

Nanoelectronics: Computation and Metrology

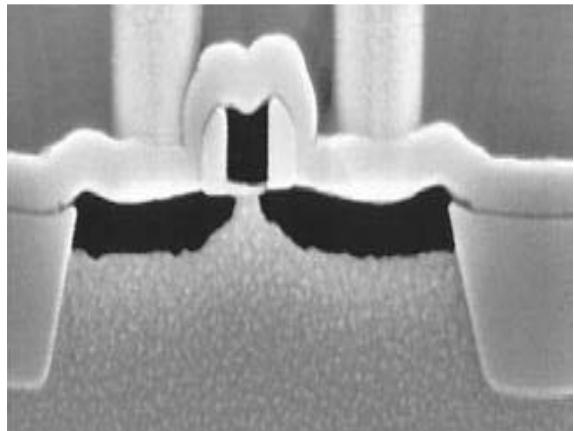
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J.C. Clark, G.K. Klimeck, and A. Raman
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West Lafayette, IN



Outline

- 1) Simulating Nanoelectronic Devices
- 2) Metrology and Computation
- 3) Role of Cyberinfrastructure

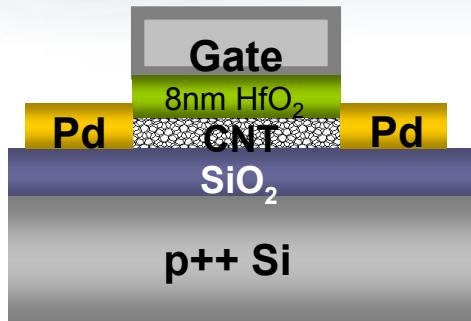
Simulating nano devices



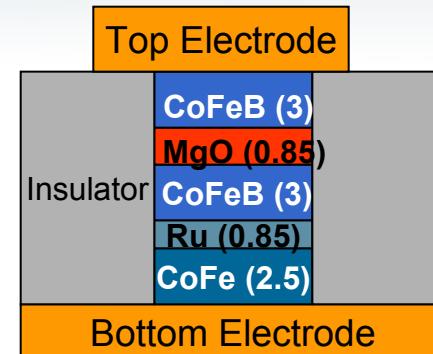
- drift-diffusion
- moments of the Boltzman Eqn.
- Monte Carlo
- full quantum

*-accurate
-fast
-useable*

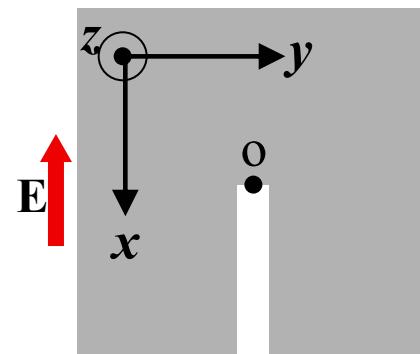
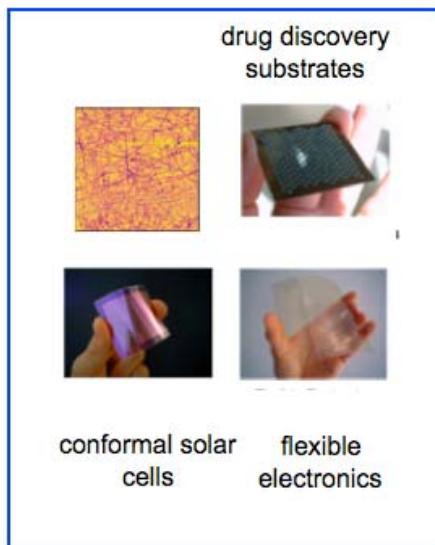
21st century electronics



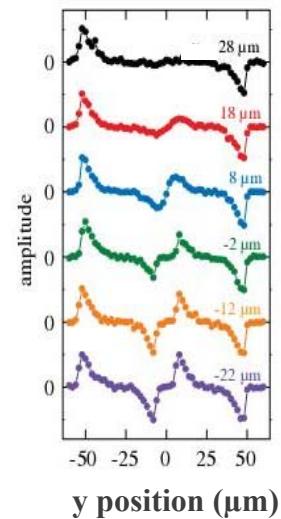
Javey, et al., *Nano Letters*, 4, 1319, 2004



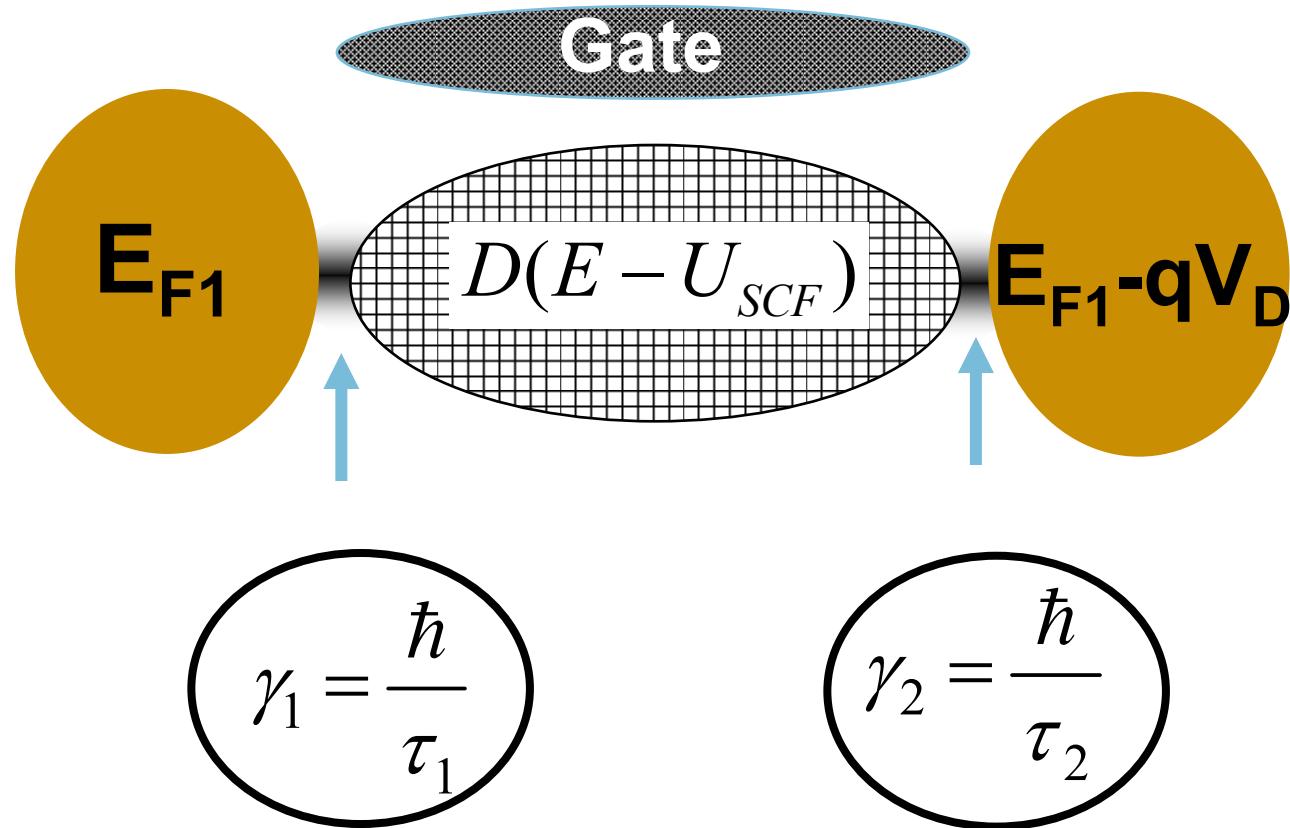
Kubota et al. , *Jap. J. App. Phys.*, 2005



