"Nothing happens till something moves"
Challenges in modeling of non-equilibrium and time-dependent material systems

Sadasivan Shankar

Senior Principal Engineer,

Technology and Manufacturing Group

Intel Corporation

Workshop*: Towards Material Design Using Strongly Correlated Electron Systems*

Kavli Institute of Theoretical Physics

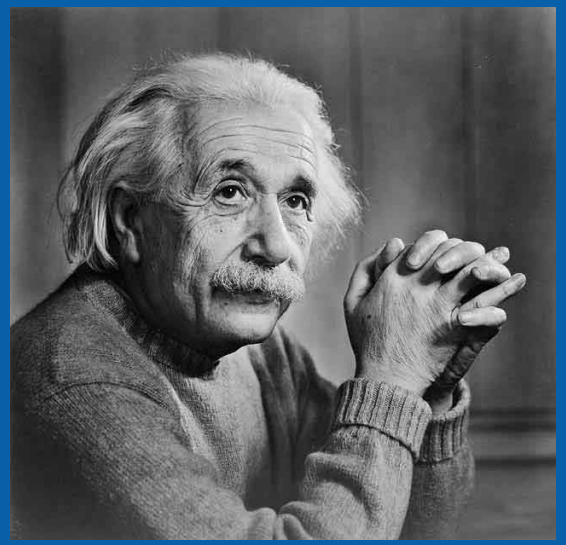
University of California, Santa Barbara

February 25-March 2, 2010

Acknowledgement

- Intel
  - M. Bohr, J. Garcia, M. Garner, M. Haverty, S. J. Park, H. Simka
- Others
  - V. Bochenkov, K. Cho, B. Feldman, J. Hutchby, N. Miller

"Nothing happens till something moves"



Non-equilibrium Systems

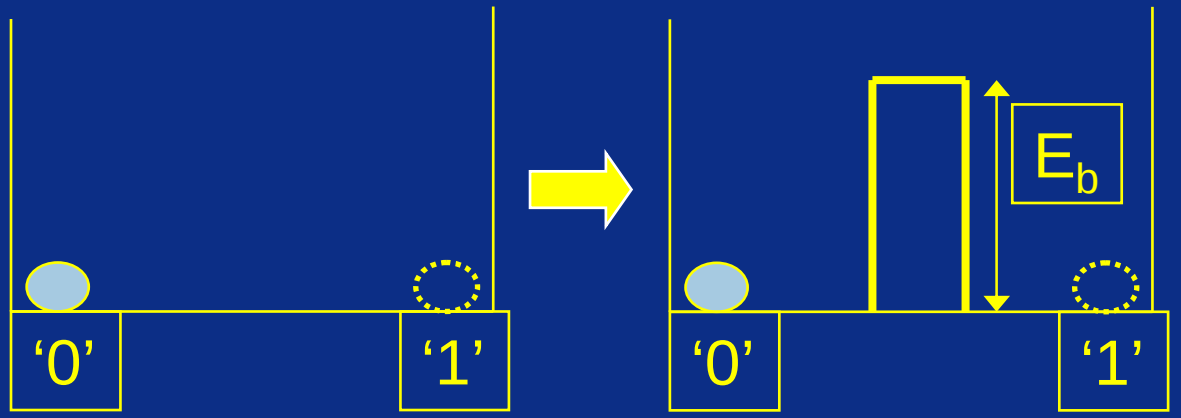
National Academies Report (1999)

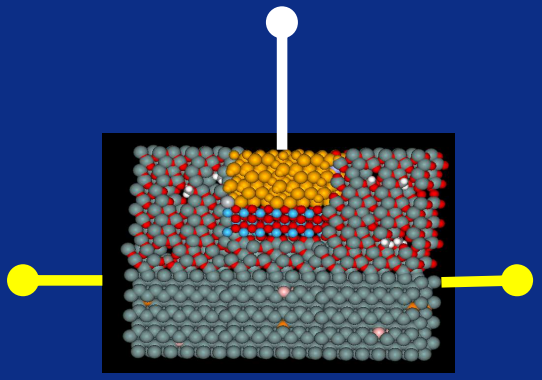
The term ''nonequilibrium physics'' means "the study of physical systems that are not in mechanical and thermal equilibrium with their surroundings…..

Time dependence of physical systems imply properties changing with time

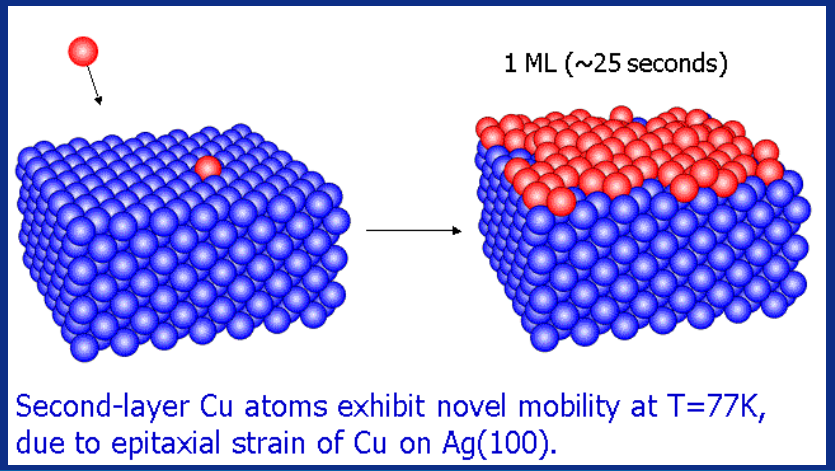
Non-Equilibrium and Time Dependence

Electronic *Switching*





M. Haverty

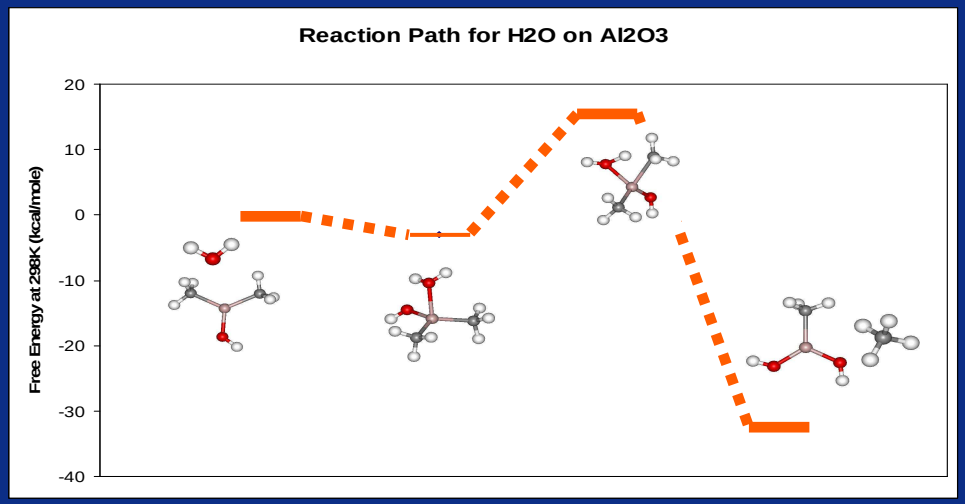


Vapor Deposited
Nucleation and
Film Growth

V. Bochenkov et.al

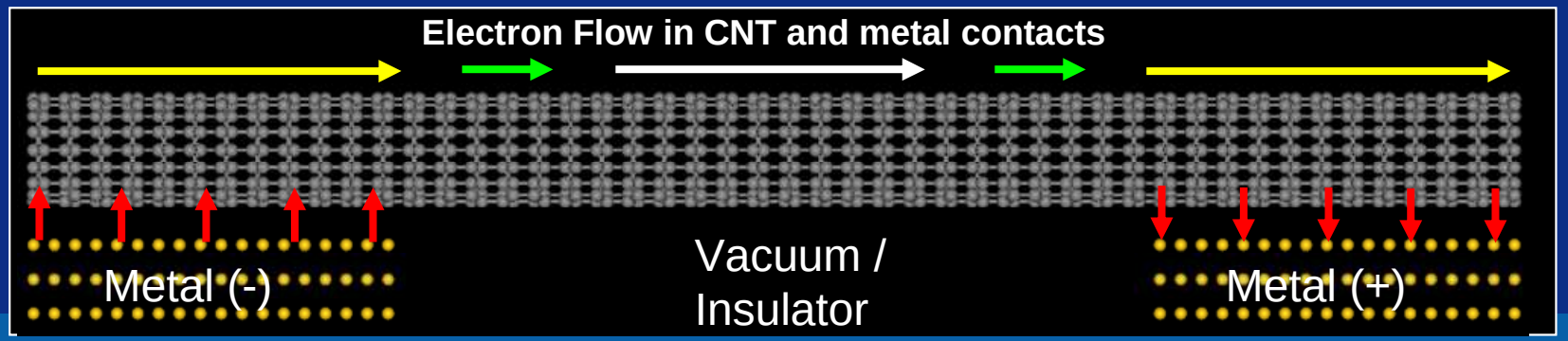
Non-Equilibrium and Time Dependence

Chemical Reactions in *Synthesis*



H. Simka et.al

Conductance in Nanostructures

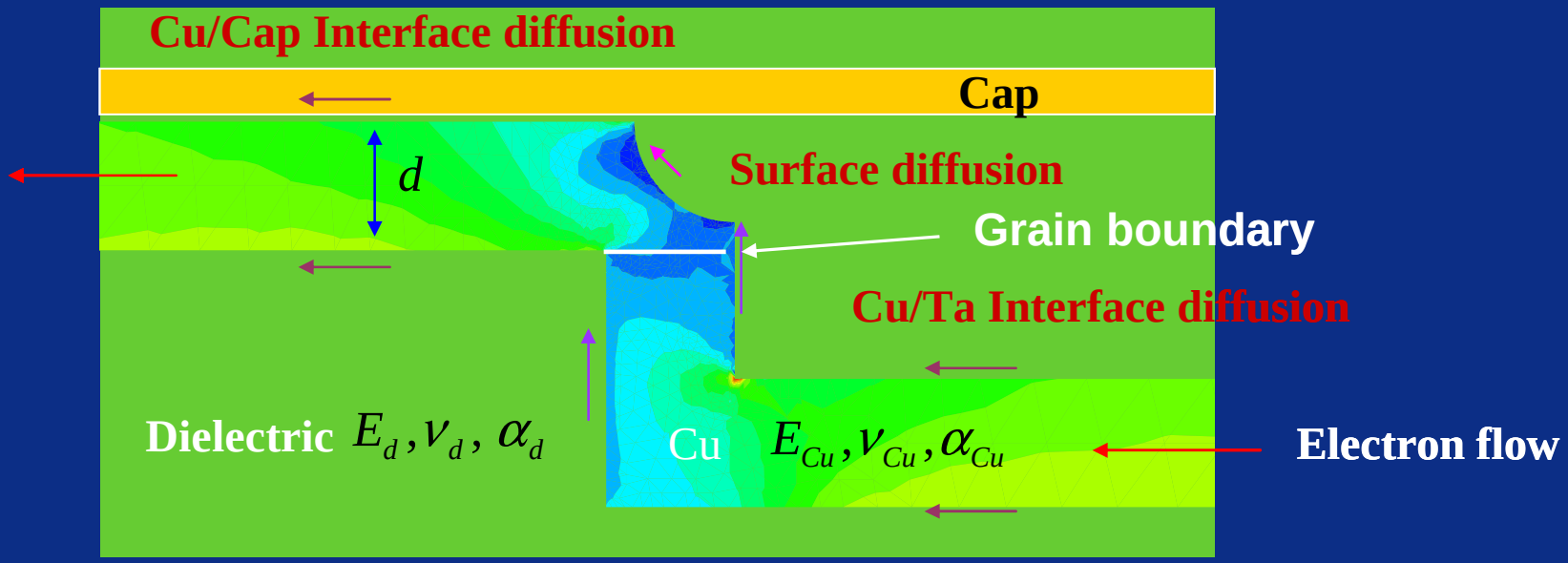


S.Shankar

S. J. Park et.al

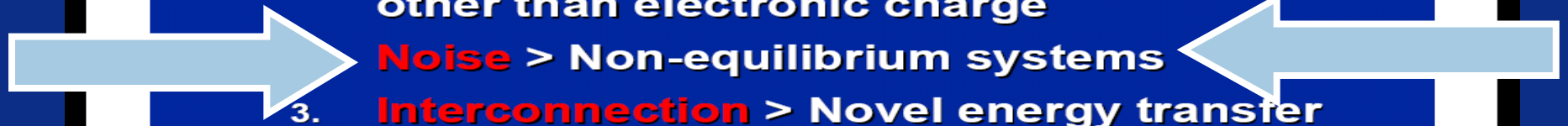
Non-Equilibrium and Time Dependence

Electron *Transport* and Atomic *Migration* = *Electromigration*



A. Bower et.al

ITRS 2007 Emerging Research Vectors



Five research vectors *

1. Energy > Computational state variables other than electronic charge
2. Noise > Non-equilibrium systems
3. Interconnection > Novel energy transfer mechanisms
4. Heat >Nanoscale thermal management
5. Manufacturing cost > Directed self assembly

