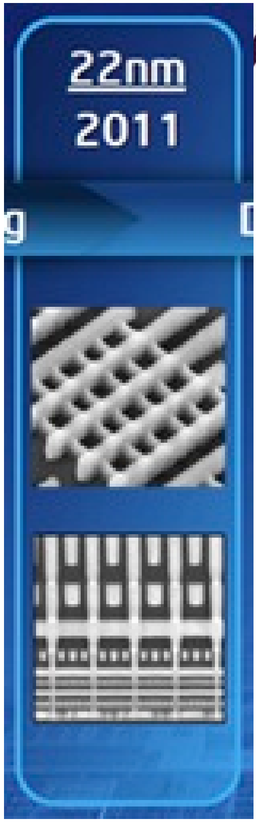
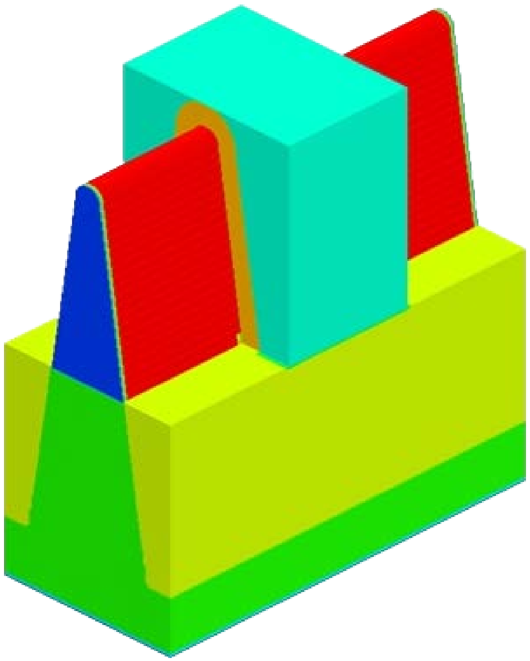
Today: non-planar 3D devices
Better gate control!

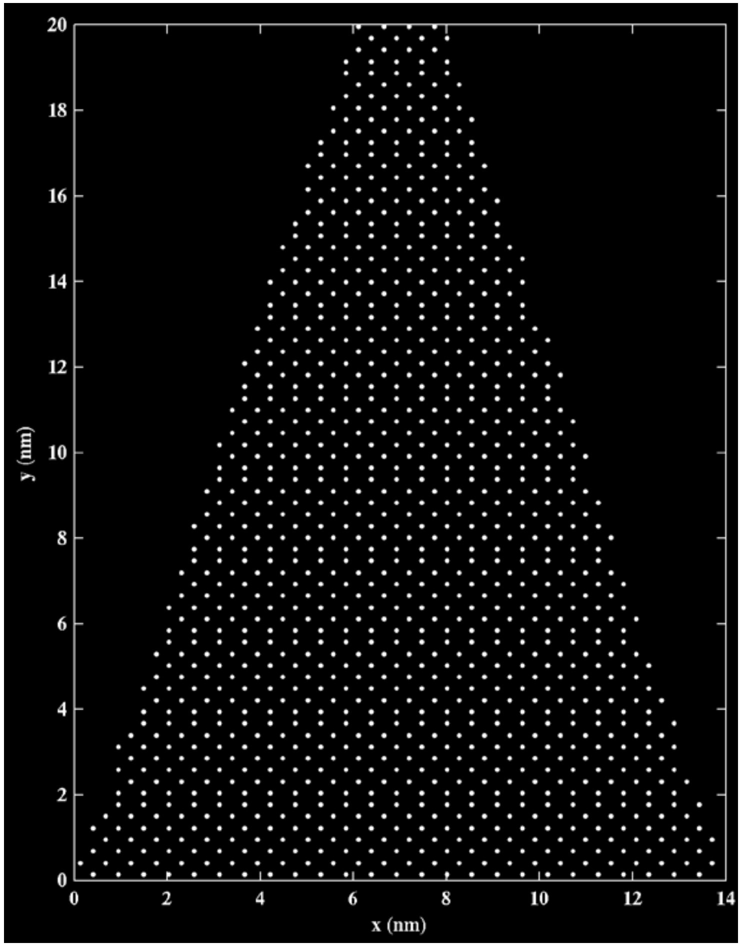




22nm = 176 atoms

8nm = 64 atoms

1,085 atoms



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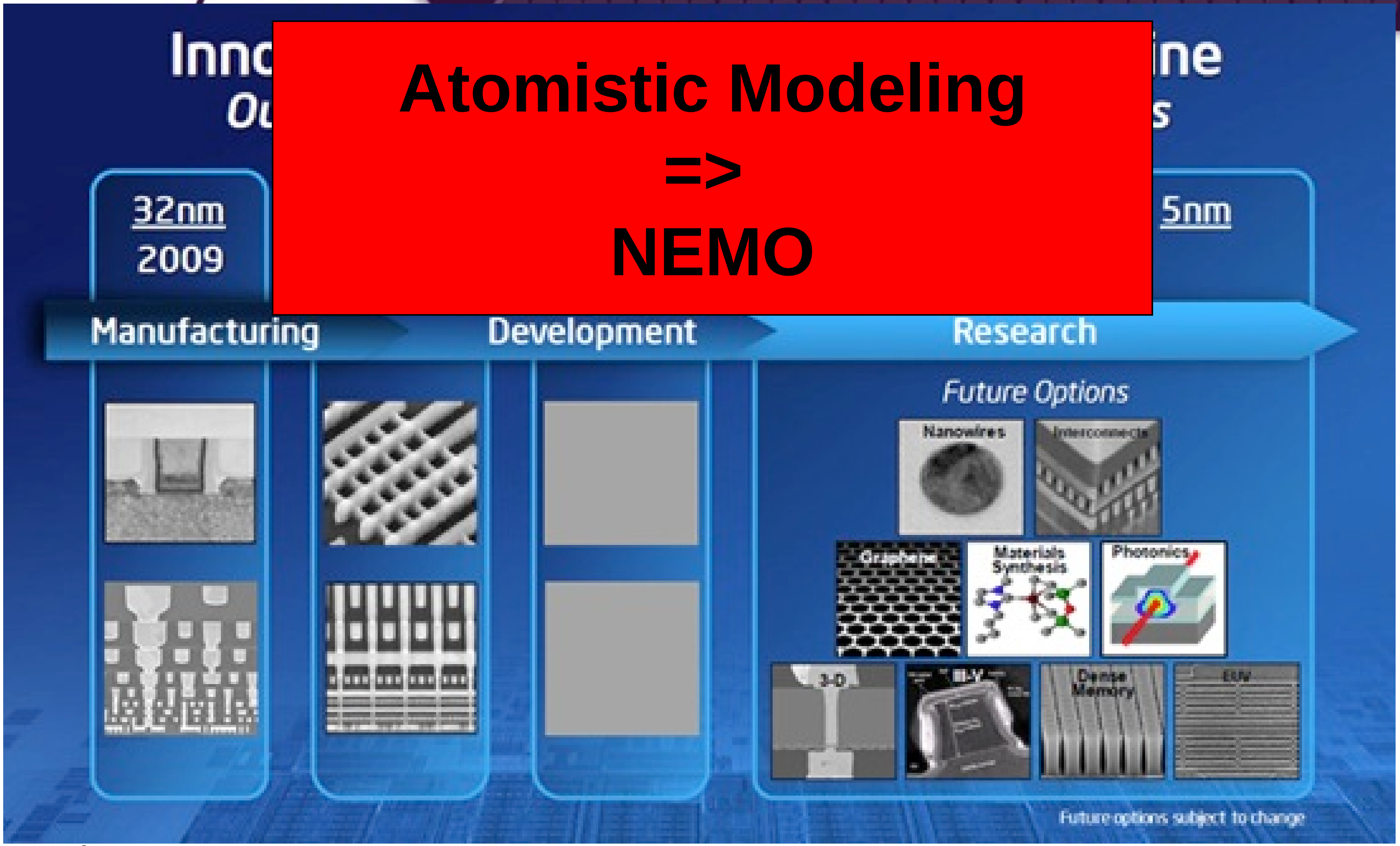
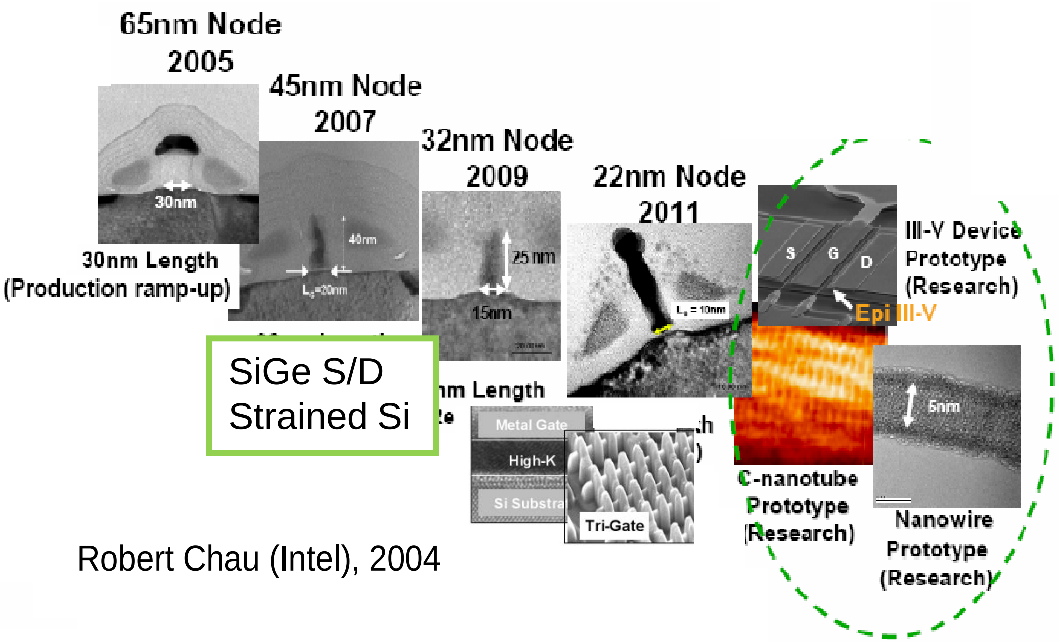
http://www.chipworks.com/media/wpmu/uploads/blogs.dir/2/files/2012/08/Intel22nmPMOSfin.jpg

Roadmap of finite atoms!



Atomistic Modeling
=>
NEMO

nm Node	22	14	10	7	5
Node atoms	176	122	80	56	40
Critical atoms	64	44(?)	29(?)	20(?)	14(?)
Electrons	160-190	64-80	30-38	18-23	11-15



Robert Chau (Intel), 2004

Observations:

- 3D spatial variations on nm scale
- Potential variations on nm scale
- New channel materials (Ge, III-V)

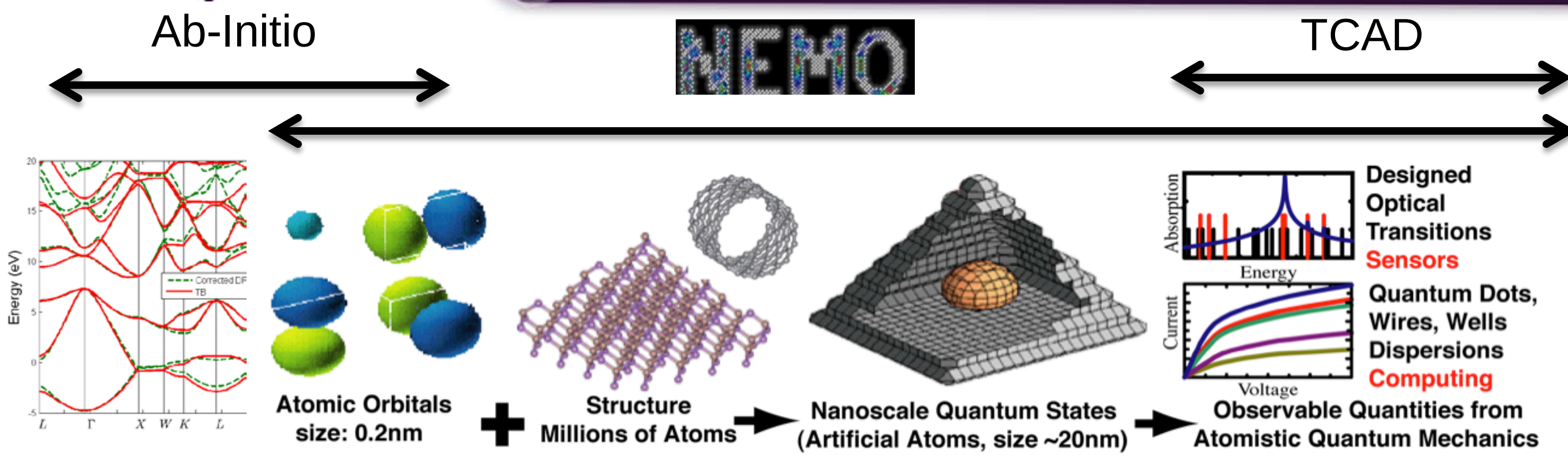
Questions / Challenges

- Strain ?
- Quantization?
- Crystal orientation?
- Atoms are countable; does granularity matter? Disorder?
- New material or new device?

Assertions of importance

- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation
  - » Band coupling, non-parabolicity, valley splitting
  - » Local (dis)order, strain and orientation

NEMO5 - Bridging the Scales From Ab-Initio to Realistic Devices



Goal:
- Device performance with realistic extent, heterostructures, fields, etc. for new / unknown materials

Problems:
- Need ab-initio to explore new material properties
- Ab-initio cannot model non-equilibrium.
- TCAD does not contain any real material physics

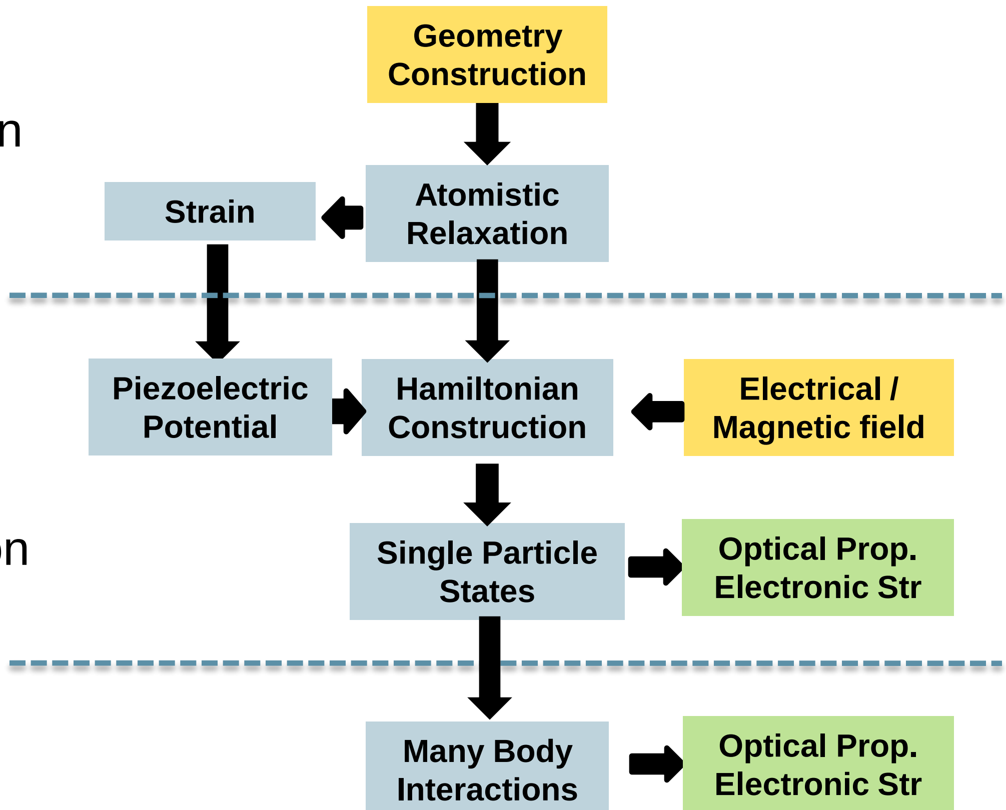
Approach:
- Ab-initio:
  - Bulk constituents
  - Small ideal superlattices
- Map ab-initio to tight binding (binaries and superlattices)
- Current flow in ideal structures
- Study devices perturbed by:
  - Large applied biases
  - Disorder
  - Phonons

NEMO - Multi-Scale Modeling

Atom
Positions
~10-50 million
atoms

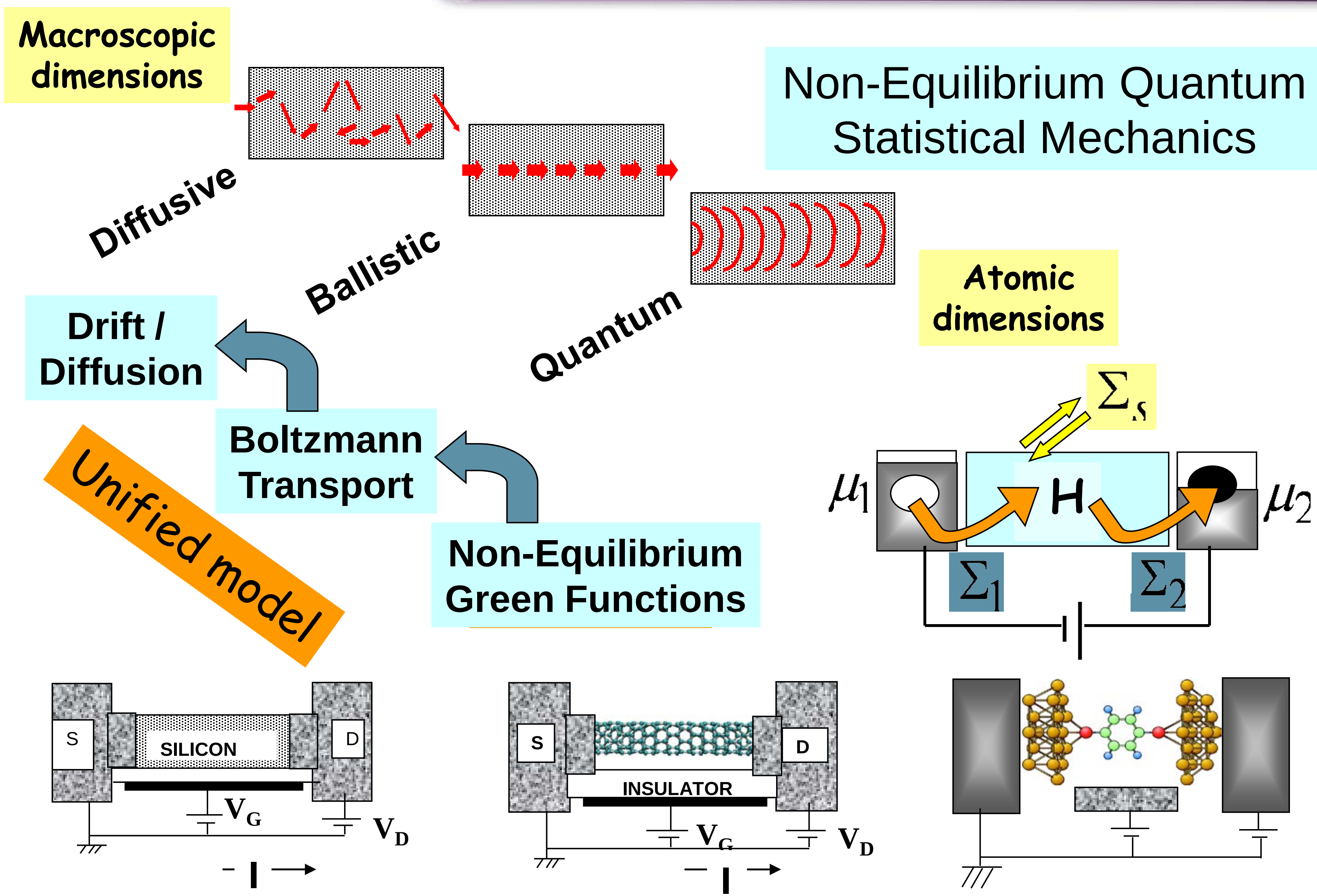
Valence
Electrons
~0.5-10 million

e-e
interactions
Few States



- Valence Force Field (VFF) Method
- Piezoelectric eff. Pol. charge density
- Empirical tight binding $sp^3d^5s^*$ + spin orbit
- SCP: Poisson + LDA
- Slater Determinants

Quantum Transport far from Equilibrium



	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Yes	-	-	Yes	Yes
Dim.	1D	any	any	any	
Atoms	~1,000	…n	100 Million	~1…0,000	
Crystal	[1… …ZB		[100], …ubi…ZB, W…		A… Any
Strain	-	V…	V…		…MVFF
Multi-physics	-				Spin, Classical
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 leve… 30,000 c…	…els …0,000 co	4 levels 100,000 cores

First predictive NEGF tool

First 10 million atom elctronic structure

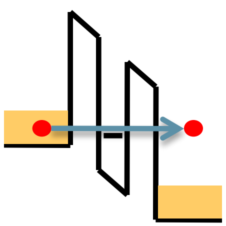
First multi-scale, multi-physics million-Electron

First peta-scale Engineering

Coming soon: Silvaco

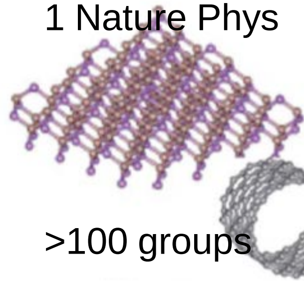
All codes:
>100,000 lines

>300 papers

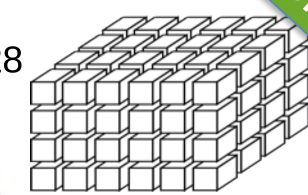


4 top pubs cites:
545,157,128,82
Patents:2

4 pubs cites:
166,157,131,128
1 Nature Phys



>100 groups

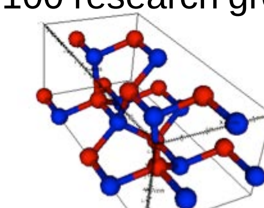


2 pubs in Science & Nature Nano 2012:
50 & 30 cites

Gordon Bell Prize

4 pubs cites
135,59,54,30
1 patent

New 2011-.
Intel, Samsung, GF, IBM, LockheedMartin
>100 research groups



NEMO5

Core Code / Theory Development

- NEMO-1D (Texas Instruments '94-'98, JPL '98-'03)
  - » Roger Lake, R. Chris Bowen
- NEMO3D (NASA JPL, Purdue, '98-'07)
  - » R. Chris Bowen, Fabiano Oyafuso, Seungwon Lee
- NEMO3D-peta (Purdue, '06-'11)
  - » Hoon Ryu, Sunhee Lee
- OMEN (ETH, Purdue, '06-'11)
  - » Mathieu Luisier
- NEMO5 (Purdue, '09-'today)
  - » Developed in a team

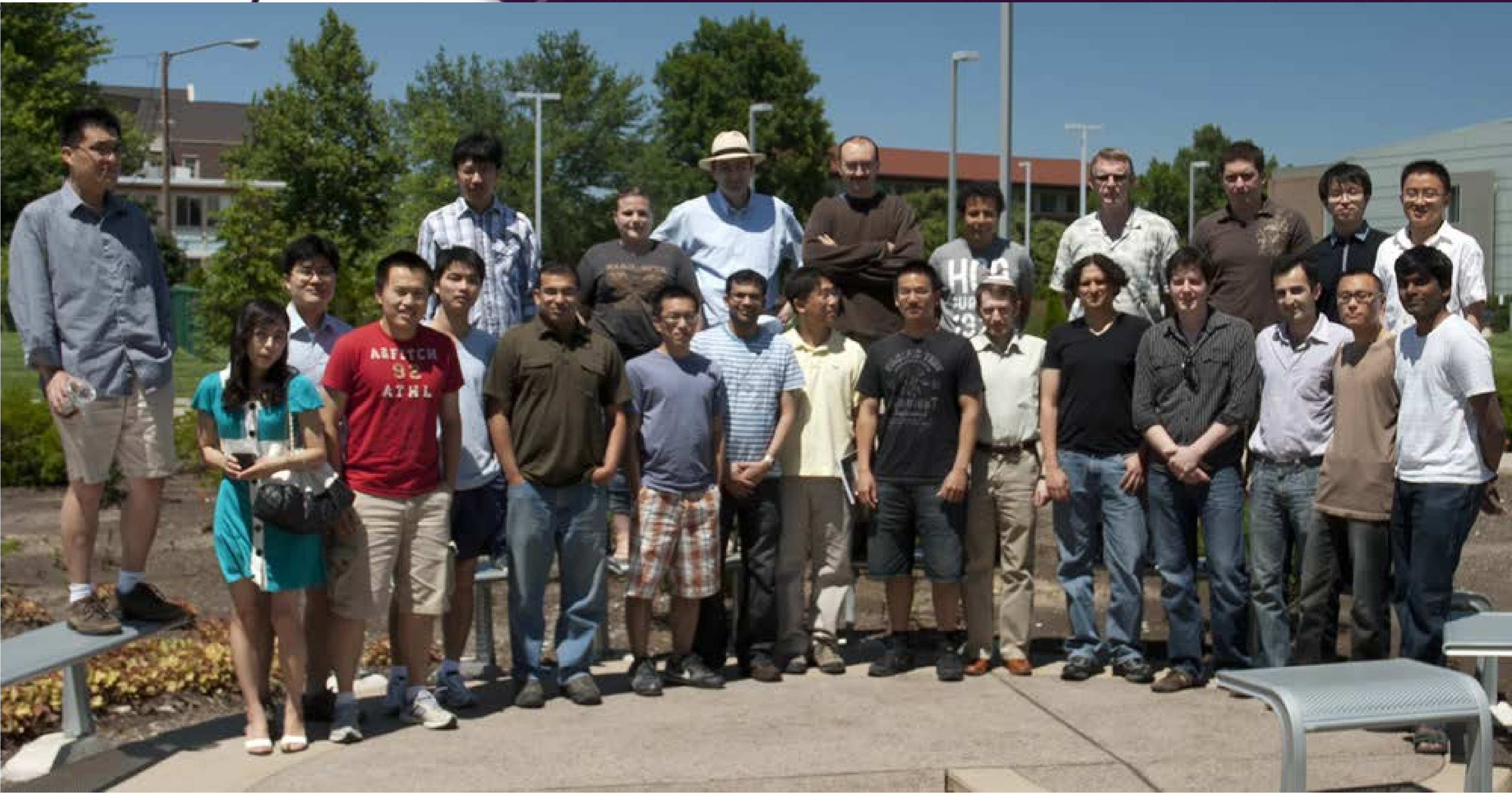
    \- professionals:

    T. Kubis, M. Povolotsky, J. Fonseca, B. Novakovic, A. Ajoy, H-H Park, S. Steiger

    \- students:

    Tarek Ameen, James Charles, Junzhe Geng, Kaspar Haume, Yu He, Ganesh Hegde, Yuling Hsueh, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Hyun Park, Ahmed Reza, Mehdi Salmani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, Evan Wilson,

Thanks to



Research Group
@Purdue
@NASA JPL 1998-2003
@Texas Instruments 1994-1998

NEMO Agenda, Funding, and Leverage

Industrial Use

GLOBAL FOUNDRIES
intel
SAMSUNG
IBM

LEAST LOW ENERGY SYSTEMS TECHNOLOGY

MIND MIDWEST INSTITUTE FOR NANOELECTRONICS DISCOVERY

NRI

Tunneling Transistors GaN, MoS_2

Industrial Development

SRC

NEMO
-Why?
-What?

FCRP

Focus Center MSD

FAME

Contacts, HEMTs

28,600 users

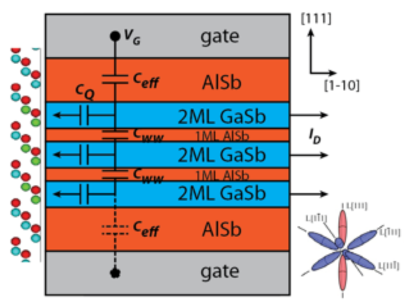
NSF-NCN

NSF

NSF-NEB

Science to Shape the Future of the Army — Army Research Office 1951

Peta-Scale NSF-OCI Computing



Quantum Computing

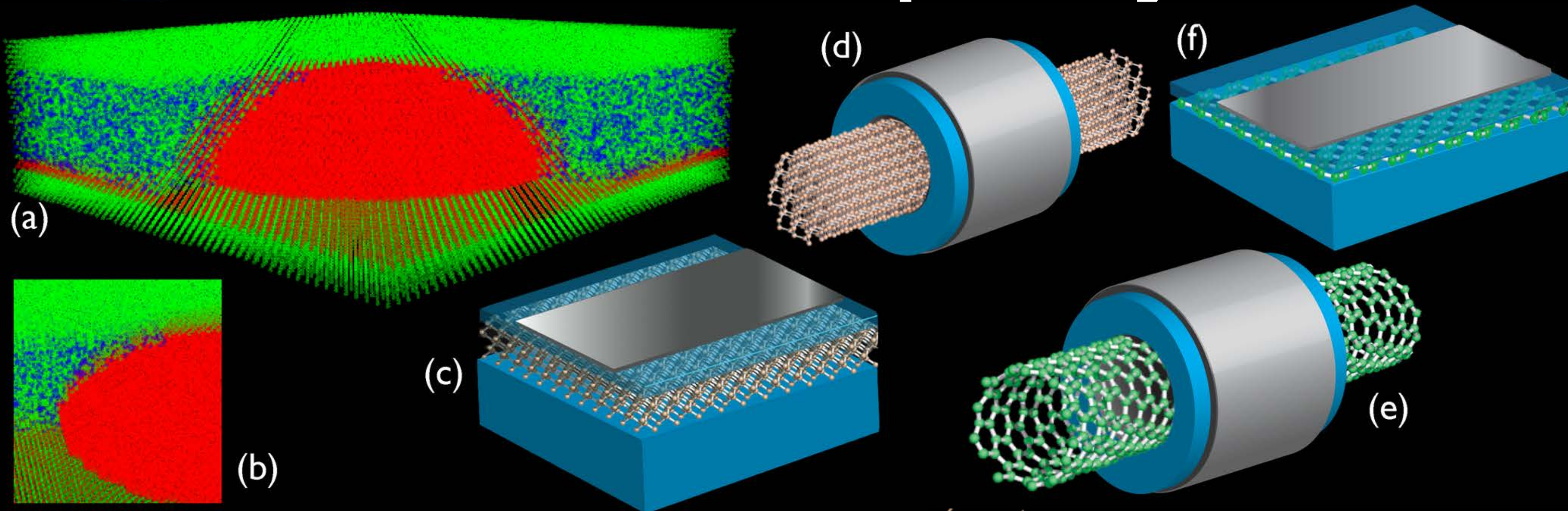
nature nanotechnology

A single-atom transist...

Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa...
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard...

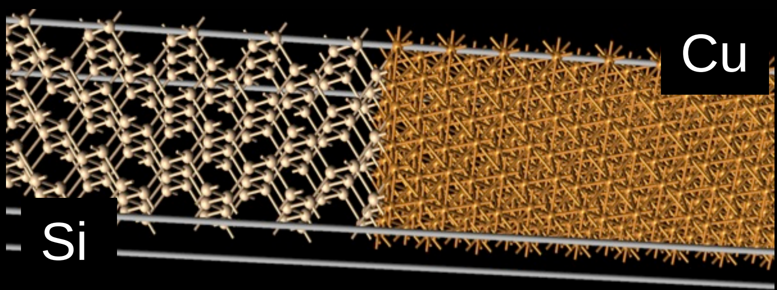
The ability to control matter at the atomic scale and build...