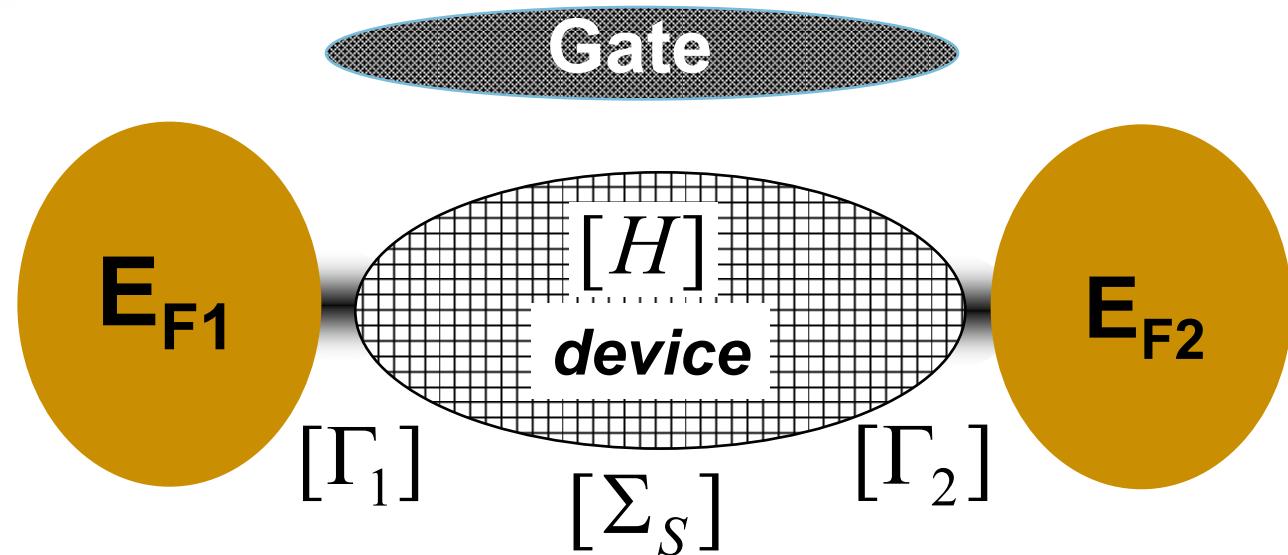
Experiment:
Awschalom et al.
PRL 97, (2006)



Generic model of a nano-device



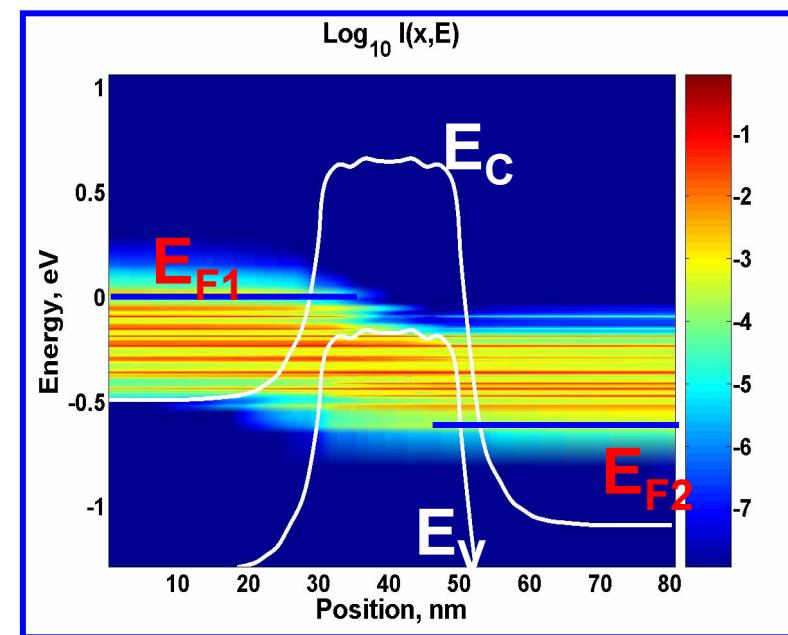
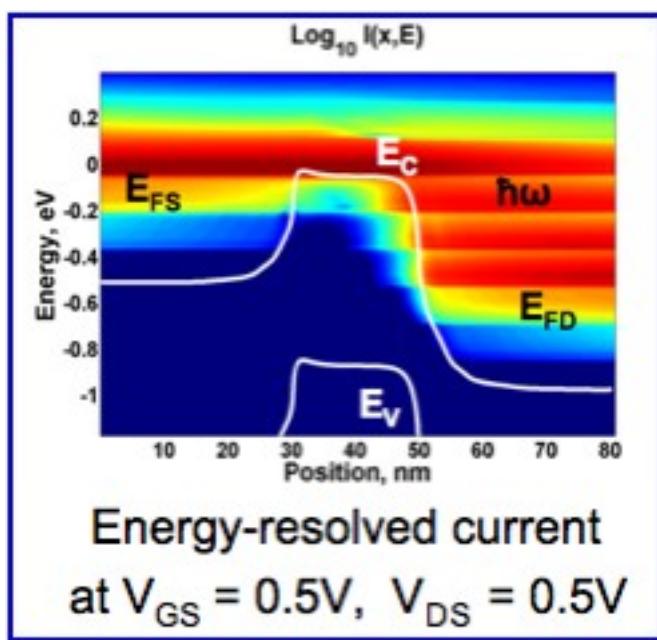
S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
(see also: www.nanohub.org)



Non-equilibrium Green's Function Approach (NEGF)

S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
(see also: www.nanohub.org)