*Adopted by the Nanoelectronics Research Initiative (NRI), And International Technology Roadmap for Silicon (ITRS)

11

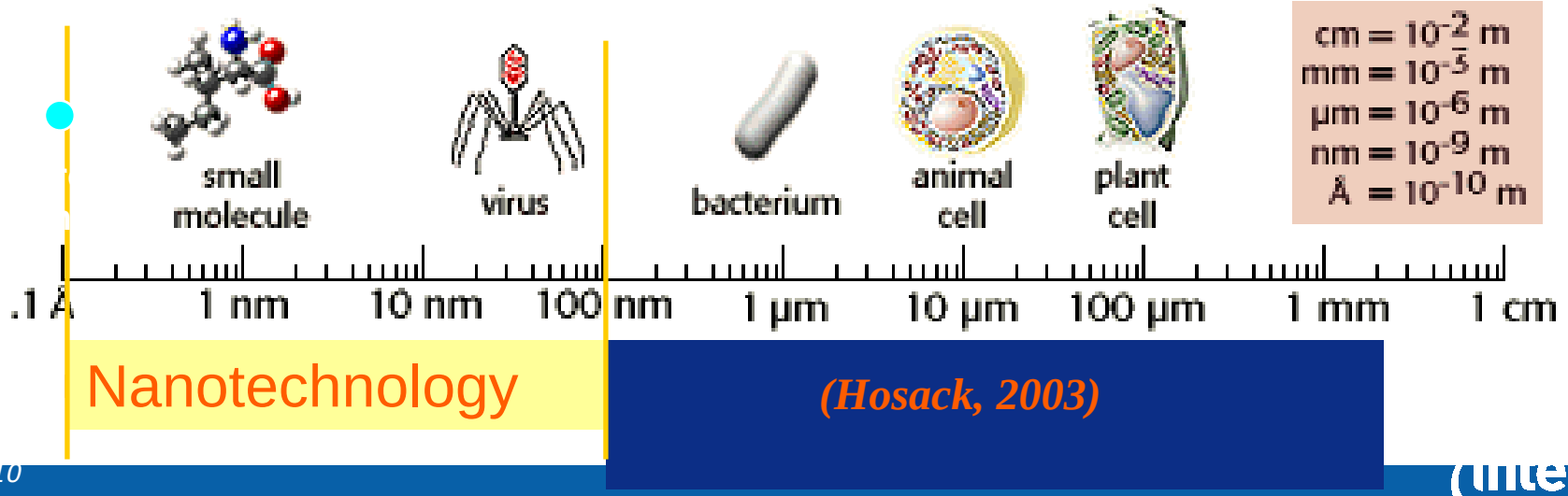
Detour: *Nanotechnology and Moore's Law*

Nanotechnology is…

Research and technology development at the atomic, molecular or macromolecular levels, in the length scale of approximately 1 - 100 nanometer range."

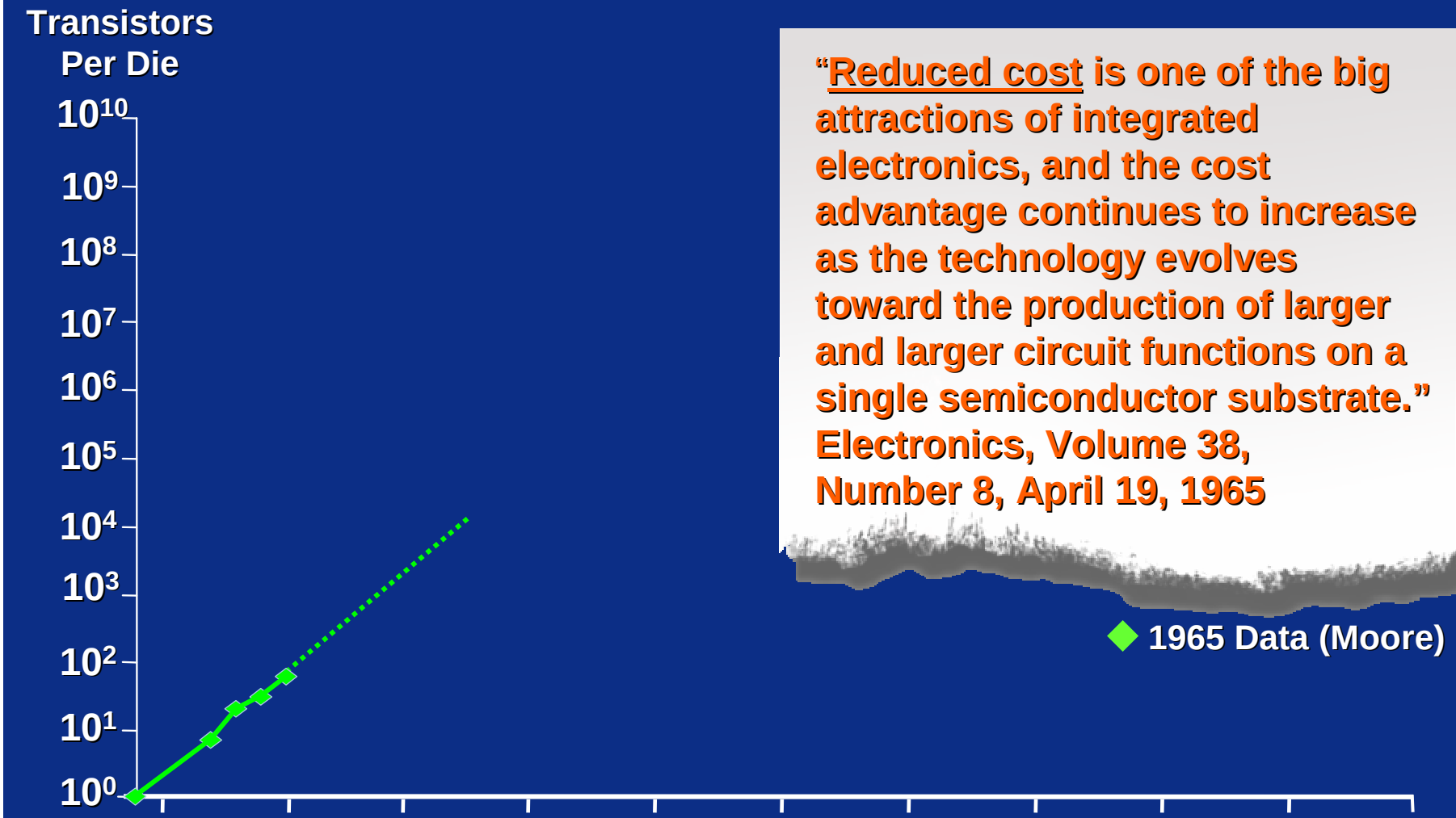
M. Roco, National Science and Technology Council, February 2000

Relative sizes of micro-and nano-objects



(Hosack, 2003)

Moore's Law - 1965

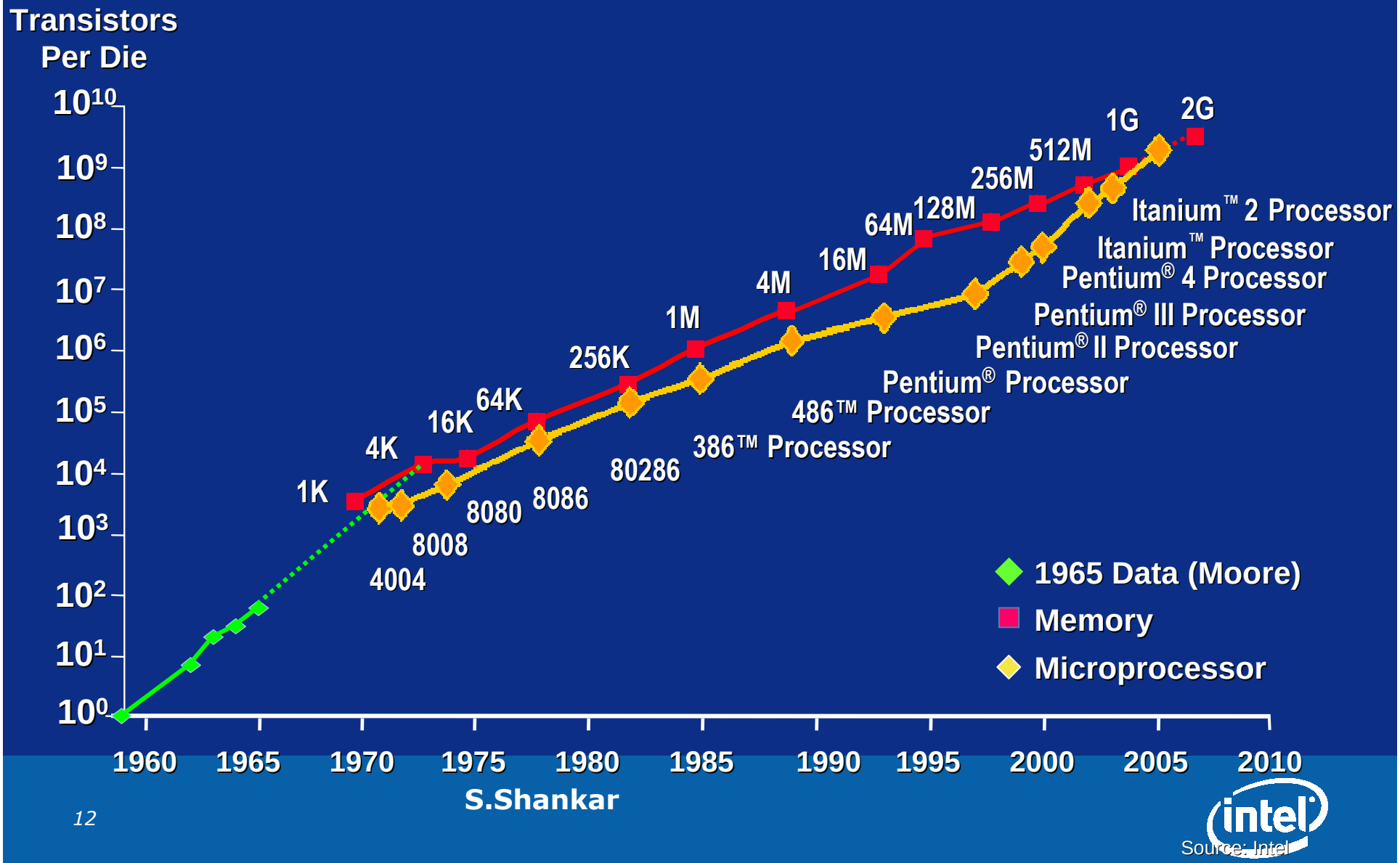


"Reduced cost is one of the big attractions of integrated electronics, and the cost advantage continues to increase as the technology evolves toward the production of larger and larger circuit functions on a single semiconductor substrate."
Electronics, Volume 38, Number 8, April 19, 1965