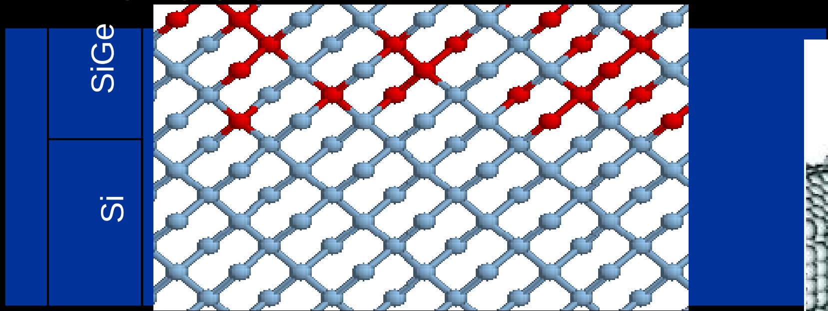
Broad Capability Overview

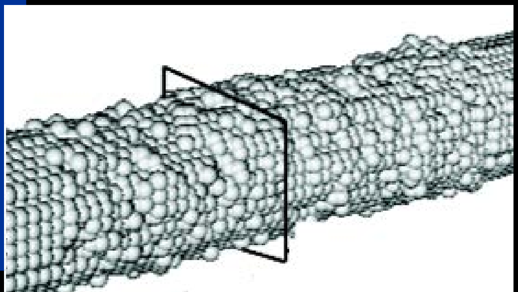


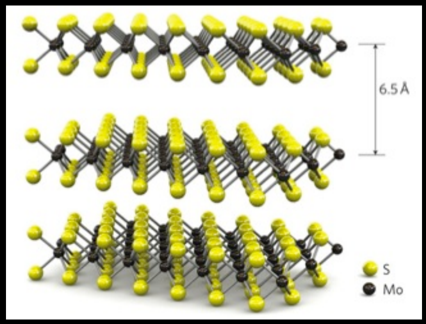
24 years development

- Texas Instruments
- NASA JPL
- Purdue

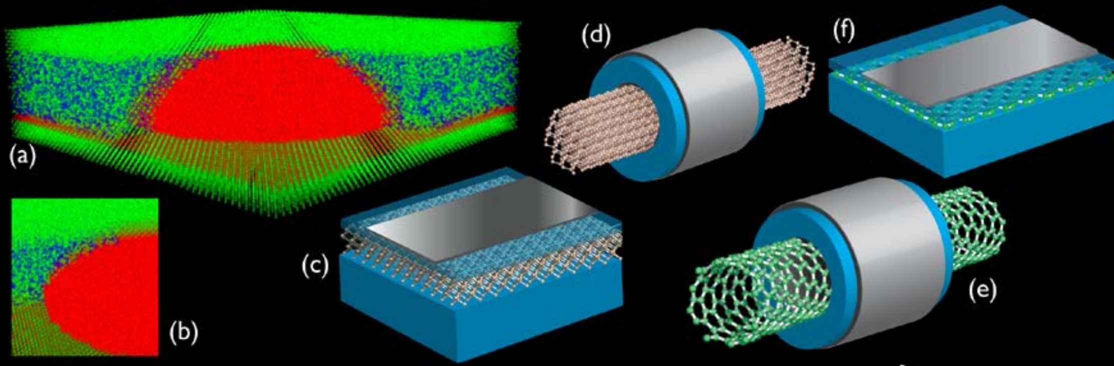






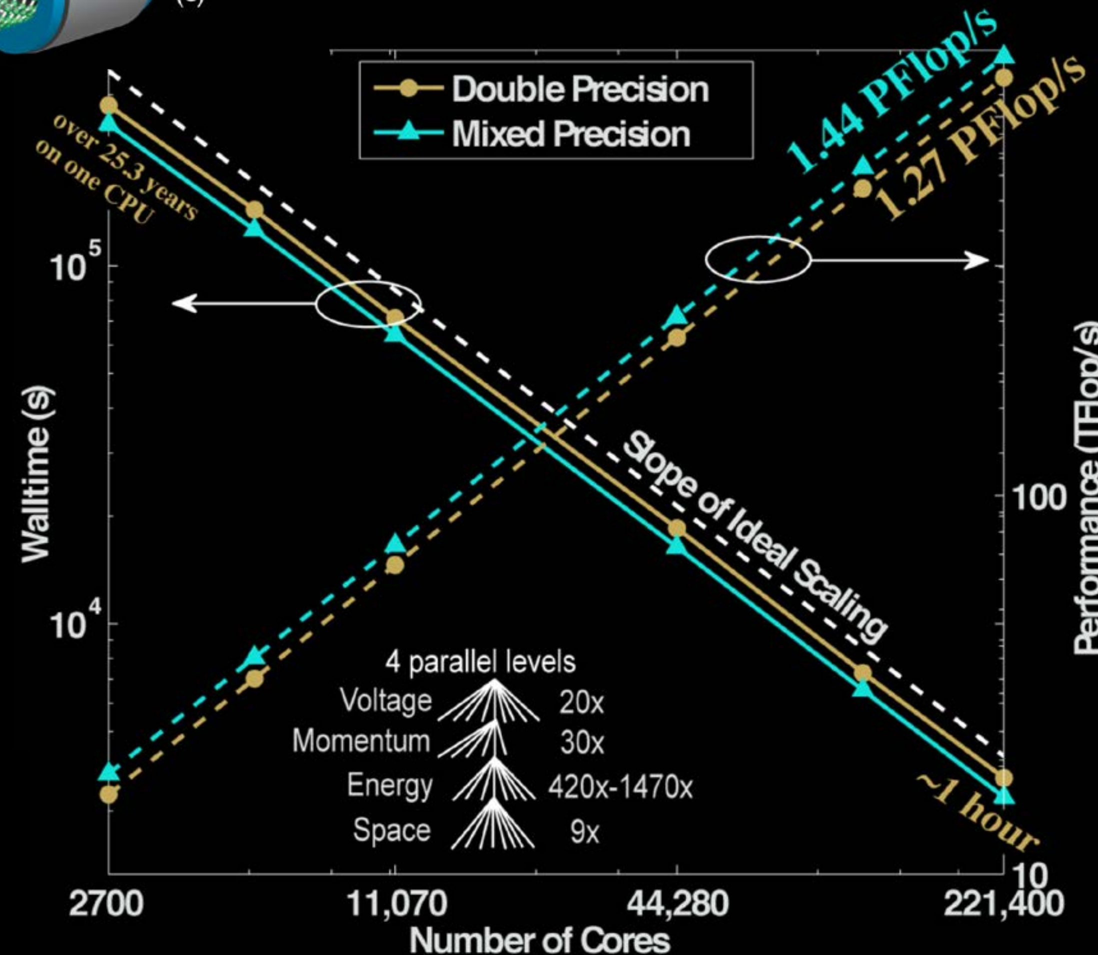


High Performance Computing with NEMO/OMEN



24 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering



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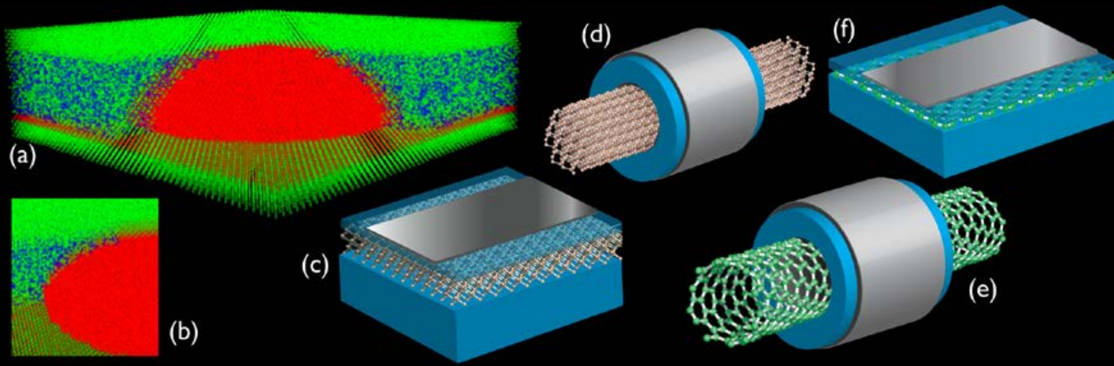
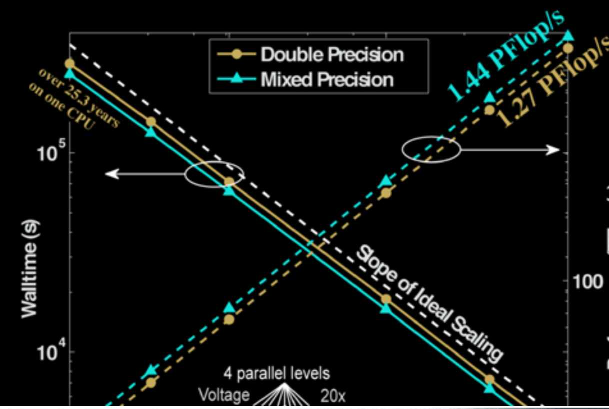
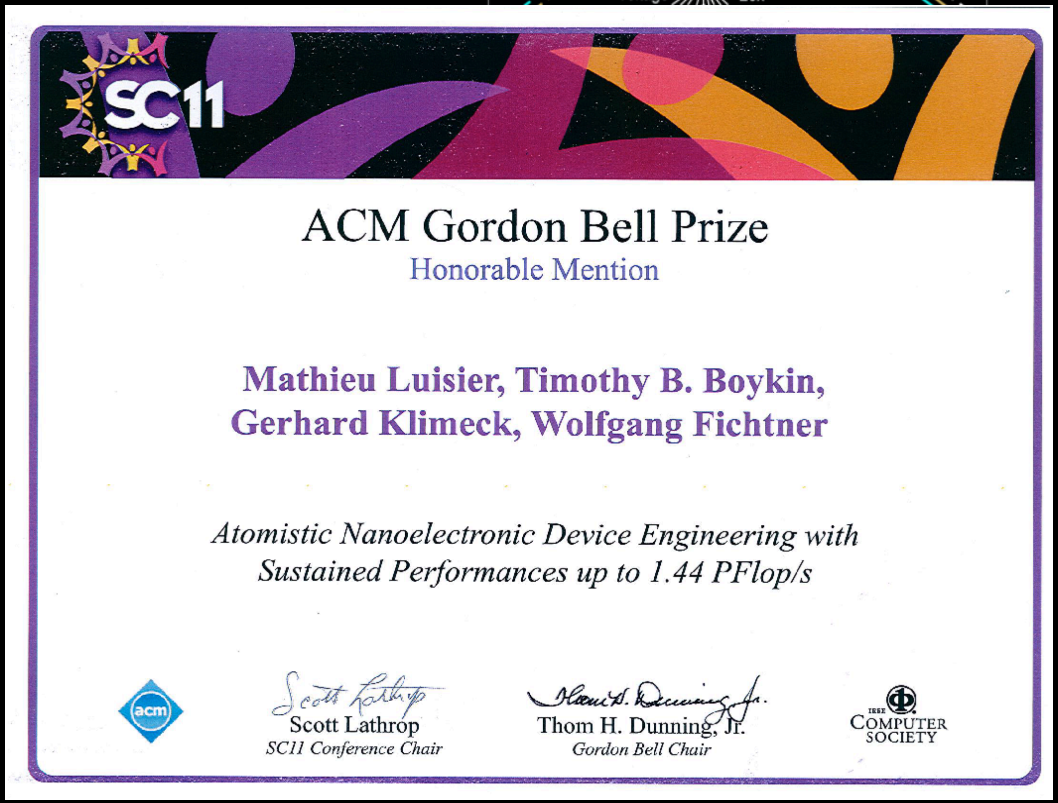


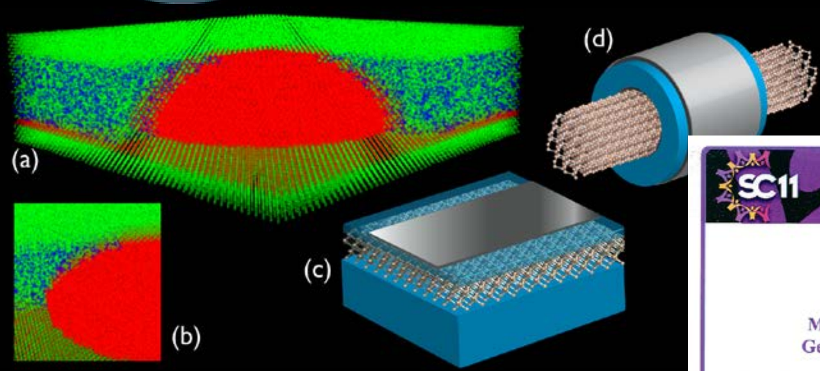


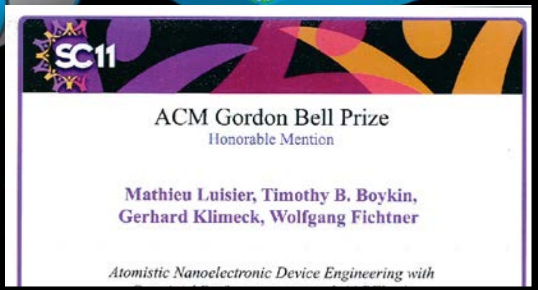
24 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell



Basic Science

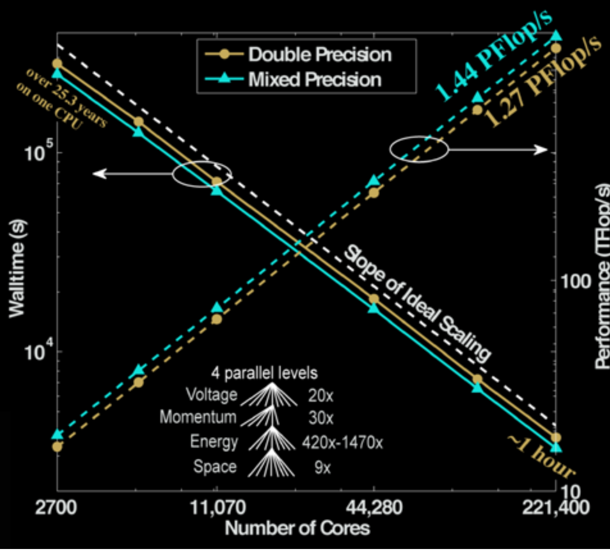


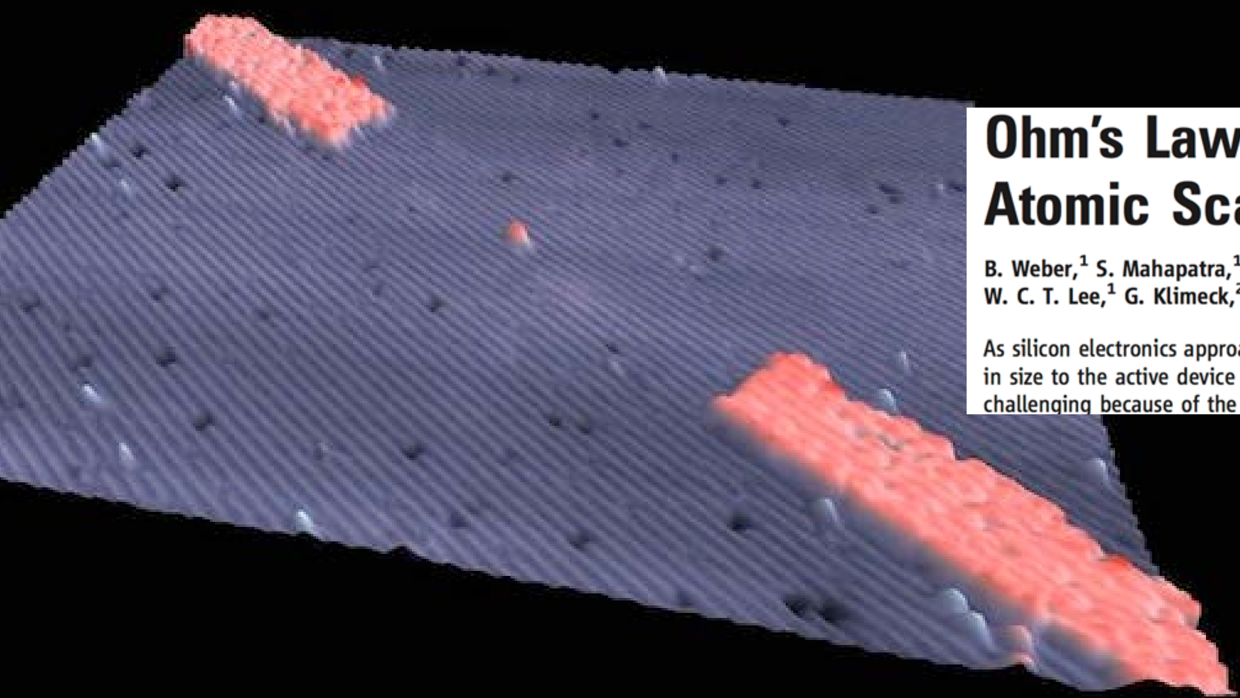


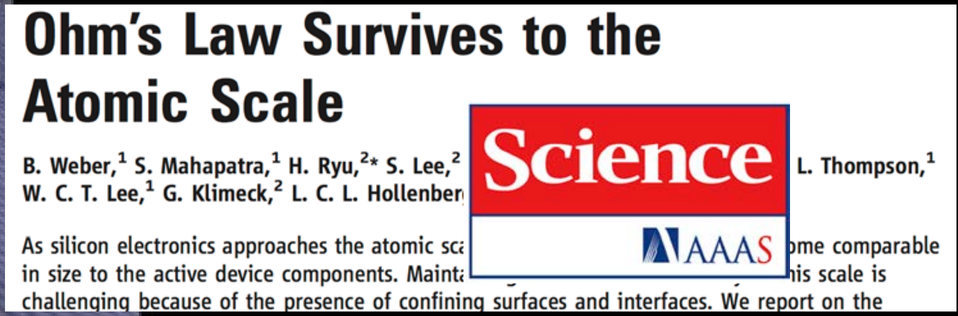
ACM Gordon Bell Prize
Honorable Mention

Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, Wolfgang Fichtner

Atomistic Nanoelectronic Device Engineering with



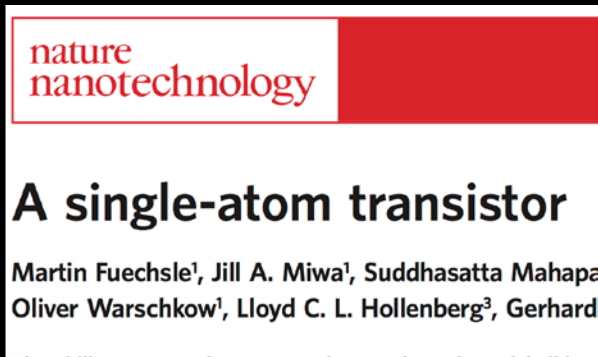




Ohm's Law Survives to the Atomic Scale

B. Weber,[1] S. Mahapatra,[1] H. Ryu,[2]* S. Lee,[2] ... L. Thompson,[1] W. C. T. Lee,[1] G. Klimeck,[2] L. C. L. Hollenber...

As silicon electronics approaches the atomic sc... ...ome comparable in size to the active device components. Maint... ...his scale is challenging because of the presence of confining surfaces and interfaces. We report on the



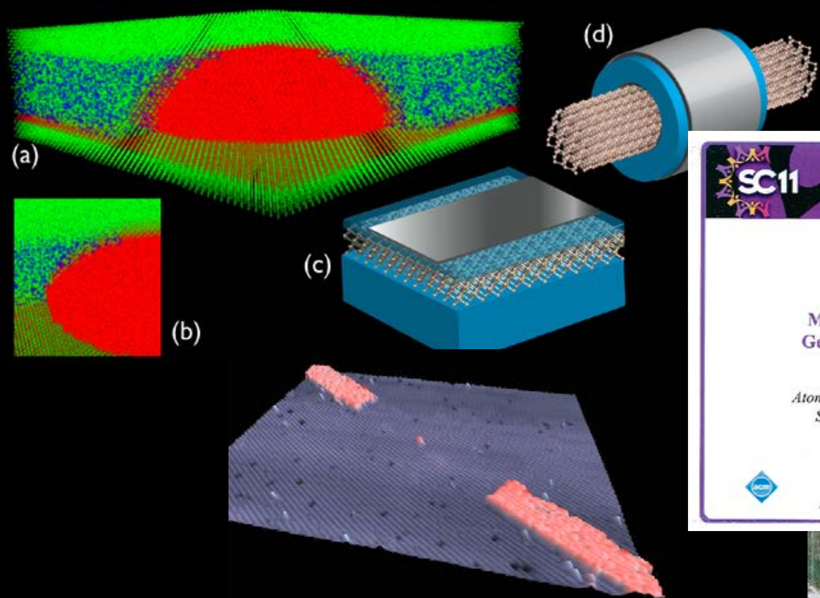
nature nanotechnology

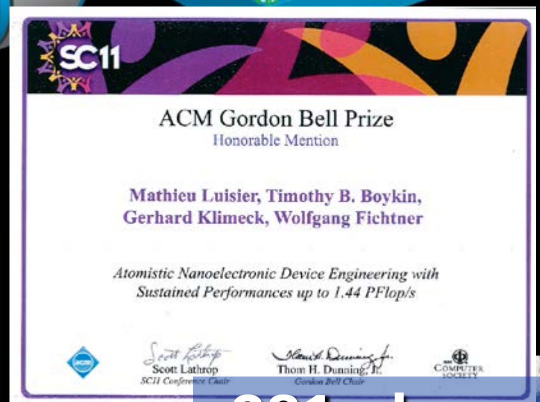
A single-atom transistor

Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa...
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard...

- Science, Nature Nano

Broad Usage



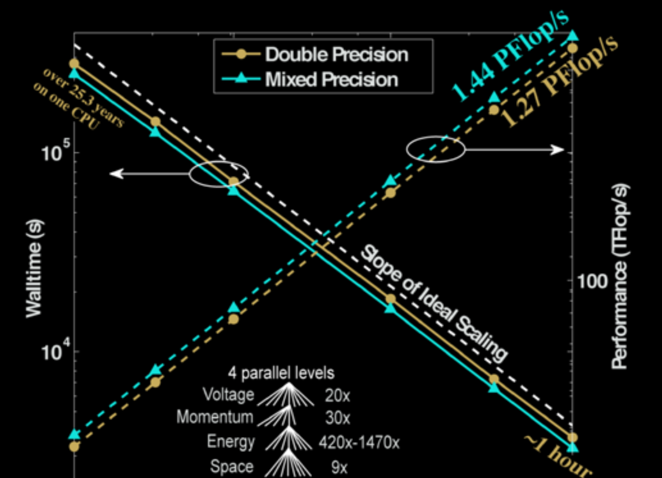

SC11

ACM Gordon Bell Prize
Honorable Mention

Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, Wolfgang Fichtner

Atomistic Nanoelectronic Device Engineering with Sustained Performances up to 1.44 PFlop/s

Scott Lathrop, SC11 Conference Chair
Thom H. Dunning, Jr., Gordon Bell Chair



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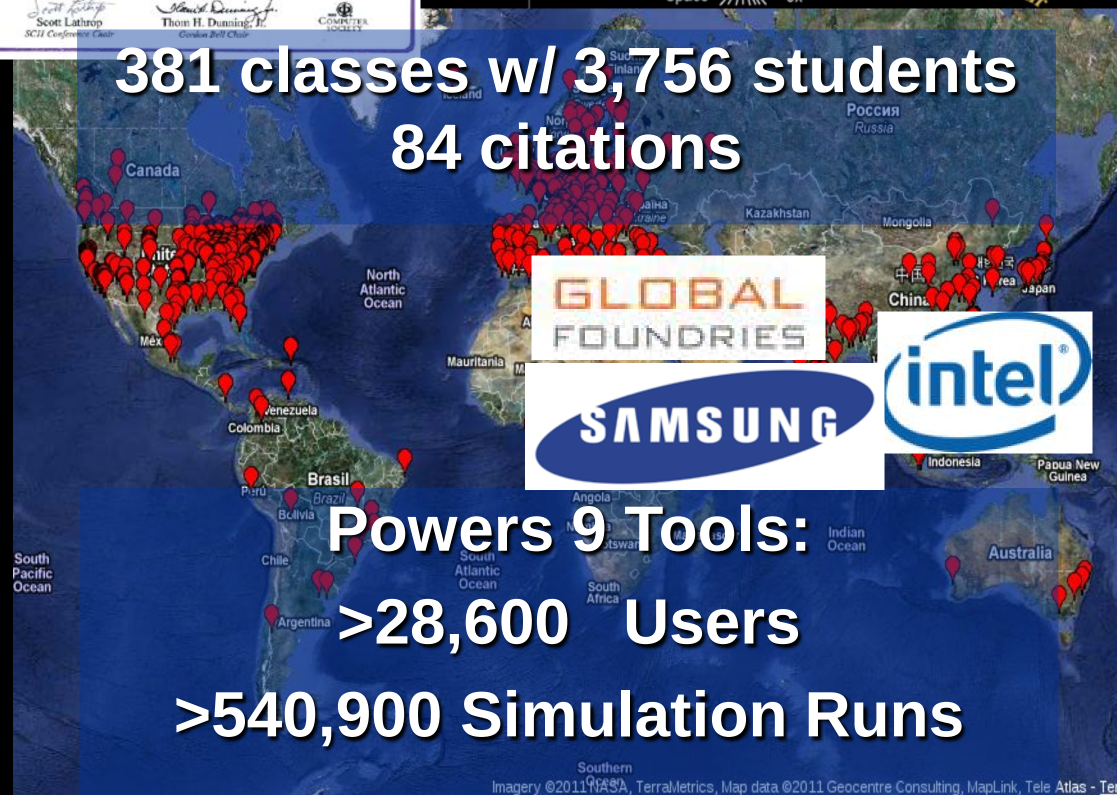
- Peta-scale Engineering
- Gordon Bell
- Science, Nature Nano



381 classes w/ 3,756 students
84 citations

Powers 9 Tools:
>28,600 Users
>540,900 Simulation Runs

Outline

- Device trends and NEMO Modeling Agenda
- Bandstructure Concepts
  - » Revisit some “old” bandstructure concepts (ancient RTDs)
  - » Bandstructure in Si nanowires
  - » Bandstructure and transport in Alloy Wires
  - » Bandstructure in SiGe wires
- Source Drain Tunneling for Lg<10nm
- Hole Mobility in SiGe nanowires / FinFETs
- Metal-Semiconductor interfaces

Lot's of Other Exciting Things but not enough time…

MOSFETs
- Bulk Scattering in NEGF
- Scattering in nanowires and UTBs

Steep SS FETs
- Tunneling FETS in III-V
- Tunneling FETs in III-N
- Superlattice FETs
- New 2D materials - TMDs

Optical Devices
- Quantum dots
- LEDs in Nitrides

Thermal transport
- Phonon transport across interfaces

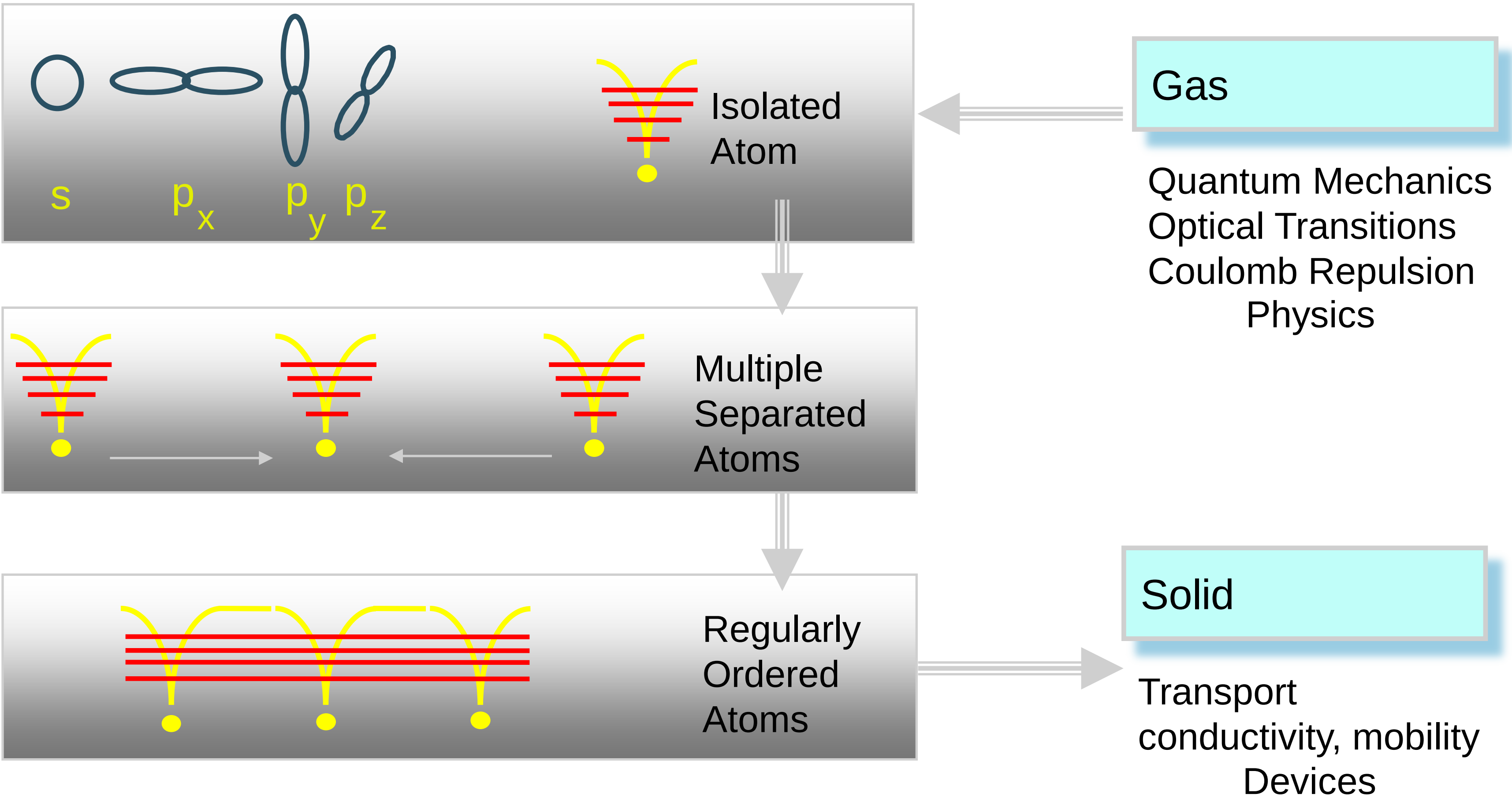
Metals
- Grain boundary scattering

Fundamental Science
- Single impurity devices
- Decoherence in quantum computing

Method Development
- Mode space
- Basis state development
- NEMO5 ⇔ Wannier ⇔ DFT
- NEMO5 ⇔ Huckel ⇔ DFT
- NEMO5 ⇔ TB ⇔
- HPC – Phi/GPU deployment
- HPC scalability

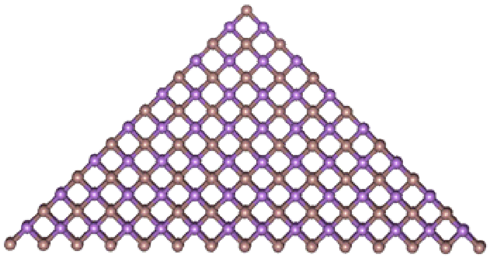
- User interface development

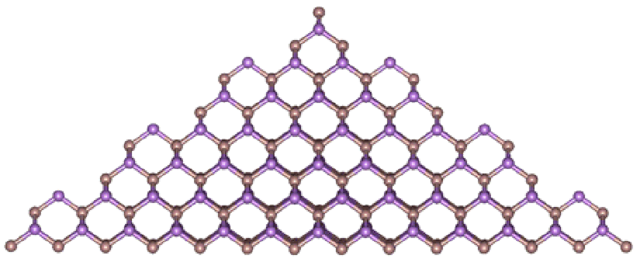
In Nanoelectronics we need to think of atoms!

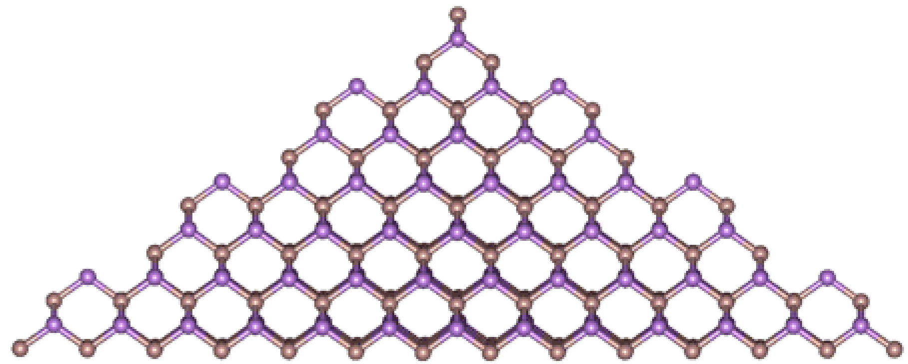


- Bands are channels in which electrons move “freely”.

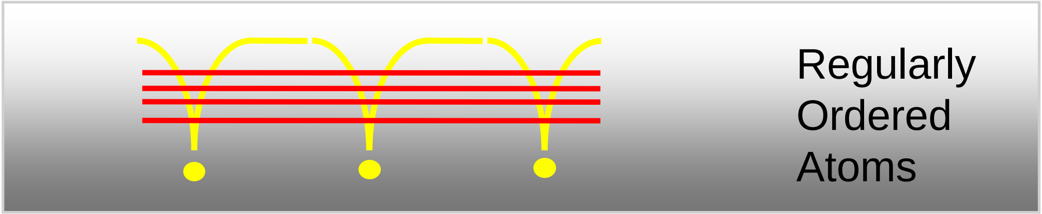
Crystals are NOT isotropic





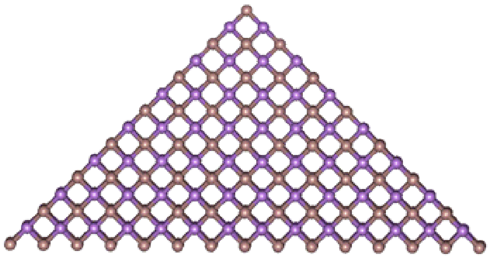


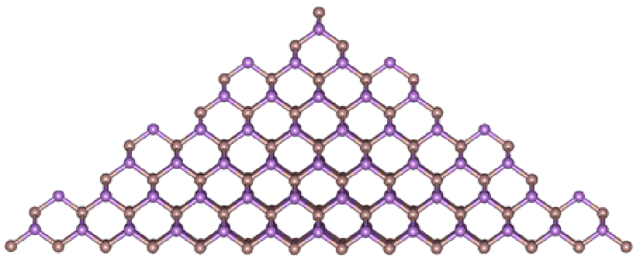
- Crystal is not symmetric in all directions!

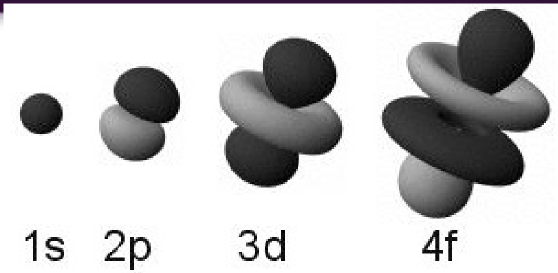


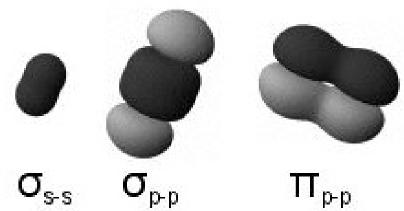
- Bands are channels in which electrons move “freely”.

NEMO5 Bonds and Orbitals are NOT isotropic

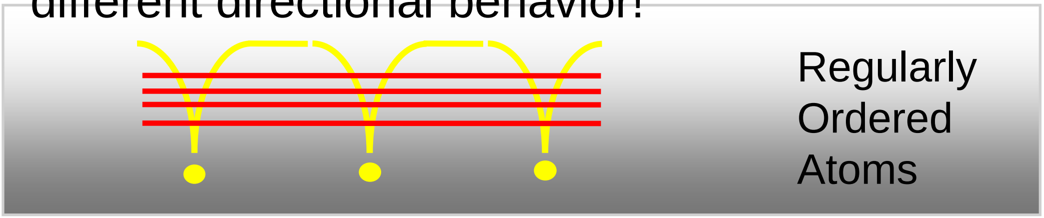








- Crystal is not symmetric in all directions!
- Orbitals on each atom give electrons different directional behavior!