NEGF simulation of CNTFETs

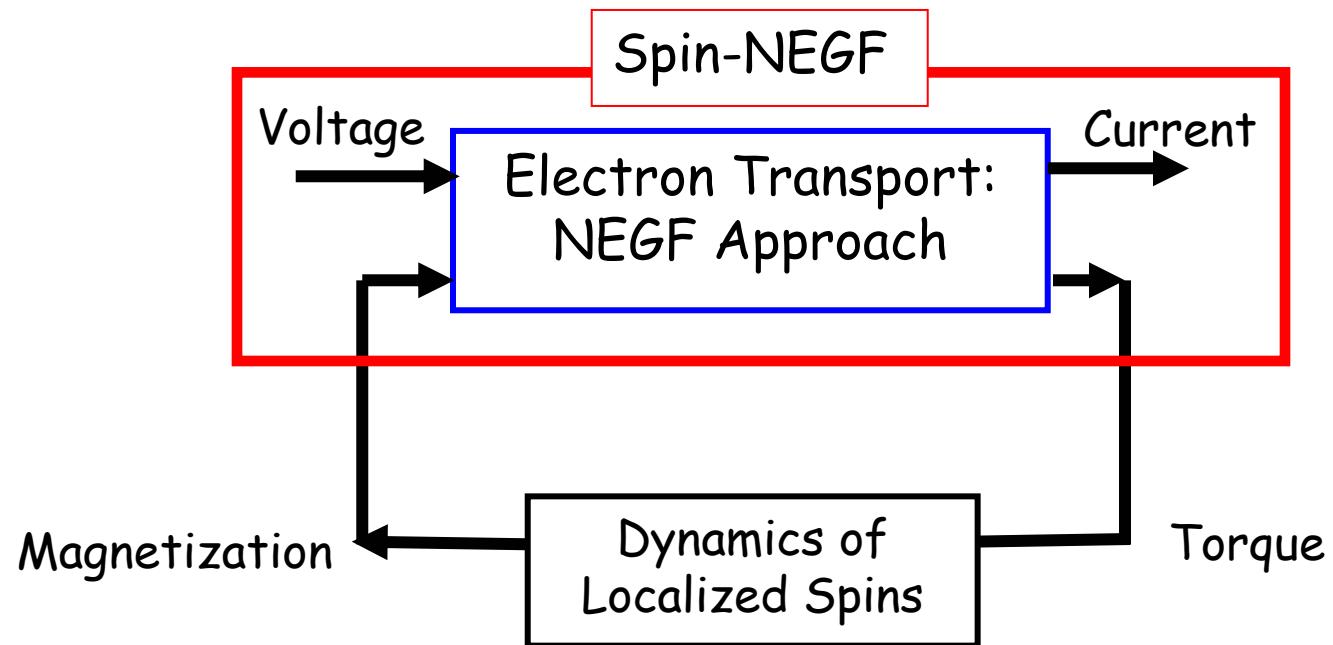


Siyu Koswatta and D. Nikonov
Appl. Phys. Lett., **89**, 021325, 2006

Koswatta, Nikonov, et al., *APL*, **87**, 2006.

(Lundstrom group)

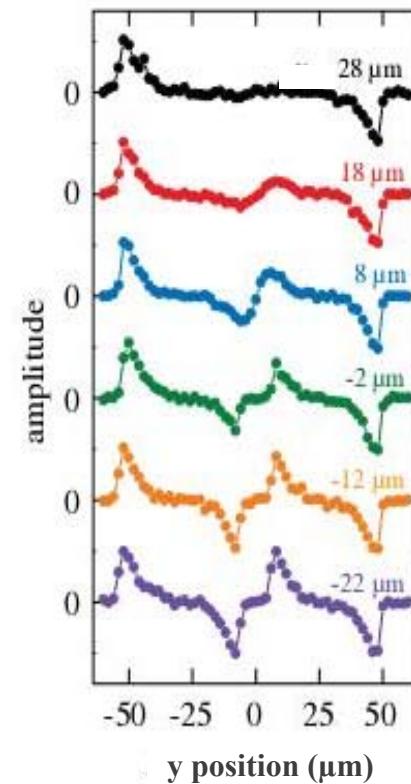
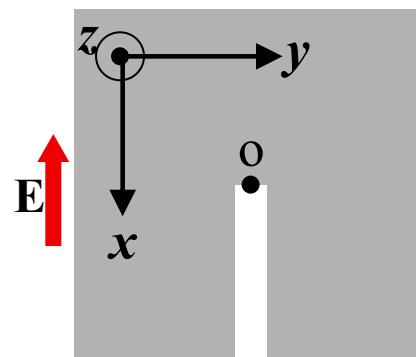
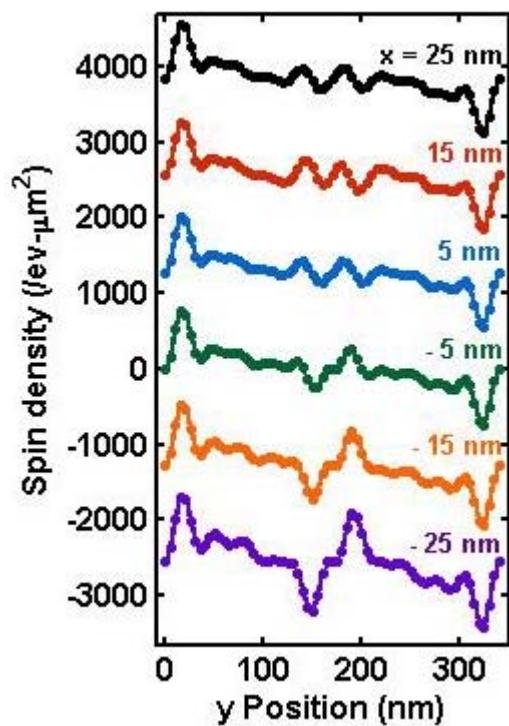
NEGF for spintronics



(Datta group)