◆ 1965 Data (Moore)

Source: Intel

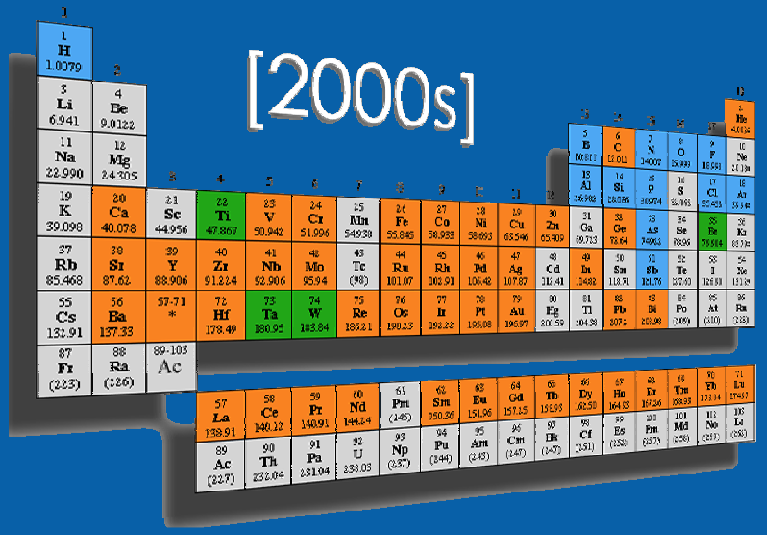
Moore's Law – 2009



S.Shankar

Source: Intel

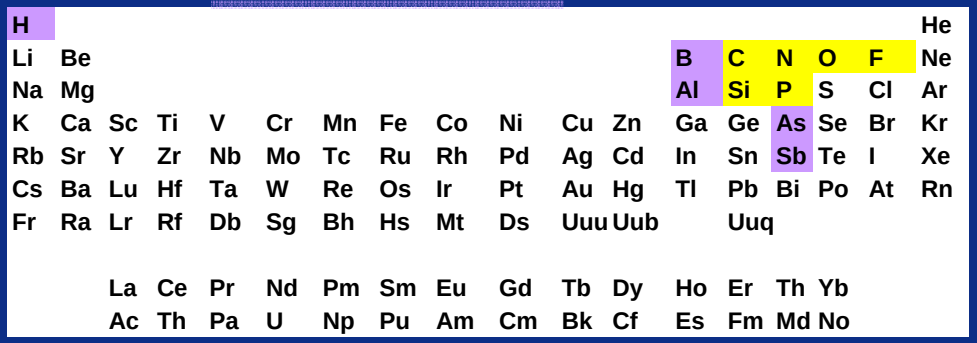
Materials World



intel Leap ahead™

Elemental Revolution

1980s CMOS

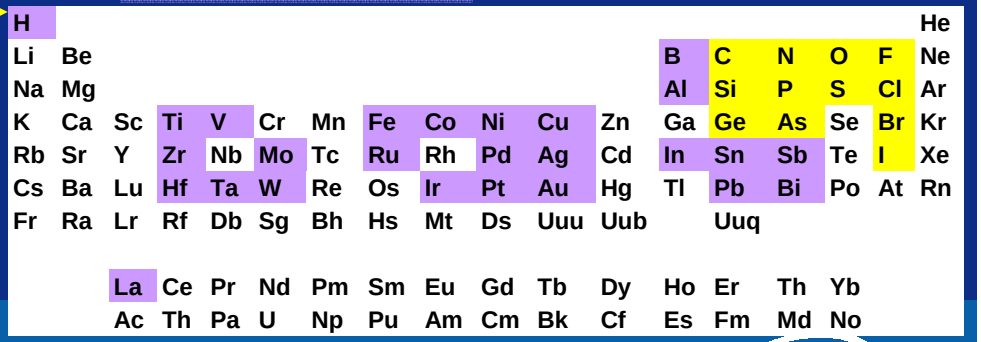


H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu	Uub		Uuq				
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Th	Yb		
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No		

- Micron-scale CDs
- Si primary substrate
- Al interconnects, 4 layers
- Transistor count, 2 million
- ~11 elements

- Nano-scale CDs => 1000x
- Flip chip plastic package
- Cu interconnects, 9-10 layers => ~2x
- Transistor count , 2 billion => 1000x
- ~38 elements => 3.5x

2000s CMOS

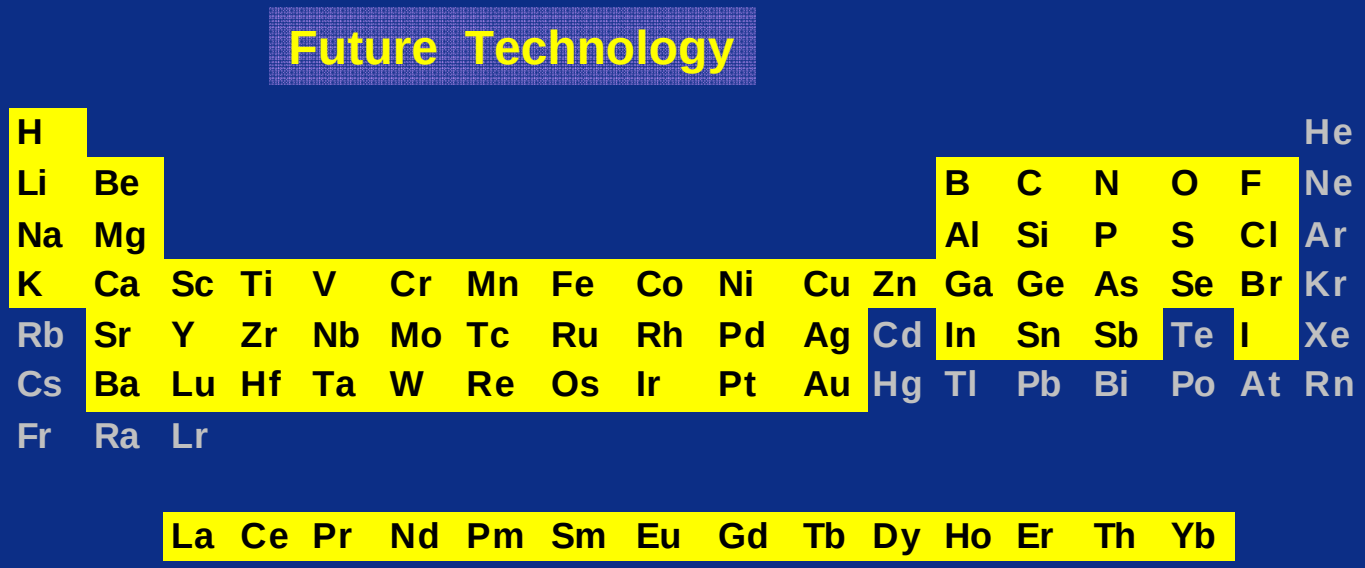


H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu	Uub		Uuq				
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Th	Yb		
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No		

S.Shankar

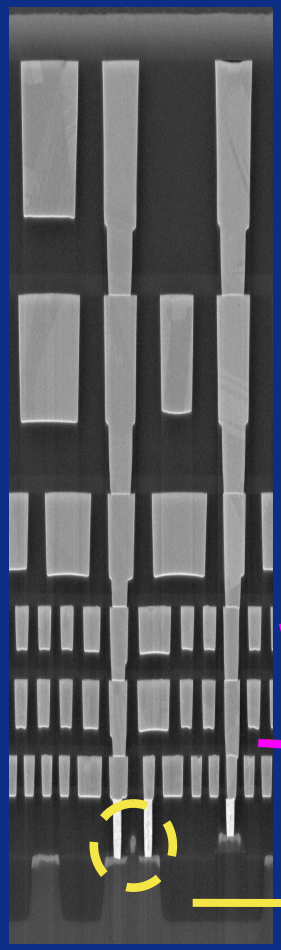
intel

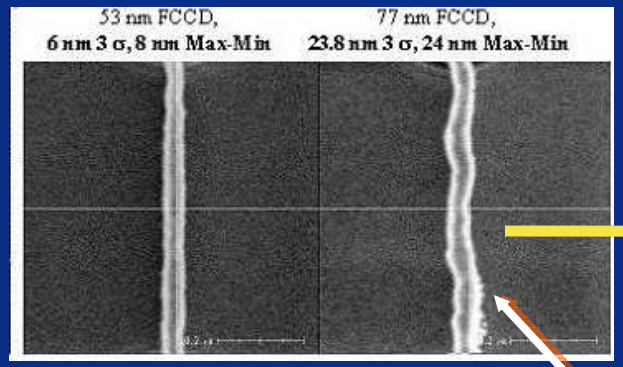
Elemental Revolution

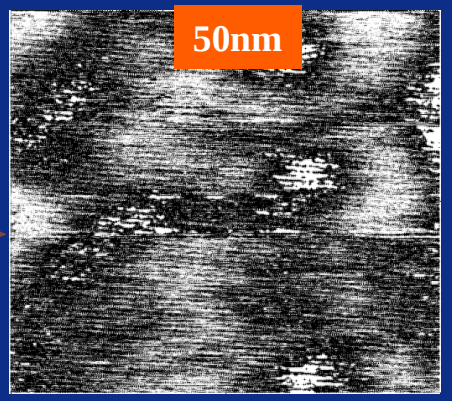


- ~ 70 elements
- But only 1/3rd of the story

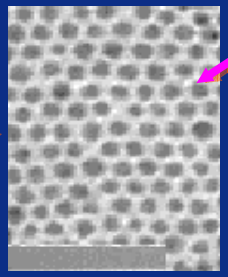
Material Revolution







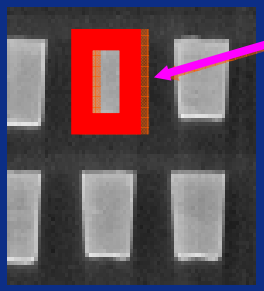
Print Features

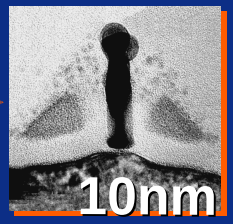


Low K Interlevel Dielectric Micelle Assembled….