Schrödinger Eq.

$$H\Psi = E\Psi$$

Ansatz: Plane Waves

$$\Psi \propto e^{ikr}$$

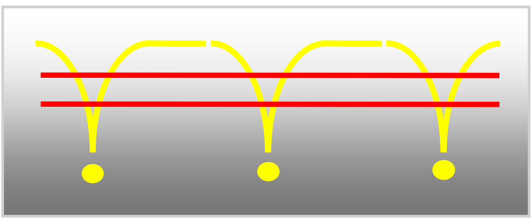
$$E = fct(k)$$

- Bands are channels in which electrons move “freely”.
- What does “free” propagation really mean?

We usually throw all details away

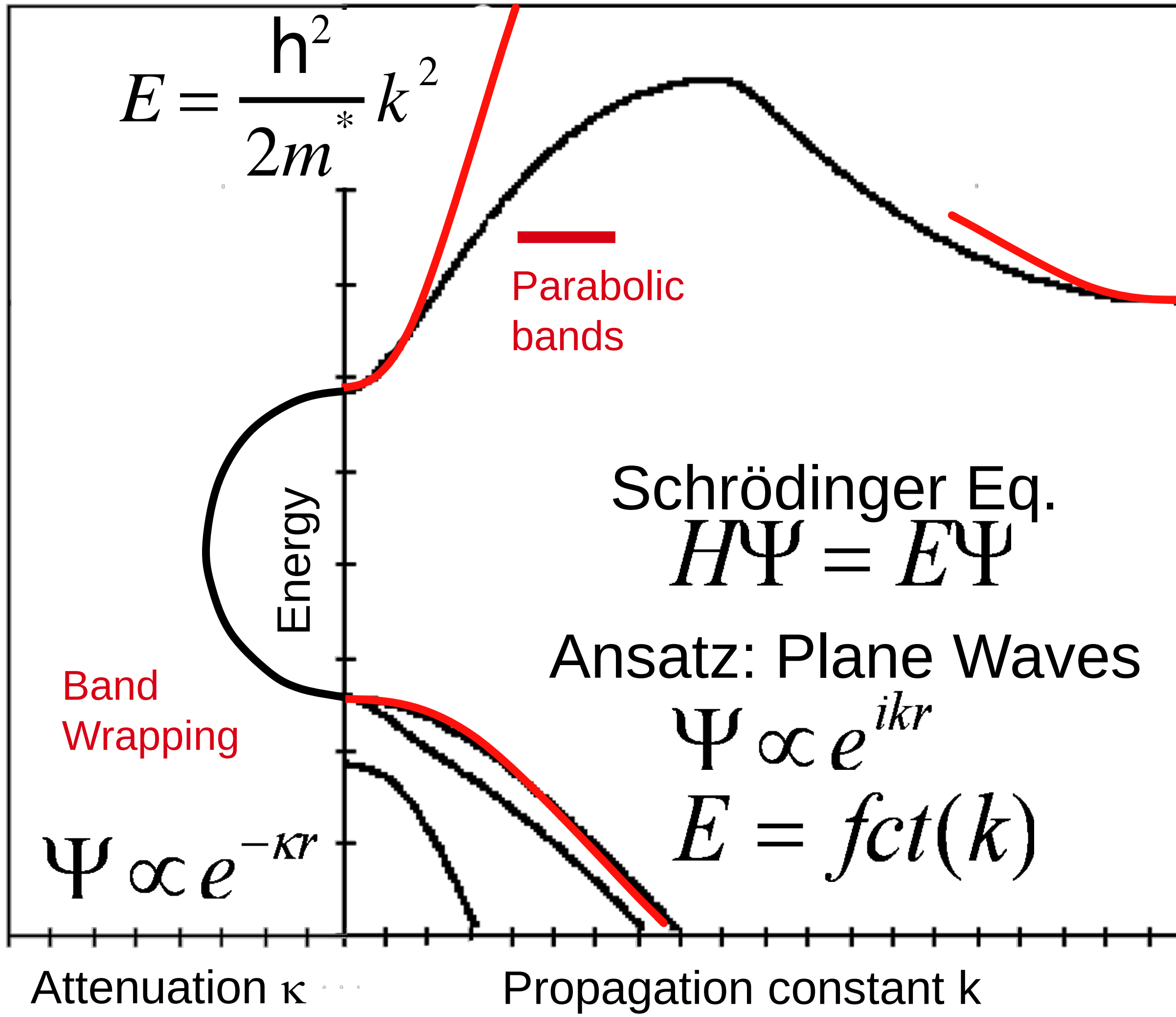
Realistic Material Properties:
- Non-parabolic cond. band
- States outside Γ at X, L
- Non-trivial valence band
- Coupled bands

Typical Assumption:
- Decoupled bands
- Parabolic bands



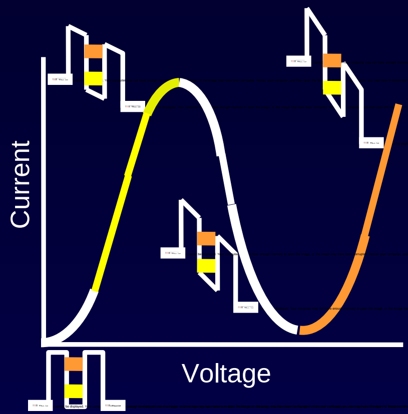
Well-Established:
- Ec, m* describes it all
  $\mu = \mu_0\ \tau\alpha\upsilon/m^*$
- Drift diffusion simulators
- Boltzmann Transport sim.
- Quantum transport sim.

Will Fail:
- Bands are coupled
- Material variations on nm-scale

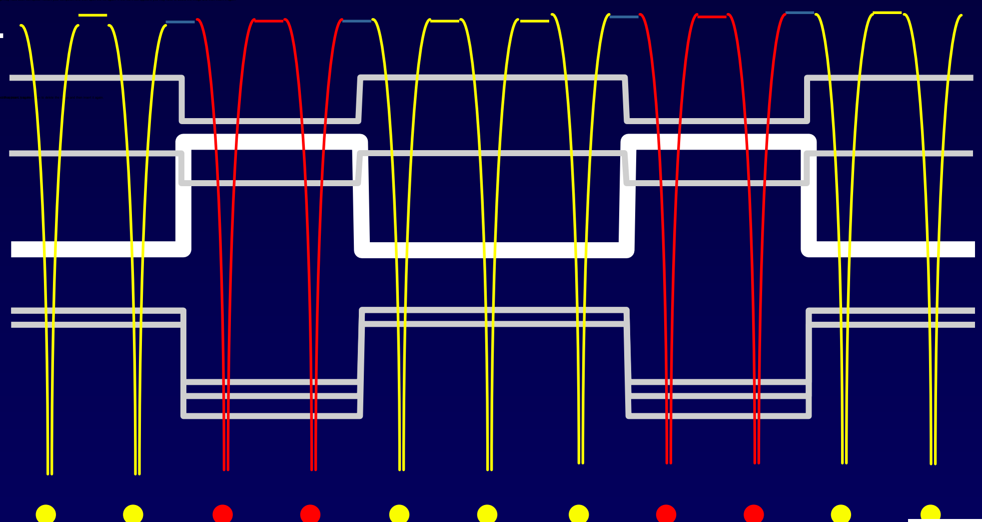


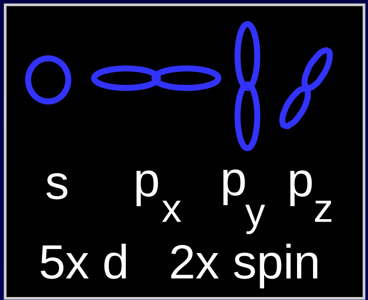
NEMO 1-D Resonant Tunneling Diode Simulation
Atomistic Representation is the Key!

Atomistic   Basis Sets



Concepts

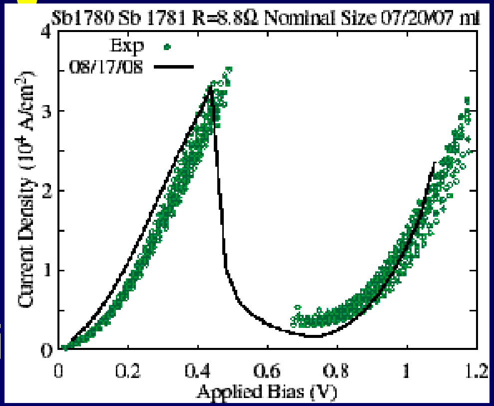




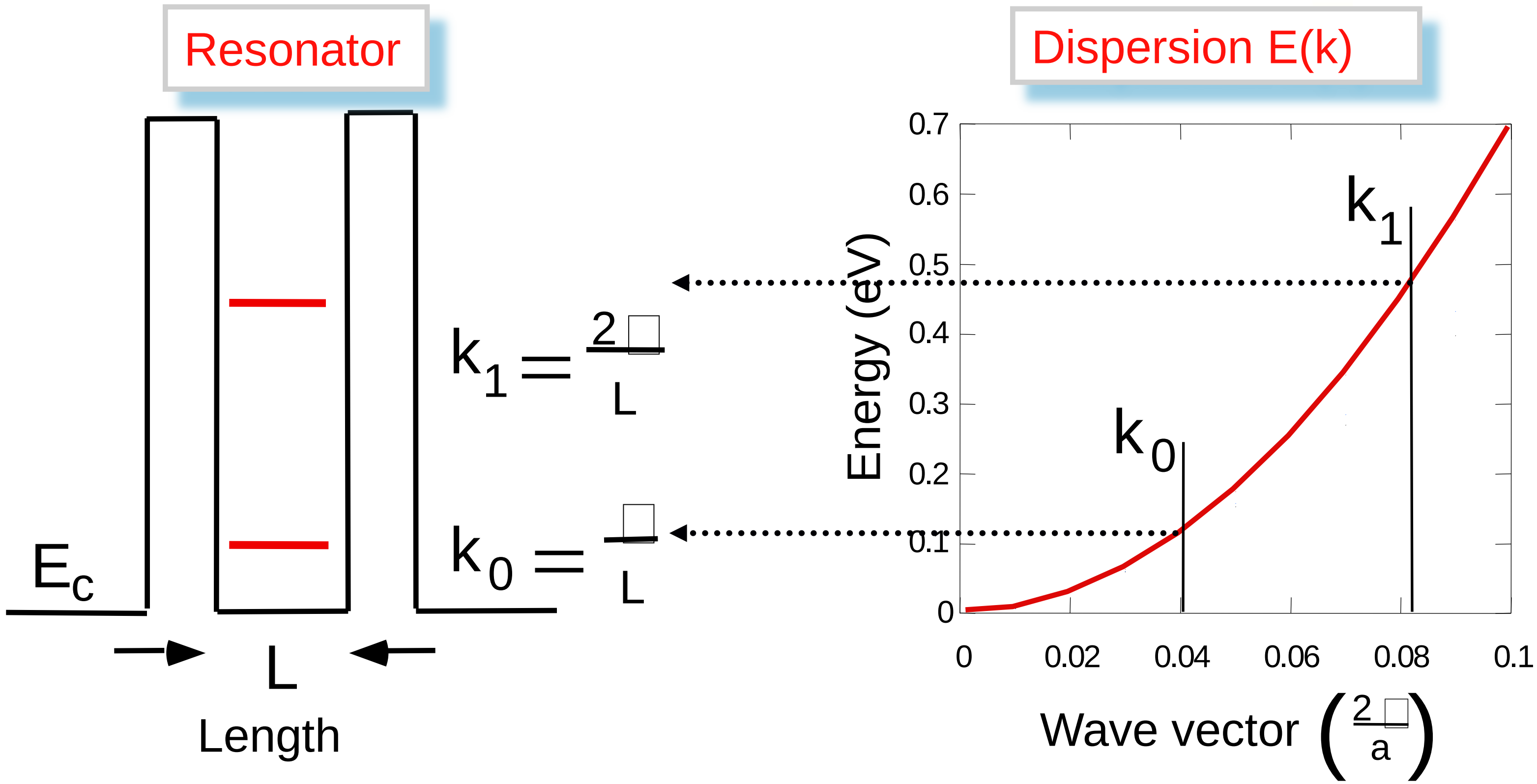
Usually considered a device
This is also a new material!

Empirical Tight Binding
makes the connection between
materials and devices!

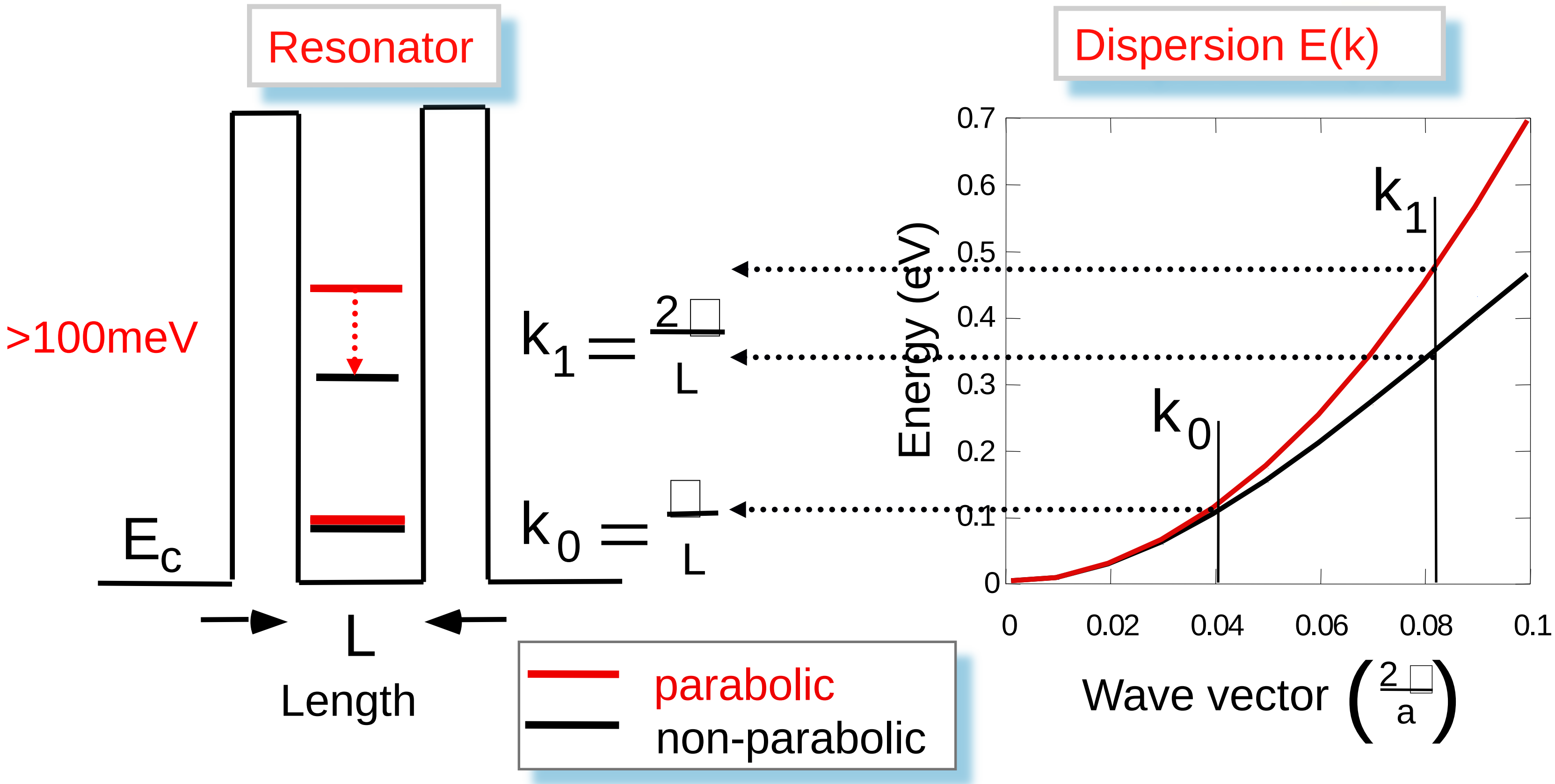
Quantitative Engineering:
Design, Analysis, Synthesi



Resonator State Quantization

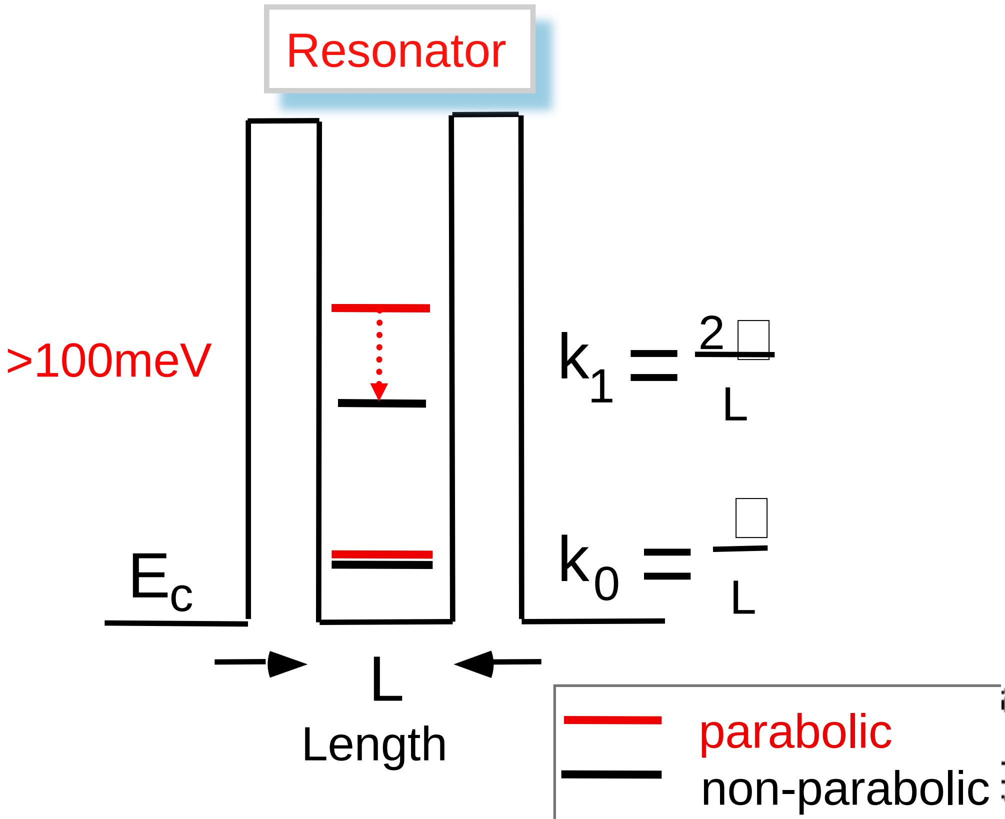


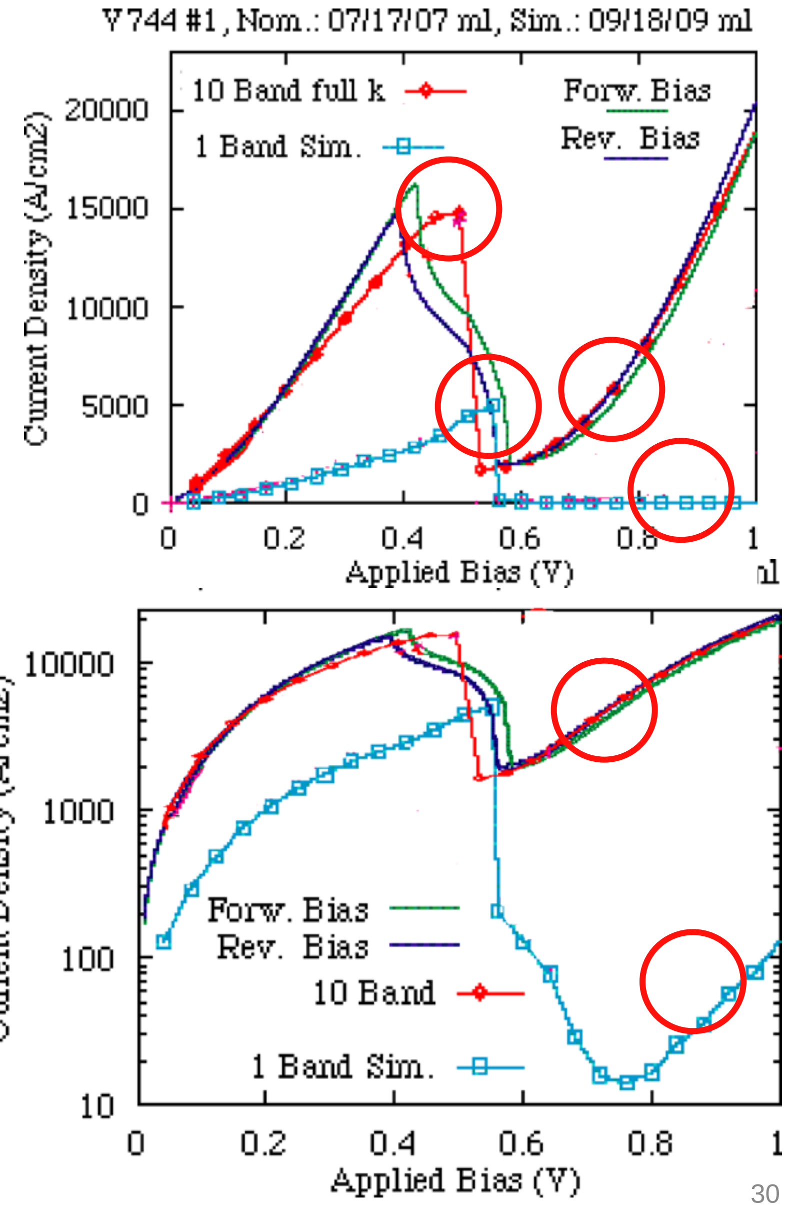
Resonator State Quantization
Effects of Band Non-Parabolicity



- Second state lowered by >100mev ~ 4kT

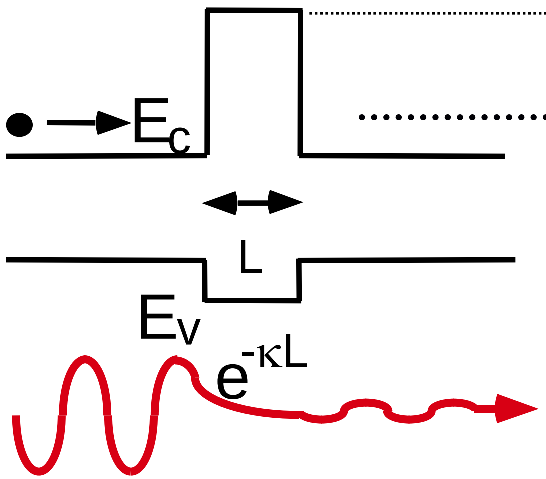
Effects of Band Non-Parabolicity on I-V Characteristics

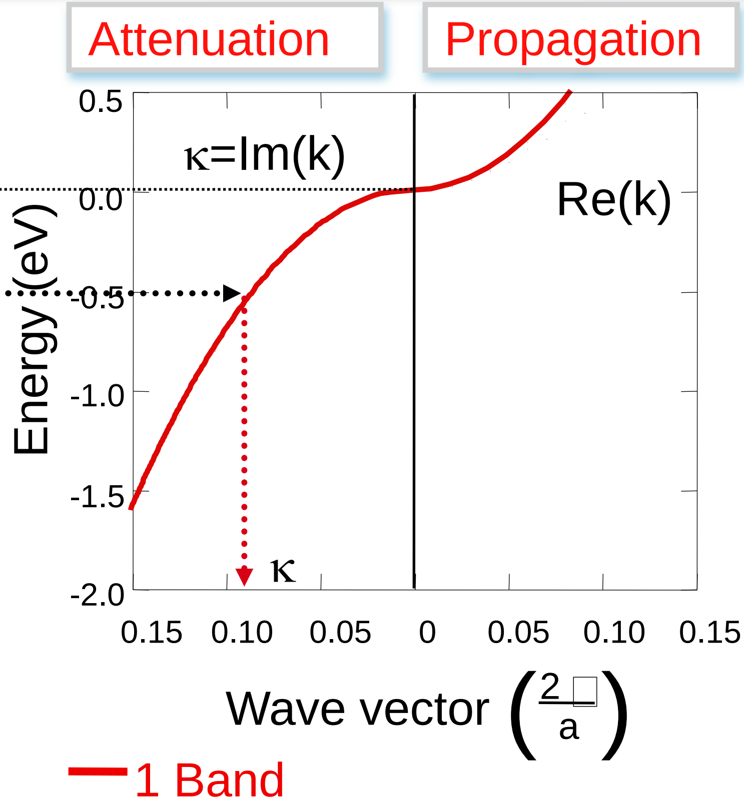




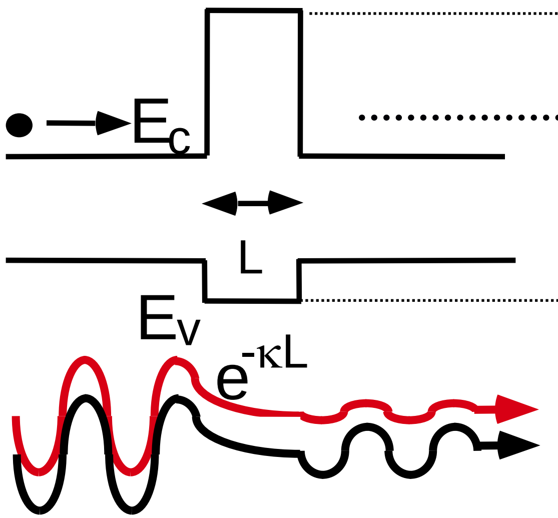
- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations
- k_0 about equal - Why is peak current different?

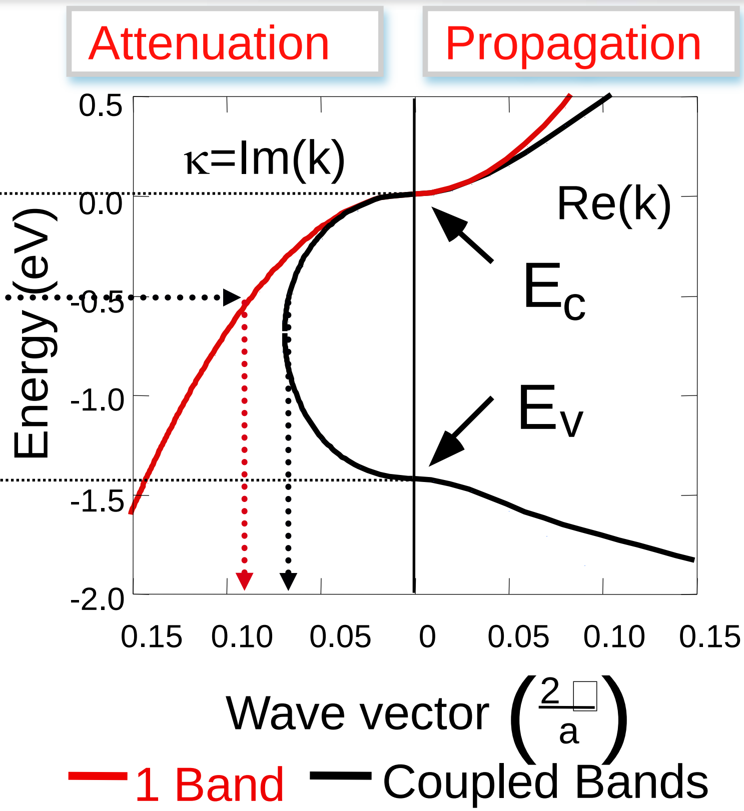
Wave Attenuation in Barriers
Single Parabolic Band



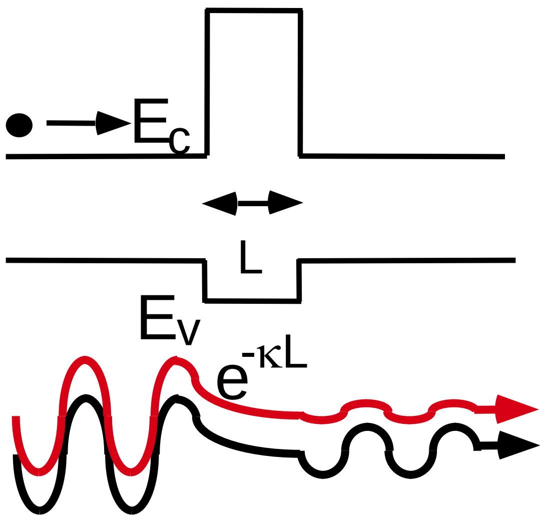


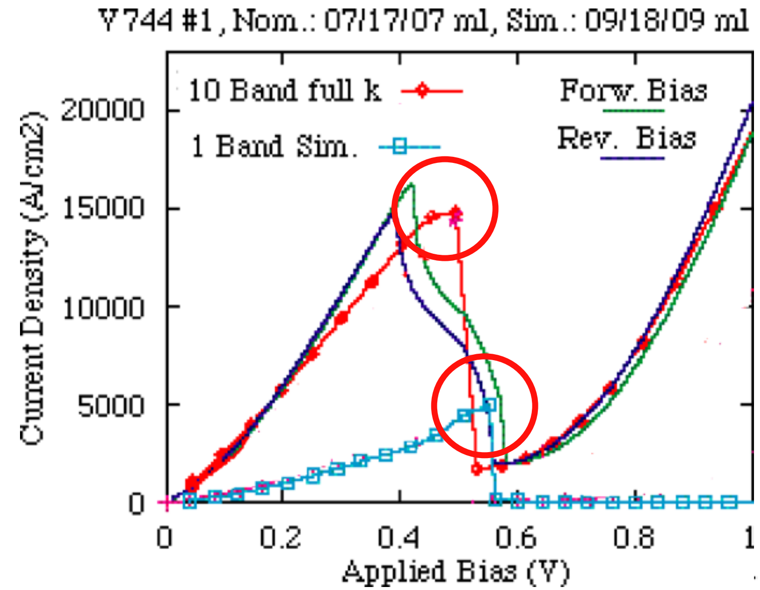
Wave Attenuation in Barriers Coupled Bands

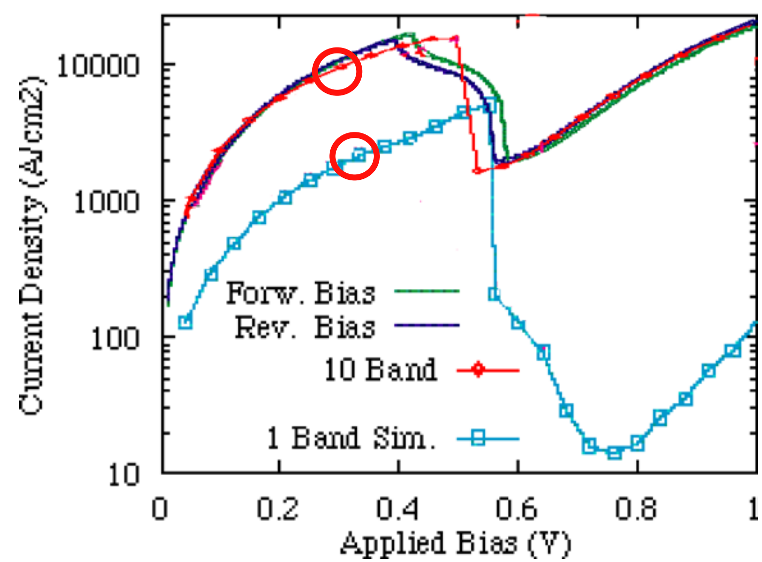




Band Warping in Barriers
Impact on I-V Characteristics







Non-Parabolicity:

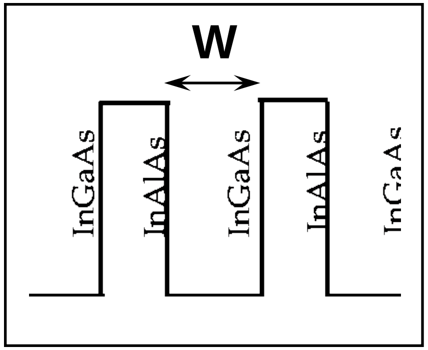
- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations

Complex Band Coupling:

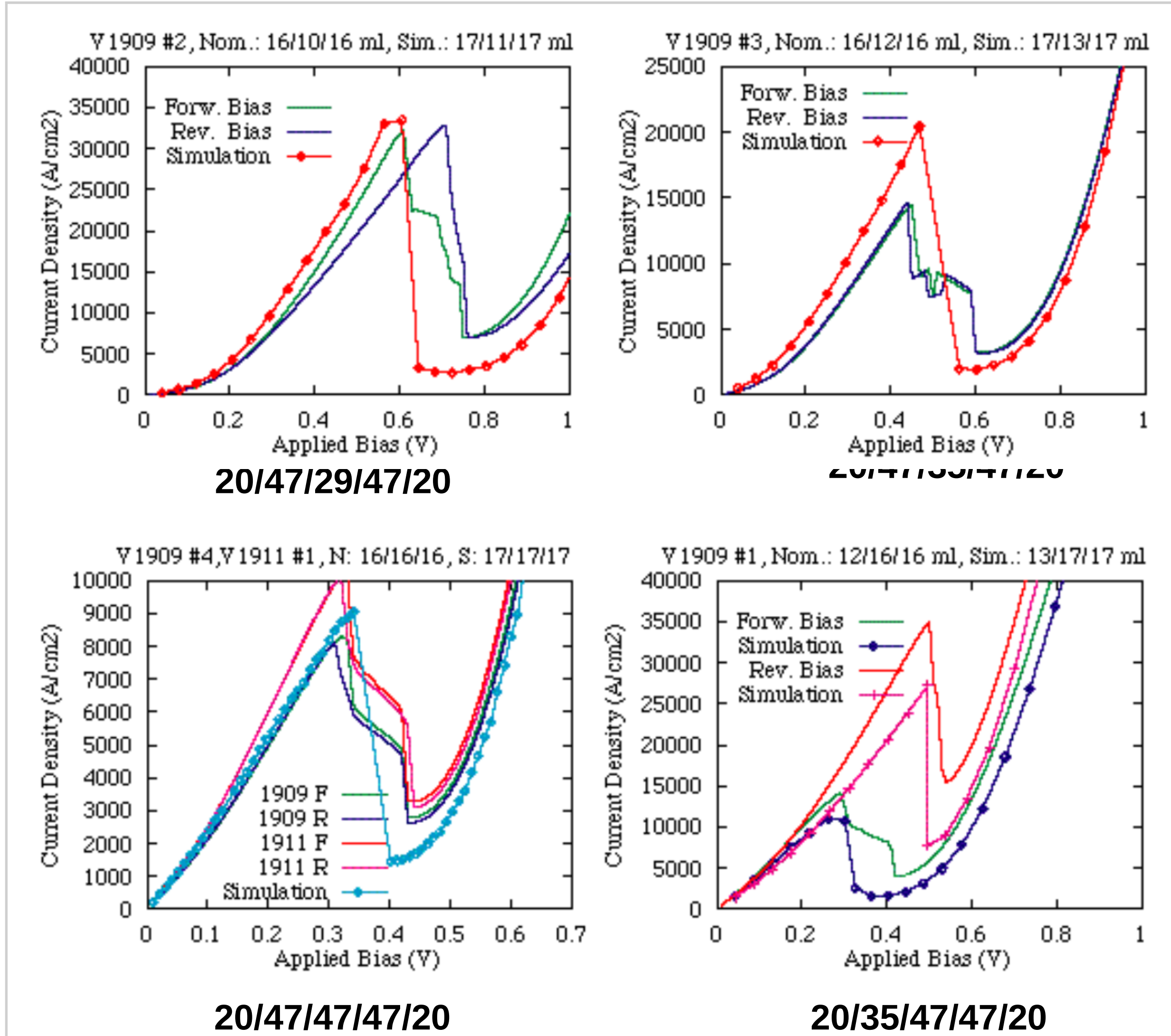
- RTD more transparent - correct peak current

4 Stack RTD with Well Width Variation

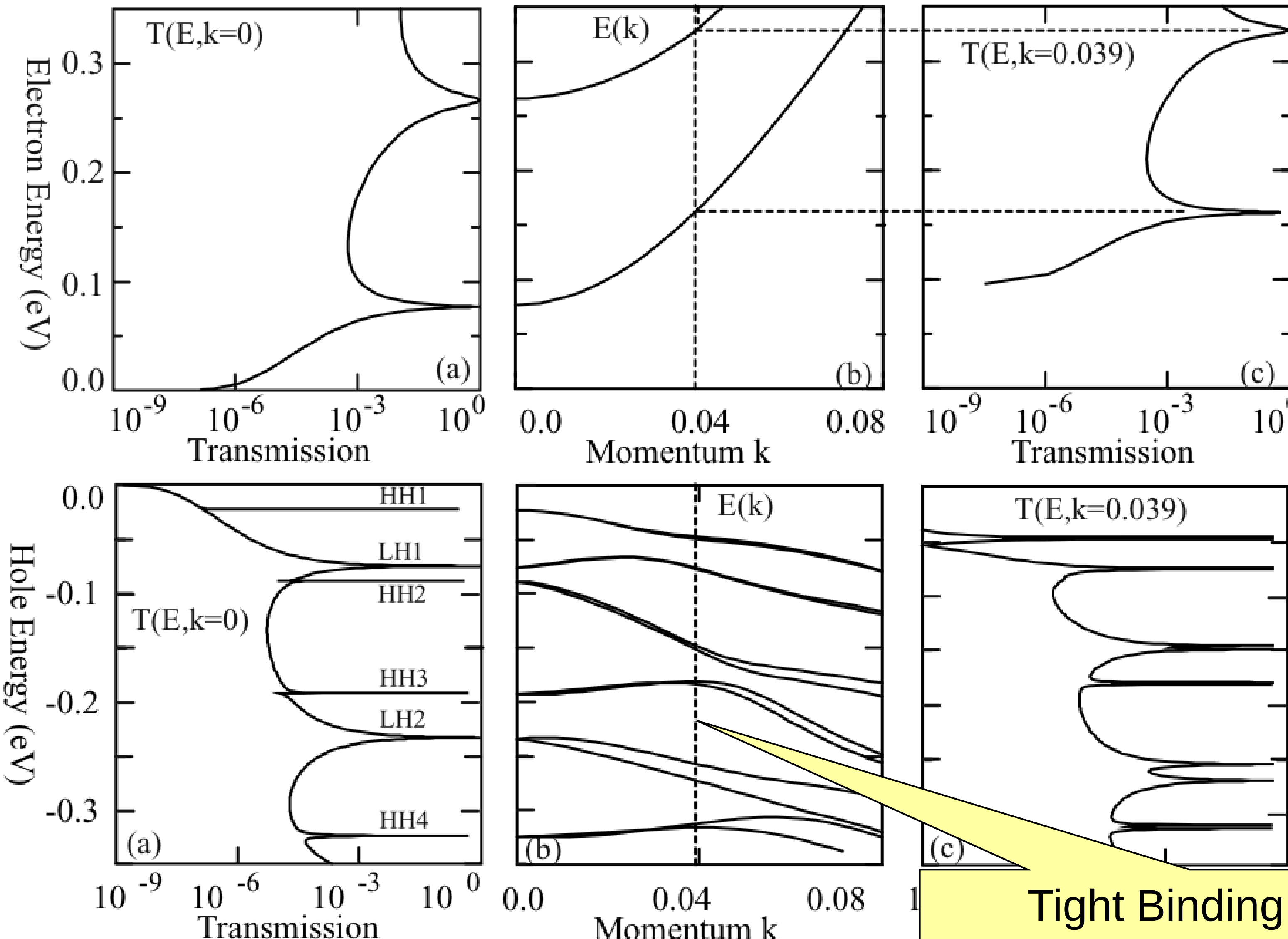
Vary Well Width

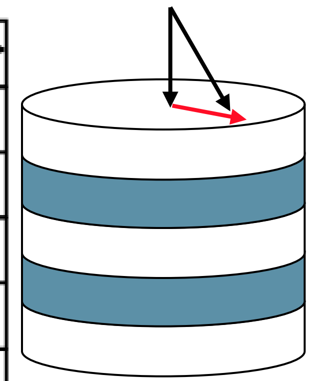


- Three nominally symmetric devices:
  47/29/47 A [1]
  47/35/47 A [2]
  47/47/47 A [3]
- One asymmetric device:
  35/47/47 A



Quantum Transport in non-parabolic, strained, and coupled bands



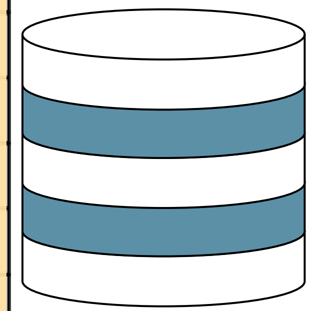


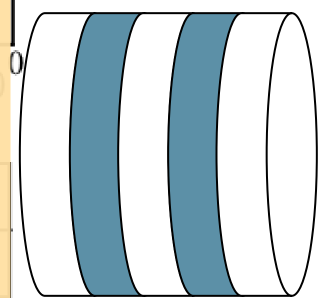
Electron:
- Dispersion looks parabolic, but is NOT
- Transmission looks replicated, but is NOT

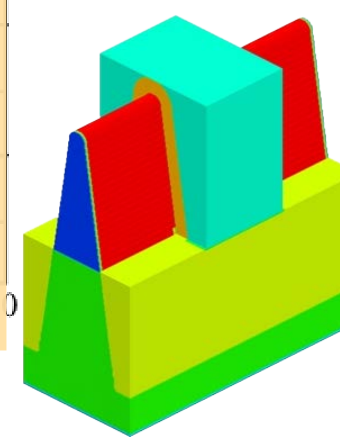
Holes:
- LH, HH, SO coupled
- Dispersion "complicated"
- Transmission dramatically

Tight Binding Handles Coupling Between Bands Strain, Non-Parabolicity

- Bandstructure – atomistic device resolution
  - »Critical for understanding room temperature, high performance devices
  - »Effective mass leads to non-predictive and wrong conclusions
  - »Tight binding can handle electrons, holes, strain, band-coupling/mixing
  - »Modern transistors (Ultra-Thin bodies, nanowires, finFETs and quantum dots) look similar to RTD







Outline

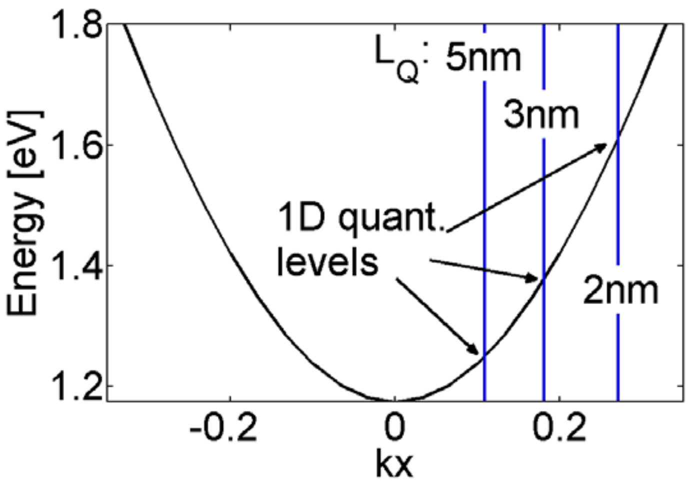
- Device trends and NEMO Modeling Agenda
- Bandstructure Concepts
  - » Revisit some “old” bandstructure concepts (ancient RTDs)
  - » Bandstructure in Si nanowires
- Source Drain Tunneling for Lg<10nm
- ~~Hole Mobility in SiGe nanowires / FinFETs~~
- Metal-Semiconductor interfaces

The effect of quantization

$$E_n = \frac{\hbar^2 \pi^2}{2 m_i L^2} \quad \text{(2D-quantization)}$$

$$E = \frac{\hbar^2 k^2}{2 m_i} \quad \text{(parabolic mass)}$$

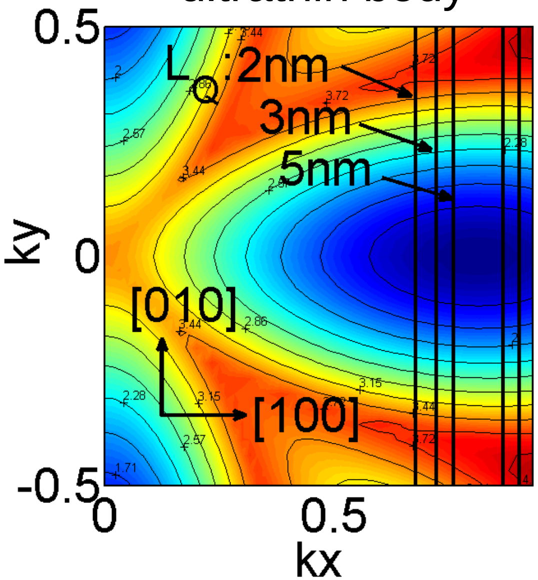
$$\rightarrow k = \frac{\pi}{L}$$



Abhijeet Paul

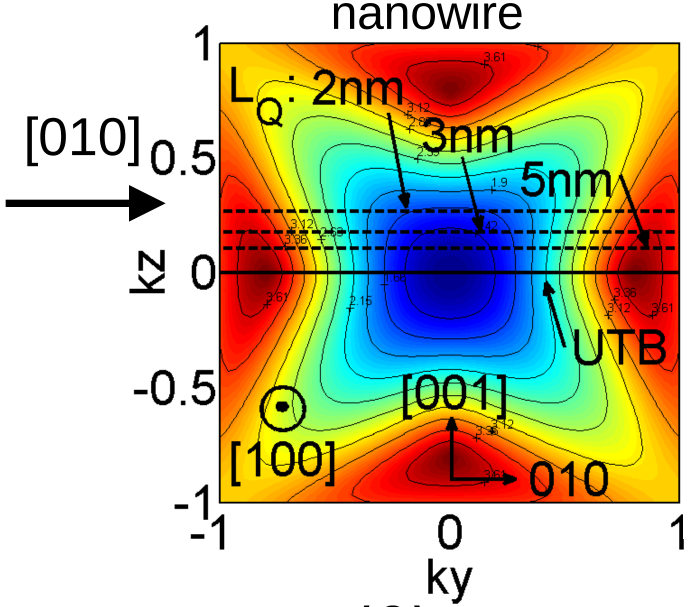
Quantization and Anisotropy

Quantized in 1 dimension
ultrathin body

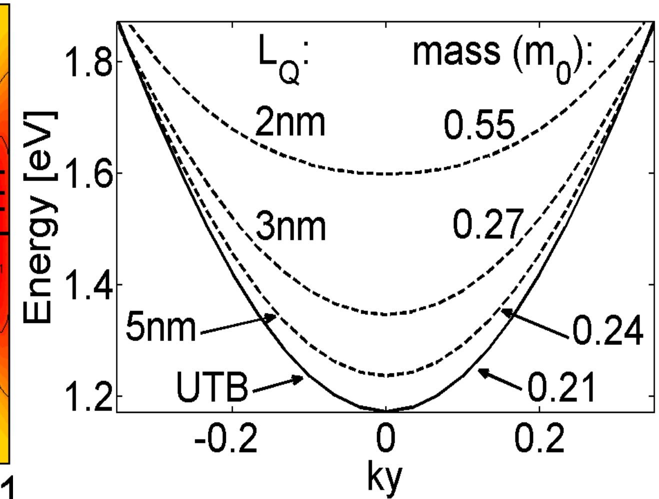


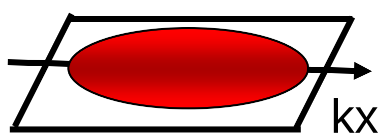
(b)

Quantized in 2 dimensions
nanowire

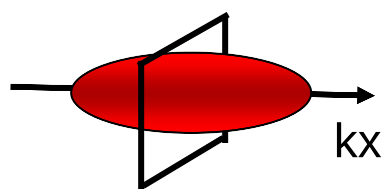


(c)

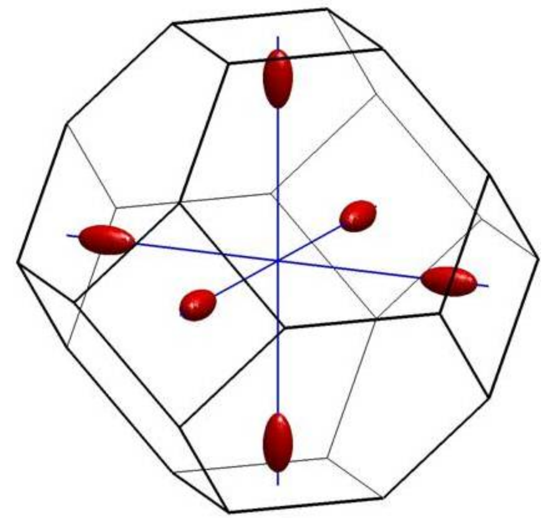




“Cut” through the ellipsoid (x-y plane)

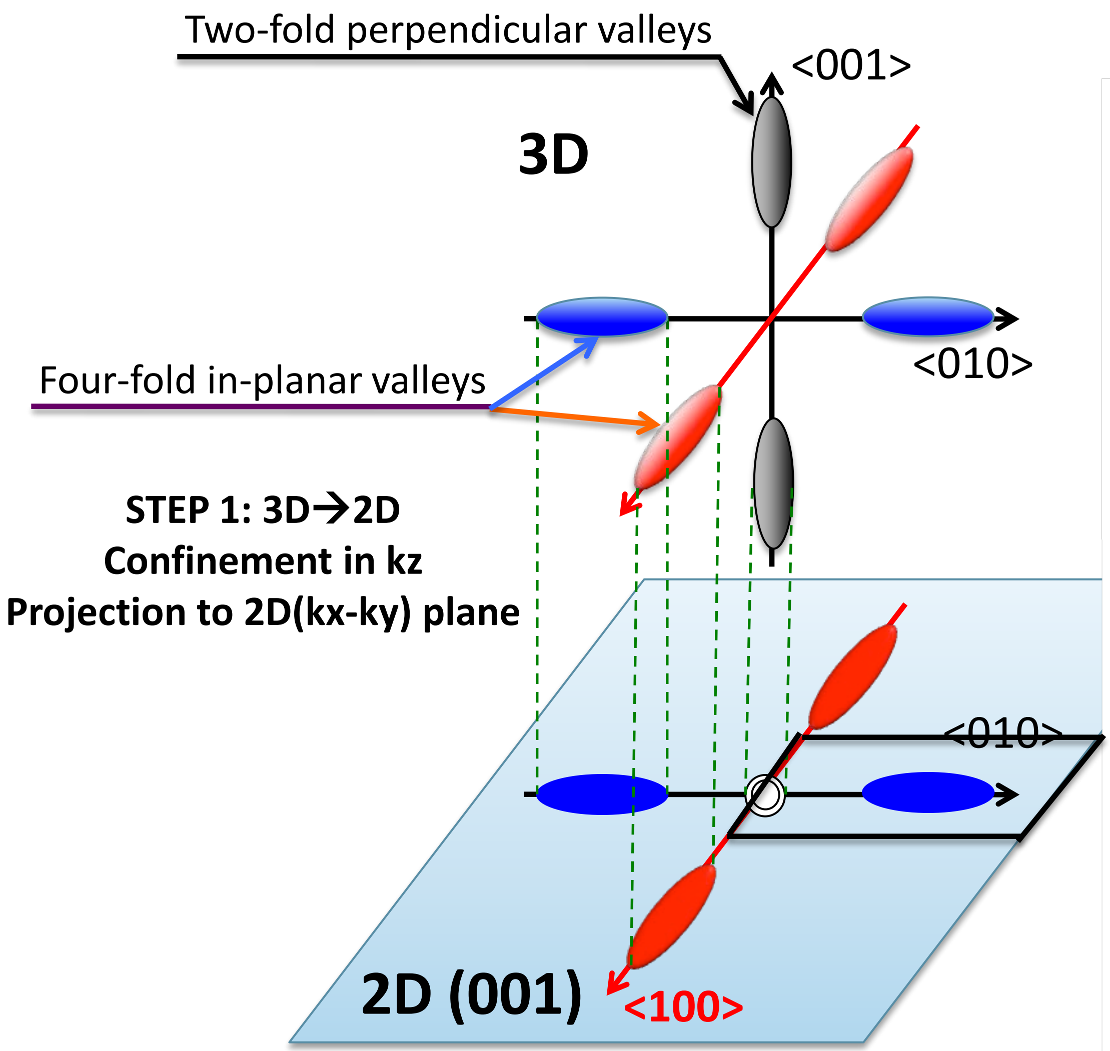


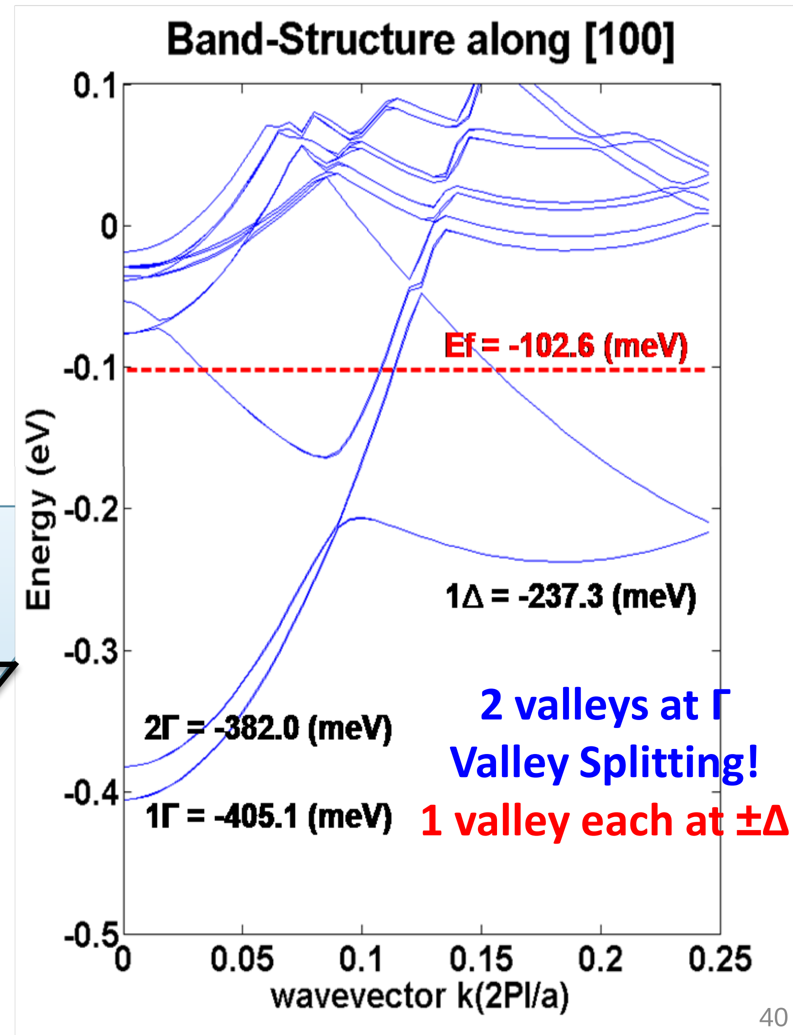
Cut through the 3nm kx line



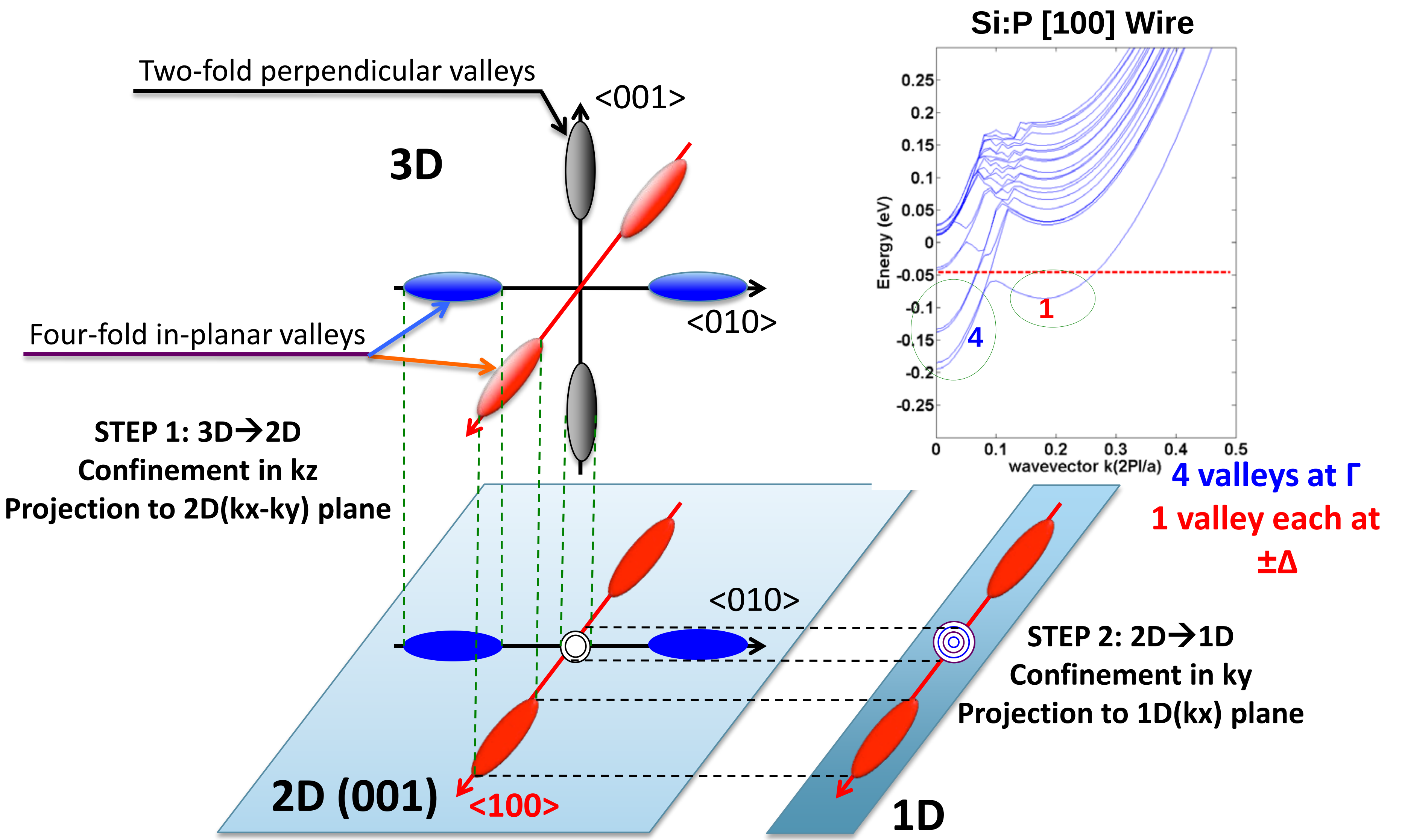
Band Projection in [100] Si:P Quantum Wells

- **3D→2D projection of Si [100] into a quantum well**



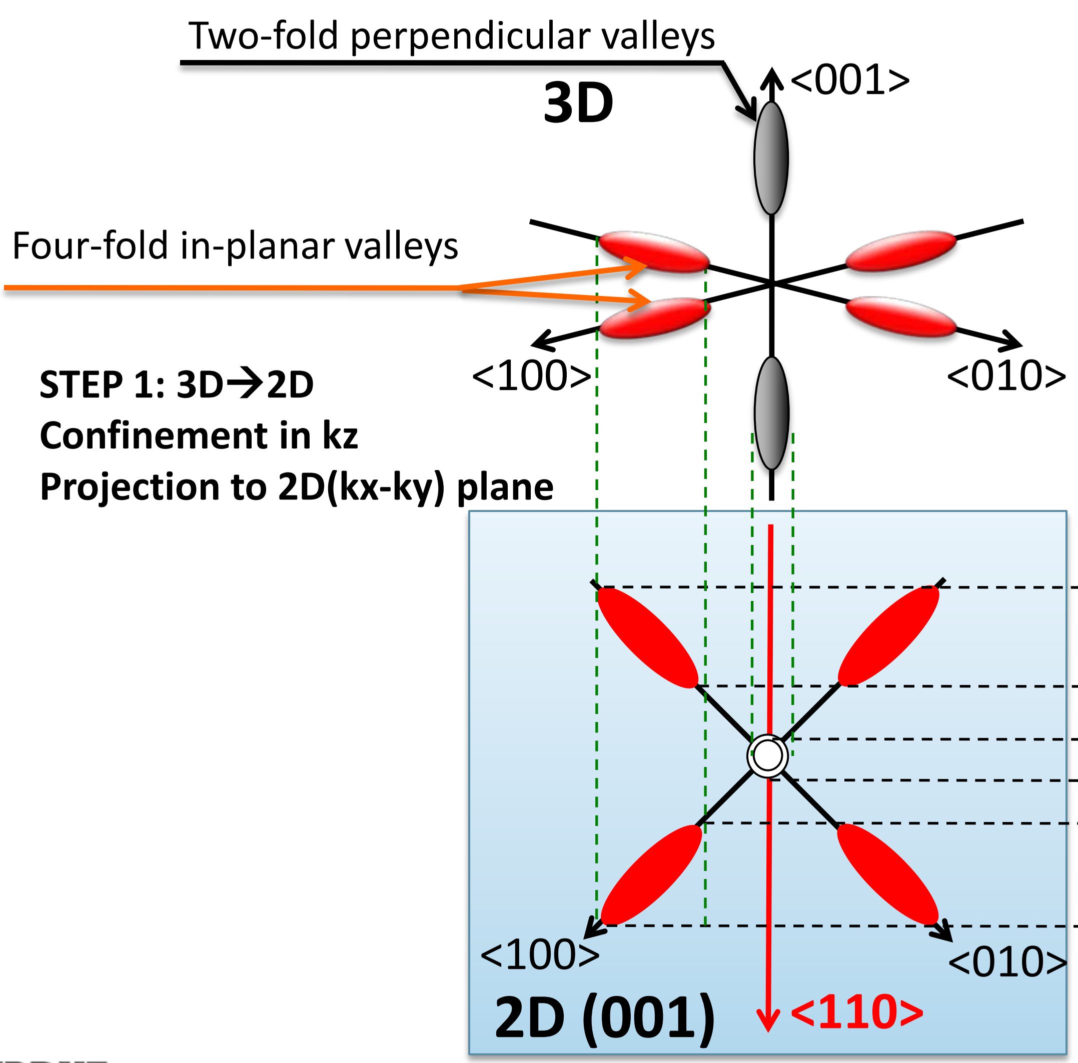


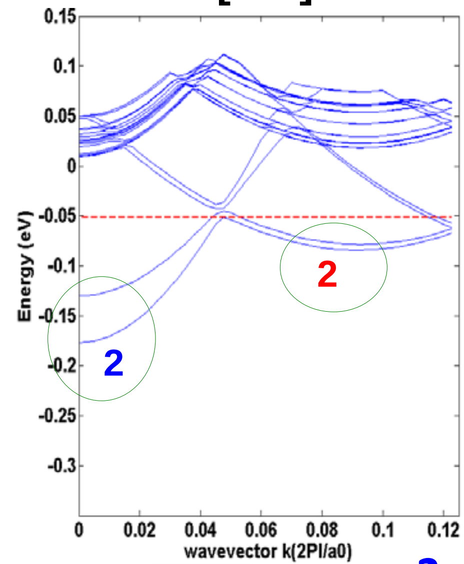
- 3D→2D→1D projection of Si [100] nanowire



Band projection in [110] Si:P wires

- **3D→2D→1D projection of Si [110] nanowire**



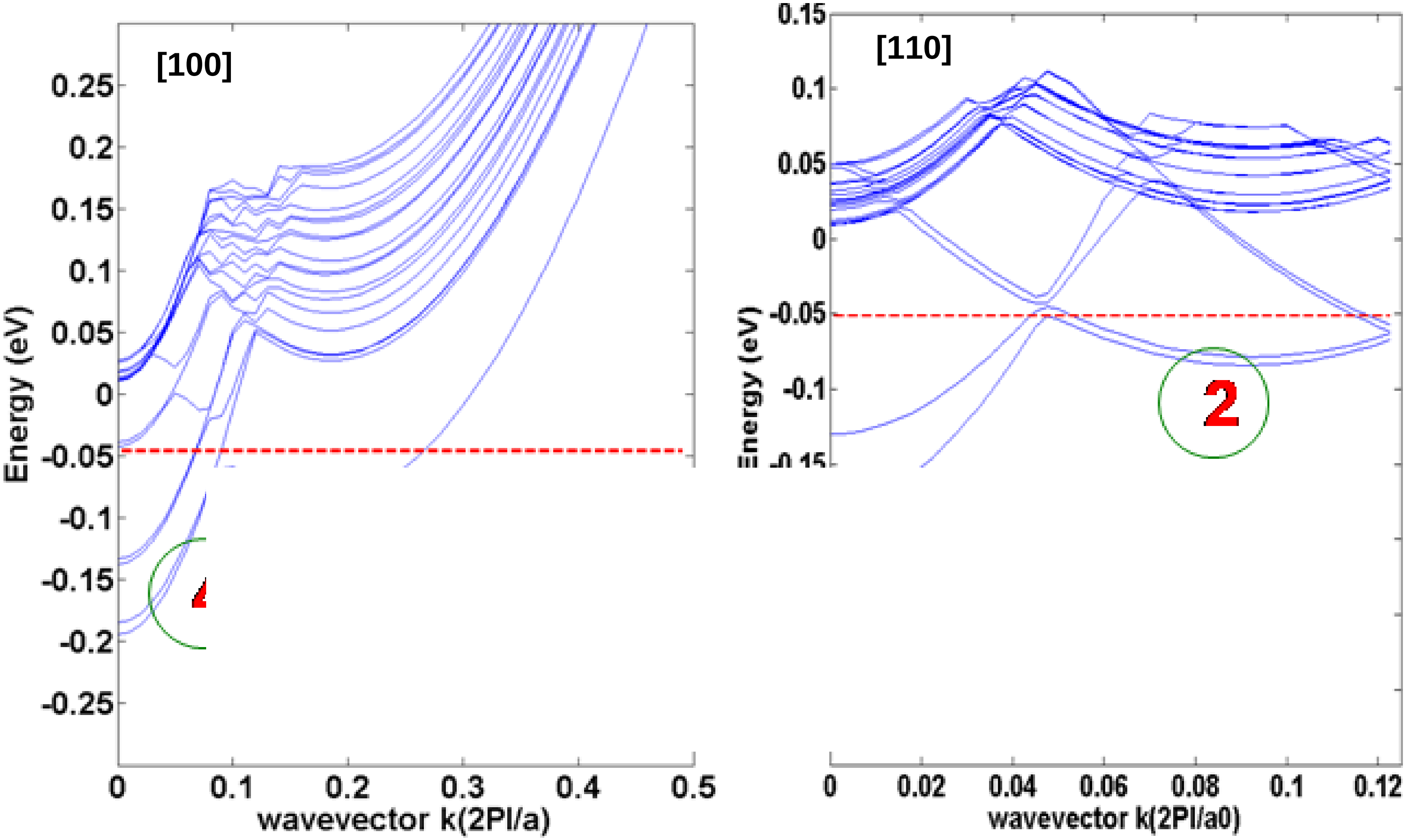


2 valleys at Γ

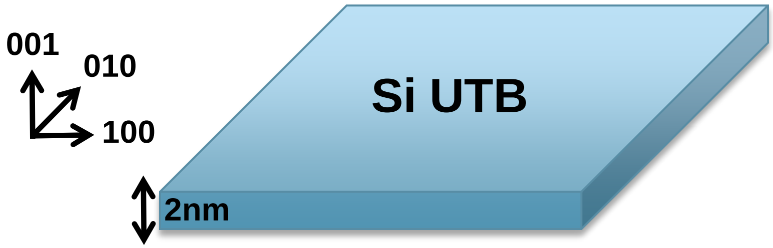
2 valley each at ±Δ

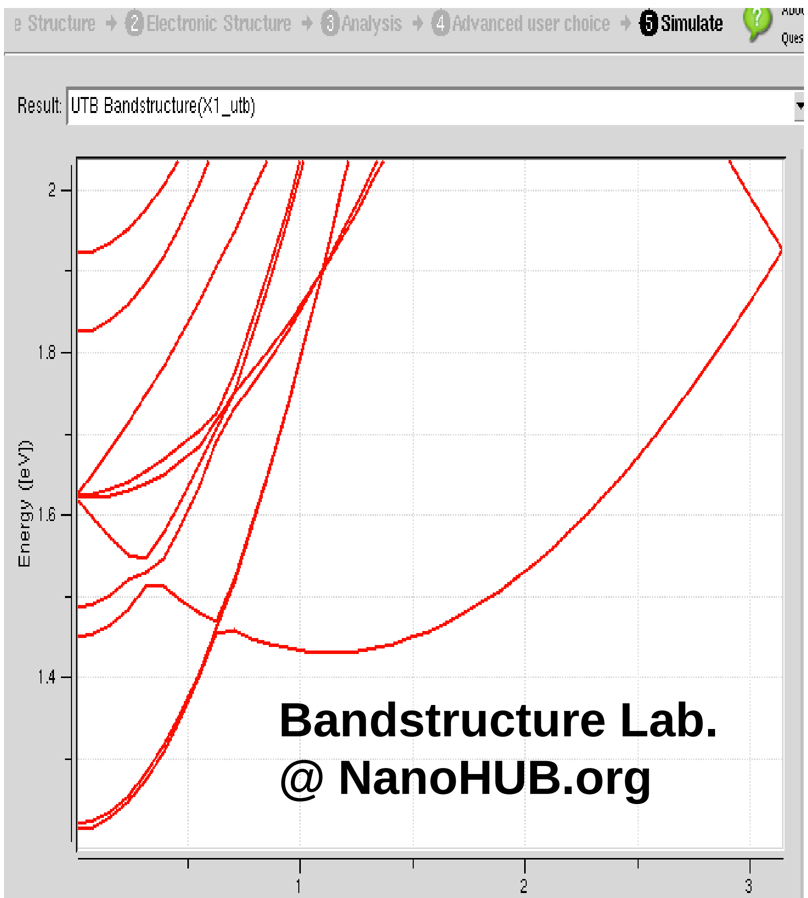
STEP 2: 2D→1D
Confinement in ky
Projection to 1D(kx) plane