NEGF for spintronics

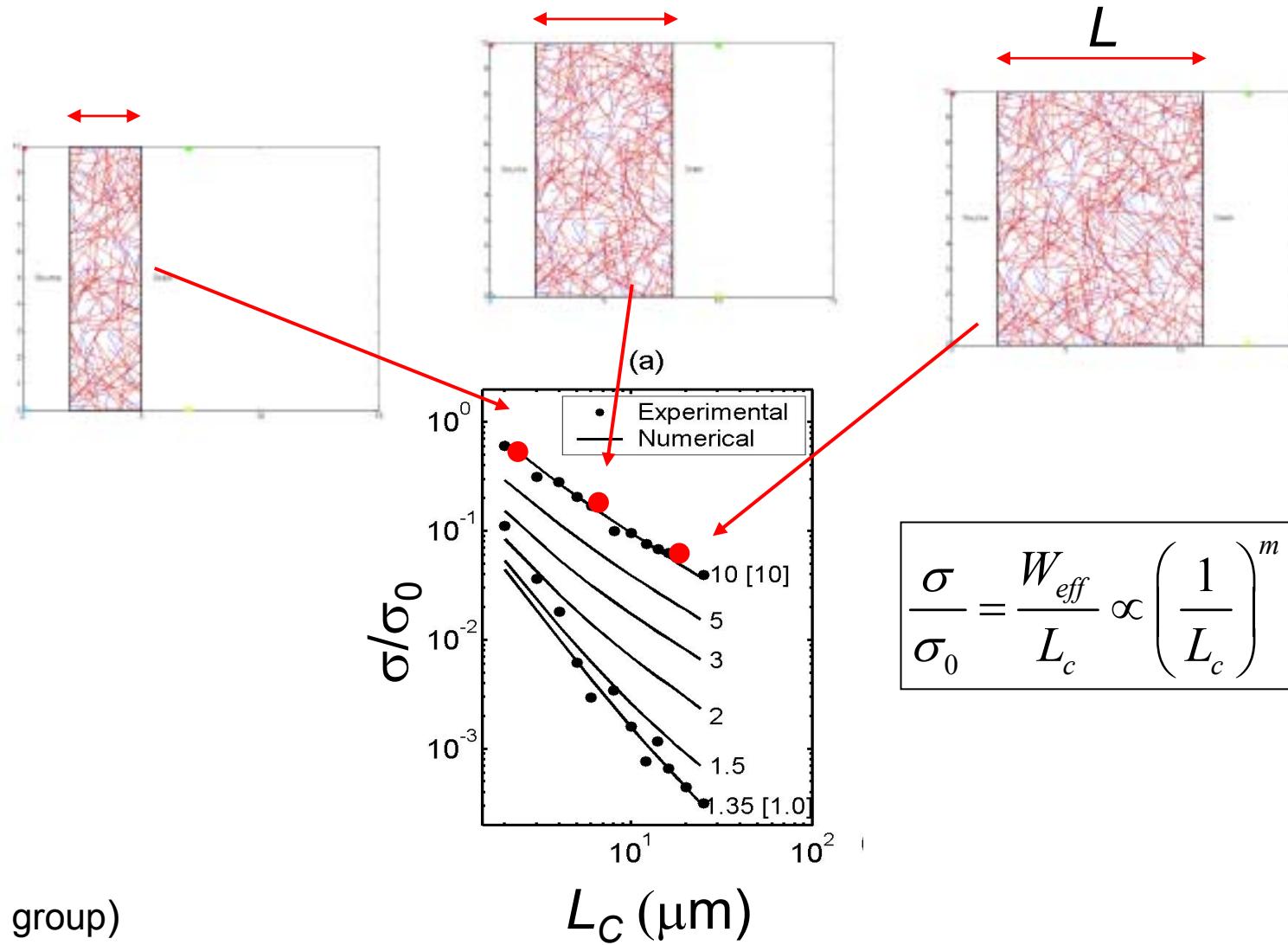
Ballistic



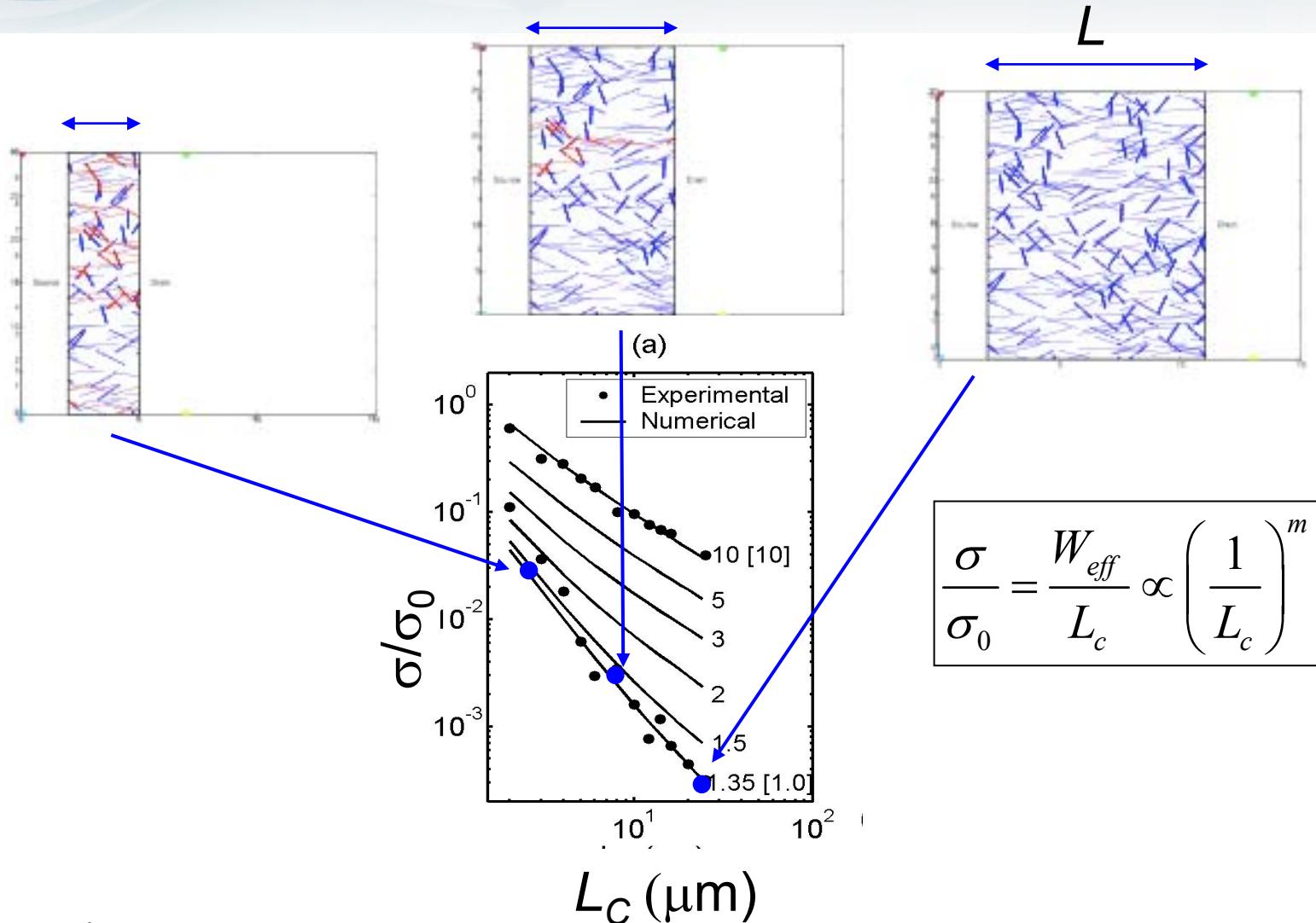
Theory:
Golizadeh-Mojarad and Datta

Experiment:
Awschalom et al.
PRL 97, (2006)

CNT networks



CNT networks



(Alam group)

nanoNet simulator at www.nanoHUB.org

Thoughts on device simulation

- 1) device simulation is being driven by new problems
- 2) the ‘bottom up’ approach adds a new perspective
- 3) it’s not just about simulation; it’s a new conceptual view

see: *Concepts of Quantum Transport*, Supriyo Datta, www.nanoHUB.org

Computation and Metrology

Three examples:

- 1) Inverse Modeling (Gerhard Klimeck)
- 2) Electro Micro Metrology (Jason Clark)
- 3) Scanning probe metrology (Arvind Rahman)

Example 1: inverse modeling of RTDs with NEGF simulation

Typical Modeling and Simulation:

- Forward Experiments:
Assume a structure =>
What is the predicted Performance?

Problems:

- Metrology:
Measured Performance =>
What is the actual structure?
- Synthesis:
Desired Performance =>
What is the best structure to be built?