Resist Nanodomains

Barrier Layer

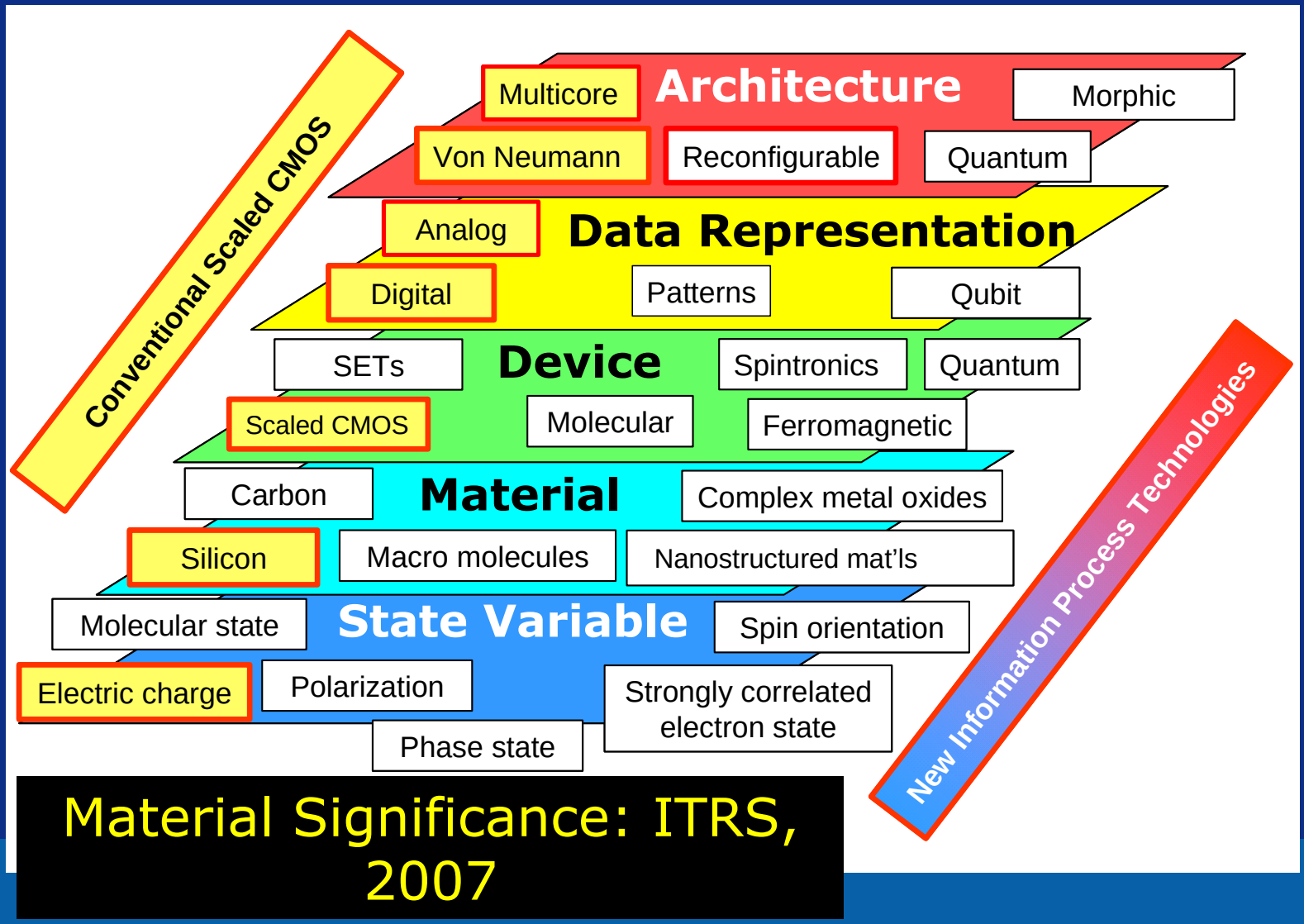




Material and Structure Dimensions Converge

S.Shankar

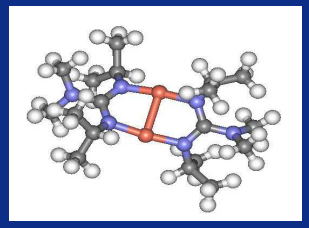
Changing Paradigm



Material Significance: ITRS, 2007

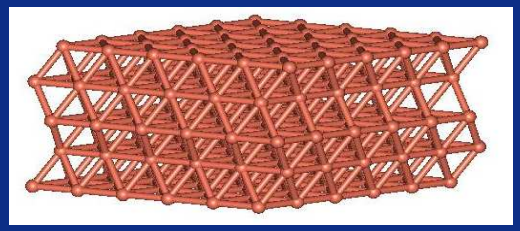
Predictive Materials Modeling

Synthesis: Precursor

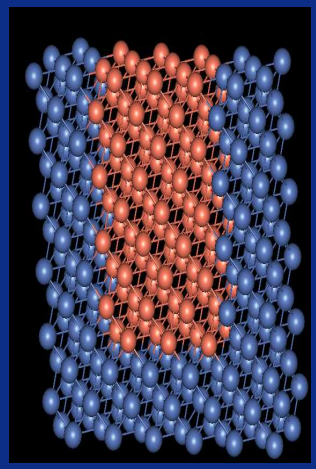


+

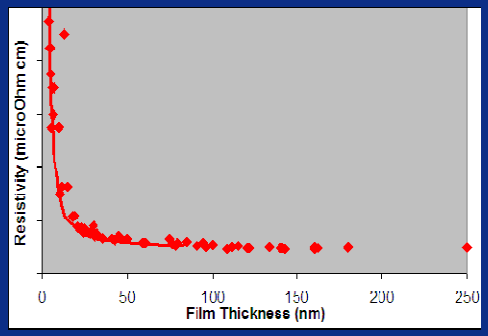
Synthesis: Substrate



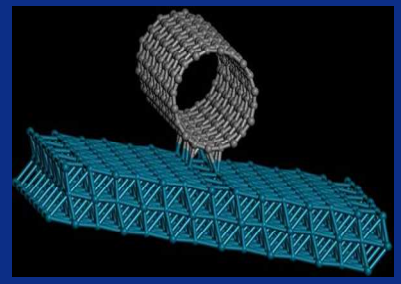
Structures and Composition



Properties



Atomic Scale Probes



Four major components on Synthesis, Structure & Composition, Probe interactions, and Properties

Complexity – A Brief Detour

Complex Systems are systems that comprise many interacting parts with the ability to generate a new quality of macroscopic collective behavior the manifestations of which are the spontaneous formation of distinctive temporal, spatial or functional structures

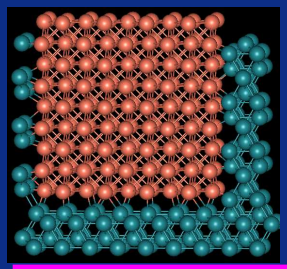
-From System Complexity to Emergent Properties, Springer (2009)

- Materials modeling (and hence *design of materials* for practical applications) of realistic structures is different than simple applications seen in literature and its "complexity" is determined by
  - Need to predict what is being measured
  - Need to address all convolutions that contribute to measurement

Materials Modeling Complexity

Computer use is increasing due to complexities

- Increasing number of materials and combinations needed by the technology
- Interfaces modulates electronic properties
  - Integration drives constraints on optimization across multiple properties
  - PPM-level concentrations of other dopants affect properties



Topography III

Schottky Barrier and Contact Resistance

I-V

Topology

Density of States II

Work Function

Interface Chemistry

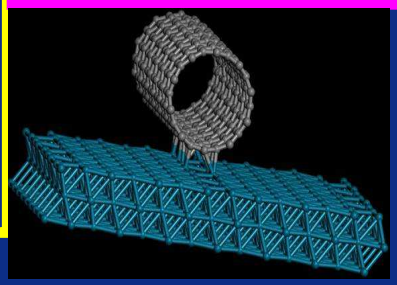
Chemical Kinetics

I

Mechanical Properties

e-Dielectric Constants

Chemical Stability



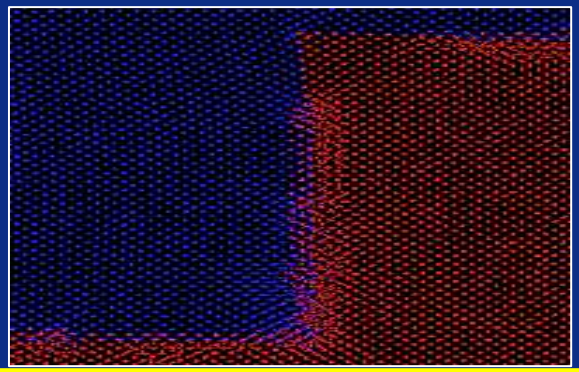
Complexity

Secondary and tertiary "properties" in nanostructures

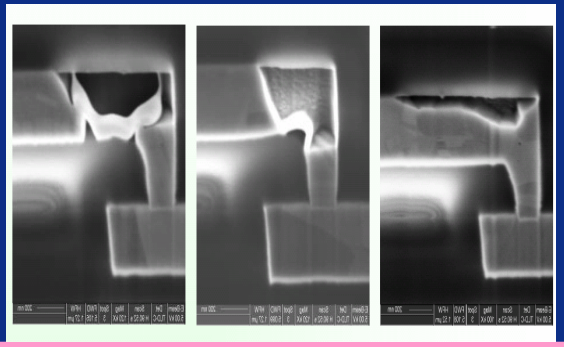
Materials Modeling Complexity (continued)

Multi-property optimization

- Interactions
- Multi-structures



e-Phonon Interactions
Atomic Diffusion IV
Time Dependence



e-Plasmon Interactions V
Multi-structures and hetero-interfaces
e-Photon Interactions

Strong Correlation VI
Domain Dynamics
Spin-Orbit Interactions

?

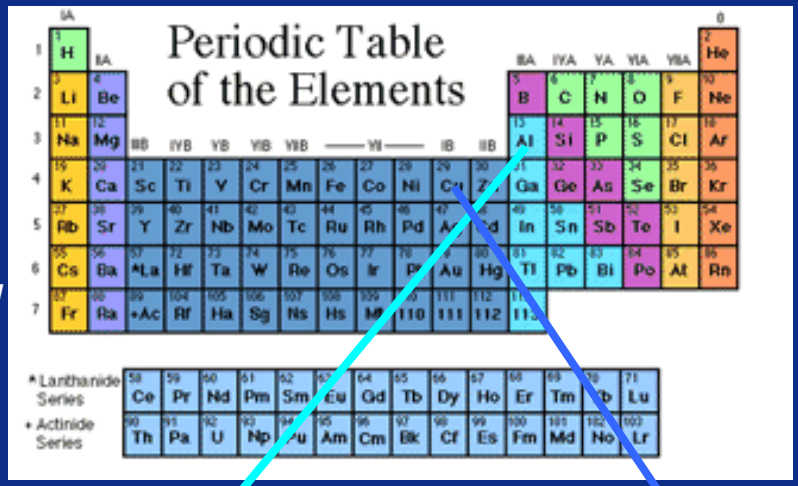
Complexity

intel

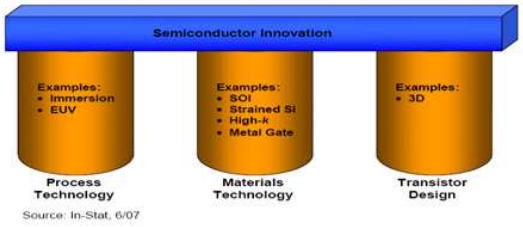
To Si or *Not to* Si is the question.....

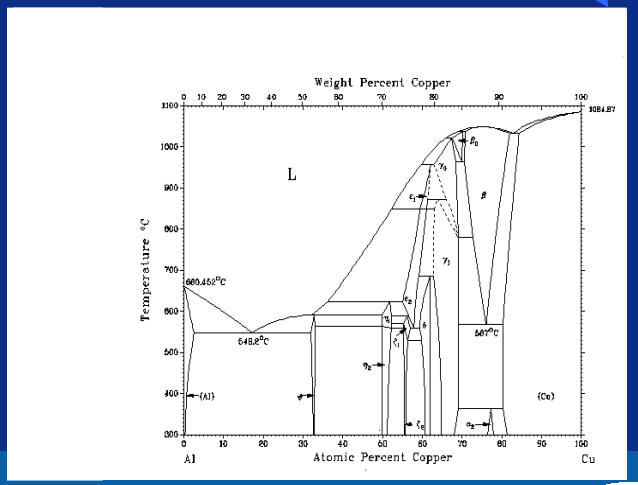
Materials technology is a key player moving forward

- According to Intel (Mark Bohr, May 2007), "*We are now in an era where we have to continue to innovate with new materials and structures. New materials have been introduced at a higher pace than a few years ago*."



In-Stat June 2007

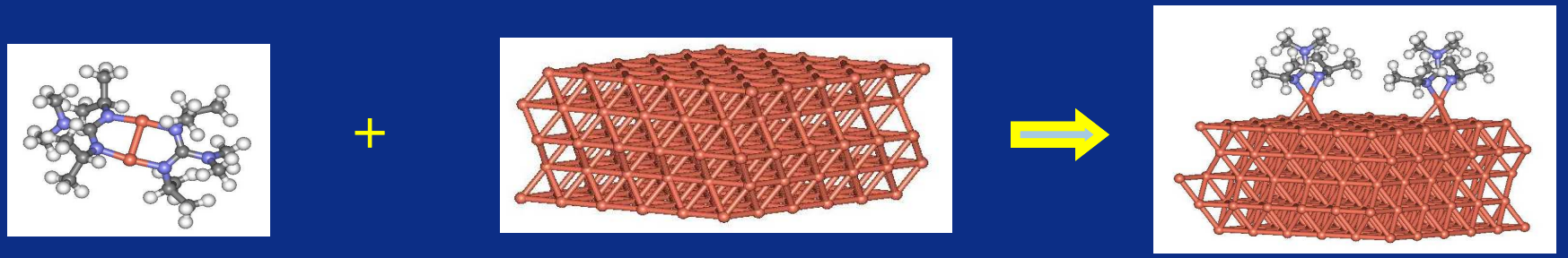




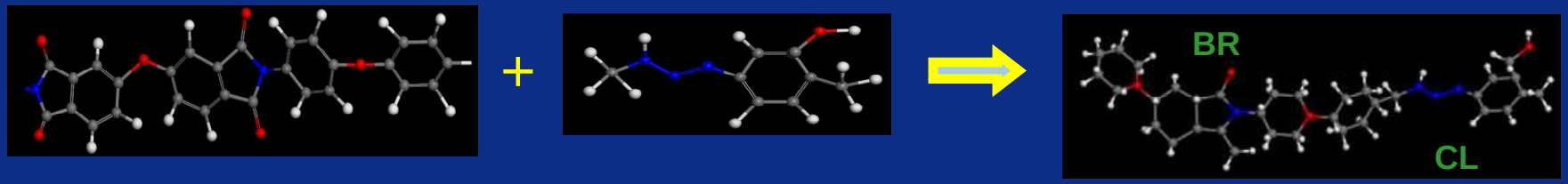
Materials Design

Materials Design

Combination of quantum methods and atomistic simulations for designing materials with desired characteristics

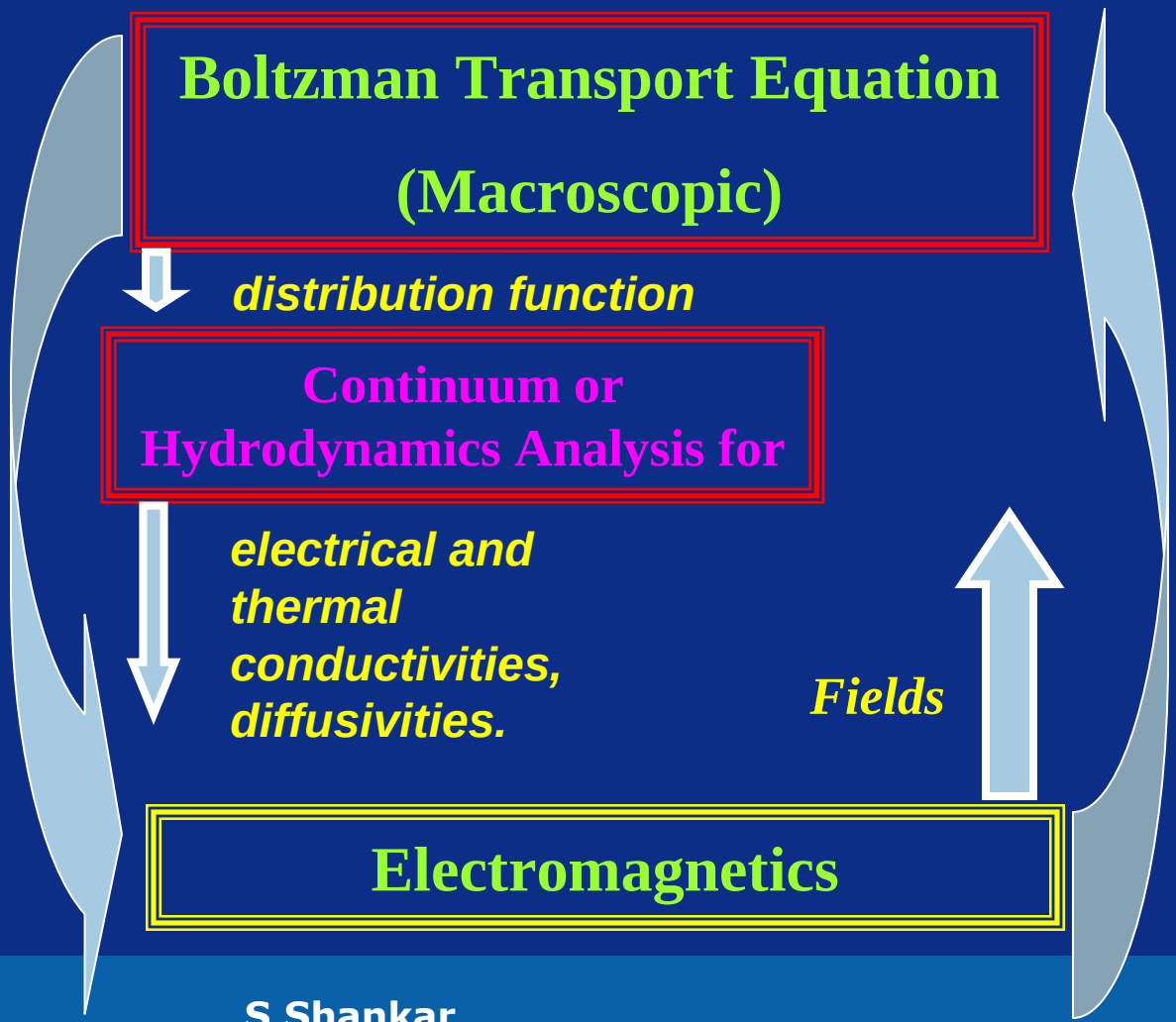


Quantum chemistry modeling applied to identify reactivity and fundamental mechanism for Cu ALD/CVD growth, not available experimentally => Contributed to first-of-a-kind 300mm ALD of pure, conformal, ultra-thin Cu

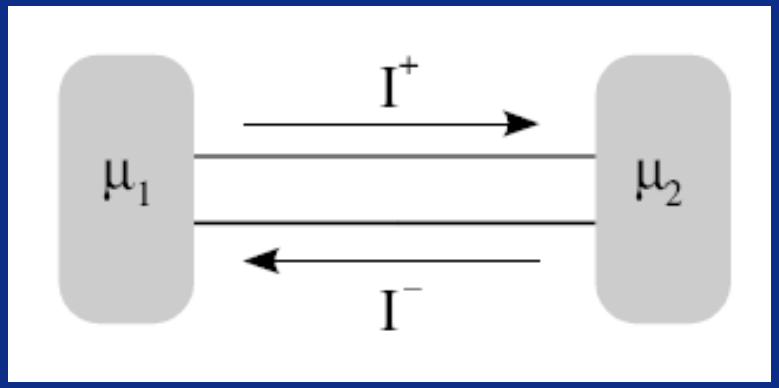


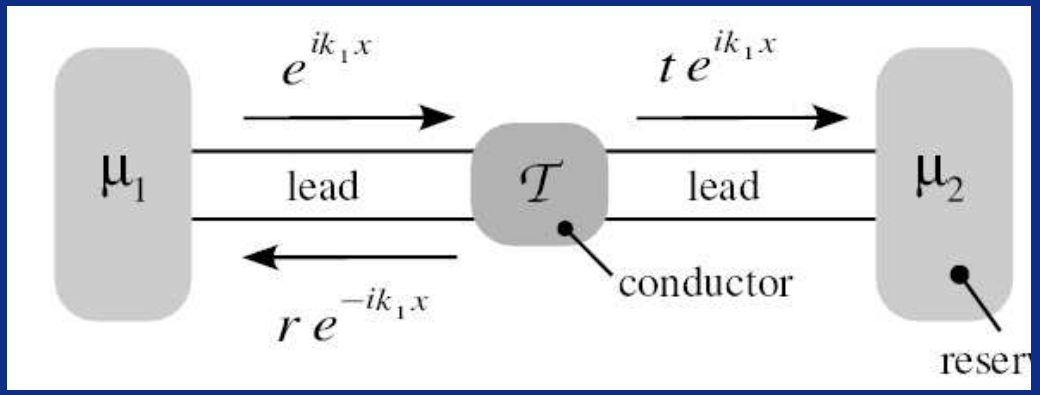
Atomistic Simulations developed and applied for engineering polymers => patent filed for tougher designed polymers with optimal thermal and mechanical properties

Classical Non-equilibrium



Quantum Non-equilibrium





Phase Coherent, Ballistic Transport:

$$I^+ - I^- = \frac{2e}{h}\int_{-\infty}^{+\infty}[f(E-\mu_1) - f(E-\mu_2)]\,dE$$

$$= \frac{2e^2}{h}\frac{(\mu_1 - \mu_2)}{e}$$

Conductance Quantum

$$G_0 = \frac{dI}{dV} = \frac{2e^2}{h} = 77.5\,\mu S$$

Landaur Formulism:

$$G = \frac{2e^2}{h}\mathcal{T}$$

$$G = \frac{2e^2}{h}\mathrm{Tr}(t^\dagger t)$$

ankar

Reference: A. Bower, P. Ho, S. Shankar (MRS, 2007, IOP, 2009)

Classical Non-equilibrium: Electromigration

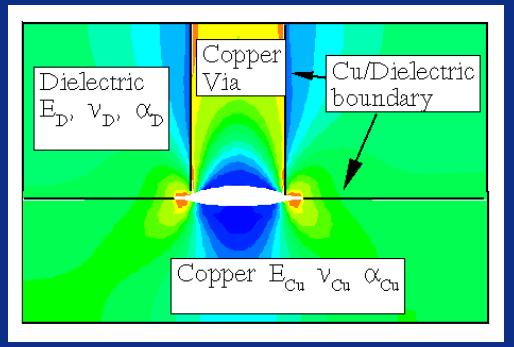
Problem

Challenges

- Cu Damascene structures are heterogeneous due to interconnect morphology and materials
- Voids nucleation and evolution are system dependent;
  - Different material properties
  - Hetero-material interfaces
  - Triple boundaries
  - Current and mass transport
  - Stress effects

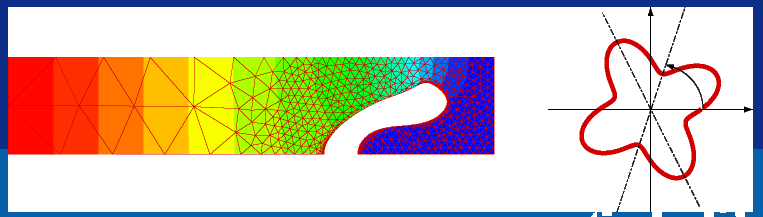
Void Nucleation

- Caused by stress induced debonding at interfaces
- Occurs early

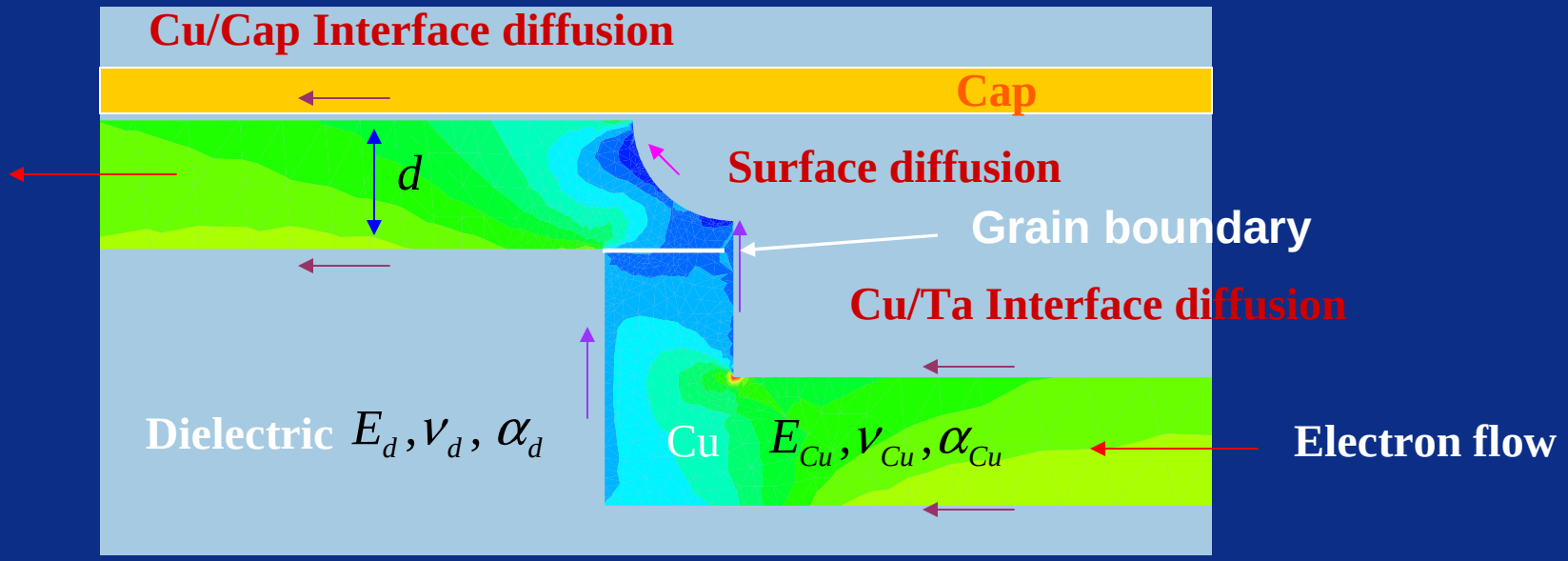


Void Evolution and Growth

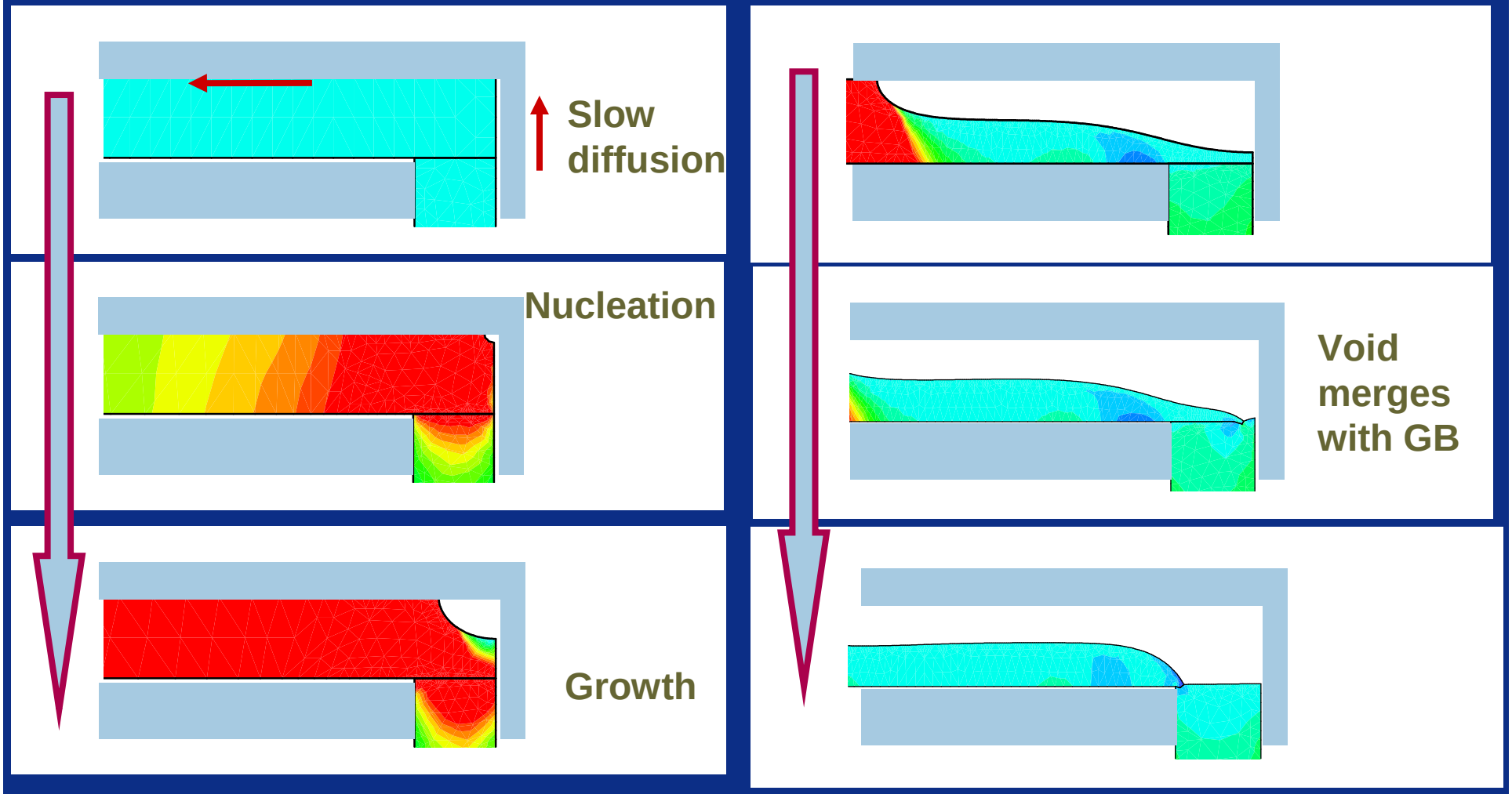
- Caused by stress and electric current induced mass transport
- Dominant part of S. Shankar



Void nucleation/growth in 2 level structure



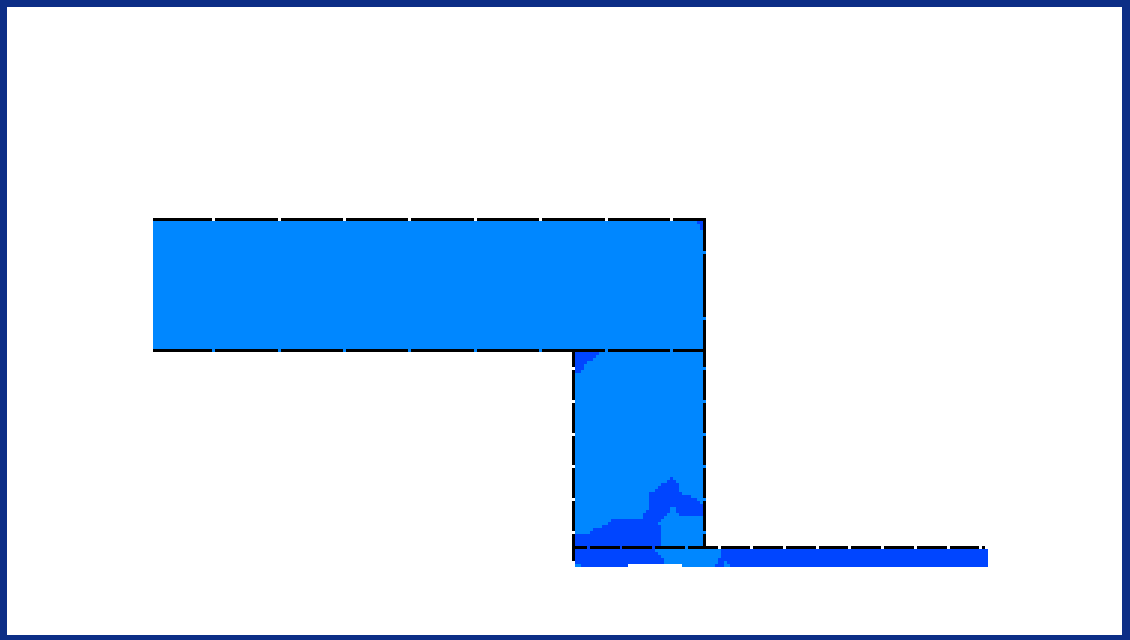
Void-grain boundary interactions



S.Shankar

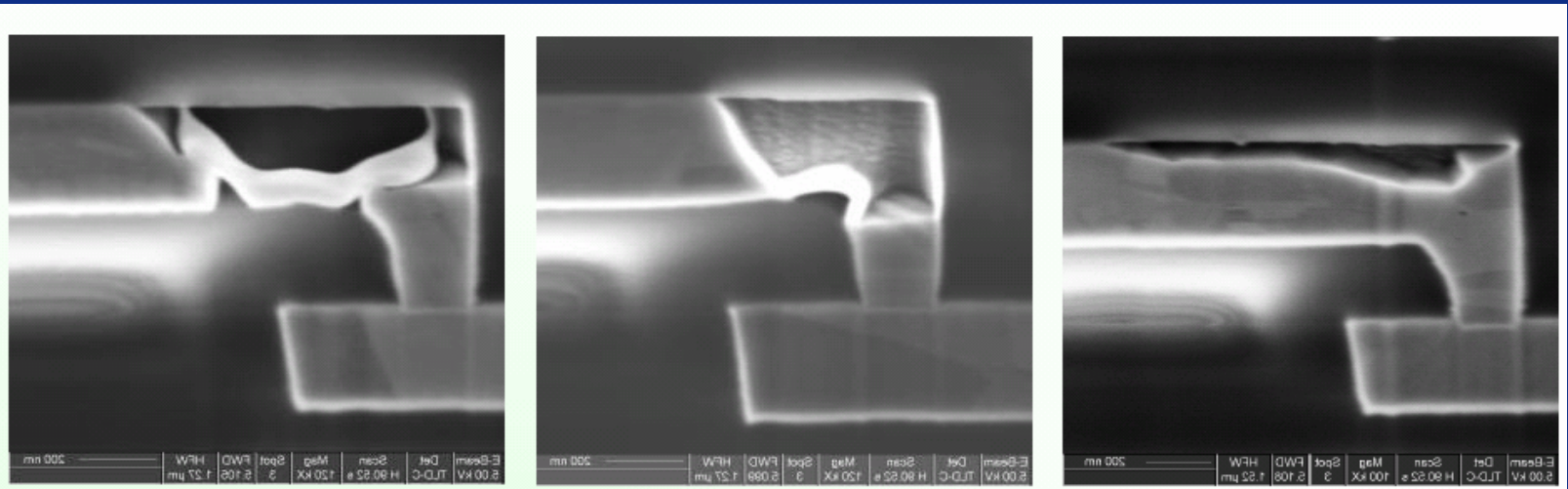
Void propagates rapidly across GB to cause failure

Void nucleation, growth and evolution



Animation showing close-up of void.
Note rapid failure after void meets grain boundary

Comparison with experiments



Hauschild *et al* (Proc AIP stress workshop, 2004)

- Void formation at interface.
- Void evolution at interface towards cathode end.
- Continuous void growth along the line with some growth into the via increasing the sigma value of void areas.

Conclusion – simulation predictions very similar to experiment. Minor differences are caused by discrepancy of grain boundaries between simulations and experiments

Quantum Non-equilbrium:
Single-walled metallic CNT

Reference: S. Park, M. Haverty, K.J. Cho, H. Dai, S. Shankar (submitted)

Introduction

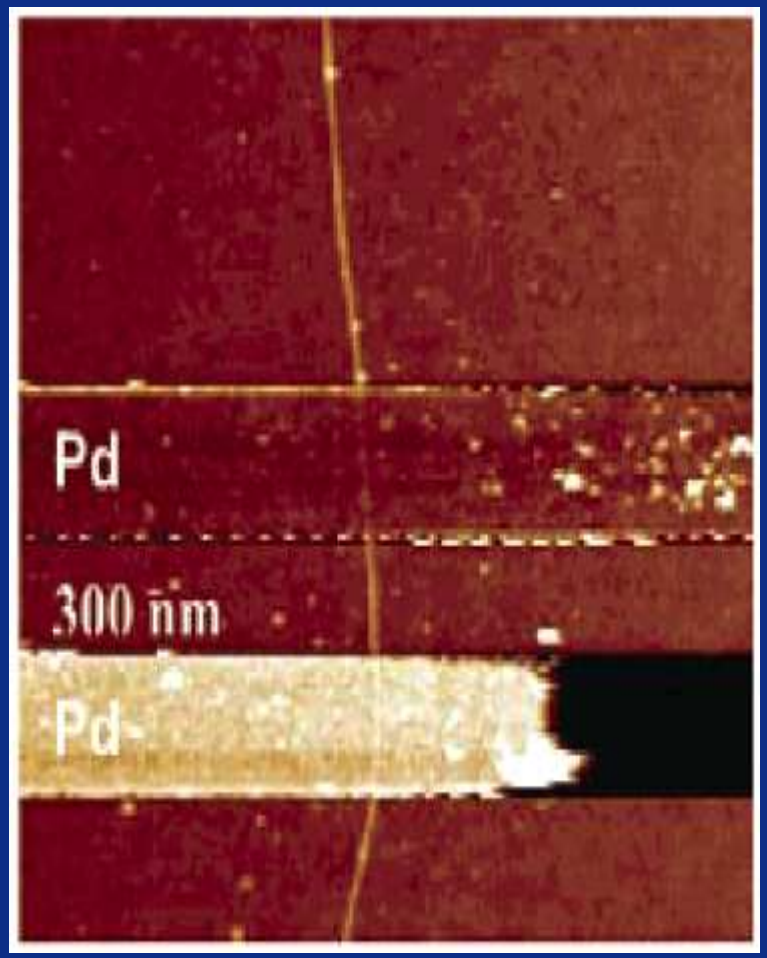
Experimental observations

- SWCNT conductance on metal electrodes < the ideal value of 4 e^2/h
- Contact resistance depends on electrode metal type
- Conductance of SWCNT on Pd electrodes depends on CNT diameter

Objectives

- Understand cause of contact

  resistance and determine the optimum metal for electrodes.
- Understand diameter dependence of contact resistance



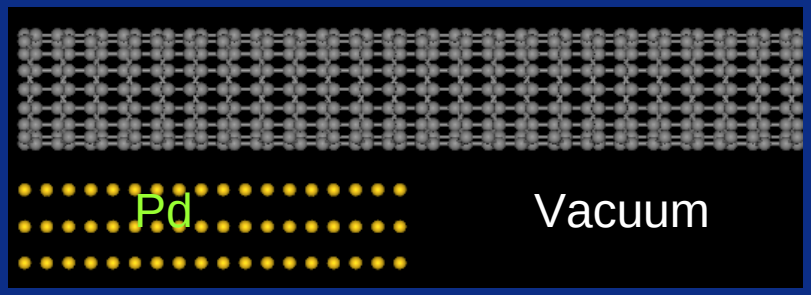
Transport Simulations for metallic CNT on Pd

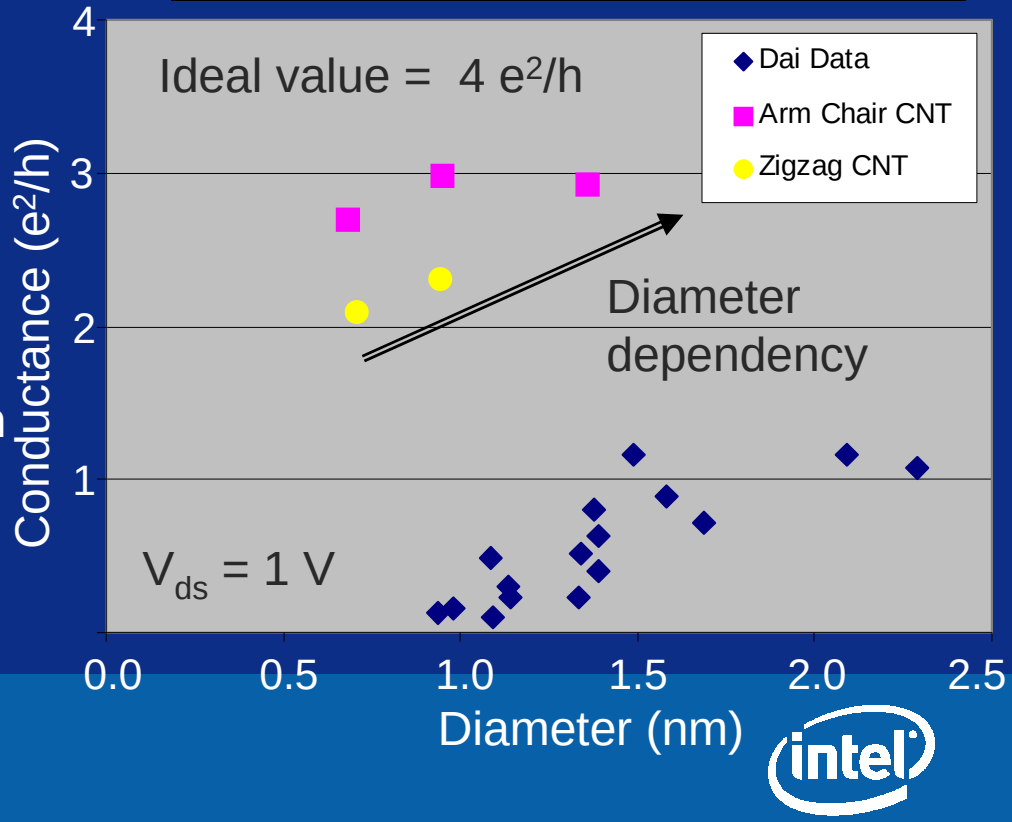
Simulation Details

- Single contact system
- Extended CNT structure on metal to vacuum
- Infinitely long metal contact
- Temperature is 0K

Simulation results

- Conductance depends on diameter
- Contact resistance occurs even with infinitely long contacts

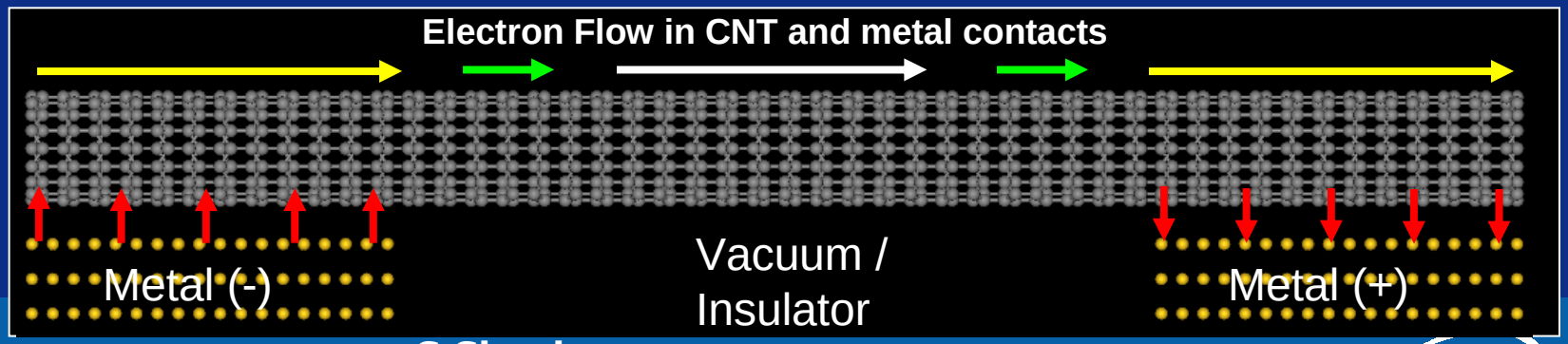




Conductance of CNT on Metal

Three possible factors for the non-ideal (reduced) conductance

- Tunneling barrier between CNT and metal (red arrow)
- CNT conductance on metal: π bond disturbance due to metal (yellow)
- Conductance between the deformed CNT at the metal contact and un-deformed CNT in vacuum/insulator (green arrow)



S.Shankar

Tunneling Barriers Effects

Simulated tunneling barrier from Fermi level and Electrostatic potential (see backup)

Influence of Metal Electrode Type

- Au tunneling barrier is high; Pd and Ti have no barrier *(negative)*

Influence of CNT Diameter

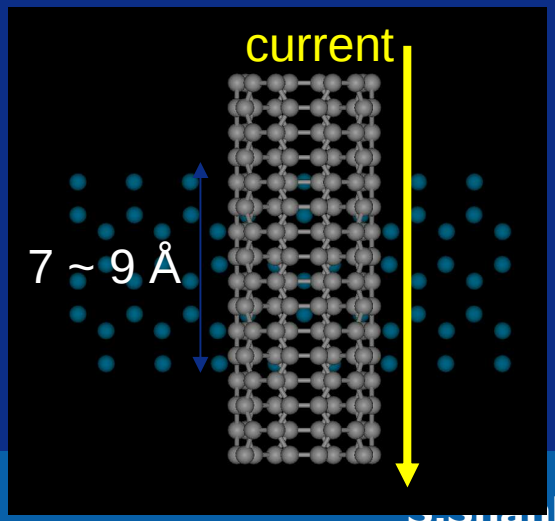
- Tunneling barriers becomes more negative as CNT diameter decreases

CNT Conductance on Metal

CNT Conductance simulation with underlying metal

- CNT on metal relaxed with ab initio simulations
- (5, 5) and (9, 0) on Au, Pd, and Ti, V_{ds} = 1V.
- Varied diameter of armchair and zigzag CNT on Pd

Conductance drop depends on type of metal and conductance increases with CNT diameter



Conductance (e^2/h)	Ti	Pd	Au
Armchair CNT (5, 5)	**1.42**	**2.86**	**3.64**
Zigzag CNT (9, 0)	**1.13**	**2.04**	**3.68**

CNT Diameter (nm)	0.68	0.95	1.36	
Armchair Conductance (e^2/h)	**2.86**	**2.98**	**3.38**	
CNT Diameter (nm)	0.71	0.94	1.17	1.40
Zigzag Conductance (e^2/h)	**2.04**	**2.16**	**2.16**	**2.43**

S.Shankar

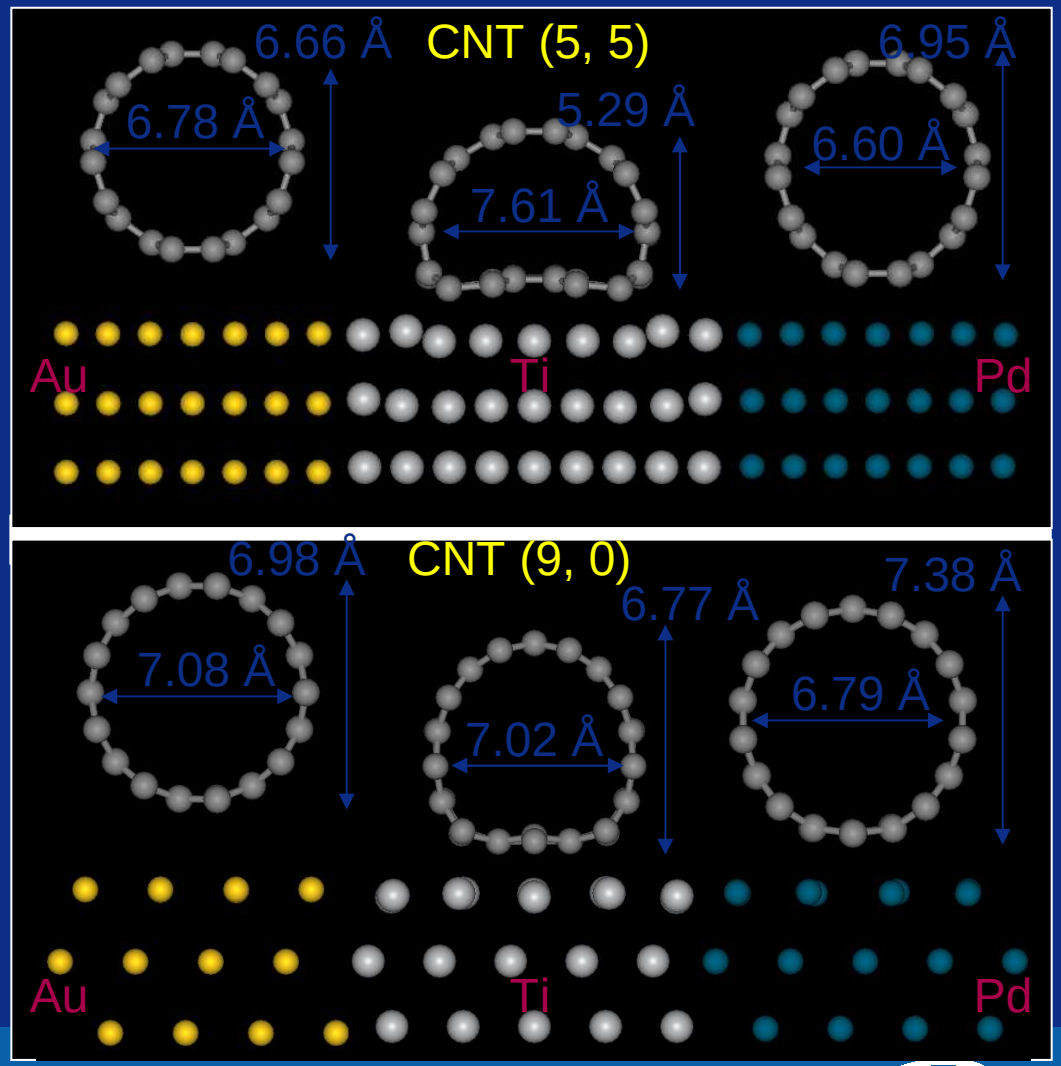
Deformation of CNT on Metal

Diameter in Vacuum

- CNT (5, 5): 6.83 Å
- CNT (9, 0): 7.09 Å

CNT on metal

- Au: small deformation
- Pd: egg-shape
- Ti: large deformation



Interaction strength vs. conductance

Tunneling barrier and Interaction strength is correlated.

- Strong interaction: Low tunneling

CNT conductance on metal and interaction strength is correlated.

- Strong interaction: Low CNT conductance

Interaction strength between CNT and metal determines conductance

- Weak interaction: high tunneling barrier & high CNT conductance
- Strong interaction: low tunneling barrier & low CNT conductance

However, good contact needs low tunneling barrier + high CNT conductance

What about Future ?

Nanotechnology – Two major paradoxes

Size in nano dimensions, but

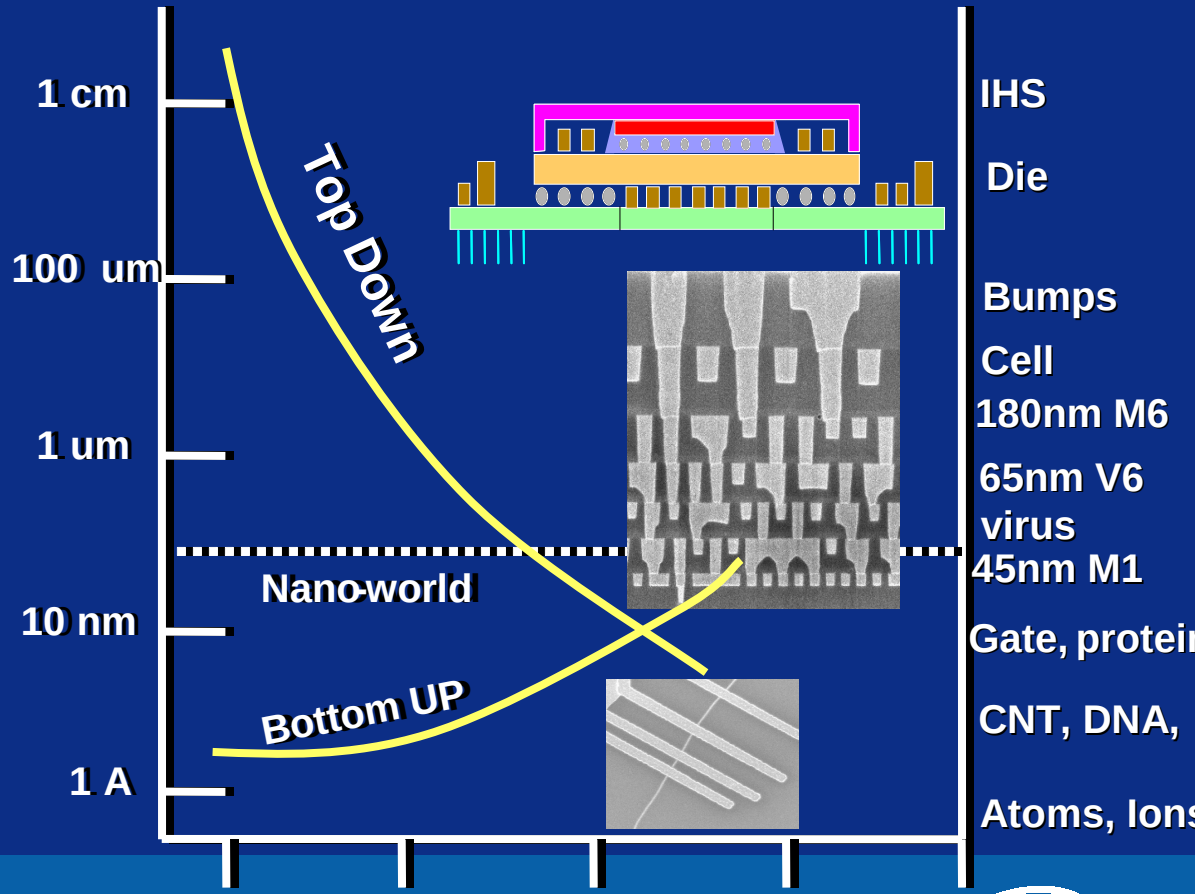
- Interfaces/bulk ratio >>1, interfaces modulate behavior (e.g pinning, voiding)
- Non-local effects manifest
  - Density of states modulated by neighboring materials and structures
- New structures or thin films which are chemically different, are integrated
  - High-k/Metal gate
  - Polymer ILD

Metrology unable to characterize precise specific effects, especially "buried" surfaces

- Use modeling to deconvolve measurement

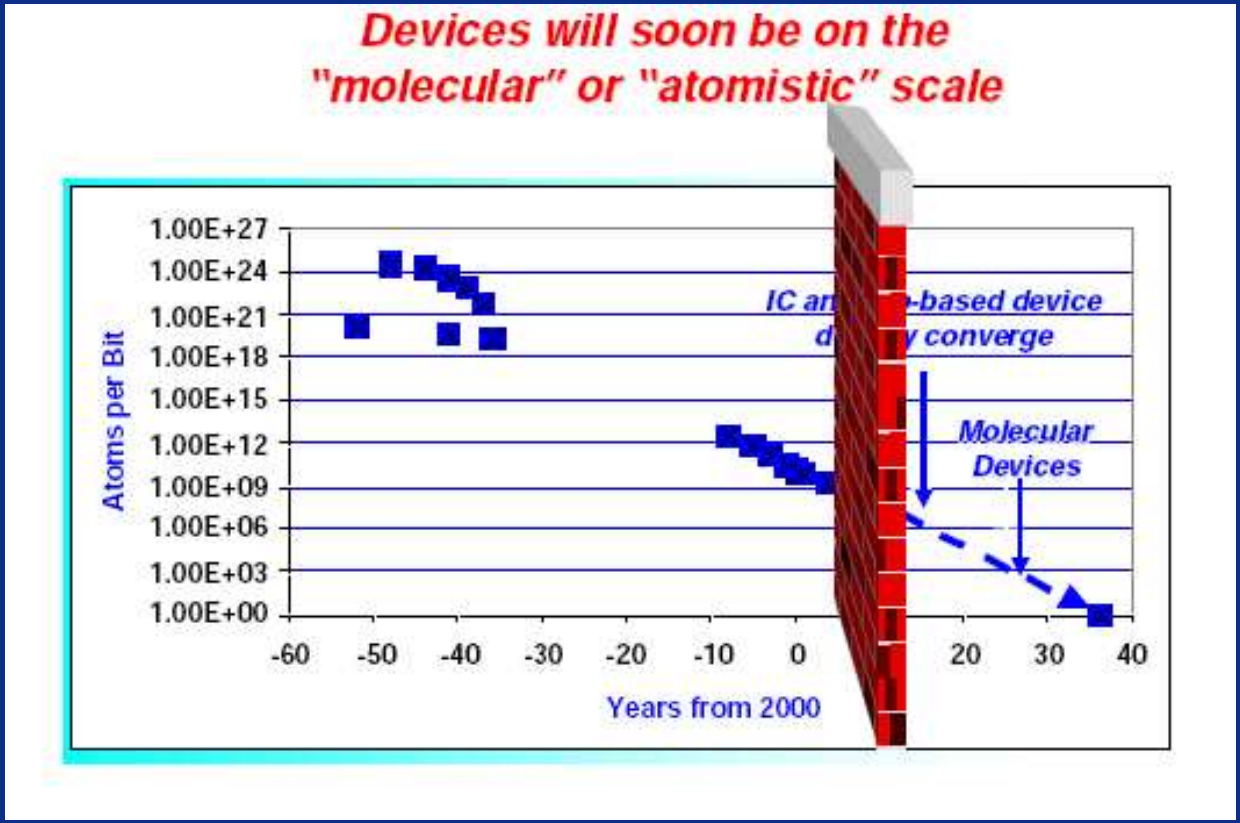
Material Dimensions falls between Molecules and Structures

The Frontier



S.Shankar

Existing Gaps



Number of atoms a state of the art density functional theory algorithm can deal with:

1985	1990	1995	2000	2005	2010	2015
	2	>10	>50	500	1,000	???

S.Shankar

Summary for Materials Modeling

Identify specific areas need further research and development

- Theory Development
  - Examples: Extension of density functional theory-based techniques, low concentration defects, time-dependent systems, lanthanide elements and complex compounds (ternary and quaternary)
- Algorithm Development
  - Bridging time scales to simulate fully dynamical systems
    - E.g. Molecular dynamics of reactions, Transport of finite systems, Quantum Monte Carlo
  - Bridging length scales for integrated systems
- Software Development
  - Scalability and Productization
- Not sure whether multi-scale techniques can be self-consistent
- We are trying to put together focus group in US for getting a common industry-academic platform for Computational Materials

Lessons for Complex System Modeling

Complex system modeling is addressed by reductionism; other holistic approaches may need to be evaluated

Identify common simulation platform

- Each research group has its own set of codes and libraries
- Evolutionary change in technique development
- Targeting niche markets, expensive software with system requirements

Semiconductor Research Corporation is evaluating functional diversification

- Integration of heterogeneous components including biological systems