Band Projection in [100]/[110] Si:P Quantum Wire

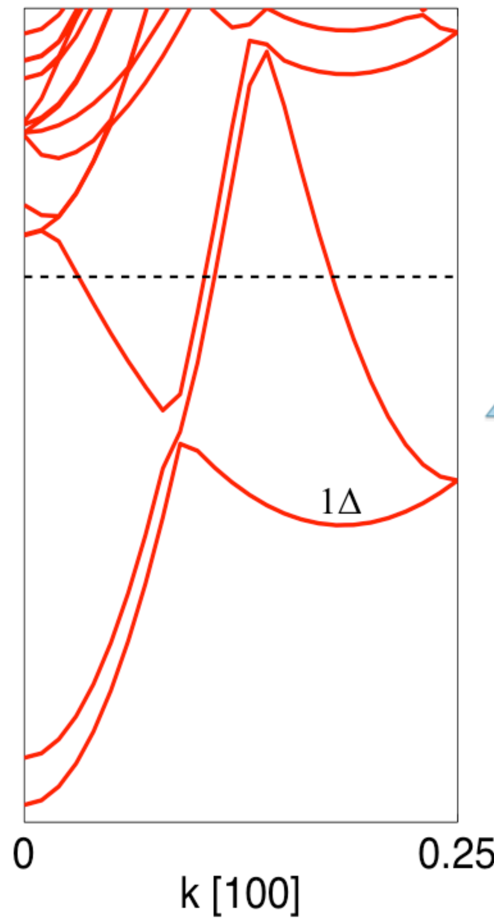


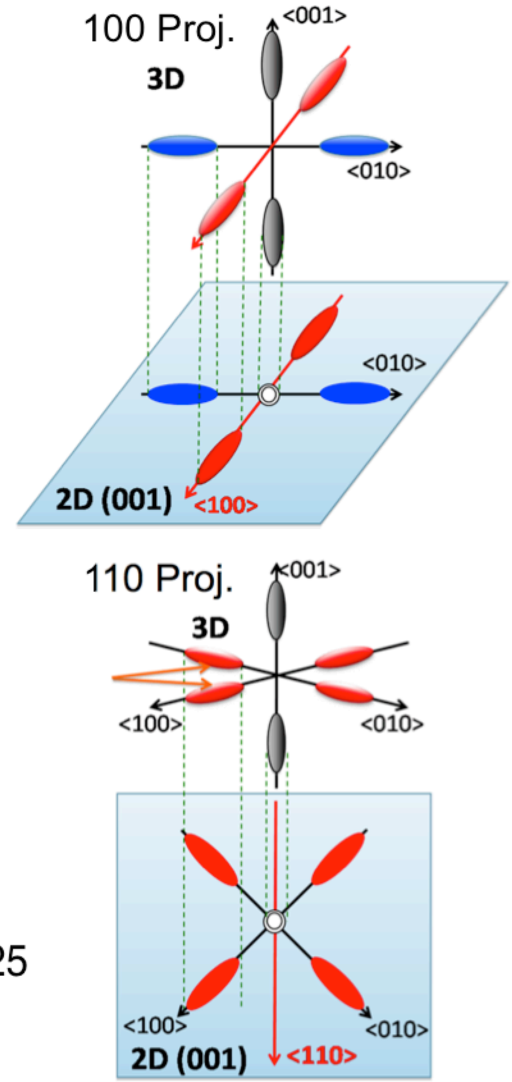
Band-Projection: A comparison to Si UTB



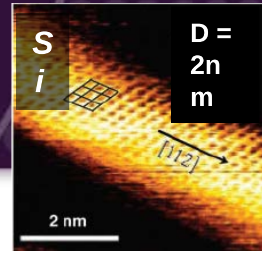


ction of 6 ellipsoids
ction band



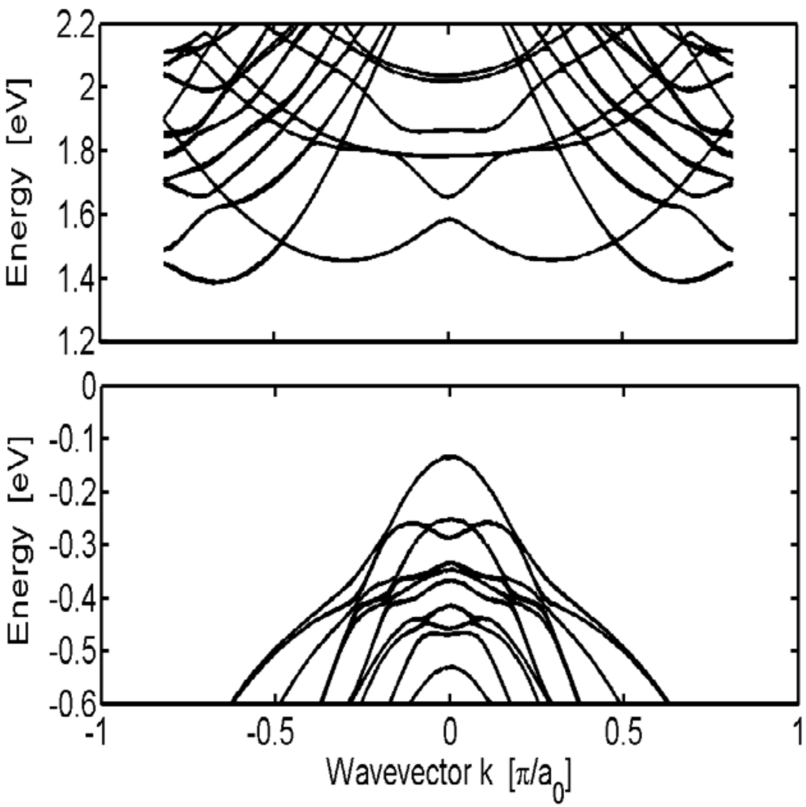


Circular 112 Wire Comparison with Experiment

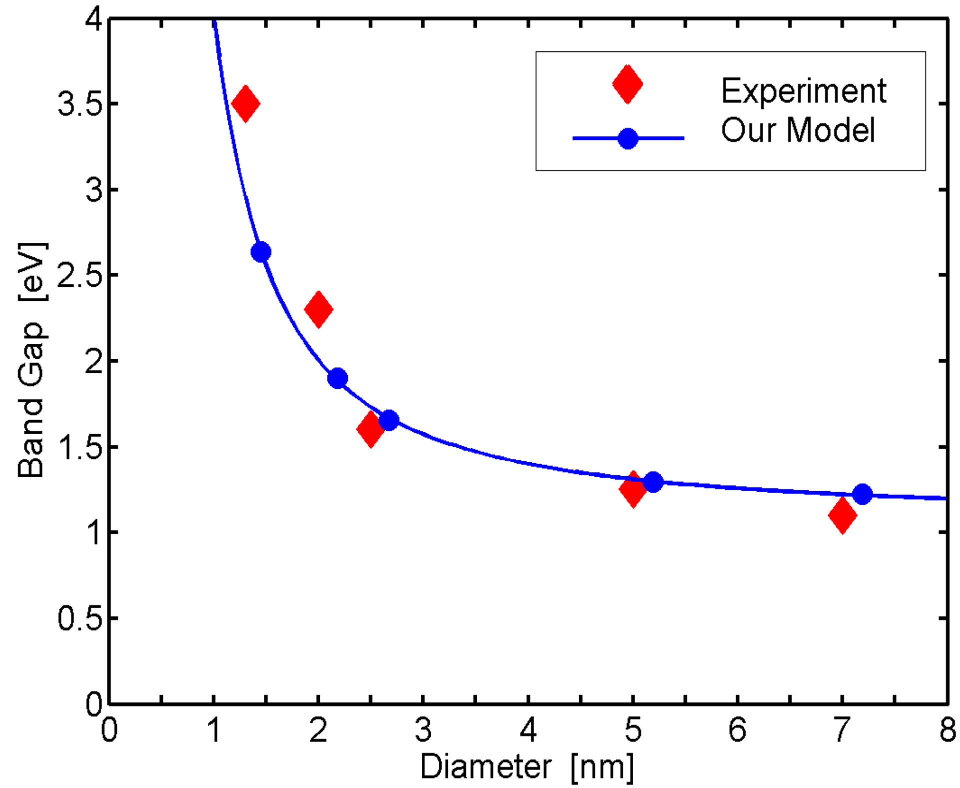


Ma et al., Science, 299, 1847, 2003

Si, CW [112], D=3.0nm



Si, CW [112]



Our tight binding calculation provides good agreement with experiment data (*Ma et al., Science, 299, 1874, 2003*.)

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  - » Bandstructure and transport in Alloy Wires
  - » Bandstructure in SiGe wires
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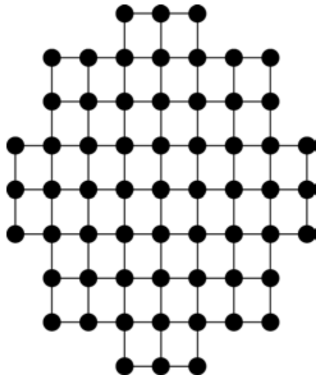
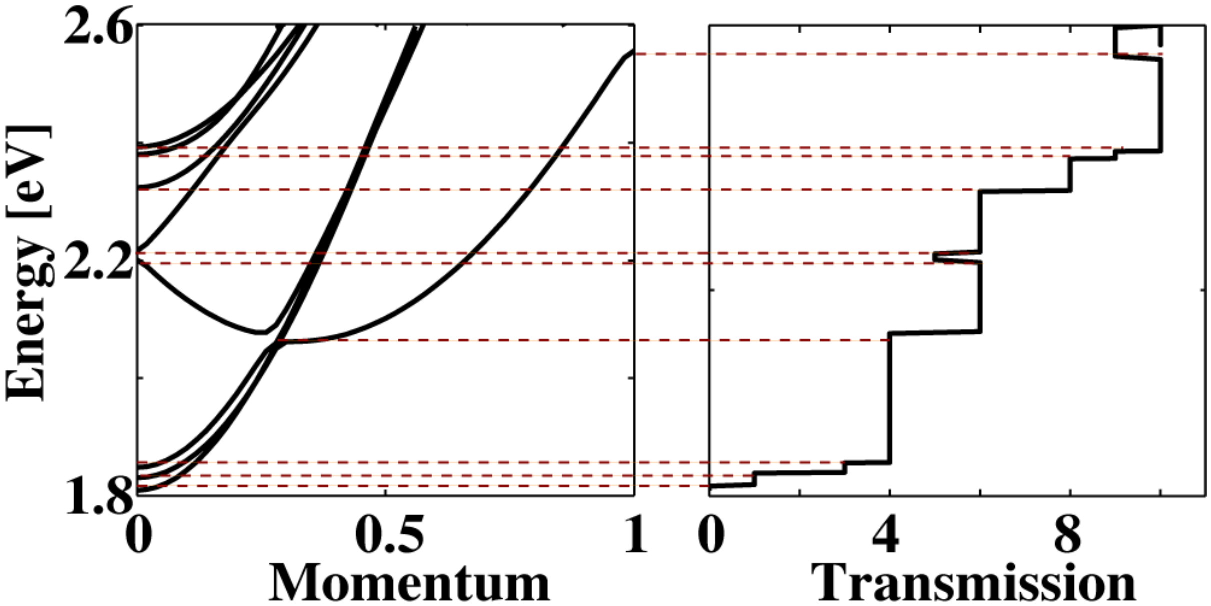
- Hole Mobility in SiGe nanowires / FinFETs
- Metal-Semiconductor interfaces
- Future NEMO5 Developments

"Perfect" Nanowires

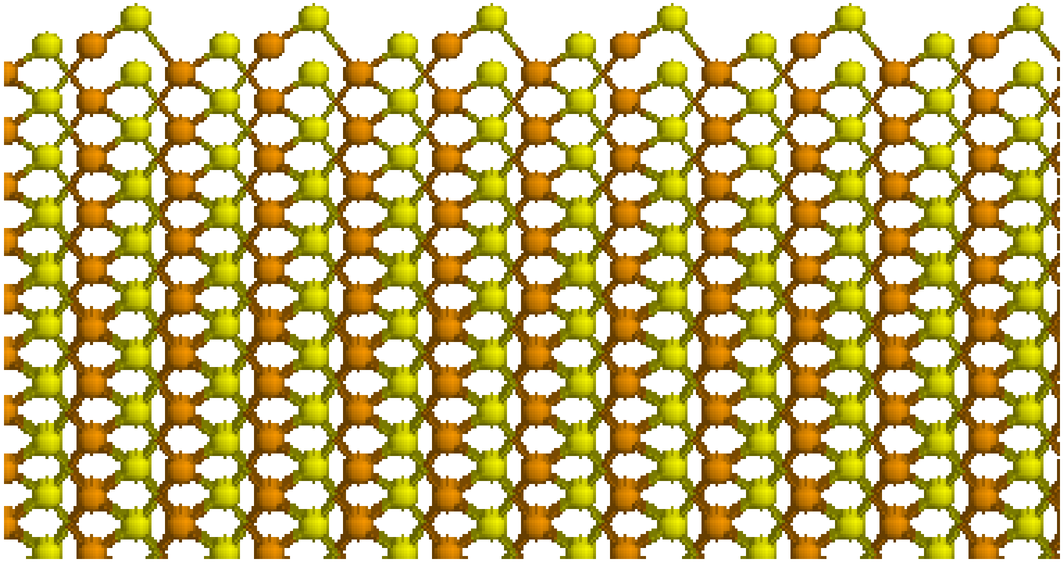


Simulated:
2nm [001] wire
infinitely long



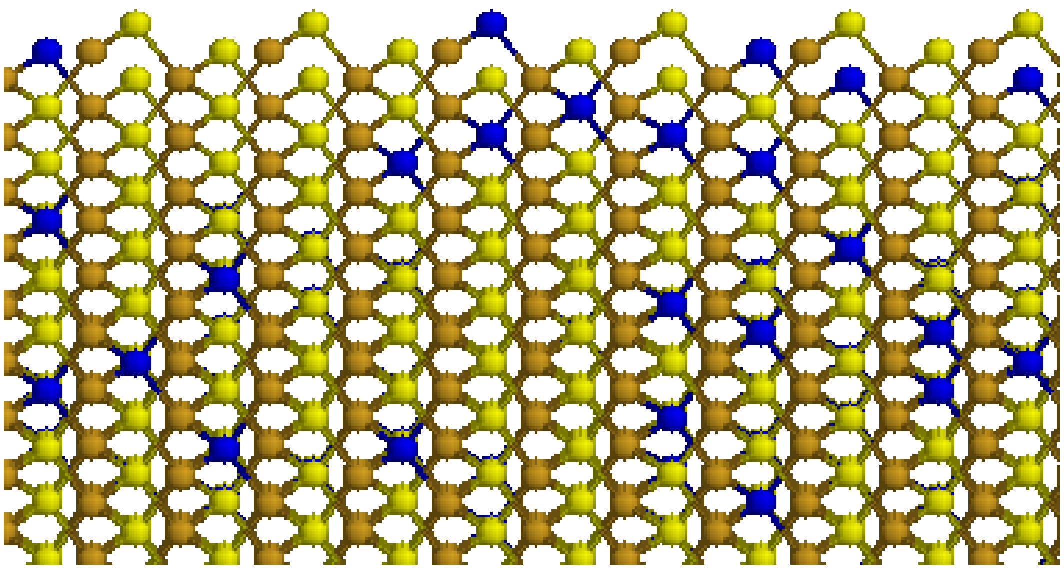
- Every band => transmission channel
- Transmission is quantized

AlGaAs alloy nanowire
Adding Al into GaAs

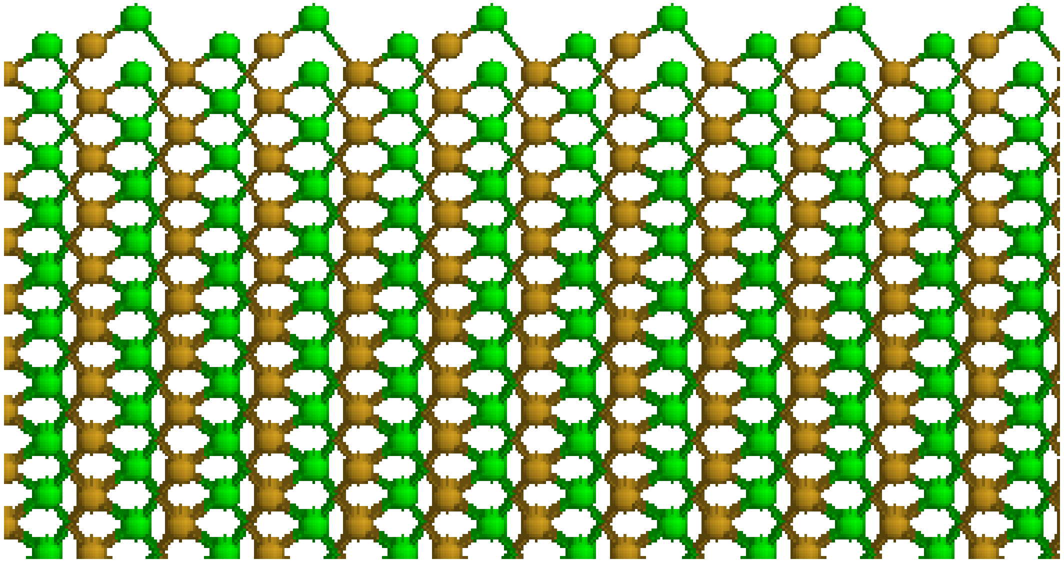


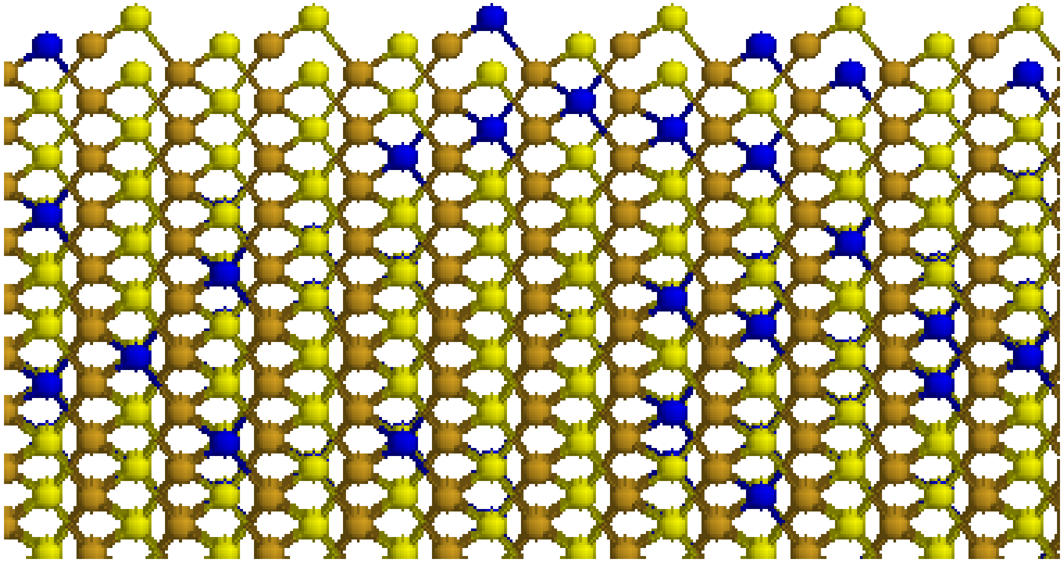
Ordered nanowire
-perfect GaAs

Insert
Al



Alloyed nanowire
-locally disordered
-Not periodic



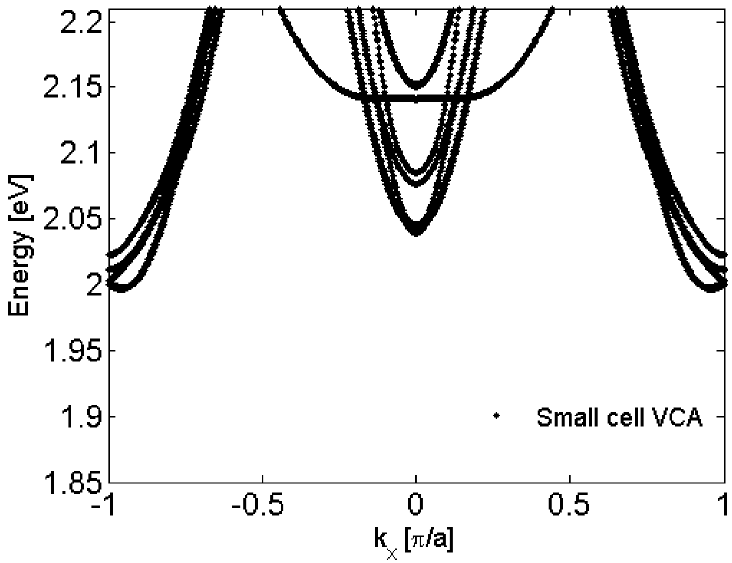


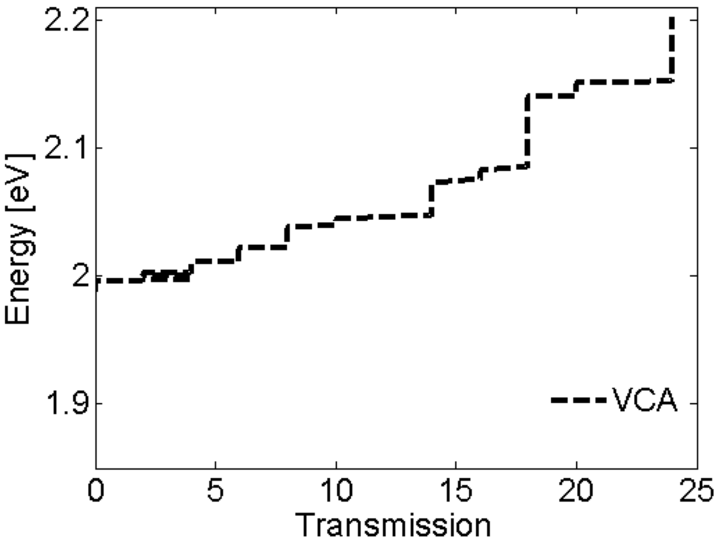
Alloyed nanowire
-Average Al and Ga
-locally ordered
-Periodic

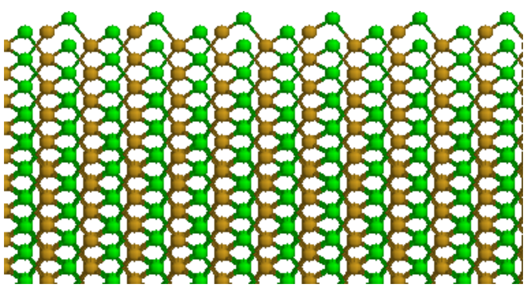
Typical Approach: VCA

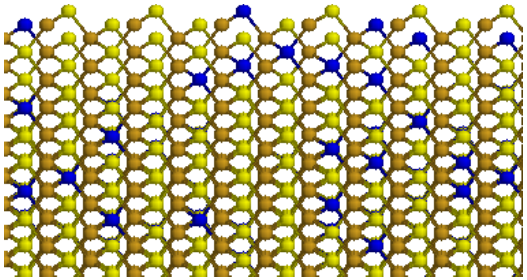
Alloyed nanowire
-locally disordered
-Not periodic

Bandstructure and transmission of VCA AlGaAs alloy nanowire







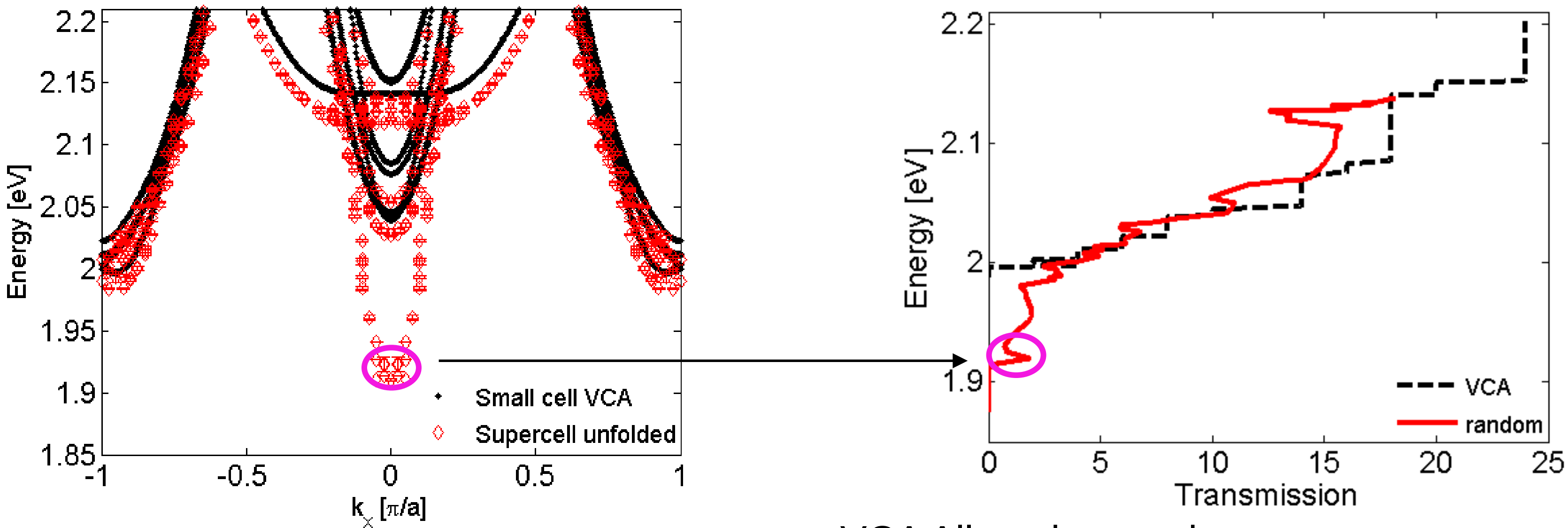


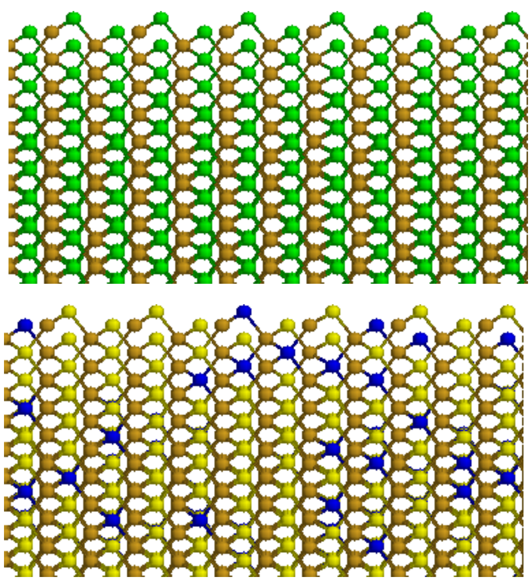
?

VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

Truly Alloyed nanowire
-locally disordered
-Not periodic

Bandstructure and transmission of VCA AlGaAs alloy nanowire

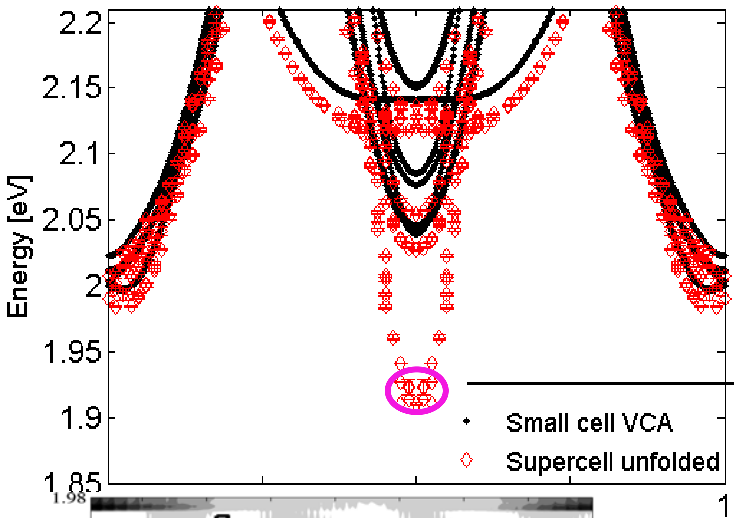


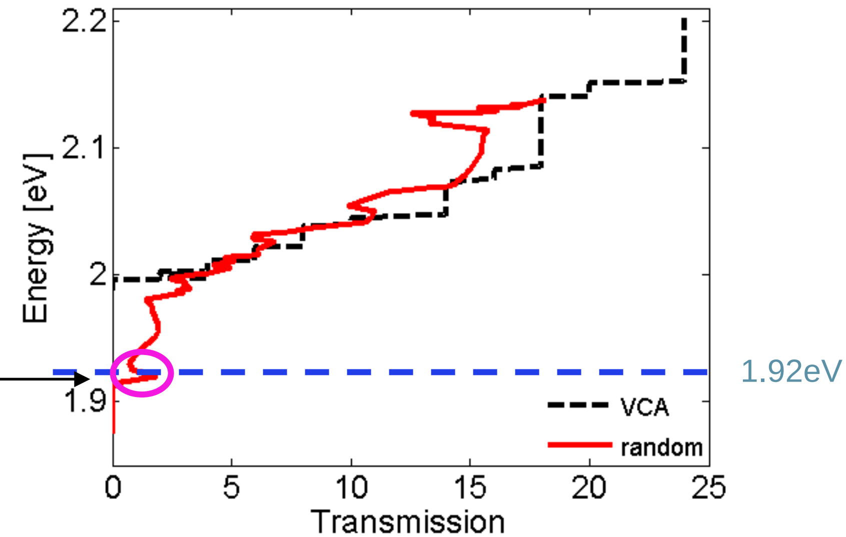


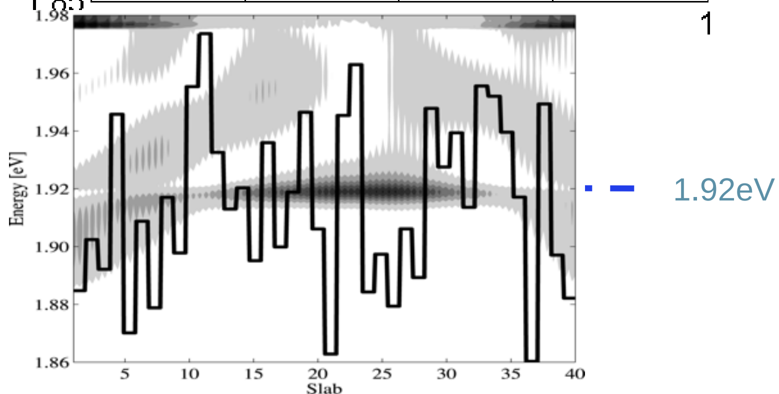
VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

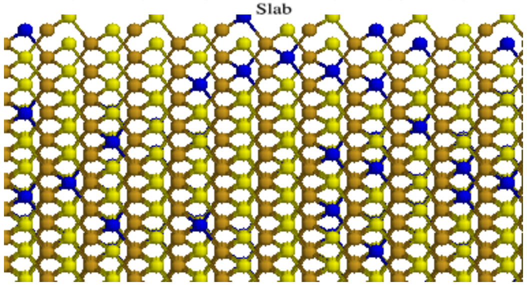
Truly Alloyed nanowire
-locally disordered
-Not periodic
-Approximate bandstructure - lower bandgap
-Transmission - no steps - resonance features

Bandstructure and transmission of VCA AlGaAs alloy nanowire









VCA Alloyed nanowire
- -Average over Al and Ga
- -locally ordered
- -periodic
- -every band has step transmission

Truly Alloyed nanowire
- -locally disordered
- -Not periodic
- -Approximate bandstructure - lower bandgap
- -Transmission - no steps - resonance features
- -Localized states - resonant tunneling

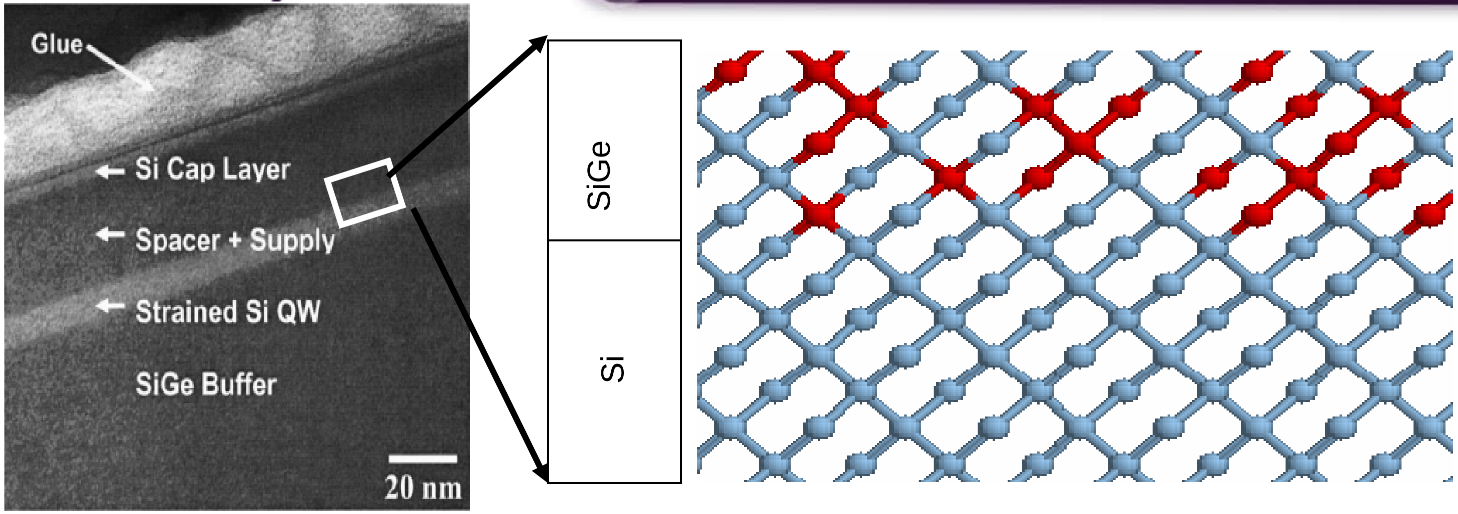
Timothy Boykin, Mathieu Luisier, Andreas Schenk, Neerav Kharche, Gerhard Klimeck
“The electronic Structure and Transmission Characteristics of AlGaAs Nanowires“
IEEE Transactions on Nanotechnology, Vol. 6, 43 – 47 (2007)

Achievements (2007):
true atomistic electronic structure model
Transport with real disordered alloy
Localization of states emerges naturally

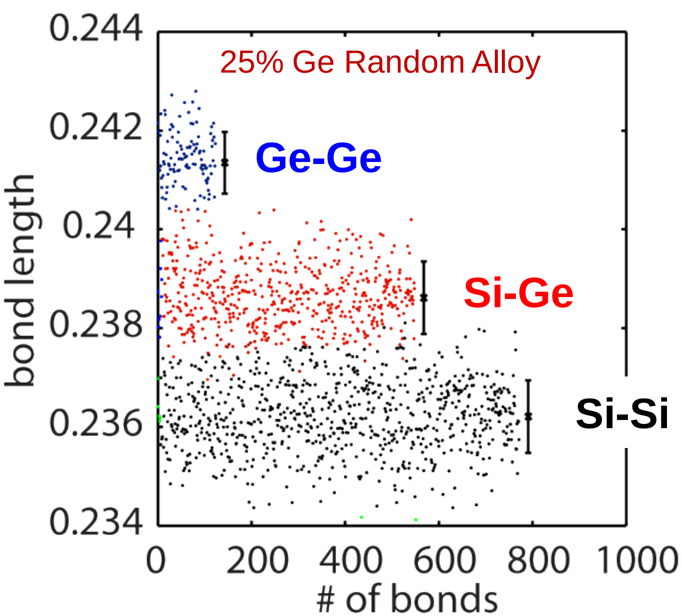
Short-Comings (2007):
No true strain model
Contacts are smooth
No I-V
No Phonon Scattering

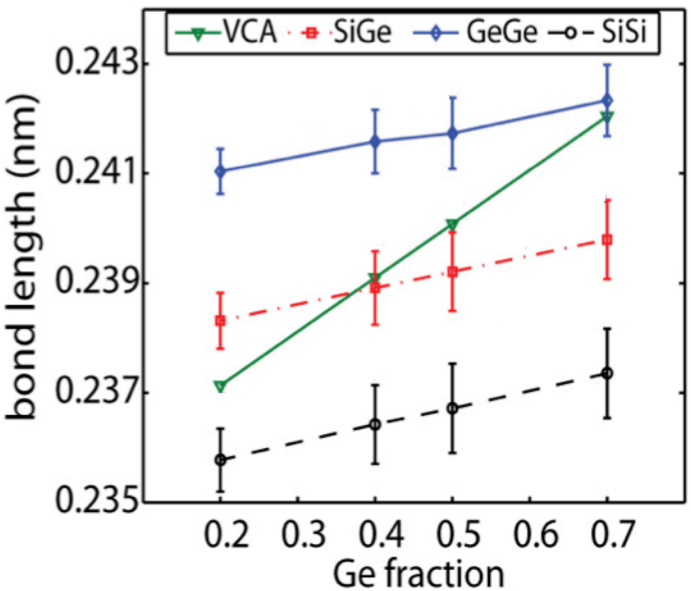
Features available today in NEMO5

Atomistic Disorder in SiGe



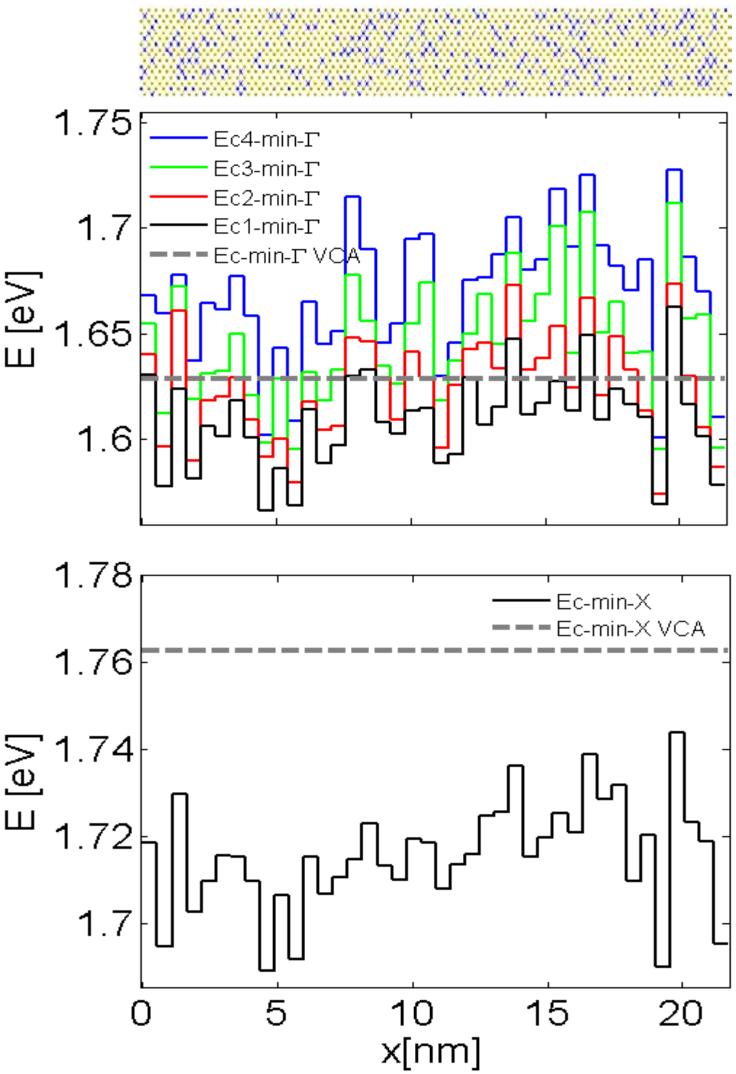
Alloy disorder
- Atom Type
- Bond Length





Atom Positions Fluctuate! => NOT a homogeneous crystal

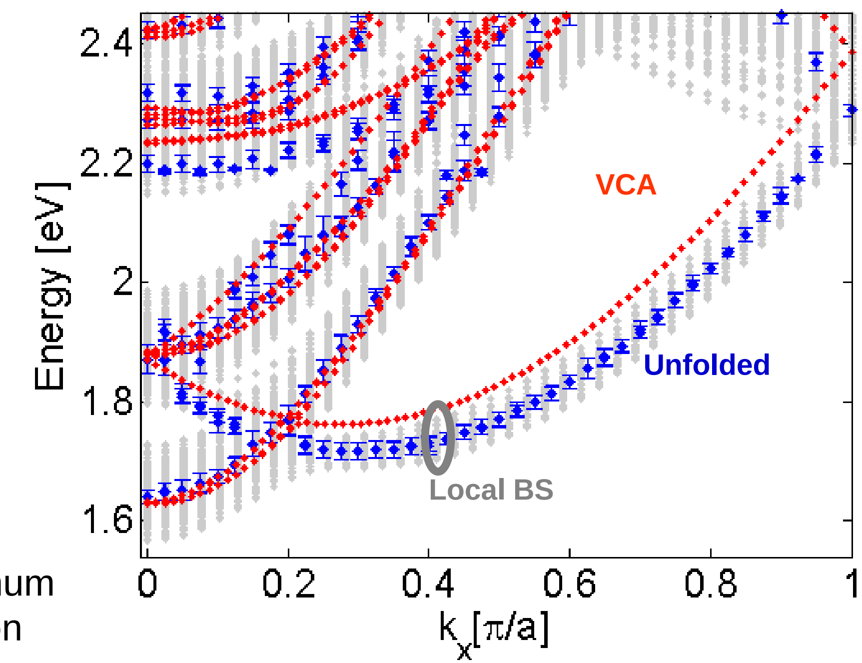
SiGe nanowire



Bandedge minima first four conduction subbands (Δ_4 valleys)

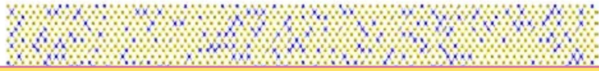
Bandedge minimum transport direction (Δ_2 valleys)

VCA is not a good approximation for Δ_2 valleys



Special Issue on Nanoelectronic Device Modeling in *IEEE Transactions on Electron Devices* (2007)

SiGe nanowire



Gerhard Klimeck, Shaikh Ahmed, Neerav Kharche, Marek Korkusinski, Muhammad Usman, Martha Prada, Timothy Boykin
"Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D: Part II - Applications"
IEEE Transactions on Electron Devices, Vol. 54, pg: 2090 - 2099, (2007), (INVITED)
Special Issue on Nanoelectronic Device Modeling; doi : 10.1109/TED.2007.904877

Achievements (2007):
true atomistic electronic structure model
true atomistic strain model

Short-Comings (2007):
Not full atomistic transport

Features available today in NEMO5

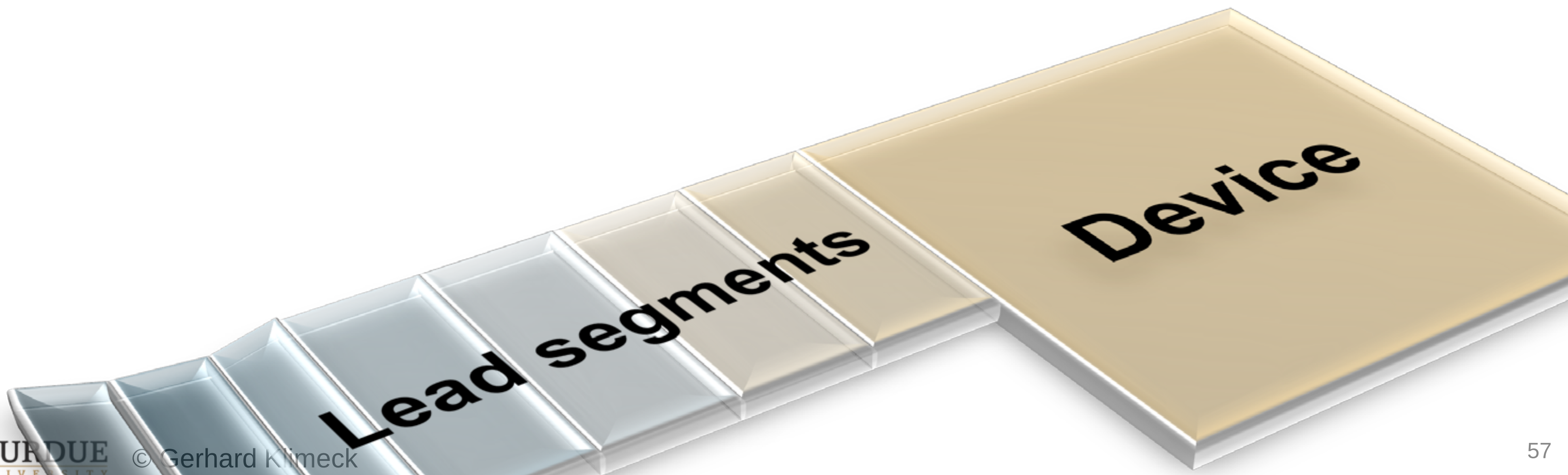
Complex Lead structures NOT infinitely periodic!

Herbert Krömer: The interface is the device

Contacts:
- Are critical to the central device behavior
- Are NOT infinitely periodic
- Have very high electron densities => significant scattering

Existing algorithms require 2 geometric extremes:
- Explicit large representation (too expensive)
- Assumption of infinite periodicity (unrealistic)

No comprehension of incoherent scattering



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Existing algorithms require 2 geometric extremes:

- Explicit large representation (too expensive)
- Assumption of infinite periodicity (unrealistic)

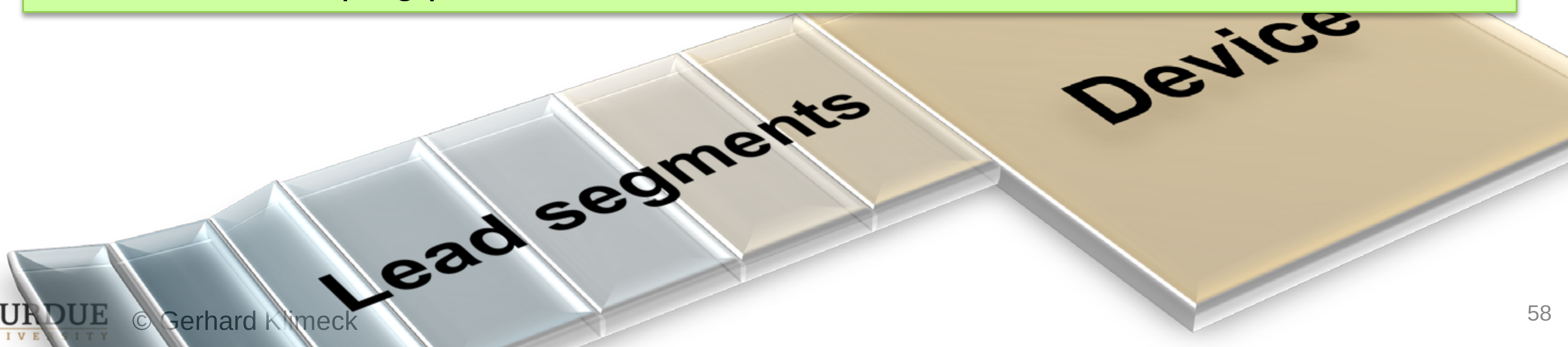
No comprehension of incoherent scattering

Lead algorithm in NEMO5:

Divide lead into segments

Apply unidirectional RGF on lead surface Green's function

Add smooth damping potential as a function of the lead/device distance

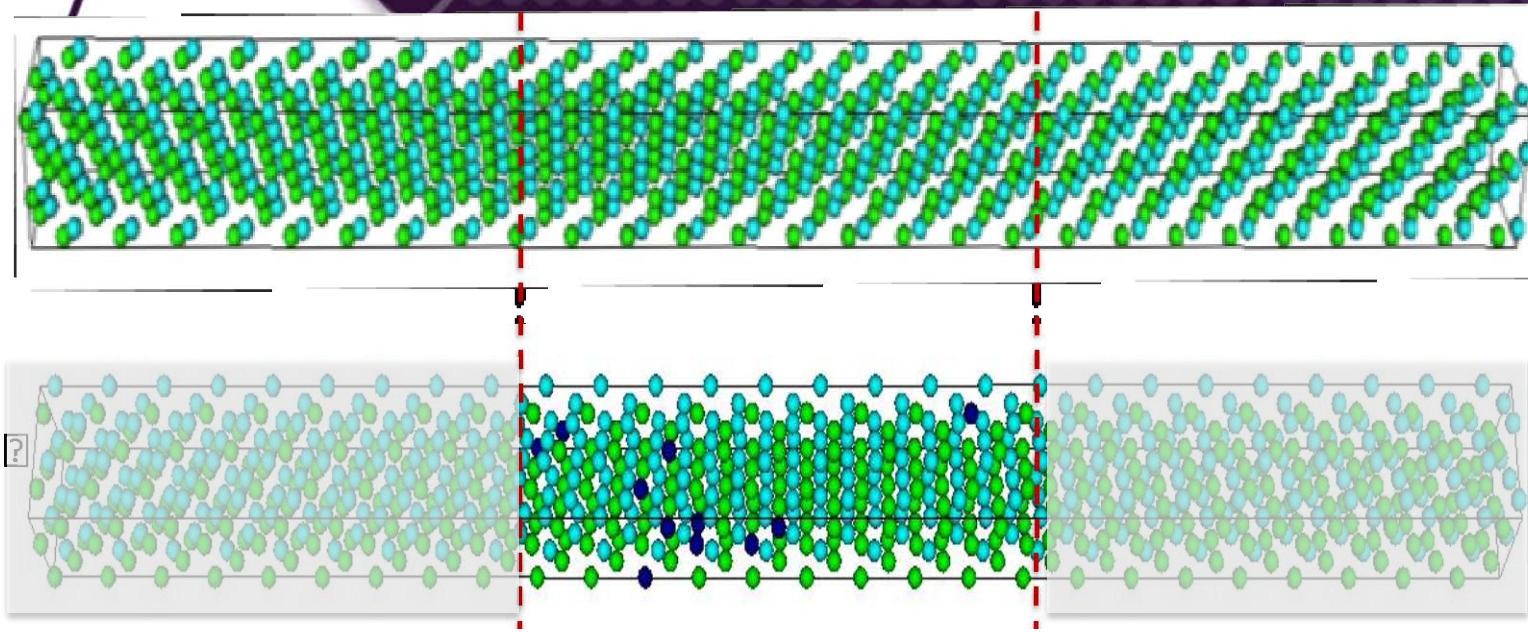


Algorithm for regular and irregular leads

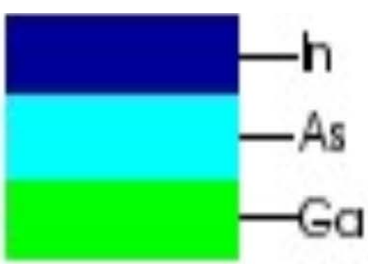
Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Pure GaAs

Alloy in device



ORDERED Contacts | **DISORDERED device** | **ORDERED Contacts**

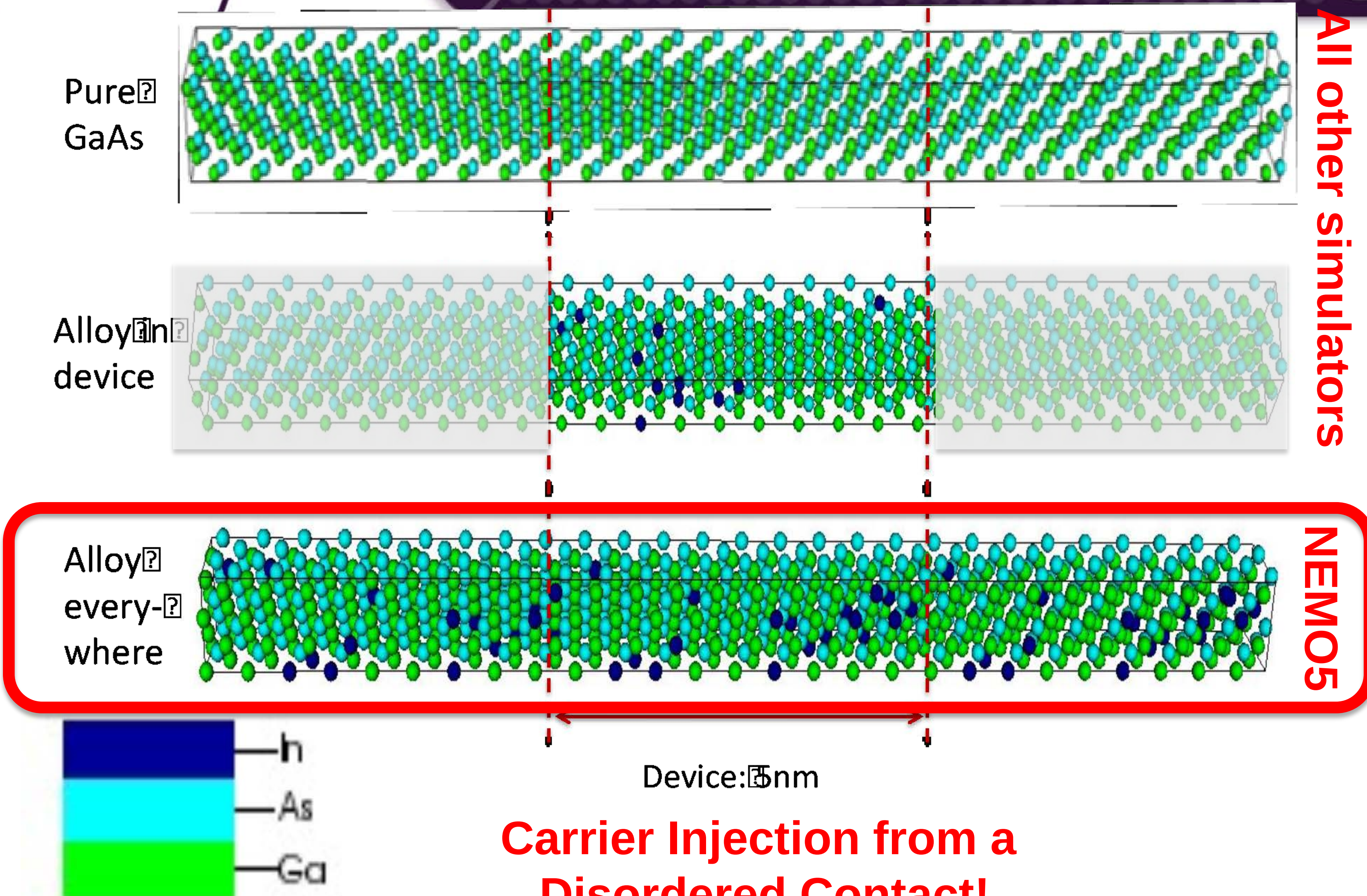


Device: 5nm

(Cross section: 2X2 unit cells)

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis



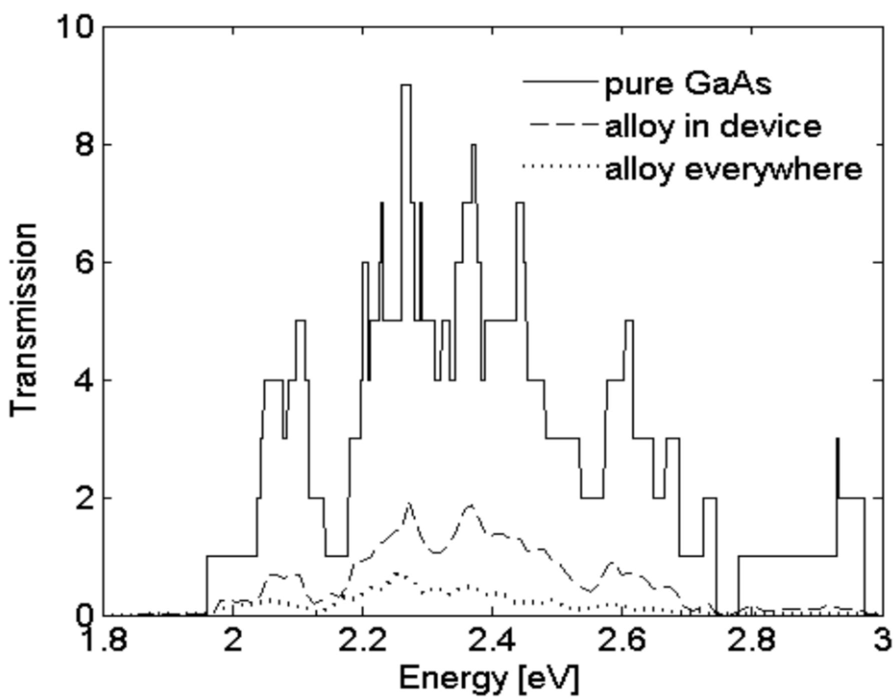
Carrier Injection from a Disordered Contact!

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Comparison with transer matrix method in regular leads.

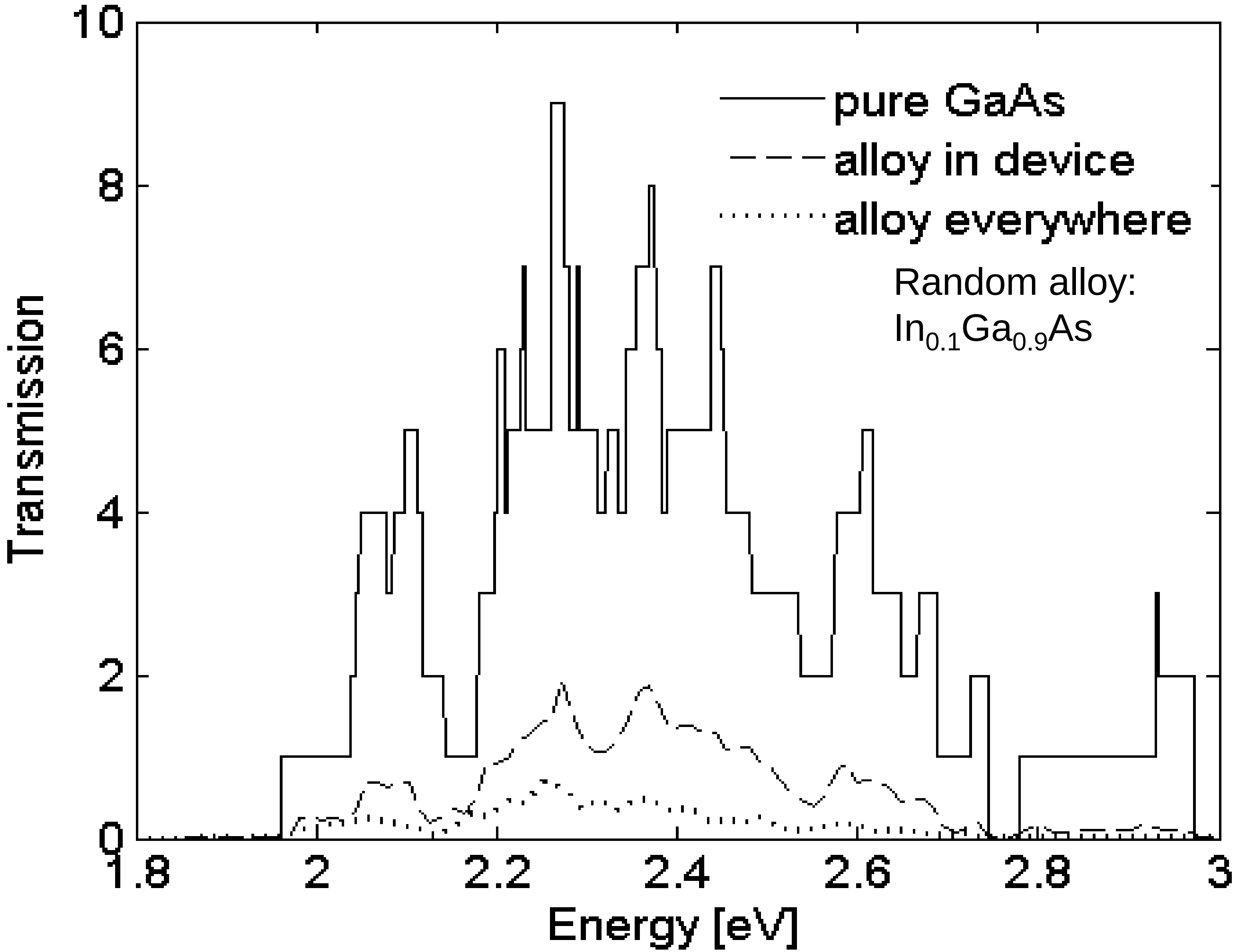
A GaAs nanowire with alloy structures:



Application in random alloy structures.