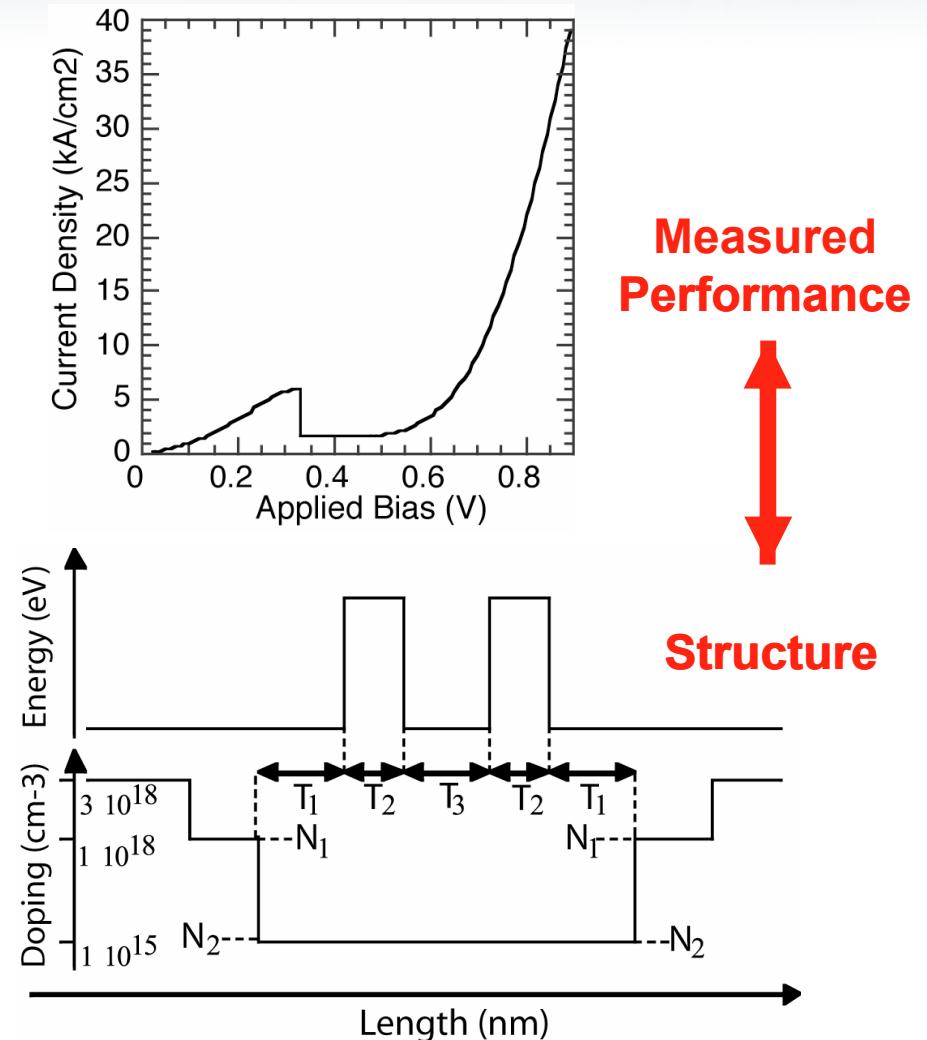
Approach:

- Use existing / verified code (NEMO)
- Genetic algorithm for global optimization
- Develop transferable fitness functions

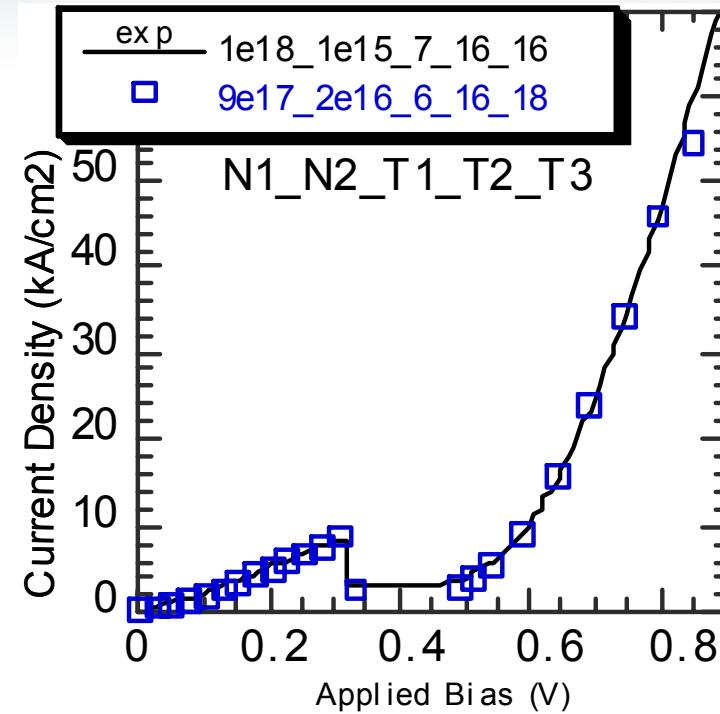
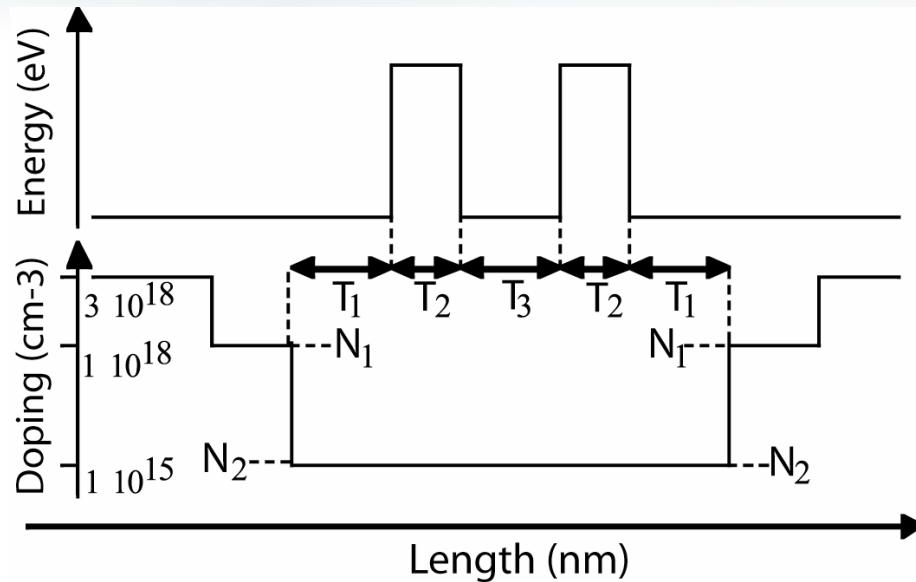
Impact:

- Demonstrate metrology of resonant tunneling diodes

(G. Klimeck group, Purdue)



Example 1: inverse modeling of RTDs with NEGF simulation



- Allow GA to vary 5 different structural parameters:
 - » 3 Thicknesses: well, barrier, spacer
 - » 2 Dopings: low doped spacer, unintentional doping in center

(G. Klimeck group, Purdue)

- GA found structure close to verified physical structure:
 - » Well thicker than intended
 - » Unintentional doping higher than expected

Example 2: electro micro metrology

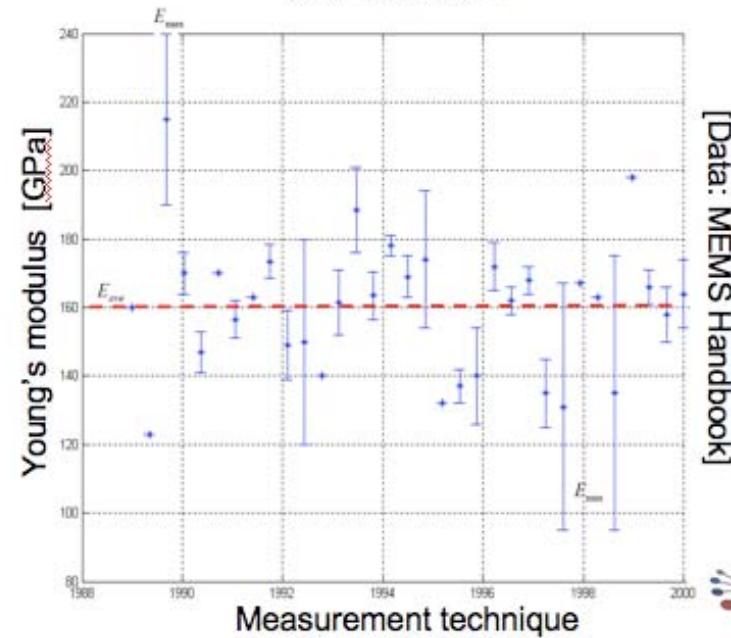
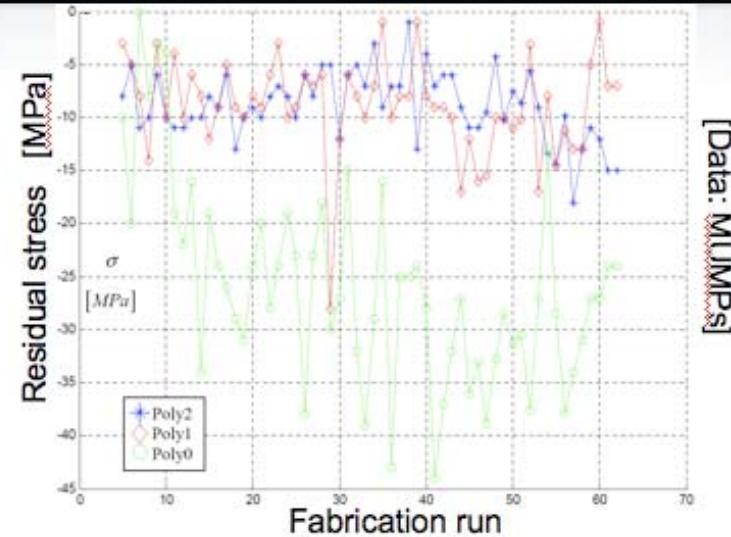
Typical design/fab process:

- Model and simulate a design
 - » Use ideal geometry
 - » Use ideal material properties
 - » Predict performance
- Fabricate the design
 - » Run a standard fabrication process
 - » Measure results

Problems:

- Process variation
 - » Geometric properties are unknown
 - » Material properties are unknown
- Conventional metrology methods
 - » Not readily accessible
 - » Time-consuming and expensive
 - » Large relative errors
 - » Few metrology standards. NIST has made 2 ASTM standards (length, strain gradient)
- Performance does not match prediction
 - » Parameters and uncertainties are not well characterized
 - » Back to the drawing board / trial and error

(J. Clark group, Purdue)



Example 2: electro micro metrology

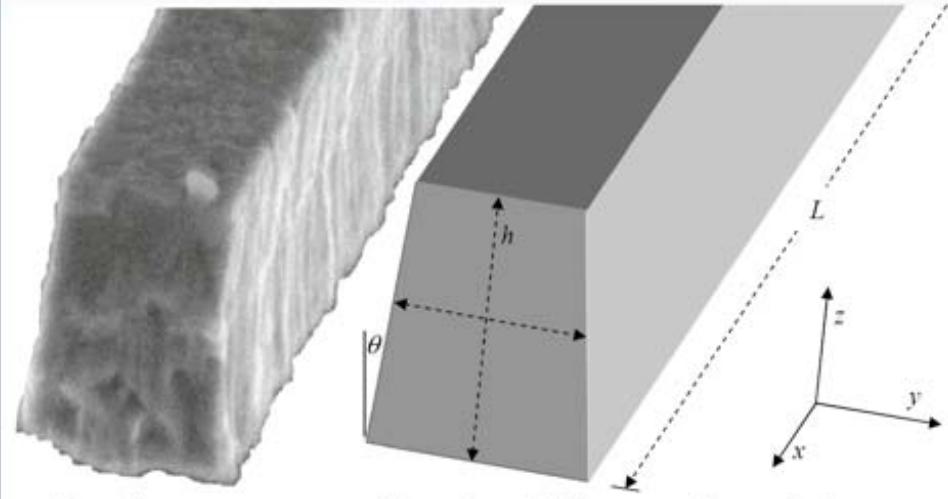
Approach:

- Leverage off of the sensitive electrical and mechanical coupling at this scale
 - » Measure over 2 dozen geometric, dynamic, and material properties by electrical probing.
 - » Greatly reduce the size of uncertainties with high-precision electrical measurands.
- Experimentally accurate modeling
 - » Verify theory and model: performance of real device versus performance of model.
 - » Replace ideal properties with precise measured properties.

Impact:

- Improved understanding of micro-nanoscale design and modeling.
- Fabrication quality control.
- Performance-based standardization.
- Improved characterization of new micro/nanoscale devices.
- Improved sensors and actuators for nanoscale phenomena.

(J. Clark group, Purdue)



True beam

Experimentally-accurate model

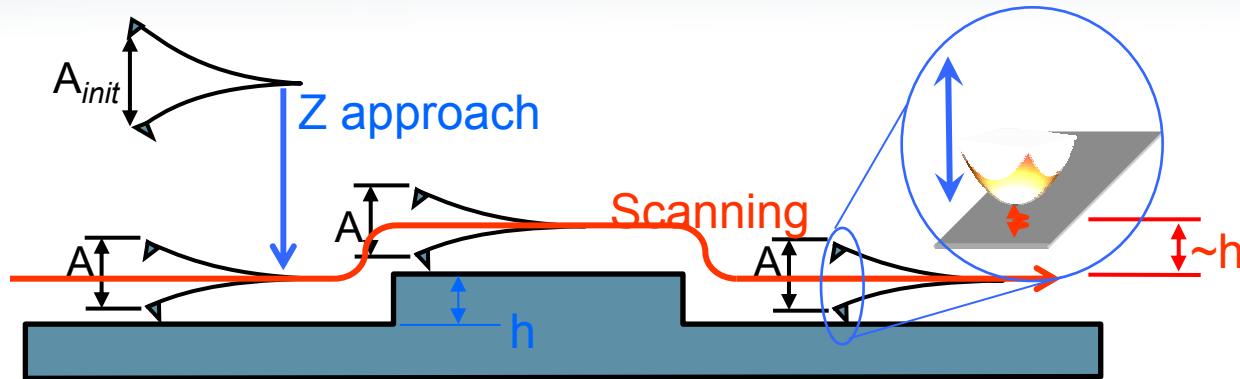
That is, the set of properties of the model that match the performance of the experiment are its effective properties.

Example: The difference between layout and fabrication is

$$\Delta w = \underbrace{\Delta w(\Delta C)}_{\text{Zero}^{\text{th}} \text{ term}} \pm \left[\frac{\partial w}{\partial \delta C} \right] \delta C$$

$O(10^8)$ Sensitivity $O(10^{-18}..10^{-21})$ Electrical uncertainty

Example 3: dynamic scanning probe metrology

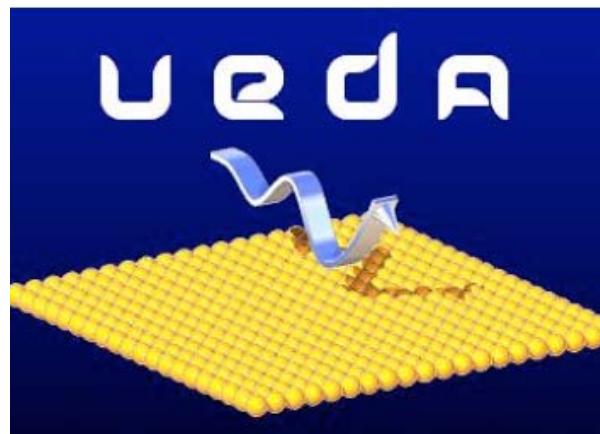


- Scanned “image” is a convolution of sample properties, tip-sample dynamics, feedback control loops, and tip geometry
- Next generation SPM nanometrology requires accurate deconvolution or compensation of each of these effects
- Tip-sample interaction physics, tip oscillations and scanning stability are very non-intuitive; a result of underlying nonlinear dynamics
- Where intuition fails, computations can offer valuable insight
- Thousands of SPM experimentalists worldwide; insight from computations **can cut training time significantly**

(A. Raman group, Purdue)

Example 3: scanning probe metrology

Virtual Environment for Dynamic AFM



www.nanoHUB.org

- State of the art simulations of AFM probe dynamics and tip-sample interaction physics
- Suite of experimentally validated code
- Tools online for force spectroscopy and scanning in air/UHV
- Future implementations for Magnetic, Electric Force Microscopy, AFM in liquid environments

(A. Raman group, Purdue)

Example 3: scanning probe metrology

Virtual Environment for Dynamic AFM

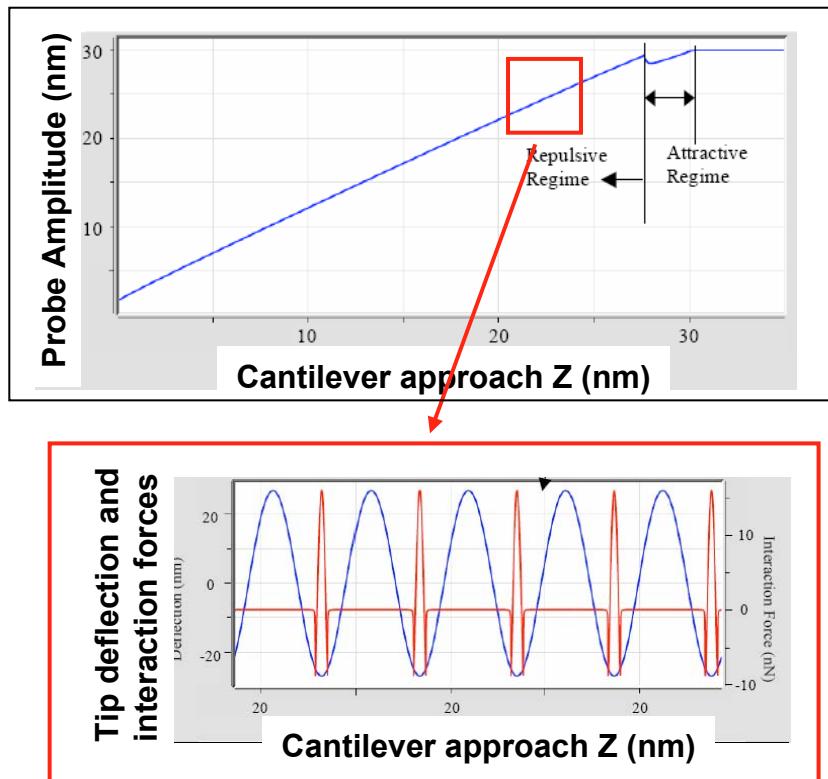


Fig. 1. Sample simulation results for Si tip, polymer sample. Computed amplitude distance curve and zoom in showing oscillation and interaction force history.

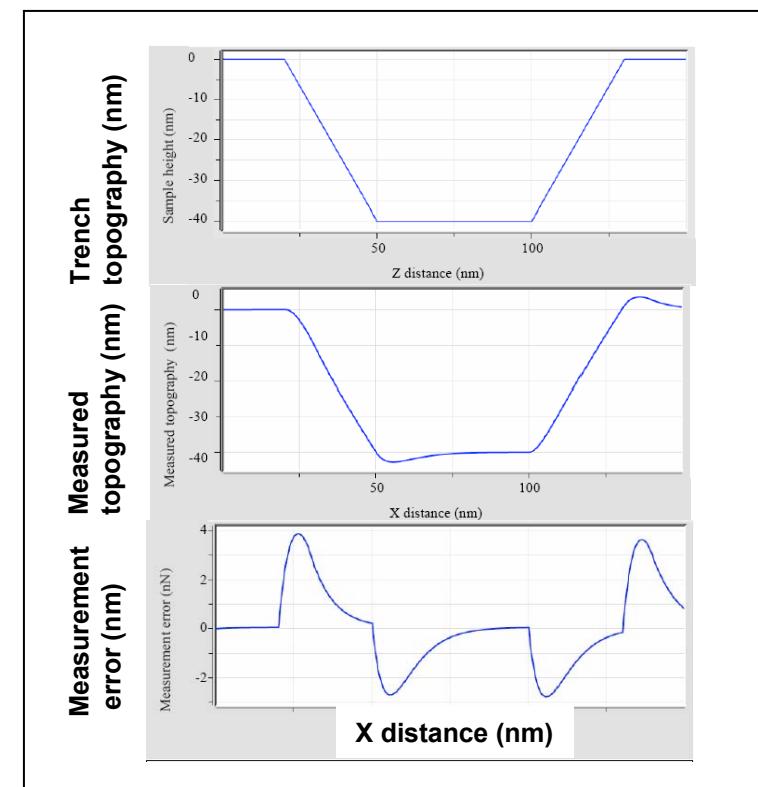


Fig. 2. Dynamic scanning simulation of a Si trench structure using a Si tip. (a) trench topography (b) the measured profile, (c) the metrology error (nm) incurred due to tip dynamics and feedback control.

Network for Computational Nanotechnology

1) people and programs



2) cyberinfrastructure

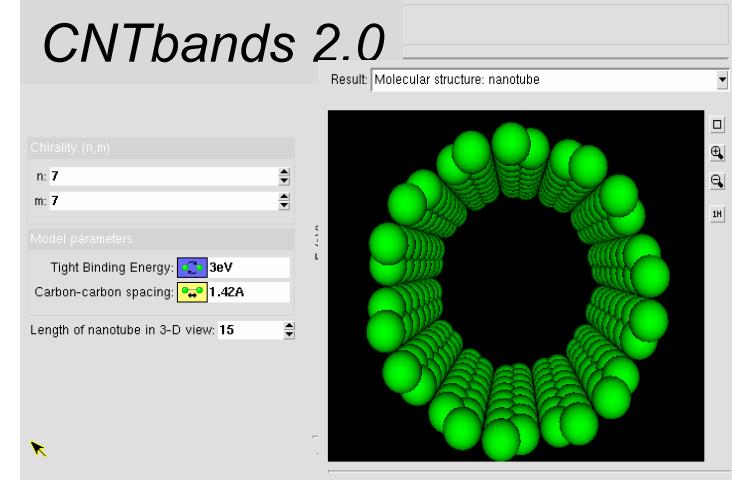
The screenshot shows the nanohUB.org homepage with a banner for OMTools 2.0. The page includes sections for News, Events, Resources, Publications, Tools, About, and Help. A prominent feature is the "Submit your manuscript" button. The footer displays the URL www.nanoHUB.org.

3) partners

Purdue, Illinois, Northwestern, Stanford, Berkeley, Florida, UTEP, Norfolk State U.

Online simulation

www.nanoHUB.org



- 1) online simulation
- 2) open source software

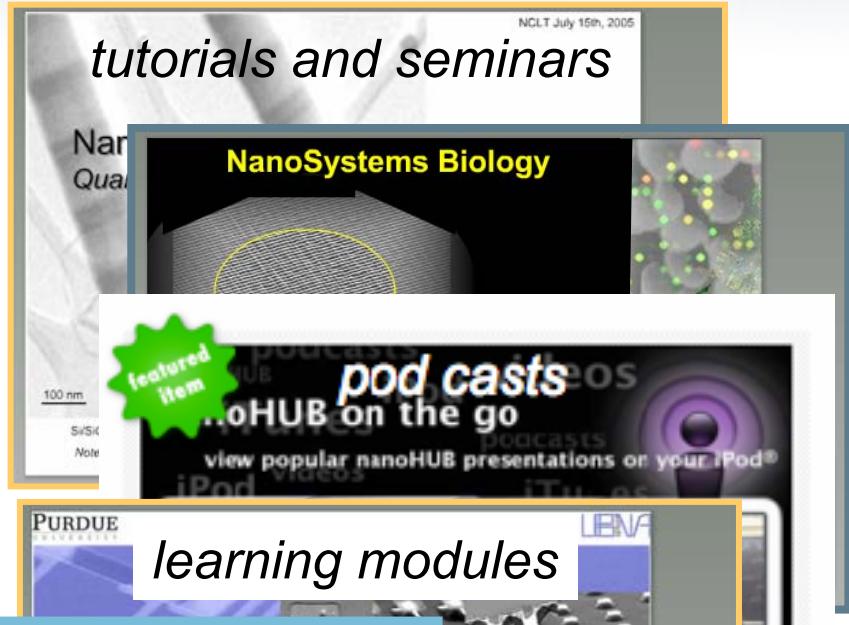
...and more



The screenshot shows the nanohUB homepage with a dark blue header featuring the logo and navigation links: Home, My nanohUB, Resources, Contributions, About, and Support. Below the header is a search bar. A large green banner at the top left promotes "CMBonds 2.0" with a small molecular simulation interface and a green molecular model. To the right of the banner is a text box about the nanohUB's mission. The main content area is divided into four sections: Simulate, Research, Teach & Learn, and Contribute. Each section has several sub-links. At the bottom of the page are news and events sections.

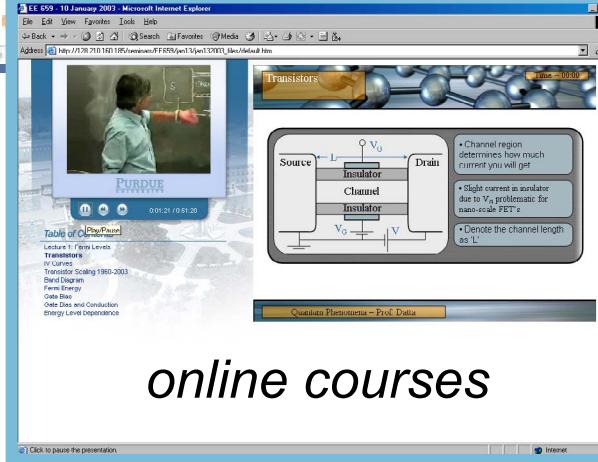
*online simulation
and more....*

tutorials and seminars



The screenshot shows a slide from a presentation titled "NanoSystems Biology". The slide features a grayscale image of a cell membrane with a yellow circle highlighting a specific area. A green starburst graphic contains the text "featured item". Below the image, the text "pod casts" and "view popular nanoHUB presentations on your iPod®" is displayed. The slide is part of a larger presentation with other slides visible in the background.

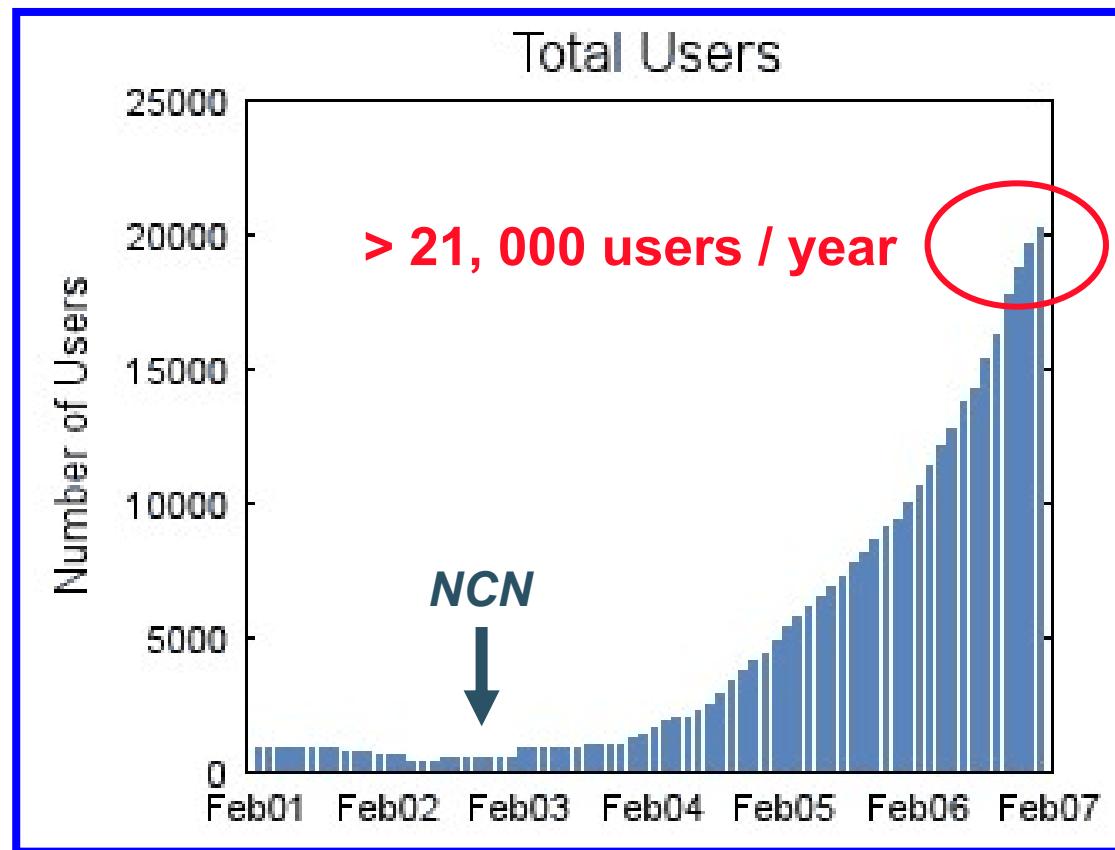
learning modules



The screenshot shows a slide from an online course titled "EE 659 - 10 January 2003 Microsoft Internet Explorer". The slide is titled "Transistors" and includes a video player showing a person in a lab coat working with equipment. Below the video is a schematic diagram of a p-n-p transistor with labels for Source, Drain, Insulator, Channel, and Gate. A table of contents for the course is listed on the left. The slide is part of a larger presentation with other slides visible in the background.

online courses

nanohUB users



- 1) device simulation is being driven by new problems
- 2) the ‘bottom up’ approach adds a new perspective
- 3) it’s not just about simulation; it’s a new conceptual view
- 4) computation will play an increasing role in metrology
- 5) cyberinfrastructure can play a role