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis



Yu Wang, Yu He, Gerhard Klimeck, Tillmann Kubis,
"Nonequilibrium Green’s function method: Algorithm for regular and irregular leads"
16th International Workshop on Computational Electronics, Nara, Japan June 4-7, 2013

Achievements (2013):
true atomistic electronic structure model
true atomistic strain model
True coherent quantum transport
Treatment of extended disordered contacts

Short-Comings (2013):
No I-V’s yet
No coupling to phonons

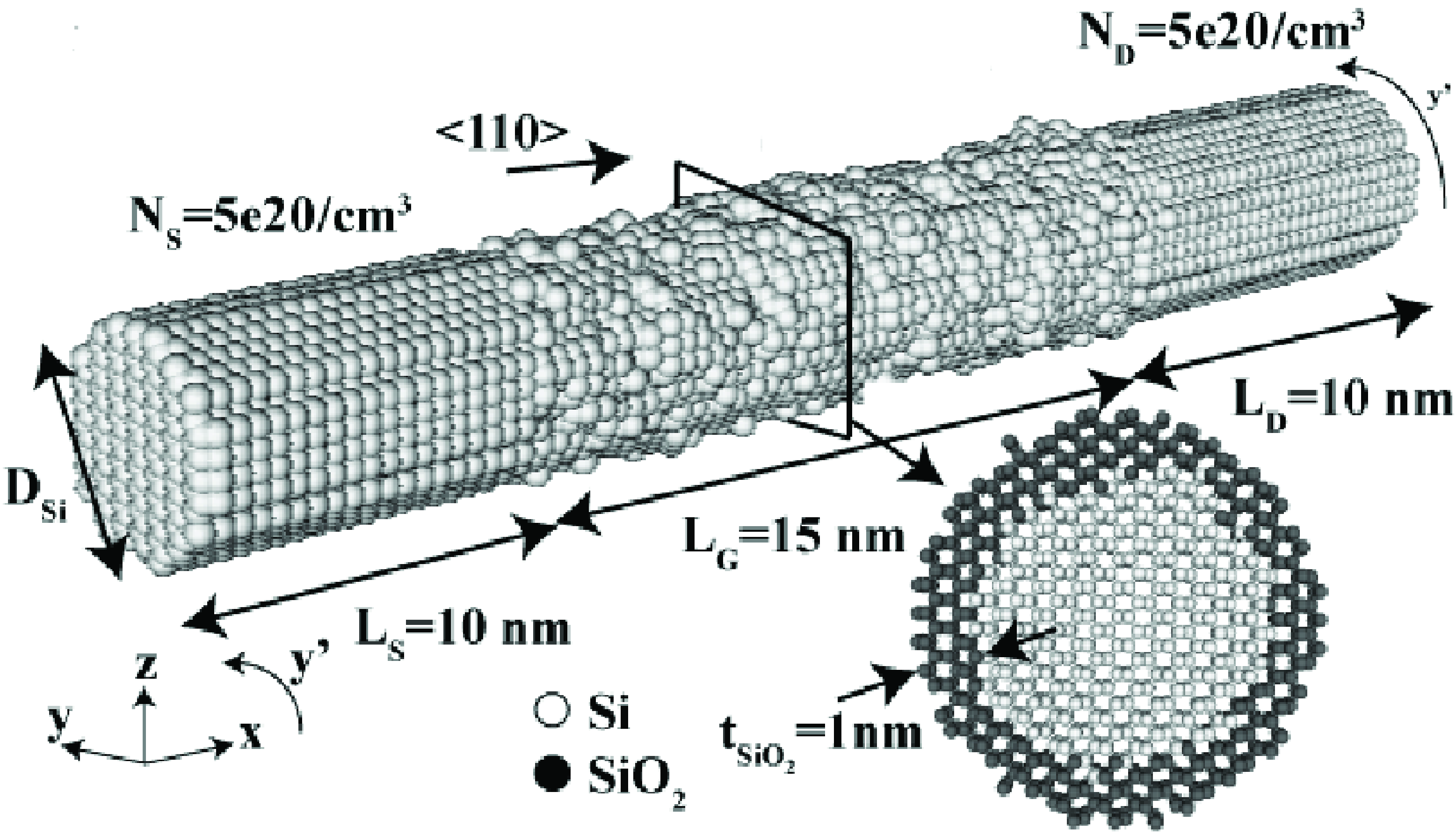
Features available today in NEMO5

Interface Roughness Effect on ON-Current in Nanowire FETs

Objective:

- Investigate the ON-current reduction at nanowire diameter below 3nm in experiment

Realistic/atomistic rough interface between Si/SiO_2



Interface Roughness Effect on ON-Current in Nanowire FETs

Objective:

- Investigate the ON-current reduction at nanowire diameter below 3nm in experiment

Approach:

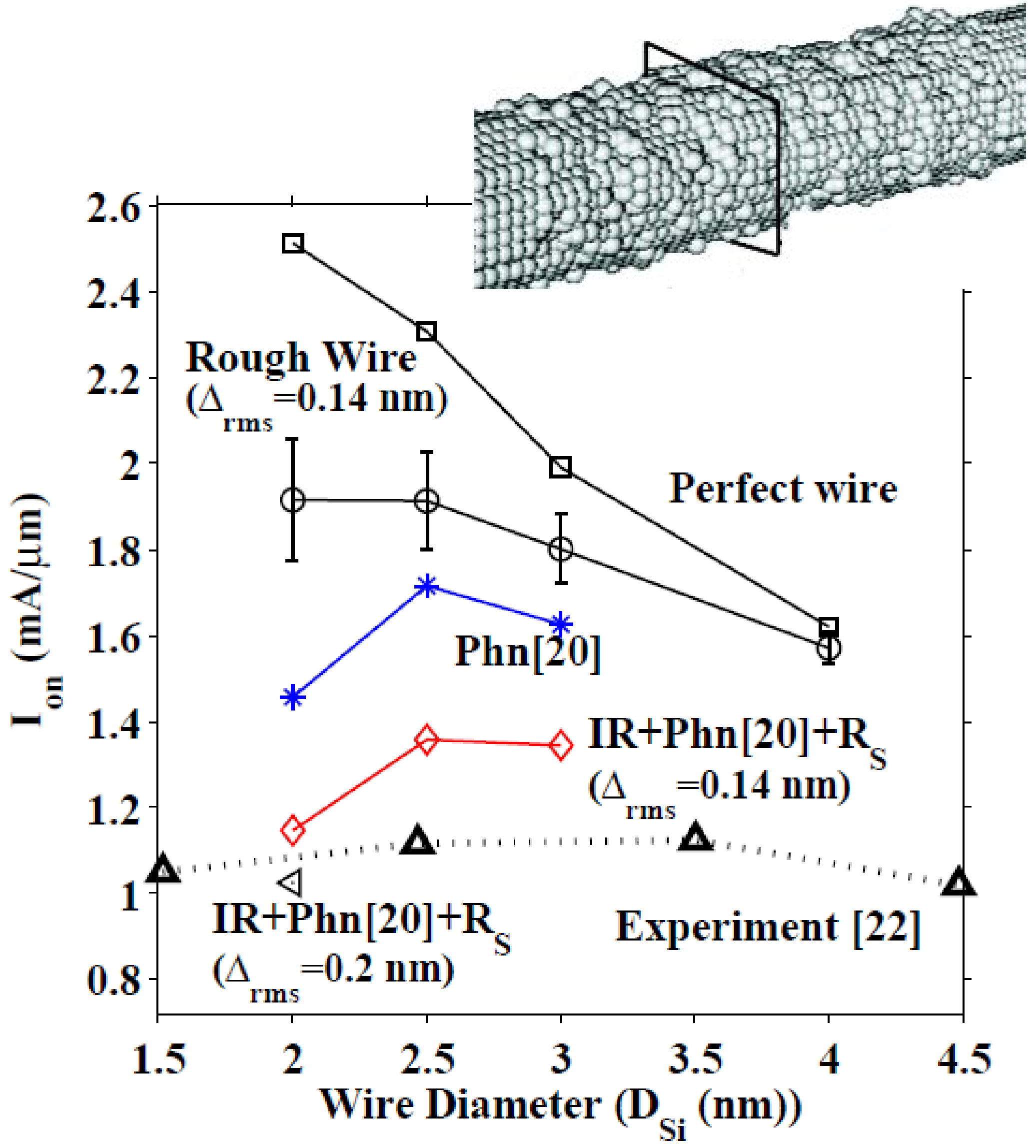
- Atomistic simulation using OMEN
- Combine the effect of phonon scattering and interface roughness scattering

Impact:

- Quantitative match of simulation with experimental data
- Significance of interface roughnes scattering and phonon scattering captured qauntitatively

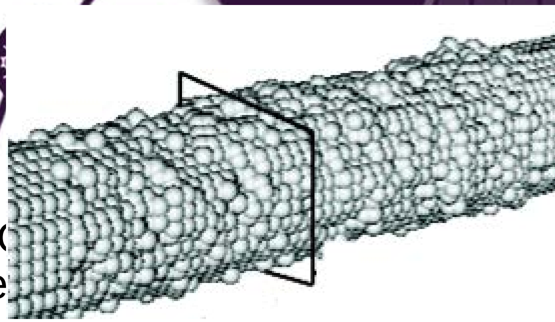
Results:

- ON-current reduction becomes significant from diameter 3 nm and below
- Phonon scattering is more important than interface roughness scattering in ON-current reduction



I_{on} is determined at V_G=Vth+2/3VDD

Interface Roughness Effect on ON-Current in Nanowire FETs



Objective:

- Investigate the (nanowire diame experiment

SungGeun Kim, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck,
"Effects of Interface Roughness Scattering on Radio Frequency Performance of Silicon Nanowire Transistors"
Appl. Phys. Lett. 99, 232107 (2011);doi:10.1063/1.3665939

Achievements (2011):
Explicit interface roughness representation
Top of barrier transport model
Phonons included through mobility model

Short-Comings (2011):
No full NEGF I-V's yet
No coupling to phonons

Features available today in NEMO5

Outline

- Device trends and NEMO Modeling Agenda
- Bandstructure Concepts
  - » Revisit some “old” bandstructure concepts (ancient RTDs)
  - » Bandstructure in Si nanowires
  - » Bandstructure and transport in Alloy Wires
  - » Bandstructure in SiGe wires
- Source Drain Tunneling for Lg<10nm
  - » Tuning the effective mass for the channel material
- Hole Mobility in SiGe nanowires / FinFETs
- Metal-Semiconductor interfaces

MOSFETs at Lg < 10 nm

ISSCC 2003 / 50th ANNIVERSARY

Forty Years of Feature-Size Predictions (1962-2002)

Christer Svensson
Linköping University, Linköping, Sweden

"It is important to note that at 8nm, we are very close to a direct source-drain tunneling limit, which, in fact, is very fundamental."

Does source-to-drain tunneling limit the ultimate scaling of MOSFETs?

Jing Wang and Mark Lundstrom
School of Electrical and Computer Engineering, Purdue University
West Lafayette, IN USA 47907-1285

IEDM 2002: "The results show that source-to-drain tunneling does set an ultimate scaling limit."

Device Scaling Limits of Si MOSFETs and Their Application Dependencies

DAVID J. FRANK, MEMBER, IEEE, ROBERT H. DENNARD, FELLOW, IEEE, EDWARD NOWAK, MEMBER, IEEE, PAUL M. SOLOMON, FELLOW, IEEE, YUAN TAUR, FELLOW, IEEE, AND HON-SUM PHILIP WONG, FELLOW, IEEE

"Estimates indicate that direct source-to-drain tunneling current limits will start to dominate the thermal OFF current somewhere in the 10–12-nm regime, thus creating the 11-nm channel length limit."

IBM, Proceedings of the IEEE, 2001

UNIVERSITY OF FLORIDA S. E. Thompson EEL 6935

"At around 10nm, direct source-drain tunneling limits present transistors."

Lecture on the Limits for Silicon MOSFETs, Fall 2004

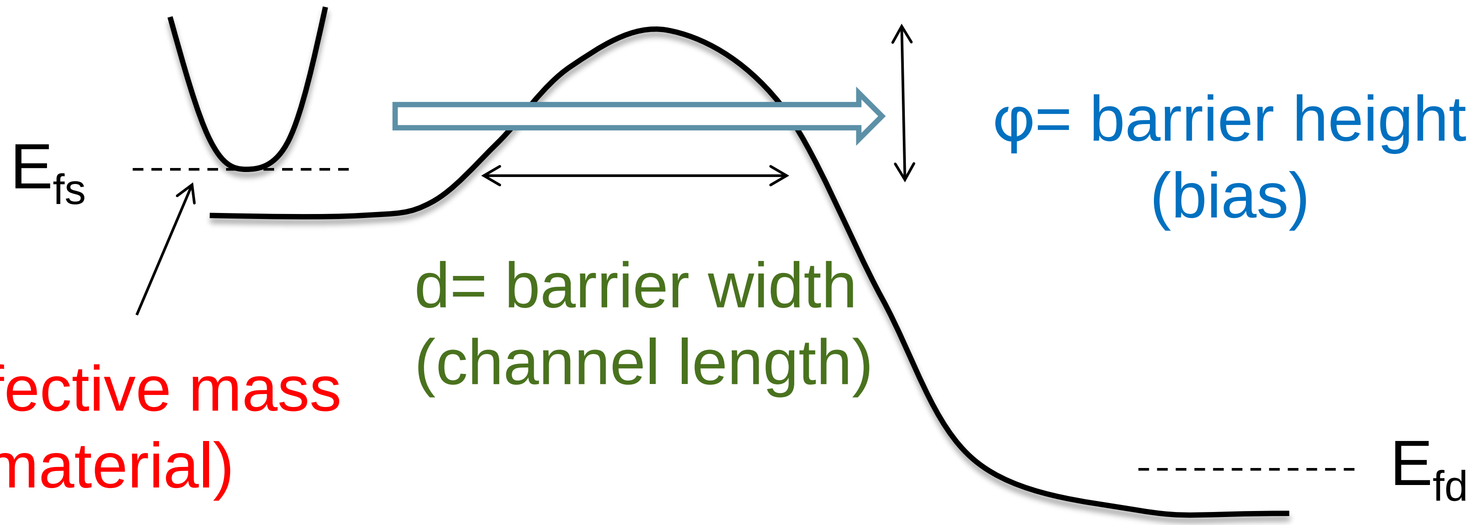
Source-drain (SD) tunneling a serious challenge L<10 nm..

Images: http://www.monolithic3d.com/2/post/2011/09/is-there-a-fundamental-limit-to-miniaturizing-cmos-transistors1.html

quantum tunneling

Tunneling probability*, T

$$T \propto \exp\left[-2\sqrt{\frac{2m^*}{\hbar^2}}\sqrt{q\varphi}\,d\right]$$



φ= barrier height (bias)

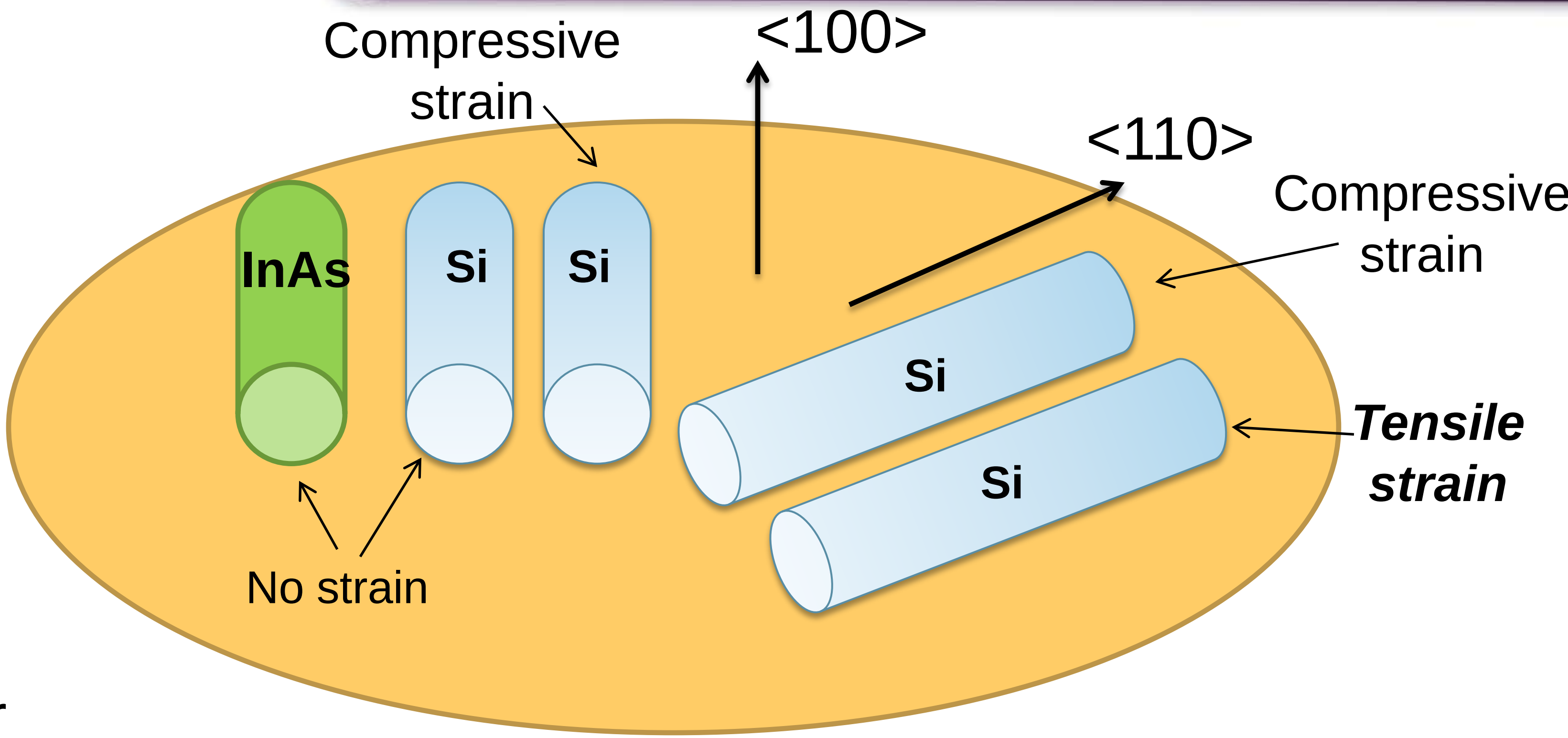
d= barrier width (channel length)

m*=effective mass (material)

Light m* (↓) → increased tunneling (↓) → limited transistor operation.

* D.J Griffiths "Introduction to Quantum Mechanics"

Different nanowire cases…



(100) wafer orientation

Saumitra Mehrotra

5 nanowire cases to be evaluated ….

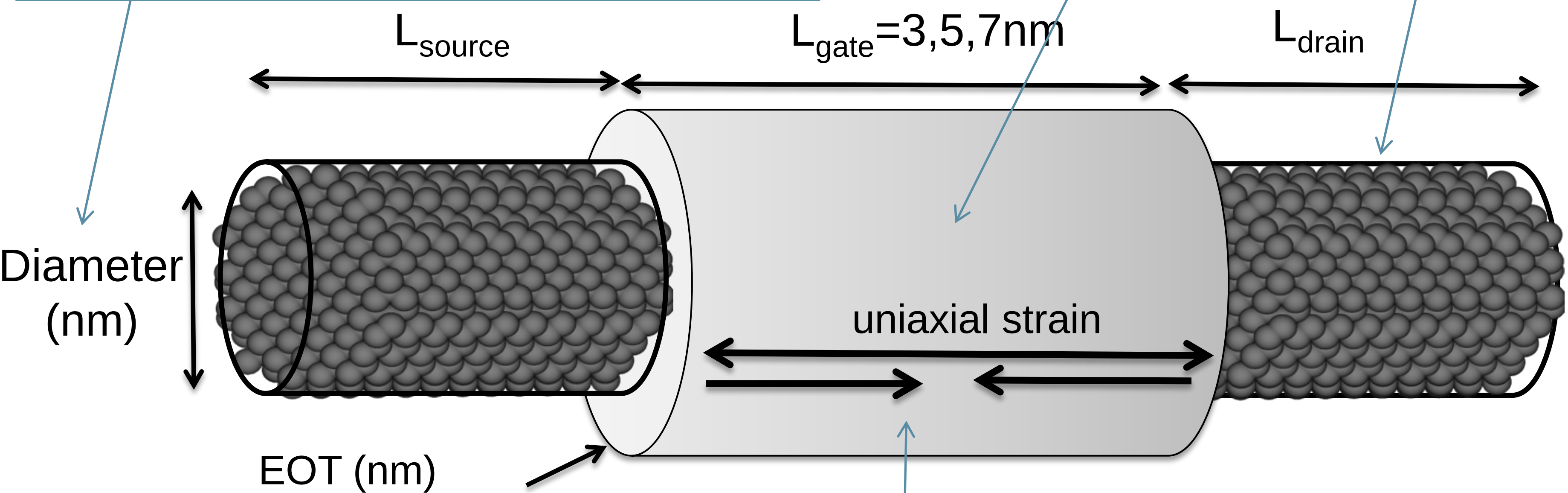
1. **InAs <100> ← current research**
2. Si <100>
3. Si <100> compressive stress
4. **Si <110> tensile stress ← current industry**
5. Si <110> compressive stress

Device geometry for L_{gate}<8nm MOSFETs

- Diameter → 3.8 nm *
  - Larger diameter → ↓gate control
  - Smaller diameter → ↑ V_{th} variability (<σ_{Vth}<20mV)

Channel Material : Si/ InAs

- N_{sd} = 1e20/cm^3 for Si and 5e19/cm^3 for InAs



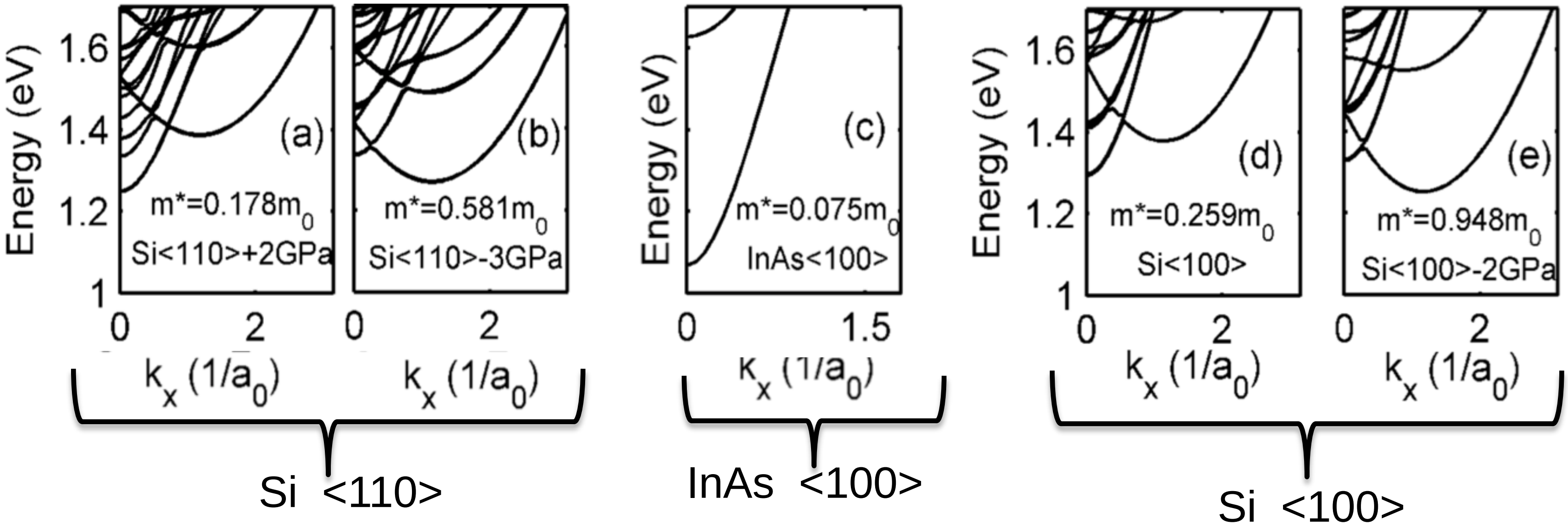
- EOT=0.5 nm (ITRS ,year 2024)

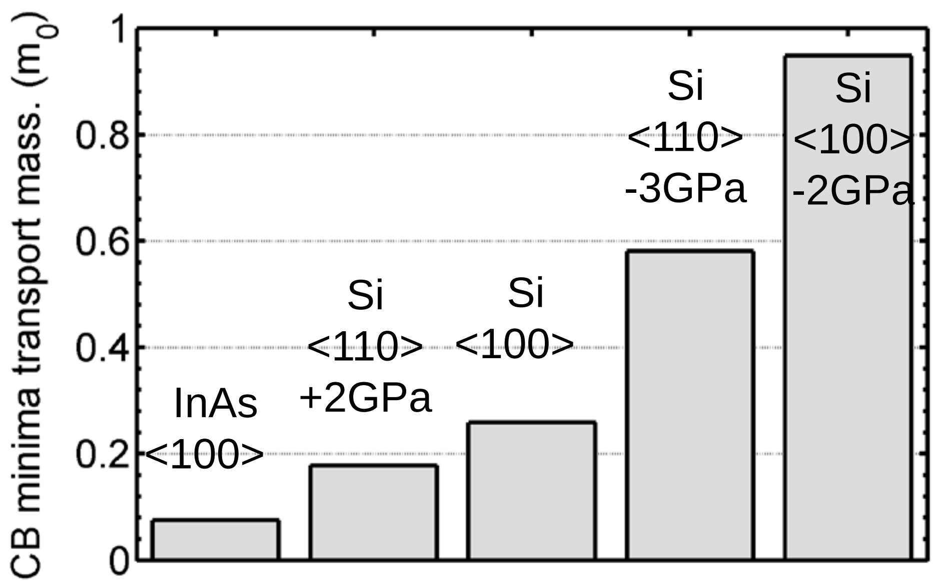
- Uniaxial strain = +(-) 2-3 GPa

Full -band atomistic quantum transport simulations

* Runsheng Wang; et al , "Investigation on Variability in Metal-Gate Si Nanowire MOSFETs: Analysis of Variation Sources and Experimental Characterization," *Electron Devices, IEEE Transactions on* , vol.58, no.8, pp.2317-2325, Aug. 2011

Si / InAs nanowires : orientation/strain effects



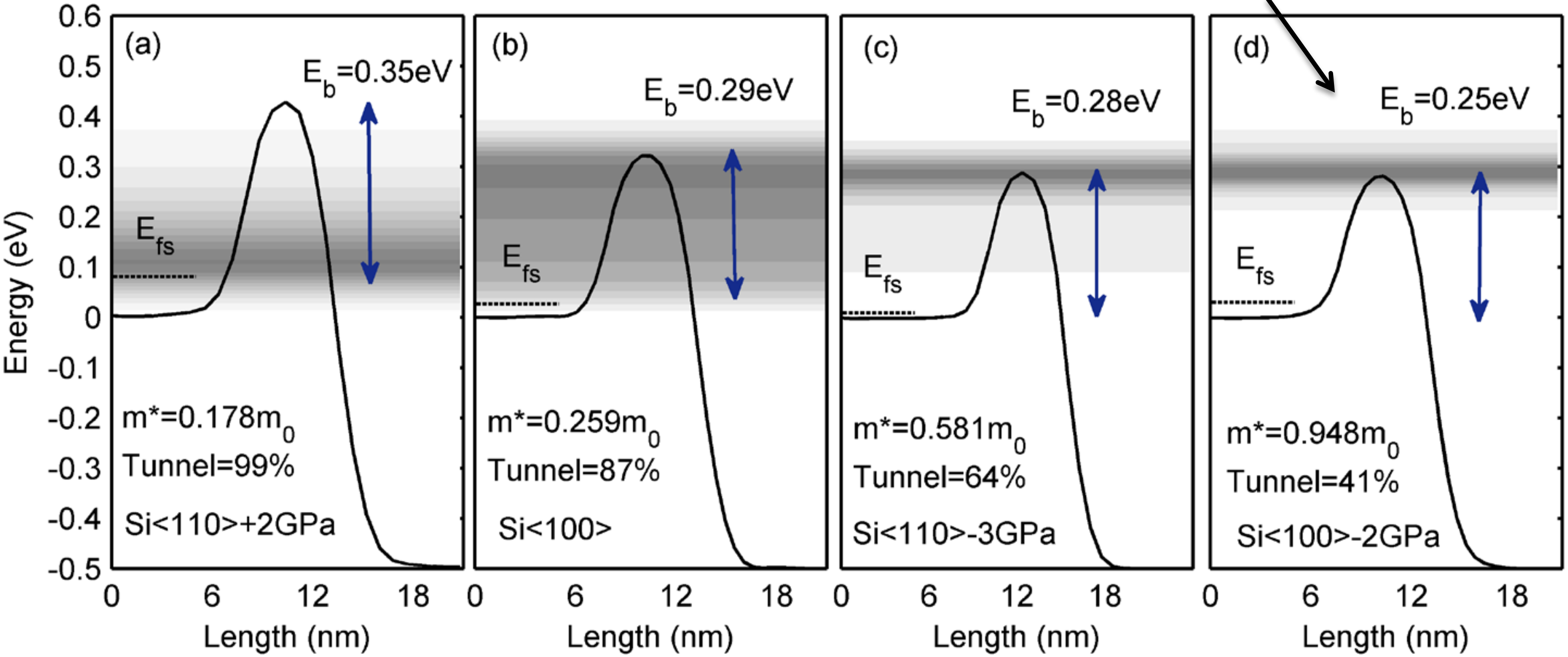


Tight-binding (sp3d5s*) E-k calculations for a D=3.8 nm diameter nanowire.

S-D tunneling : OFF state at Lg=5nm

IOFF=0.1uA/um
(norm. by Dia.)

Classical MOSFET operation where current flows over the barrier below the threshold point.

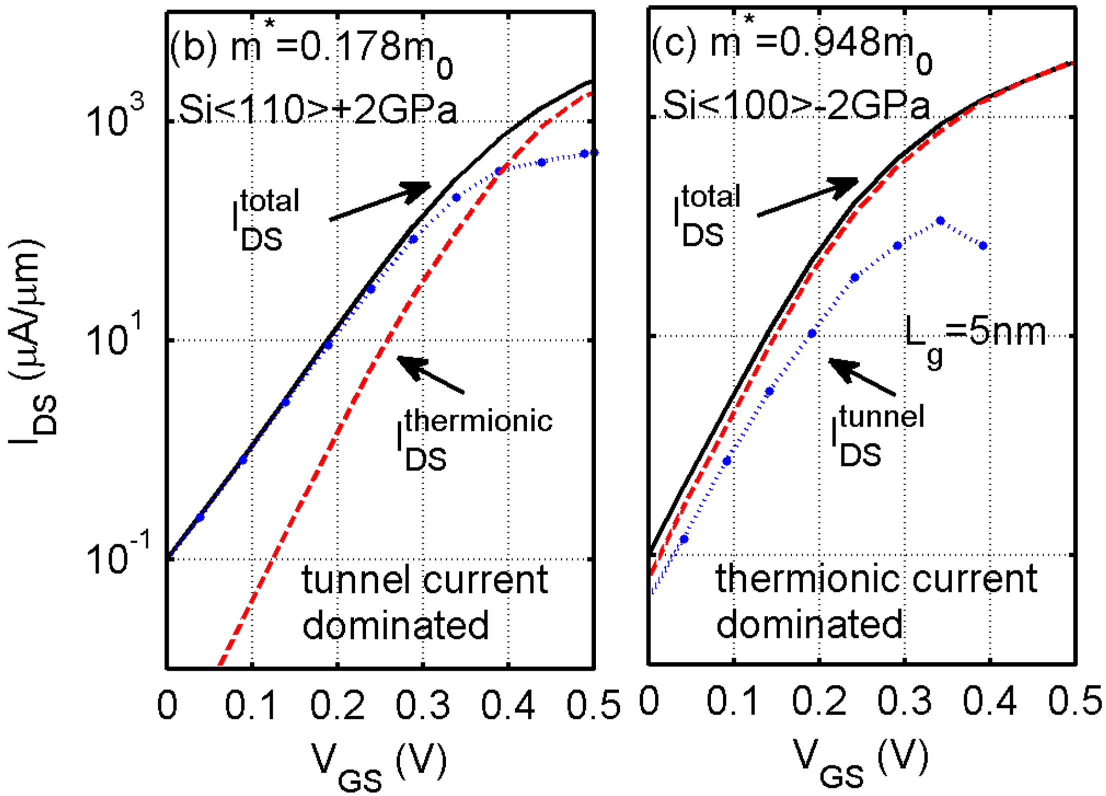


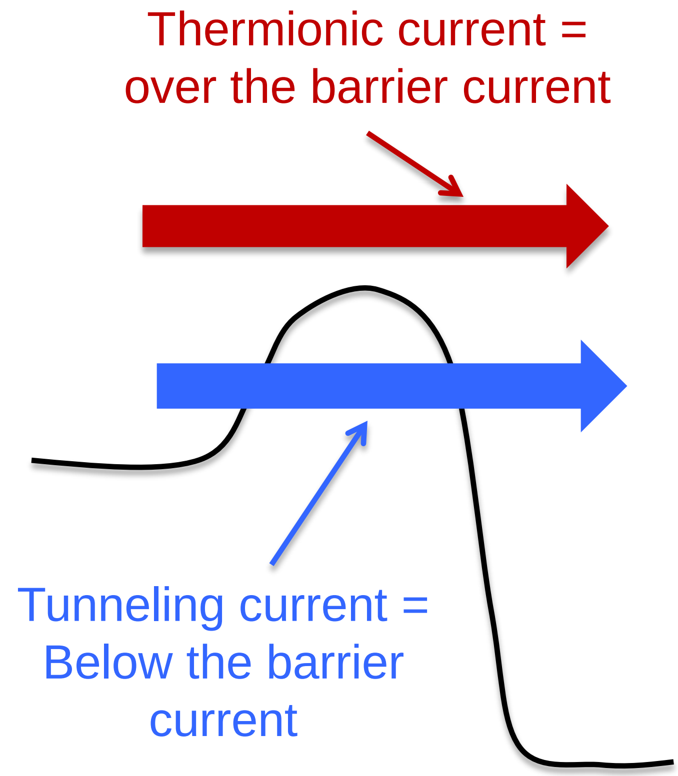
- Source-drain tunneling reduces with increasing mass (m*) .
- Barrier height at OFF state increases with reducing m* → degraded sub-threshold slope.

Thermionic and Tunneling currents

Light mass → tunnel current dominated

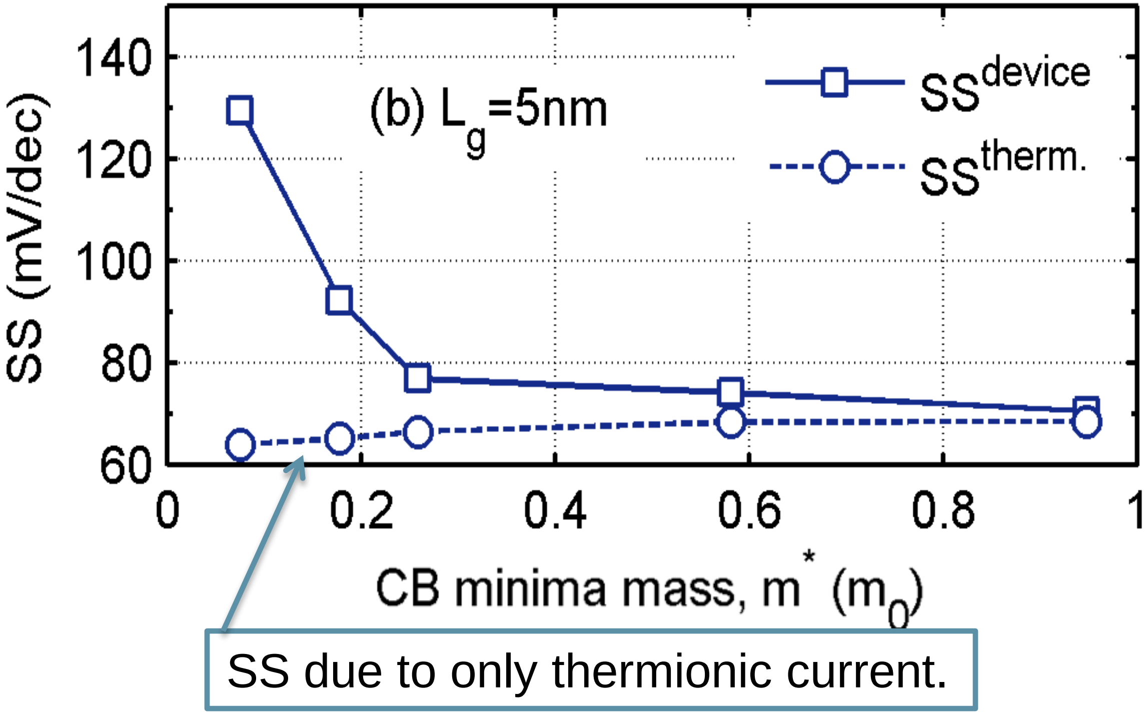
Heavy mass → thermionic current dominated

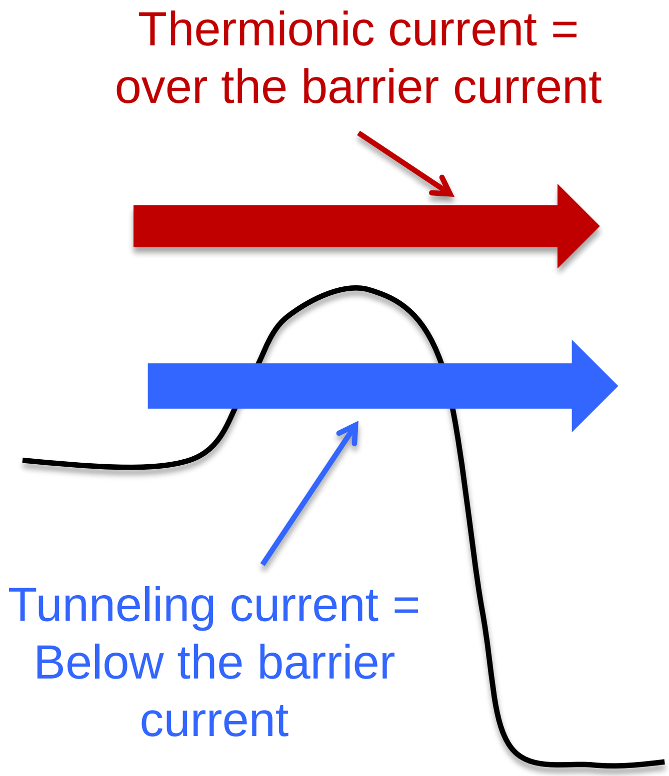




- Calculated tunneling & thermionic current contributions for heavy and light mass.

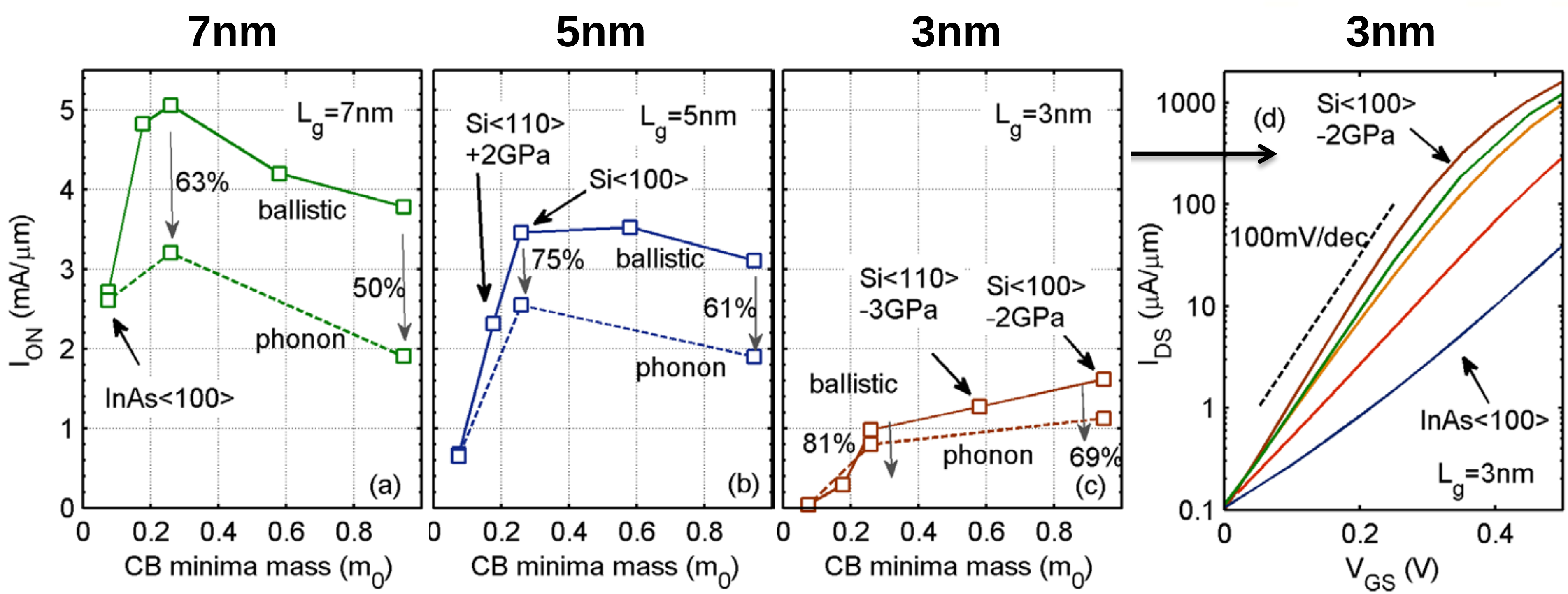
Decoupling tunneling and electrostatics





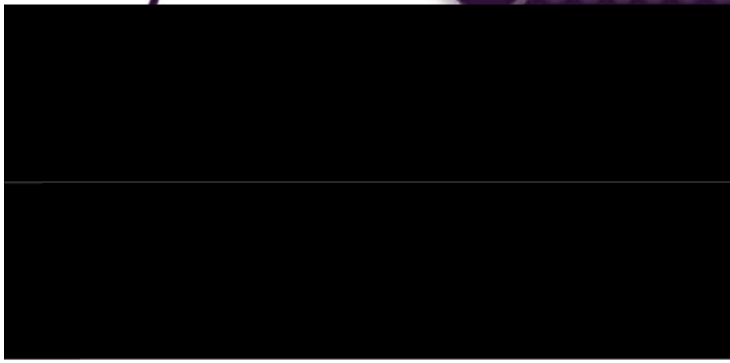
- Light transport mass degrades the SS of the device due to excessive S-D tunneling.
- The lower limit of SS is defined by electrostatics → For the geometry considered in this work electrostatics lead SS ~ 70 mV/dec.

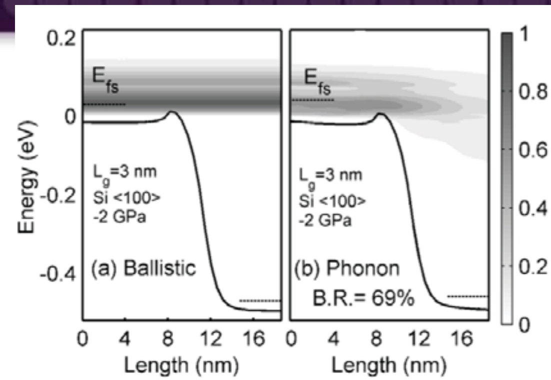
ON state performance
Strong Gate and Mass Dependence



- Ballistic ratio for InAs assumed = 90%. ON state recalculated in presence of phonon scattering for Si<100> (OMEN).
- Current normalized by diameter = 3.8 nm.
- **For a given channel length highest ON state performance shows a peak like nature because of the trade off -> m* ↓=v_{inj} ↑ but m* ↑=SS ↓**

Engineering Nanowire n-MOSFETs at Lg < 8nm





Saumitra Mehrotra, SungGeun Kim, Tillmann Kubis, Michael Povolotskyi, Mark Lundstrom, Gerhard Klimeck,
"Engineering Nanowire n-MOSFETs at Lg < 8nm"
IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 60, 2171 - 2177, (2013)

Achievements (2013):
true atomistic electronic structure&strain model
Full I-V transport simulations

Effective masses can be tuned –
Effective Mass it is NOT just a material property

Features available today in NEMO5

Outline

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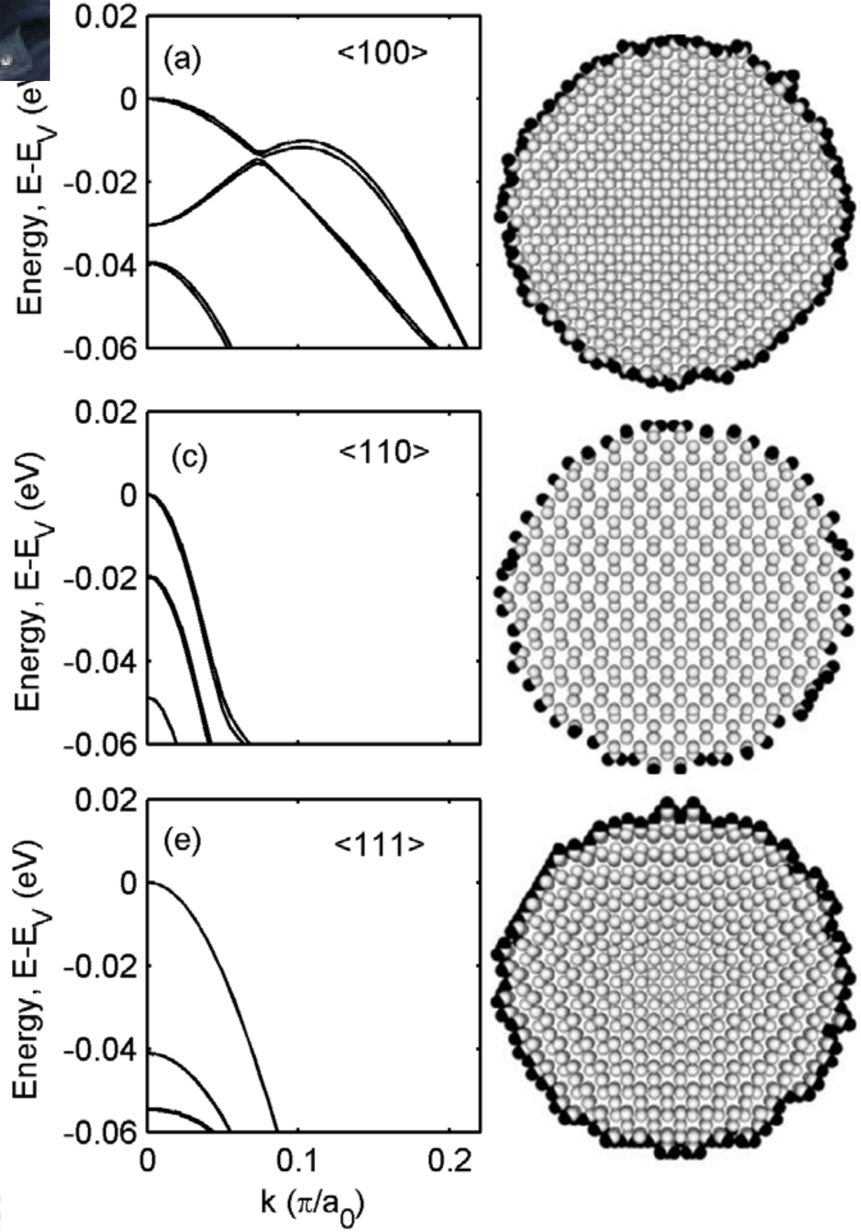
- Bandstructure Concepts
  - » Revisit some “old” bandstructure concepts (ancient RTDs)
  - » Bandstructure in Si nanowires
  - » Bandstructure and transport in Alloy Wires
  - » Bandstructure in SiGe wires
- Source Drain Tunneling for Lg<10nm
  - » Tuning the effective mass for the channel material
- Hole Mobility in SiGe nanowires / FinFETs
  - » SiGe nanowires: Scattering calculations
- Metal-Semiconductor interfaces

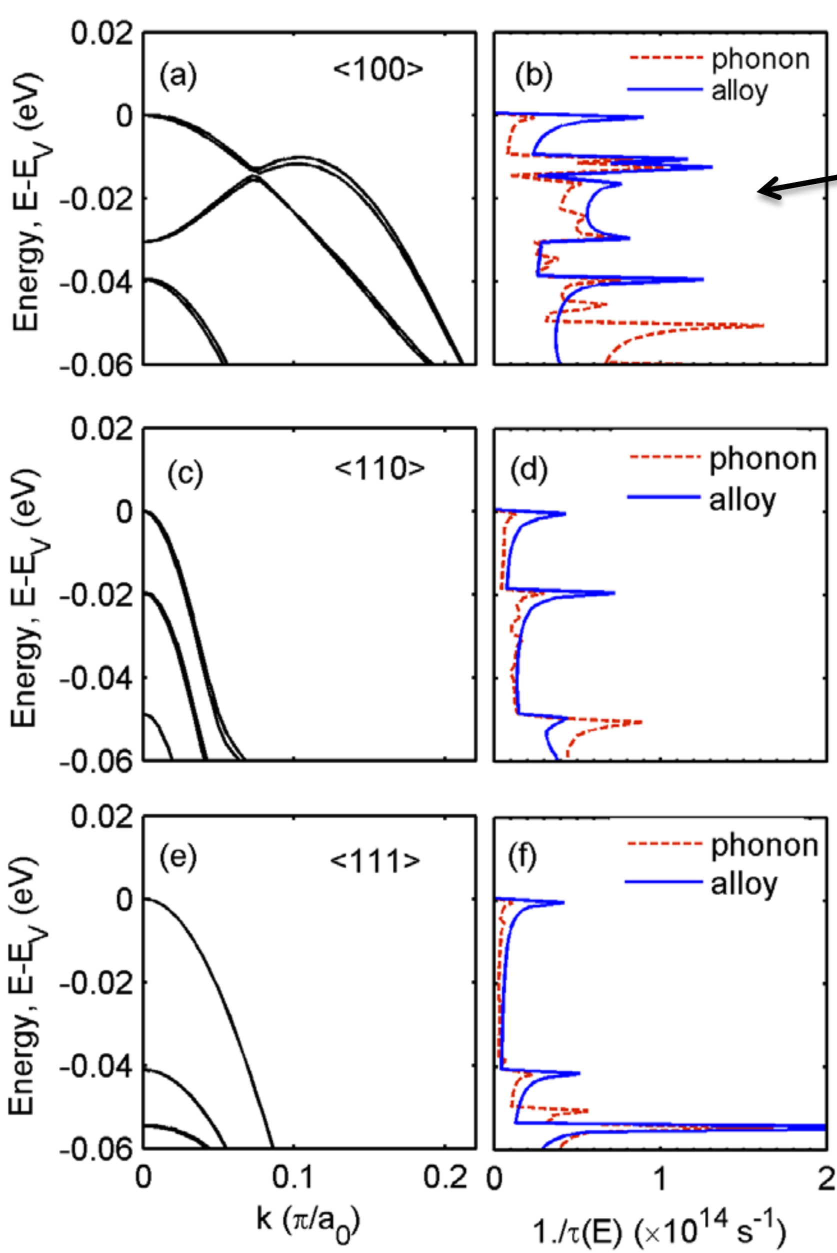
5nm diameter $Si_{0.50}Ge_{0.50}$ nanowire

Saumitra Mehrotra



- **Bandstructure is HIGHLY direction dependent!**

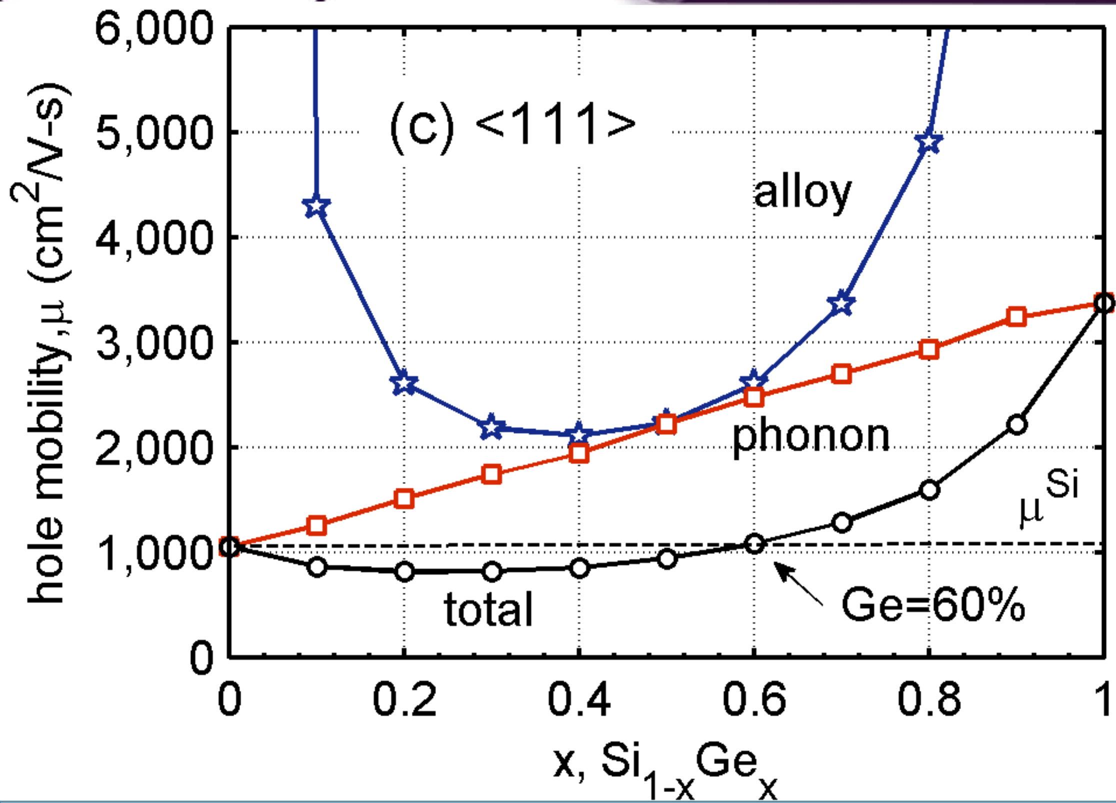
5nm diameter $Si_{0.50}Ge_{0.50}$ nanowire

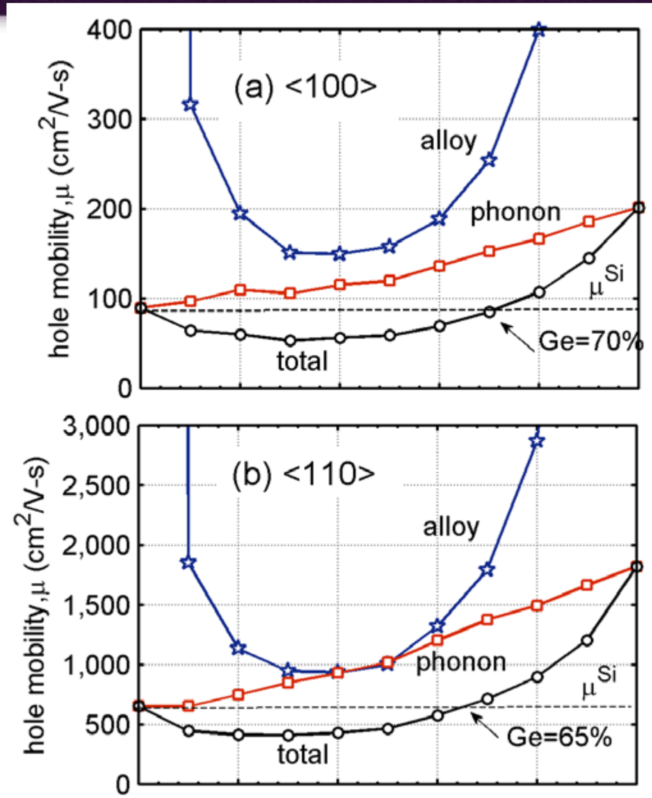


Scattering rate ↑ due heavy bands for <100>

- **Bandstructure is HIGHLY direction dependent!**
- **Scattering rates are also direction dependent**
- **Alloy and phonon scattering rates comparable**

Hole Mobility results for SiGe nanowires





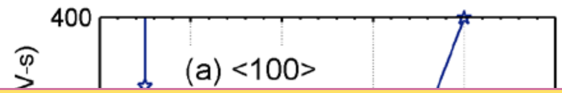
- 5nm diameter at low carrier concentration of p=5e18/cm3.
- Alloy scattering critical
- <111> has the highest mobility
- <100> has the lowest hole mobility.

- **To improve upon Si , >60% Ge in SiGe is needed.**

Atomistic simulation of phonon and alloy limited hole mob. in SiGe nanowires

rotra, P. Long, M. Povolotskyi & G. Klimeck

on



lichael Povolotskyi, Gerhard Klimeck,
limited hole mobility in Si1-xGex nanowires"
7, No. 10, 903–906 (2013)

ents (2013):
odel to classical alloy model
tradeoff space

ings (2013):
stic strain model
ctronic structure model,
tion (not true transport)

Features available today in NEMO5

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  - » Tuning the effective mass for the channel material
- Hole Mobility in SiGe nanowires / FinFETs
  - » SiGe nanowires: Scattering calculations
  - » ~~Experimental Ge slabs and wires - Multi-scale model MD-NEMO5~~
  - » ~~SiGe FinFETS – collaboration with GLOBAL FOUNDRIES~~
- Metal-Semiconductor interfaces

Objectives

- Fit Tight-binding parameter to ATK bandstructure
- Preliminary simulation to show the capability of NEMO5

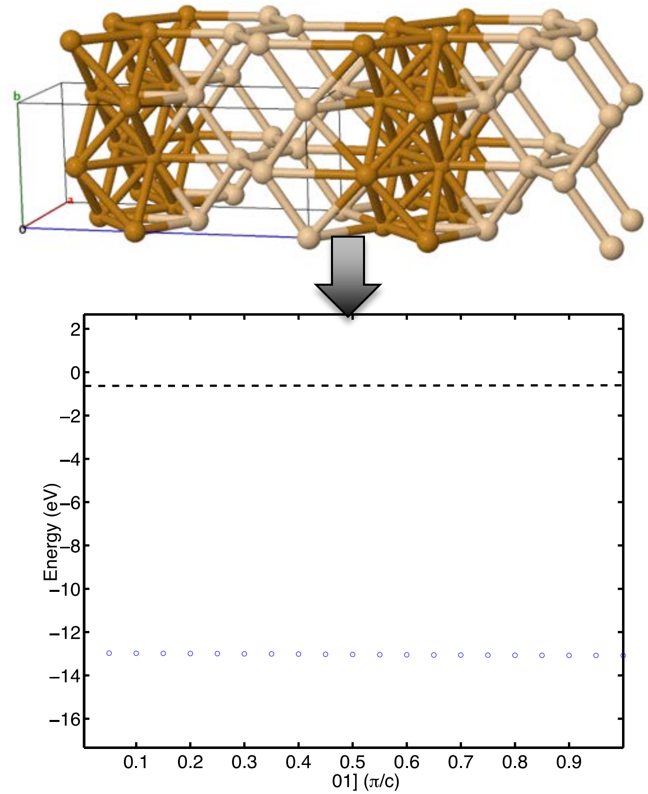
Methods

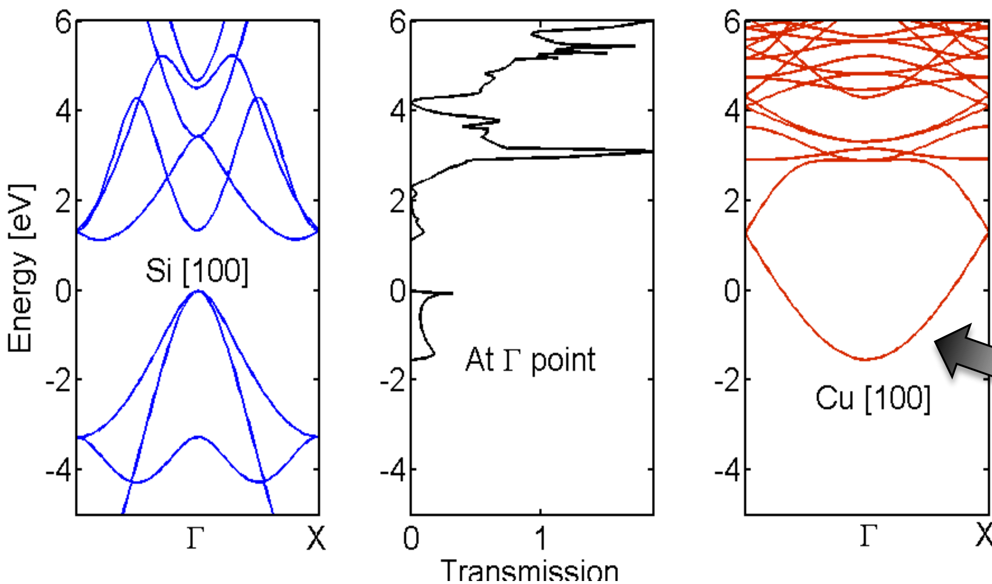
- DFT+ tight-binding model+ NEGF

Results

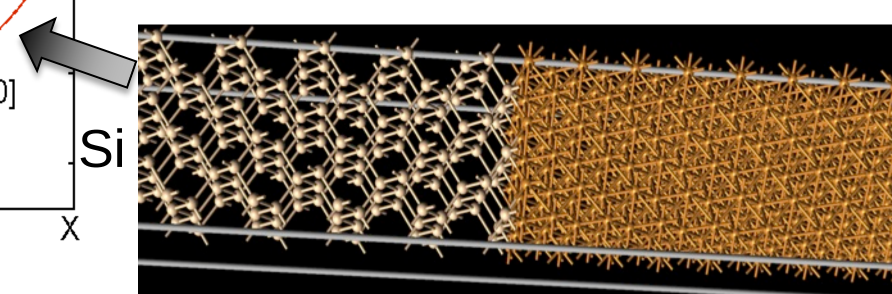
- Band structure calculation using TB parameter fits well with ATK calculation
- Transmission calculation is done by using NEGF method

Cu/Si superlattice





Si



Cu

Lot's of Other Exciting Things

MOSFETs
- Bulk Scattering in NEGF
- Scattering in nanowires and UTBs

Steep SS FETs
- Tunneling FETS in III-V
- Tunneling FETs in III-N
- Superlattice FETs
- New 2D materials - TMDs

Optical Devices
- Quantum dots
- LEDs in Nitrides

Thermal transport
- Phonon transport across interfaces

Metals
- Grain boundary scattering

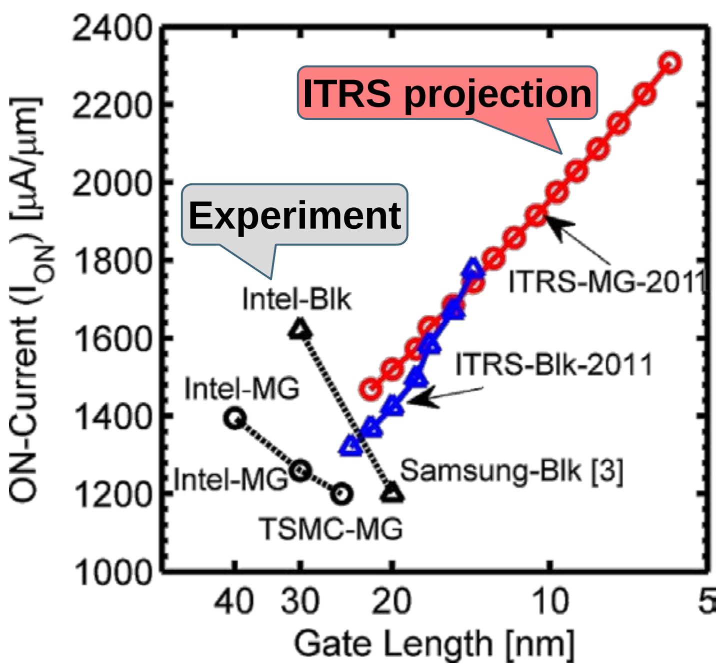
Fundamental Science
- Single impurity devices
- Decoherence in quantum computing

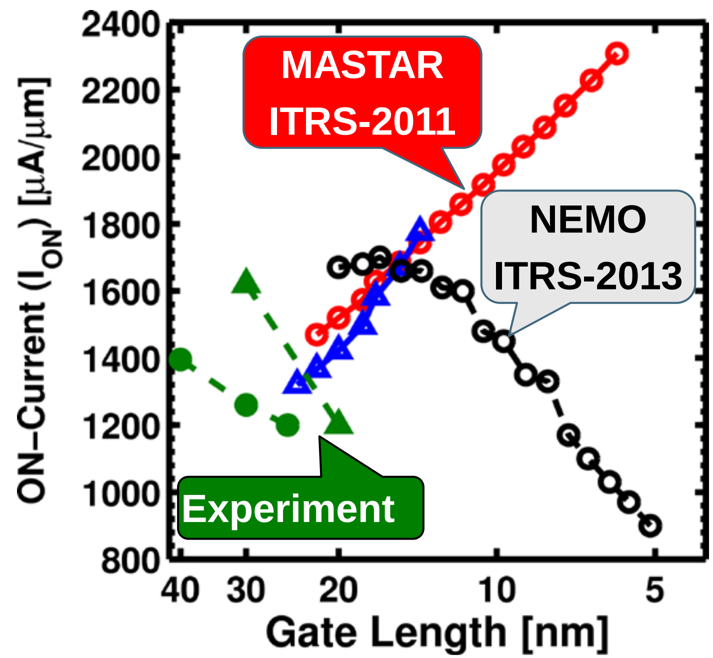
Method Development
- Mode space
- Basis state development
- NEMO5 ⇔ Wannier ⇔ DFT
- NEMO5 ⇔ Huckel ⇔ DFT
- NEMO5 ⇔ TB ⇔
- HPC – Phi/GPU deployment
- HPC scalability

- User interface development

NEMO results for ITRS projections (2014)

Analytical model only → **NEMO atomistic model**

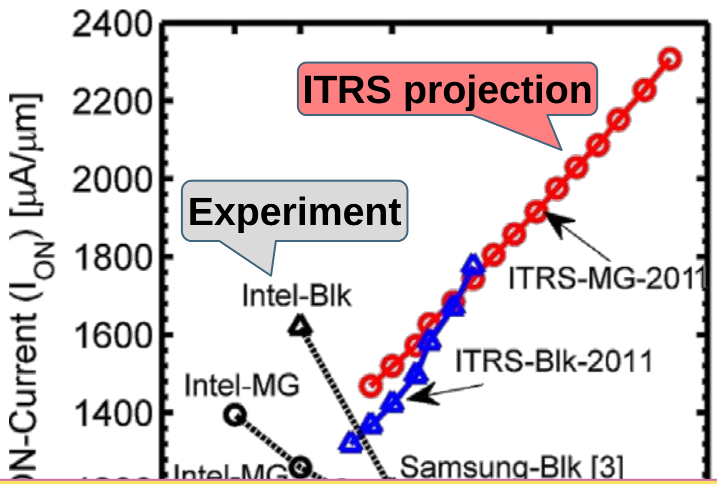


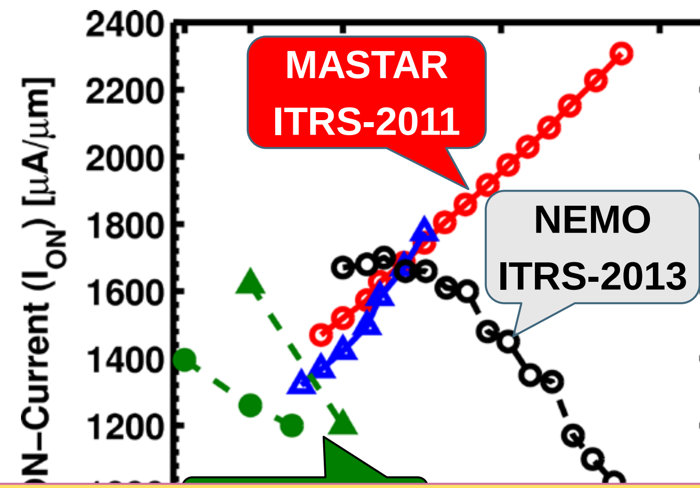


ITRS problem shows growing relevance of atomistic modeling

NEMO results for ITRS projections (2014)

Analytical model only | **NEMO atomistic model**





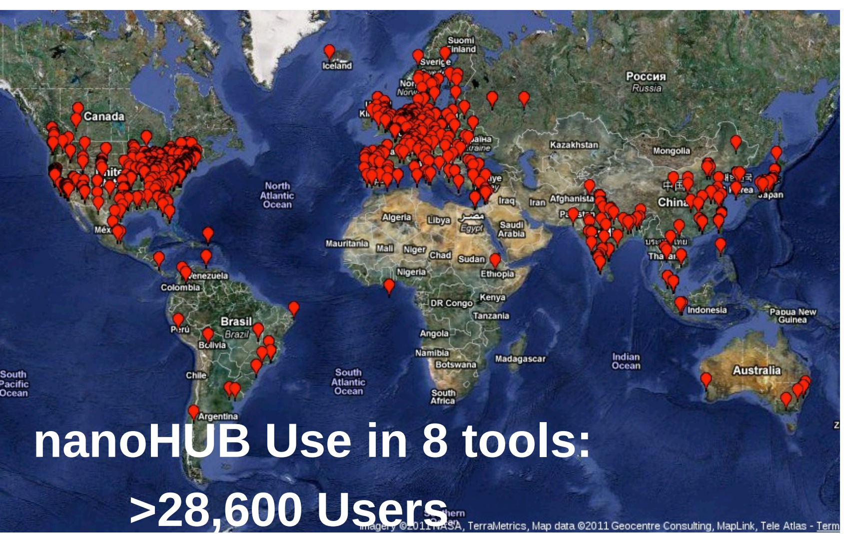
Mehdi Salmani-Jelodar, S. Kim, K. , Gerhard Klimeck,
"Transistor roadmap projection using predictive full-band atomistic modeling"
Appl. Phys. Lett. 105, 083508 (2014)
doi:10.1063/1.4894217

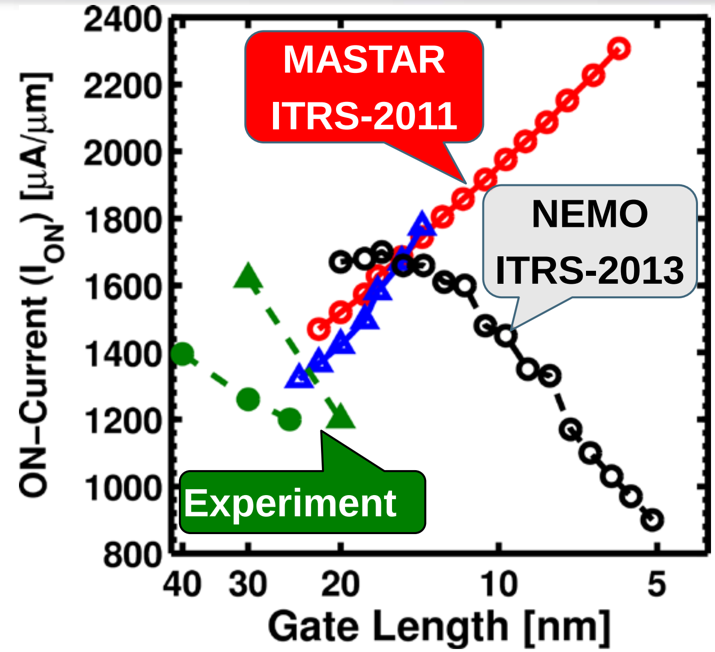
Achievements (2014):
ITRS / IRDS changes model basis
Analytical Scaling with MASTAR =>
Physics-based atomistic model / simulation with NEMO

Typical publications:
- 500+ around NEMO technology
- 7 patents

New type of publications
- Apps on nanoHUB

Published Software
- 200+ research groups
- Industry partners
- Silvaco





Observations:
- 3D spatial variations on nm sca
- Potential variations on nm scale
- New materials / devices

Assertions of importance
- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation