Materials Characterization in Nanodomains and Interfaces

Challenges for Modeling and Metrology

Sadasivan Shankar[1], Kevin Jonhston[1], Dan Herr[2]

[1] Technology and Manufacturing Group, Intel Corporation, Santa Clara, California

[2]Semiconductor Research Corporation, North Carolina

Invited Talk for The 2011 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics

May 24-26, 2011

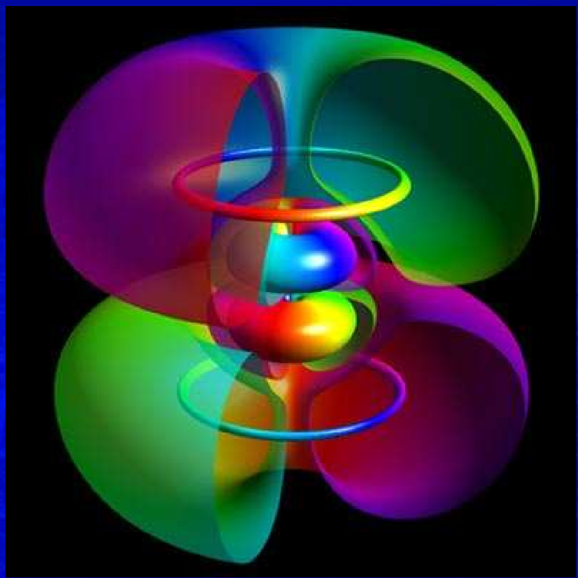
Three-fold aim of the current presentation

- ***Outline*** **Drivers of Nanodomain and Problems**
- ***Illustrate*** **modeling and metrology applications with specific examples**
- **Acknowledgement**
  - **M. Haverty, H. Simka, M. Bohr, J. Garcia**
  - **A. Bower, P. Ho**

Background on Nanoscience and Technology

Nanoscience is…

- **Understanding of science at the nano level**
  - **Quantum mechanics provides self-consistent explanation**
  - **Overlap of Molecular and Structural scales where the material behavior is due to collective behavior of nano-structures**

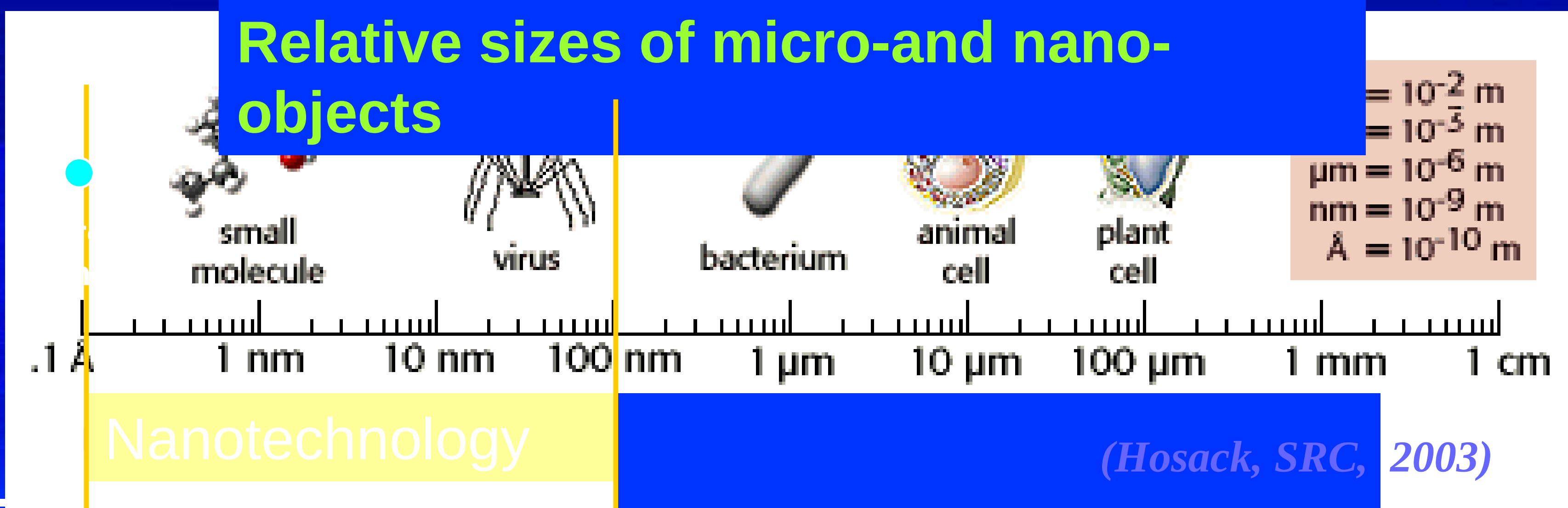


Nanotechnology is…

- **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



Nanotechnology

(Hosack, SRC, 2003)

Some key drivers of Nanotechnology

New Information Technology Components

SENSORS

DISPLAYS

OUTPUT CHANNEL

MASS STORAGE DEVICES

LOGIC

LOCAL MEMORY

- ***Information Output***
- *LCD*
- *Organic LEDs*
- *FE and Plasma Displays*
- *Optical and IR imaging*

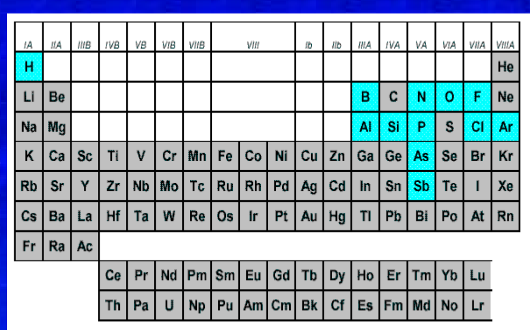
- ***Information Transmission***
- *Photonic Networks*
- *Neuroelectronic*

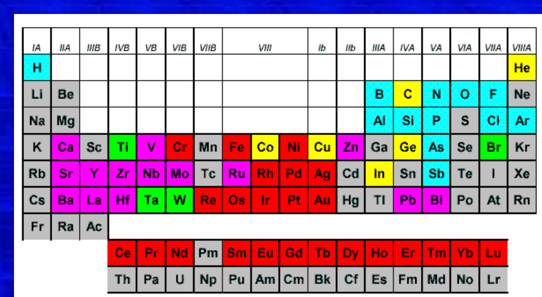
- ***Information Processing***
- *Ferroelectric DRAMS*
- *Single electron*
- *Nanotubes*
- *Molecular electronics*

(Waser, 2003)

Tipping Forces (1)

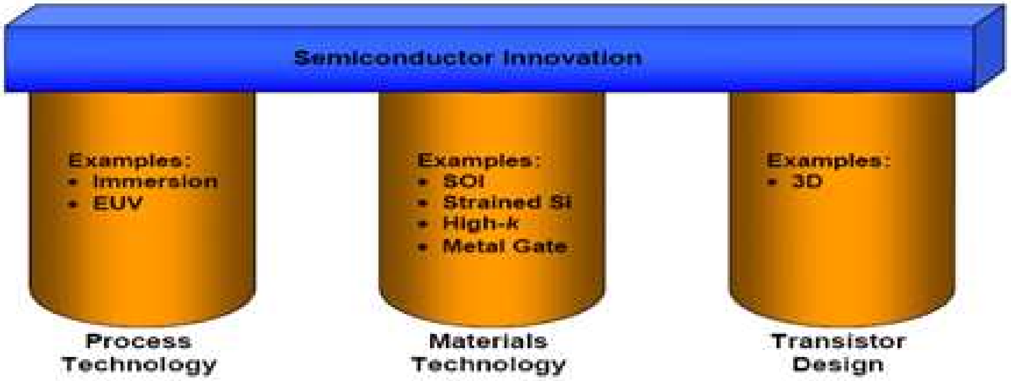
- Dimensions reduced to nano-dimensions
  - Material domains of same dimensions
  - Effect of Interfaces
- Increasing number of materials in smaller dimensions
  - 130 nm introduced Copper
    - Transition metal
  - 90 nm introduced low-k dielectric
    - Pores several nanometers
  - 45 nm introduced high-k/metal gates
    - Non-Si, polymer





Tipping Forces (2)

Modern CMOS scaling is as much about material innovation as dimensional scaling



Source: In-Stat, 6/07

ITRS Emerging Research Materials Matrix

Mat. / TWG	Low Dimensional Materials	Macro-molecules	Spin Materials	Complex Metal Oxides	Hetero-structures & Interfaces	Directed Self-assembly	ESH	Metrol. & Model'g
ESH	Detailed	General				General	Detailed	General
ERD	Detailed	Detailed	Detailed	Detailed	Detailed	General	Detailed	Detailed
FEP	General		General	General	General	General	General	General
INT	Detailed	Detailed				General		General
LIT	General	Detailed		General		Detailed	General	Detailed
MET	Detailed	General	General	Detailed	Detailed	General	Detailed	Detailed
M&S	General	Detailed	Detailed	General	General	General		
PIDS	Detailed	Detailed	Detailed			General		
PKG	Detailed	Detailed	Detailed	General		General		General

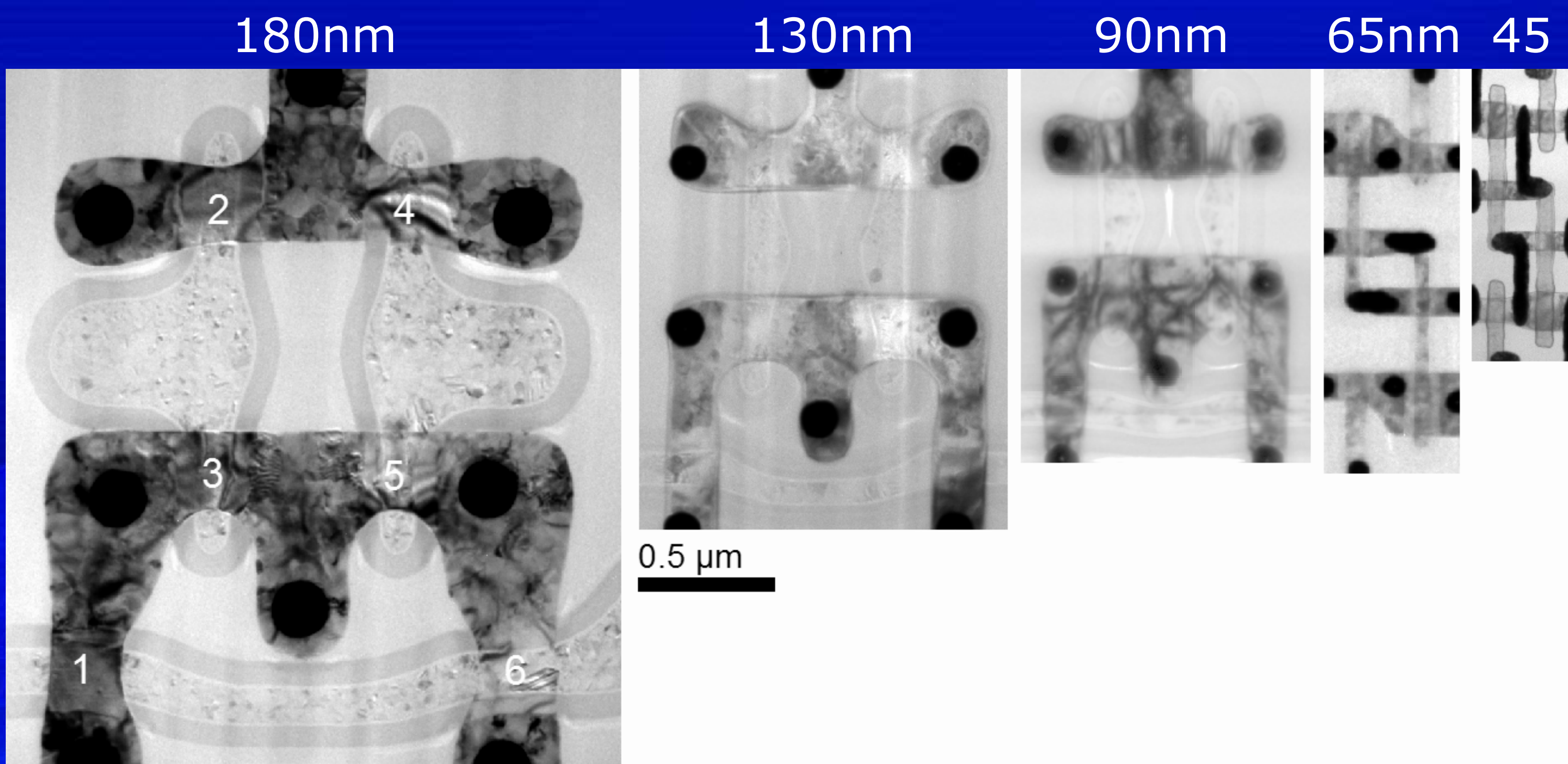
Detailed TWG requirements or alignment | General TWG interest or alignment | No TWG interest to date

TWG ≡ Technology Working Group

TWG ≡ Technology Working Group
10

Moore's Law - SRAM Cell Size

- Each cache cell has 6 transistors that together store "1" or "0" and allow the value to be changed.



Research Focus in Materials:

New Behavior not seen in traditional bulk materials

NATURE|Vol 441|18 May 2006

Ack: J. Wells, 2006

TOP FIVE IN PHYSICS

Are you working on the hottest topic in your field? Many scientists may think so, but it has been a tough assertion to prove — until now, that is. A German physicist has devised a way of answering the 'Hot or not?' question for his discipline. If it stands up to scrutiny, it could be used to rate topics across the sciences. In physics, the results show that hotness — measured by a parameter known as *m* — correlates well with the promise of future wealth… and that promise is greatest in nanotechnology.

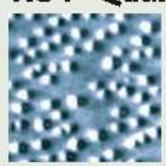
12.85 Carbon nanotubes

Super-strong materials and blisteringly fast electronic circuits: the potential applications of these tiny carbon tubes, discovered in 1991, are so enticing that everyone is pouring money into the field.

8.75 Nanowires

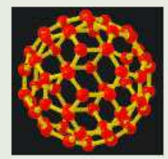
Less well studied than nanotubes, but the possible uses are similar. Nanowires could eventually prove more useful than nanotubes, because their chemistry is easier to tailor and they can be used to create nano-sized lasers.

7.84 Quantum dots



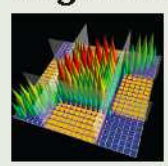
Another nanotechnology with a huge range of potential applications. These tiny specks of semiconductor material, measuring as little as a few nanometres across, have already been used to create dyes for cell biologists and new kinds of laser. Physicists hope they might one day form the basis of a quantum computer.

7.78 Fullerenes



These spheres of carbon atoms are attracting significant research interest. But the latest ranking rewards newness, so the topic may have slipped down the list because it predates nanotubes by around six years. The discovery of fullerenes earned a Nobel prize and spawned studies of numerous potential uses, such as drug delivery agents.

6.82 Giant magnetoresistance



Not a new topic, but still hot because of its economic importance. Modern hard disk drives were made possible by the discovery of giant magnetoresistant materials, which show marked falls in electrical resistance — more than around 5% — when a magnetic field is applied. Researchers are now aiming to make hard disks even more powerful.

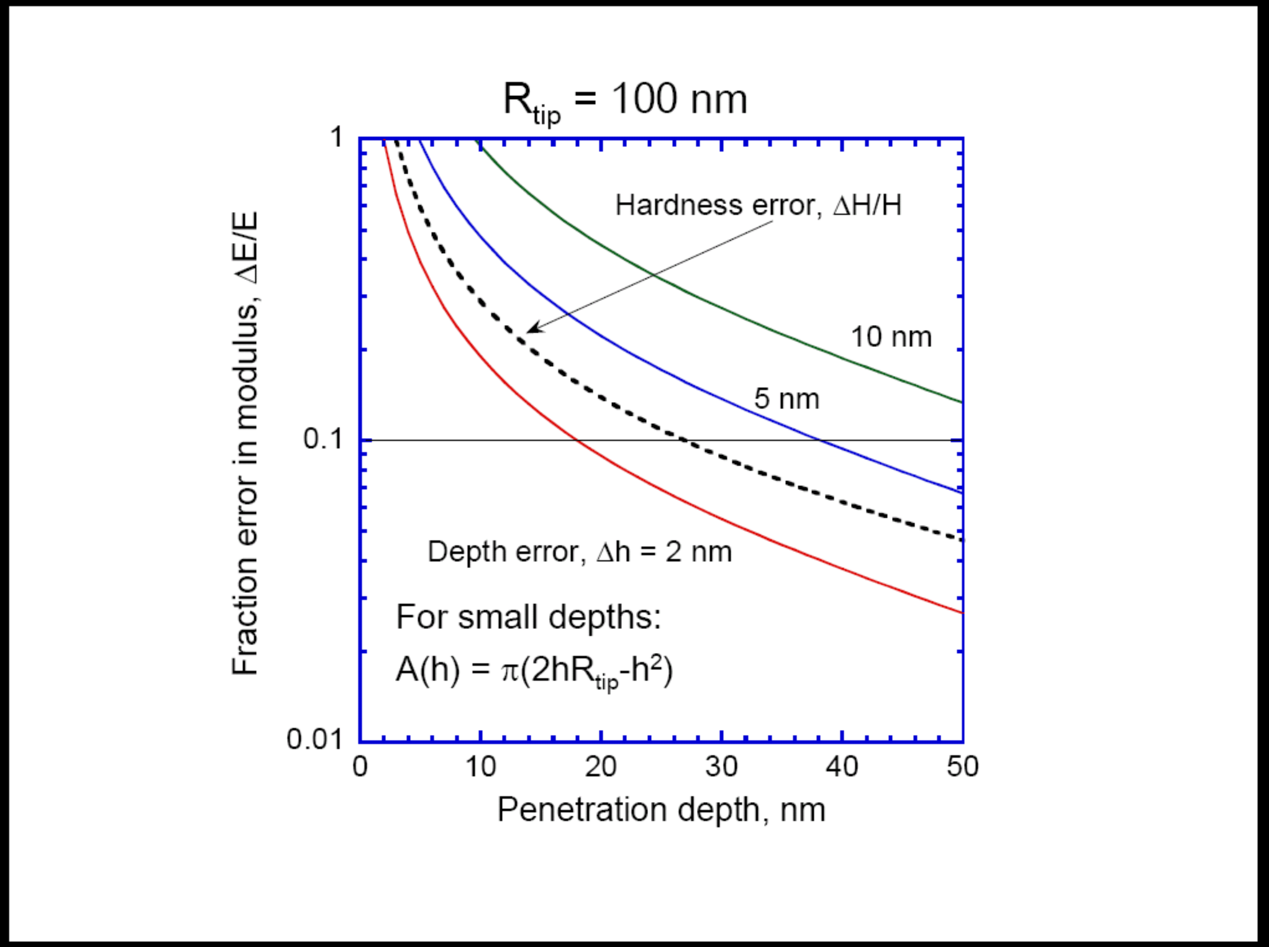
M^2: Modeling and Measurement

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

Nanotechnology Paradoxes

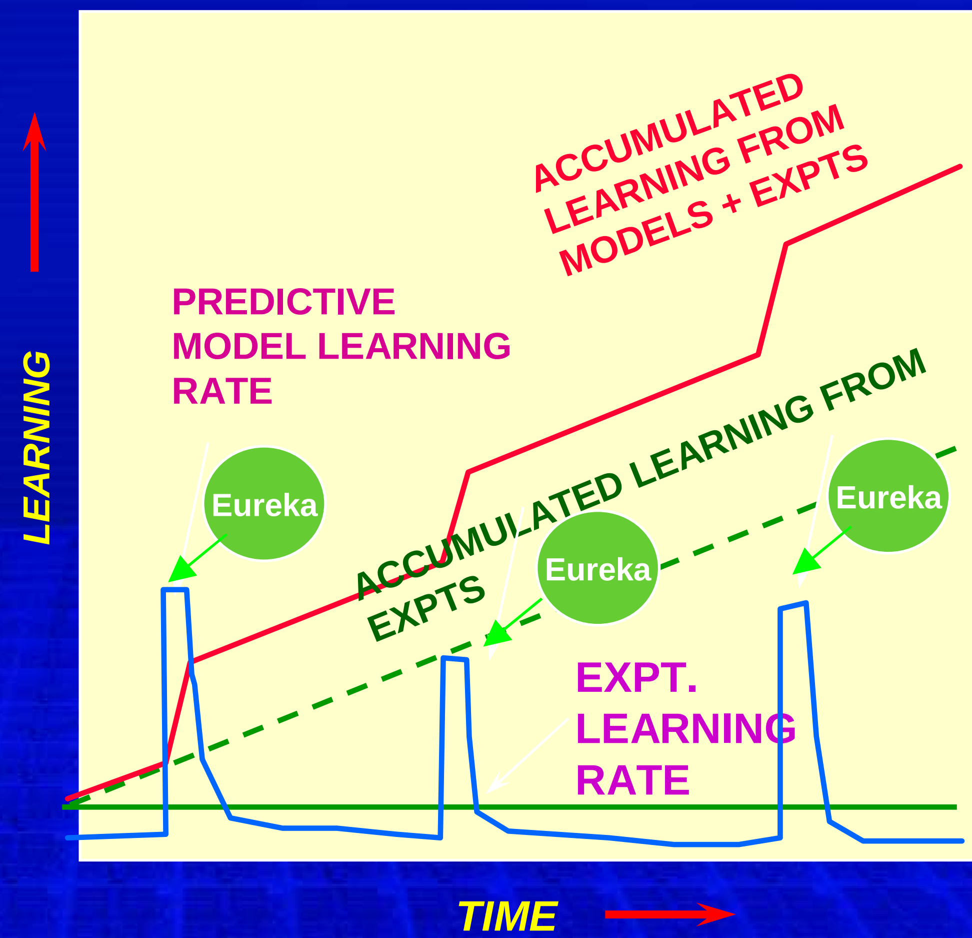
(M. Begley, 2006)



Motivation for Modeling

(Ack: J. Mar, 1998)

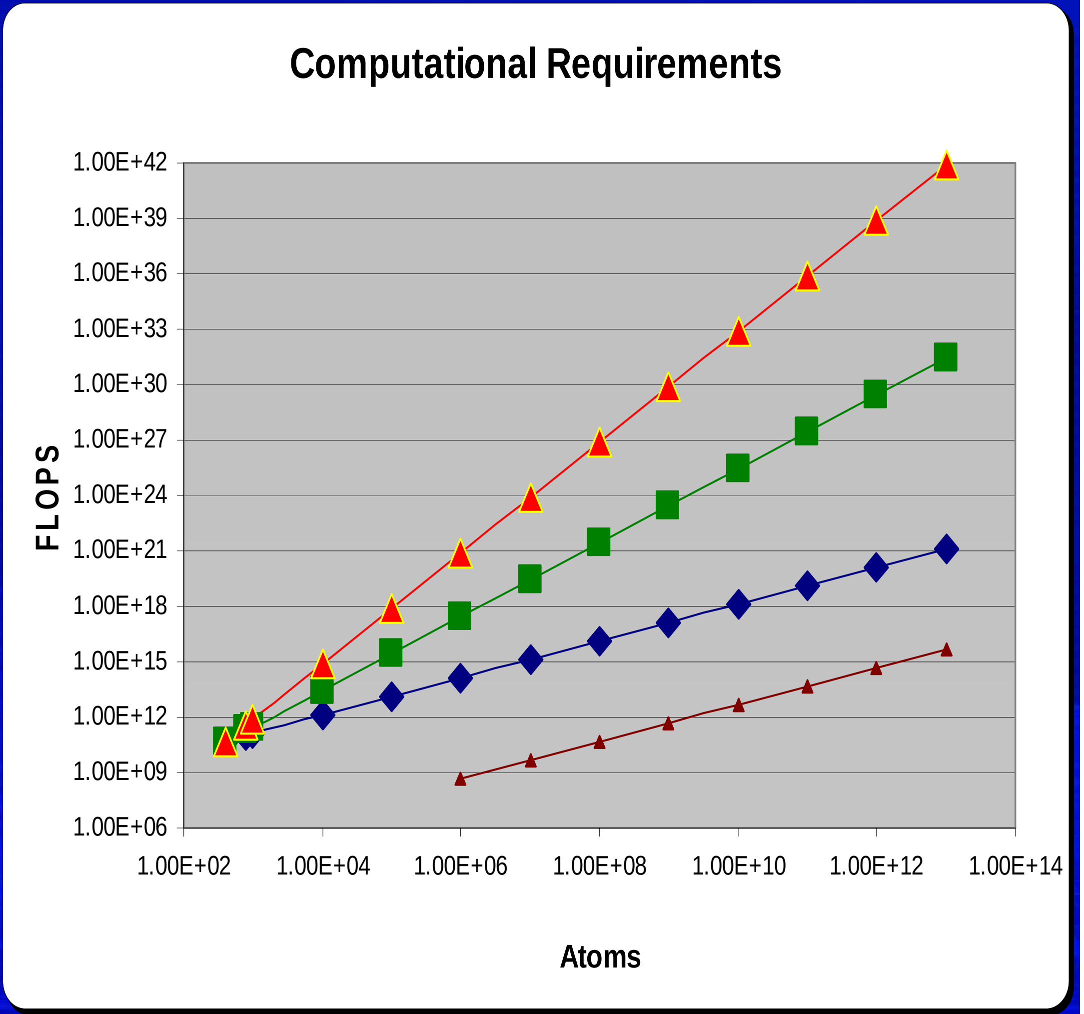
- ***Efficient and effective way of engineering material performance in devices***
- ***Multiple "Eureka" moments aid in evaluating directions***



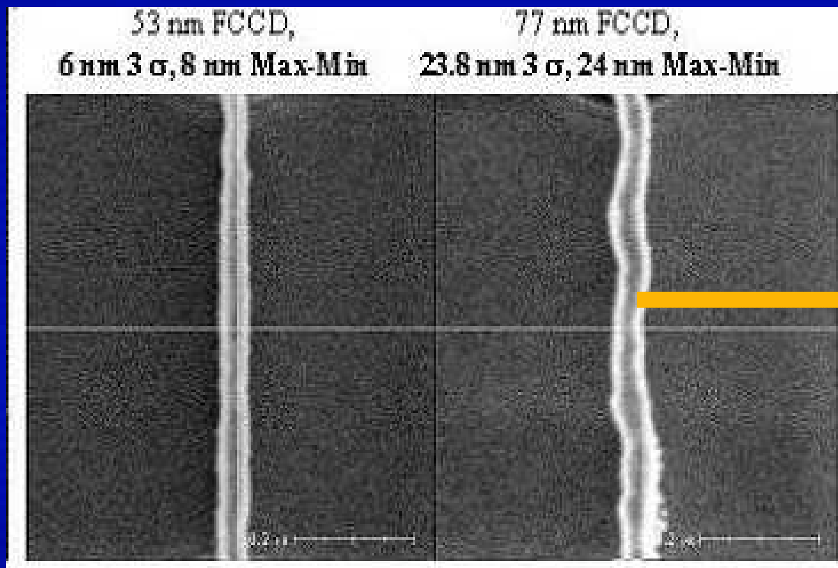
Use Modeling to Accelerate Learning Curve

Fundamental Problem in Modeling

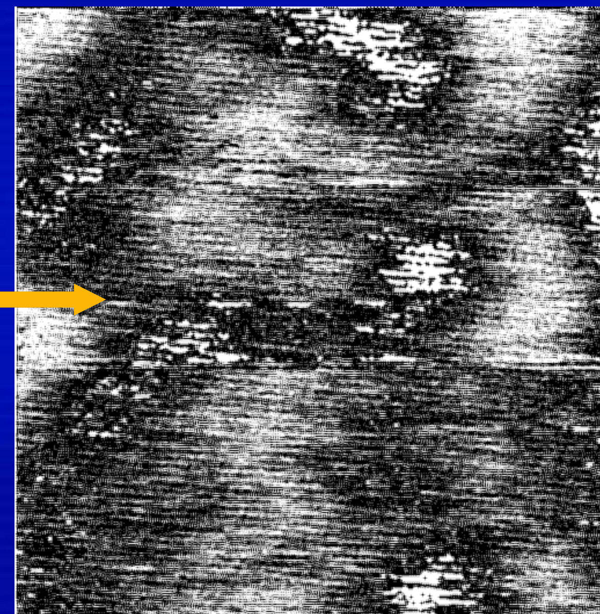
- Use of first principles is information limited
  - O(10^{23}) ~10 trillion x trillion
  - Mining & post-processing are limiting
- GIGO
  - Structure, characterization, and interface conditions need to be precise



Motivation for Metrology



?



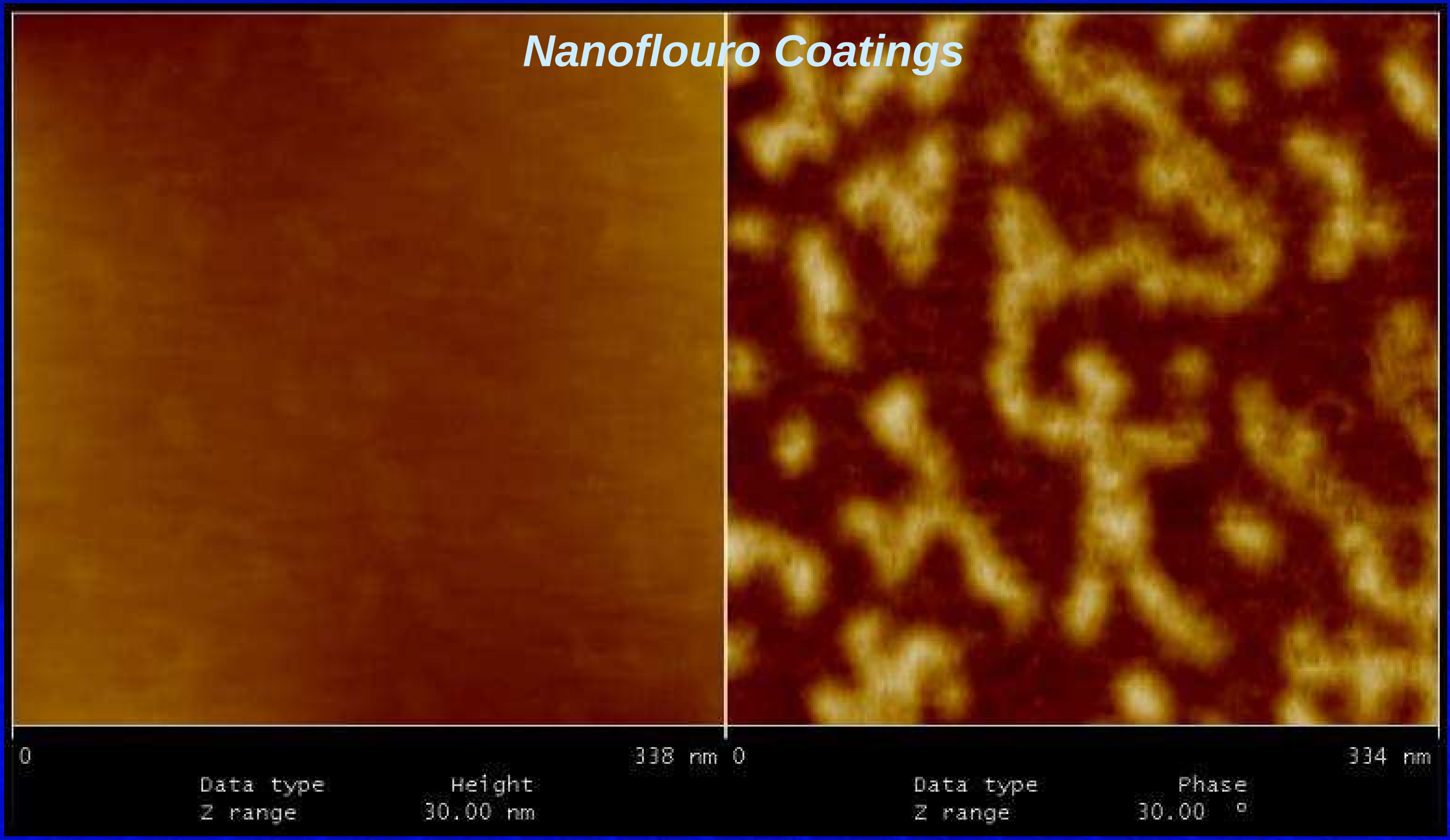
Line Edge Roughness(LER)

Ack: M. Garner

Atomic Force Microscope Picture of Resist Nano-domains

- **Use Metrology to understand structure, composition, and function**
- **2D/3D chemical, bonding, Electronic DOS, and structural characterization**
  - **Functional property characterization - Metrology & test structures to separate functional properties**

Problem in Measurement



Topography **Phase** ***(G. Blackman, 2006)***

- How do you interpret measurement ?
- What are you looking for ?

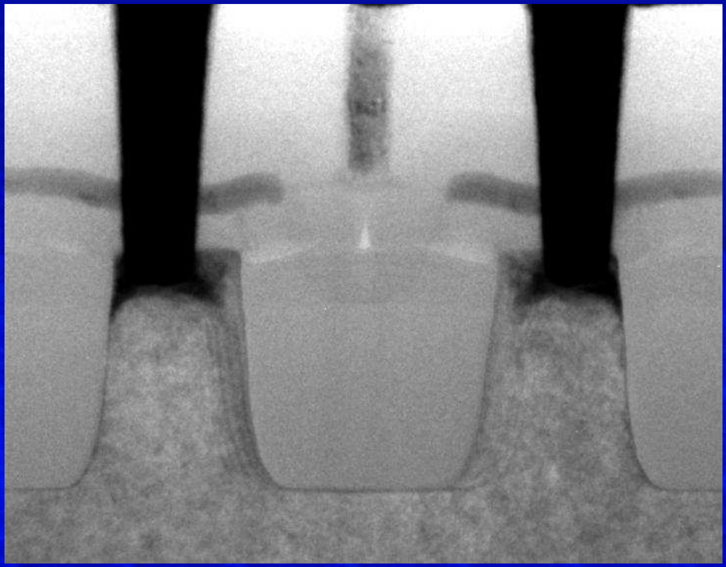
S. Shankar

Blackman, Brill, Wysong

Metrology Challenge

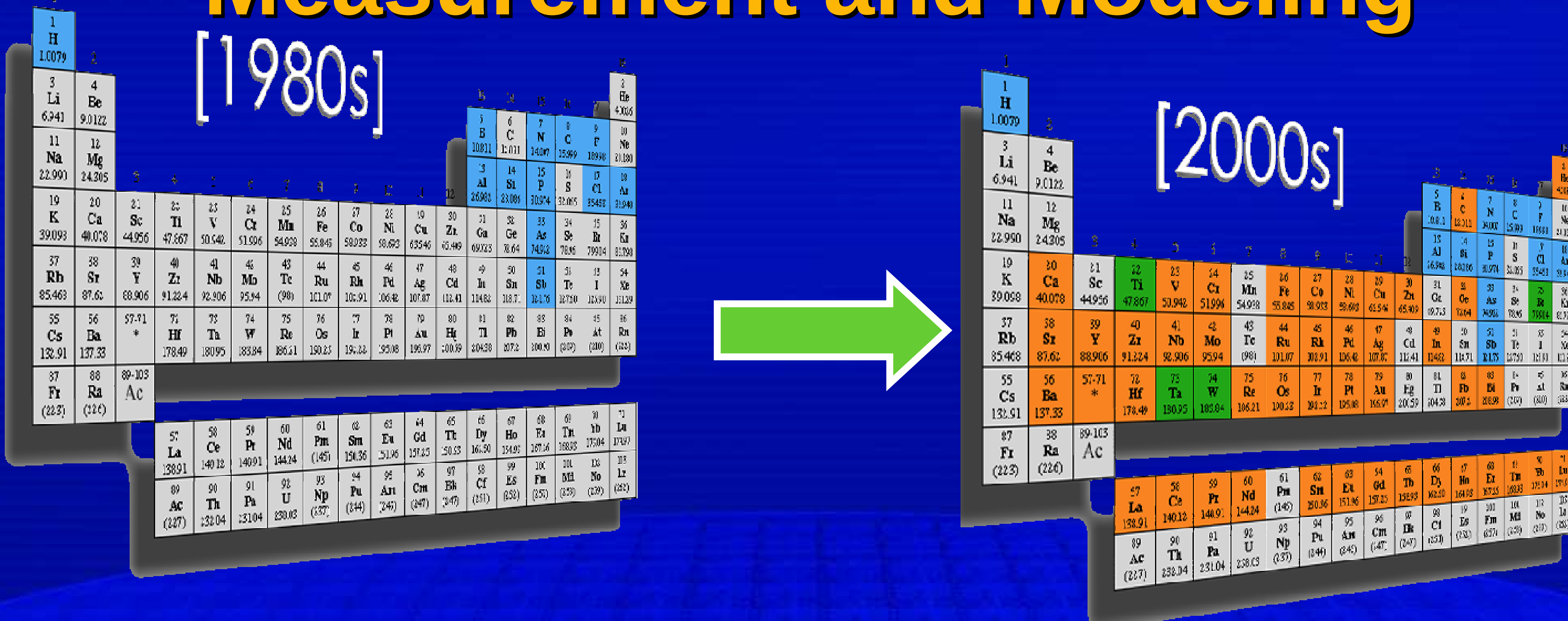
- **Dimensions of integrated devices are increasingly below the interaction volume of standard metrologies, such as SIMS, SCM, XPS, Auger, TEM**

- **Modeling is needed to deconvolute analytical results from integrated geometry**



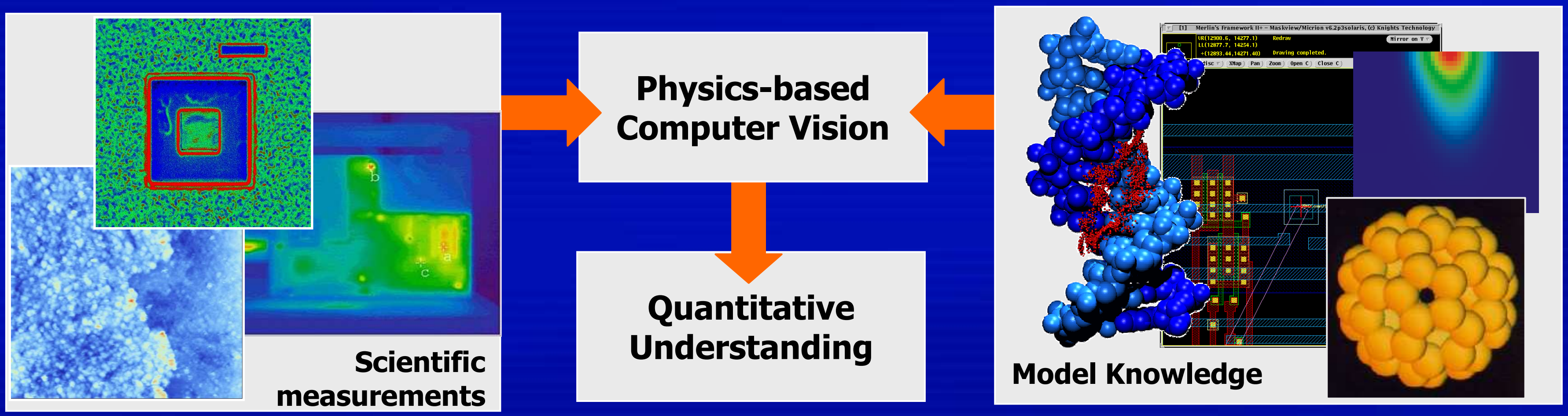
Projection image of gates and contacts – bright field TEM

Fundamental problem of Measurement and Modeling



- Presence of multiple interfaces
- Ternary compounds and higher
- Both modeling and metrology are convoluted and are up against combinatorics

Symbiosis between Modeling and Metrology



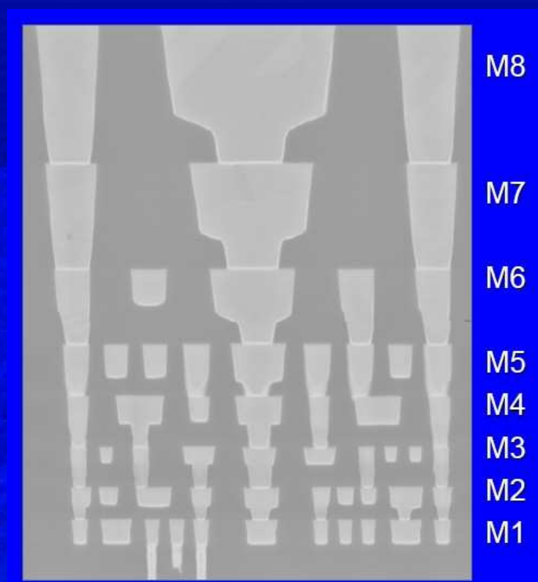
- **Model necessary to interpret a physical or electrical measurement.**
- **Physical or electrical characterization necessary to confirm a model of a novel material, device structure**

Interface Reliability

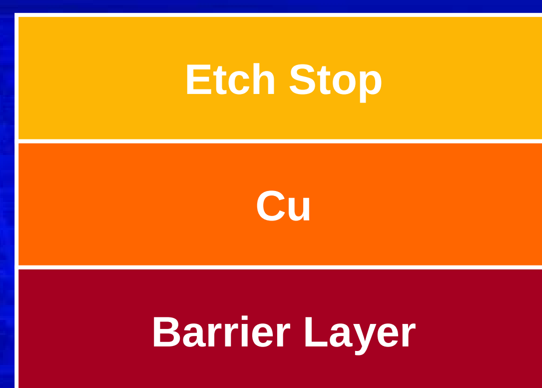
Reference: H. Simka, S. Shankar, C. Duran, and M. Haverty (MRS Symposium Proceedings, Vol 863, B9.2, 2005)

Interface Property

- **Advanced back-end interconnect technologies contain dual-damascene Cu layers and numerous interfaces:**
  - ***Intel 65nm logic technology features 8 Cu interconnect layers with CDO low-K ILD and SiCN etch stop layers (P. Bai et al,* IEEE International Electronic and Device Meeting, 2004)**
- **Understanding the interface is critical to optimize and ensure the desired properties and device reliability**

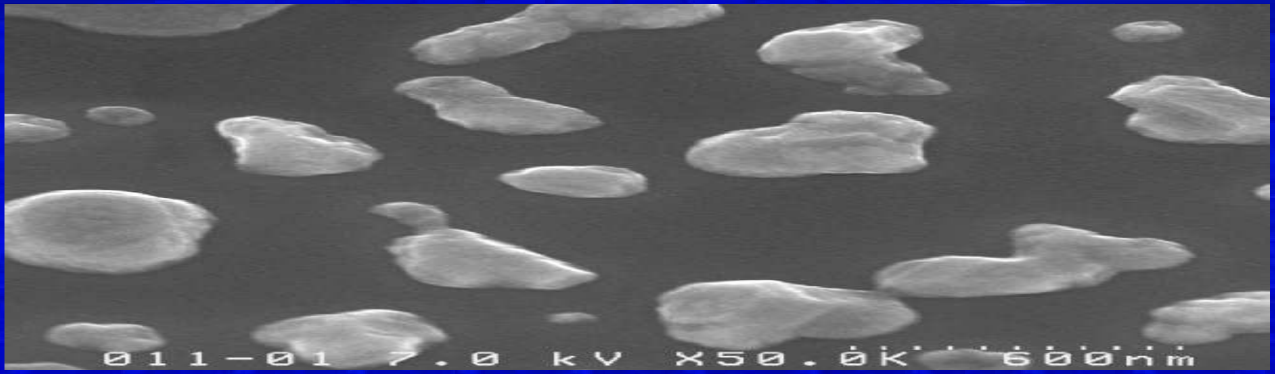


Focus of this work:



Challenges and Goals

- ***Challenges:***
  - Adhesion strength depends on many factors (materials, process conditions)
  - Lack of detailed characterization of interfaces (composition, structure, etc)
  - Adhesion measurements are often complex and time-consuming
  - Multiple effects are difficult to deconvolve and evaluate separately
- ***Goals:***
  - Develop a fundamental model for Cu interface adhesion for screening materials and guiding experiments



Agglomeration

M^2 Methodology

- **Modeling:**
  - Periodic supercell model of interfaces:
    - Typical Cu(111)slab: A few atomic layers each with 4 or 16 atoms. Atoms in the 2 layers farthest from the dielectric fixed at their bulk positions
  - Energies calculated using DFT
  - Adhesion energies determined using:

$$E_{adhesion} = (E_{stack} - E_{slab1} - E_{slab2}) / A$$

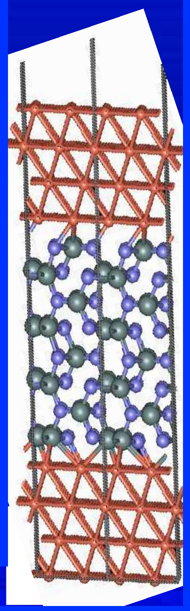
E_{stack} = total energy of relaxed stack

E_{slab1} = total energy of slab1

E_{slab2} = total energy of slab2

A = cross sectional area of interface

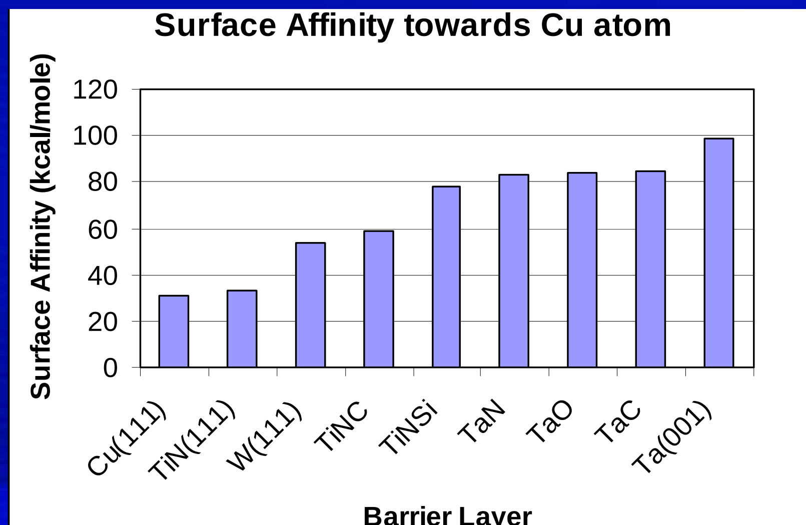
- **Metrology:**
  - Wetting experiments



Interface Adhesion

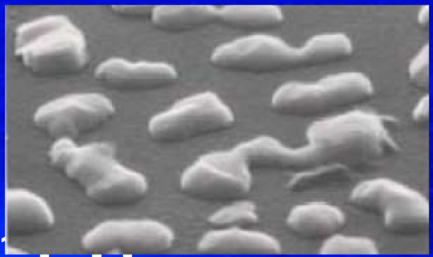
- **Modeling showed that surface affinity towards Cu increases in the order of**

TiN(111) < W(111) < TiNC < TiNSi < TaN, TaC, TaO < β-Ta(001)

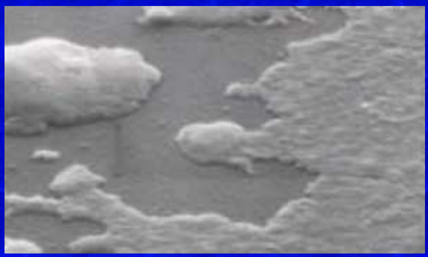


- **Results consistent with de-wetting experiments for 100Å Cu on various barrier layers, annealed at 380°C for 15 minutes**

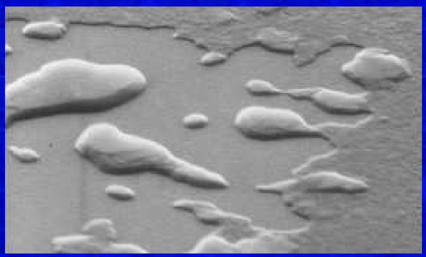
TiN



TiNSi



TaN



Ta

Classical Open System: Electromigration

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

Problem

Challenges

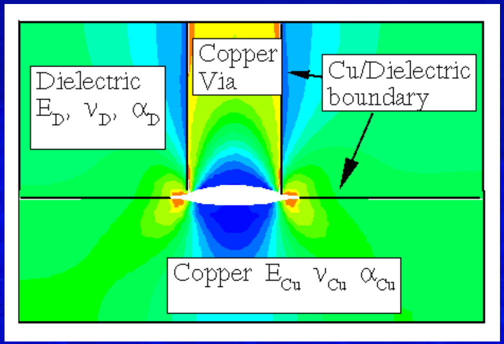
• Cu Damascene structures are heterogeneous due to interconnect morphology and materials

• 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

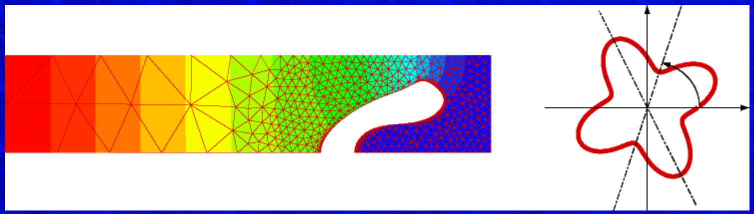
• Occurs early



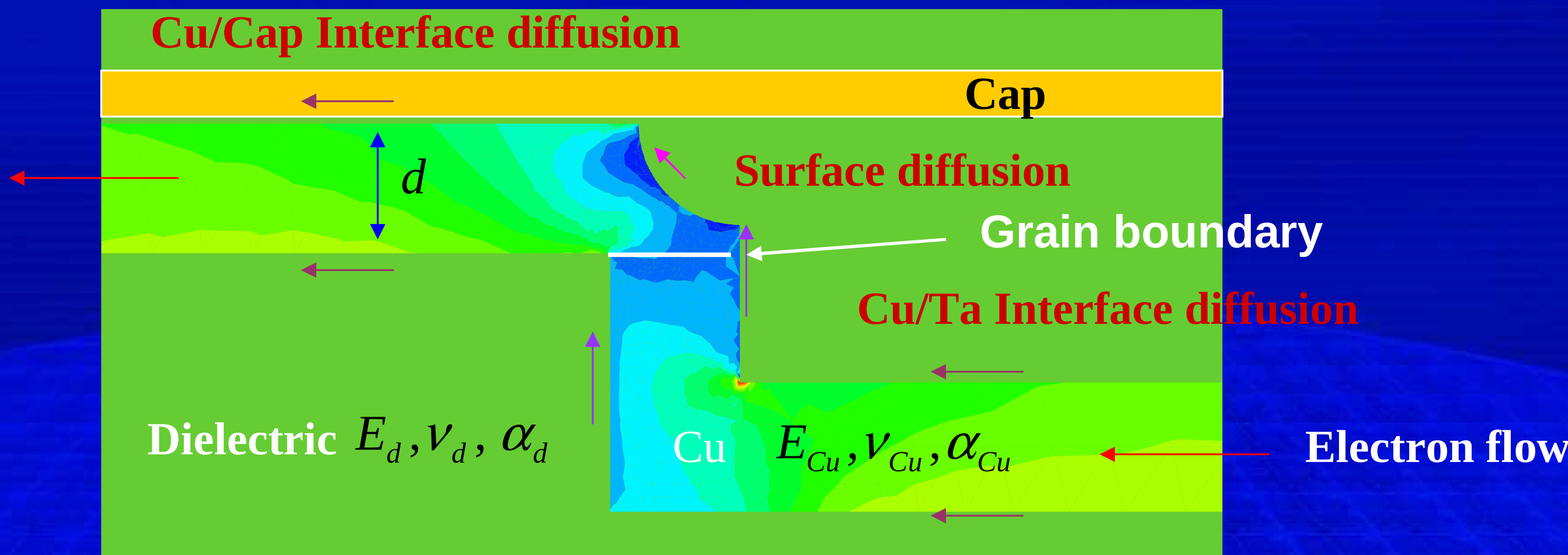
Void Evolution and Growth

• Caused by stress and electric current induced mass transport

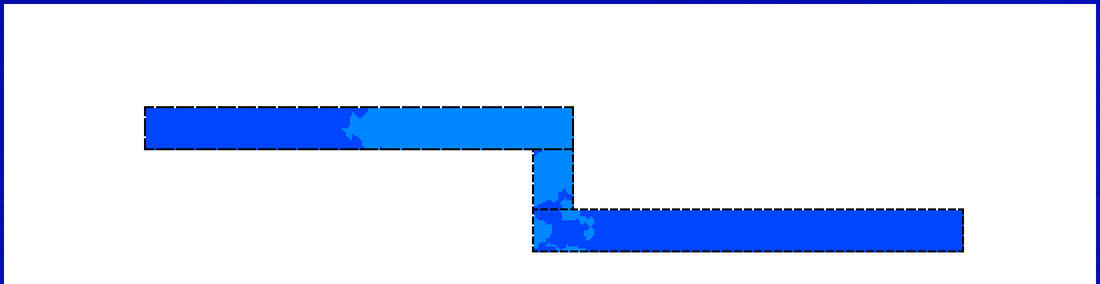
• Dominant part of interconnect life



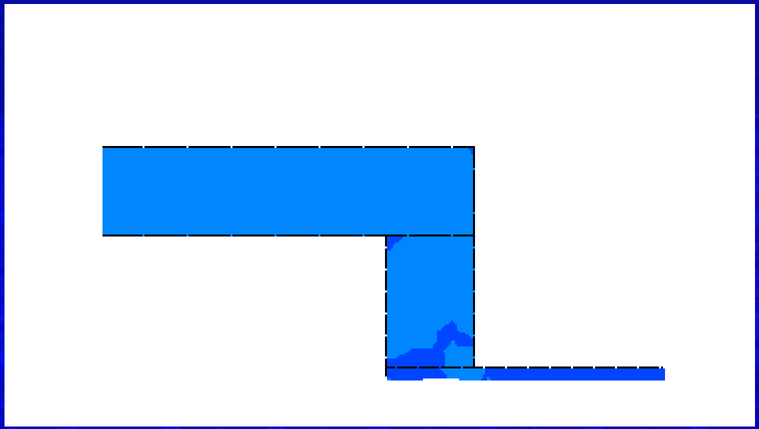
Void nucleation/growth in 2 level structure



Void nucleation, growth and evolution

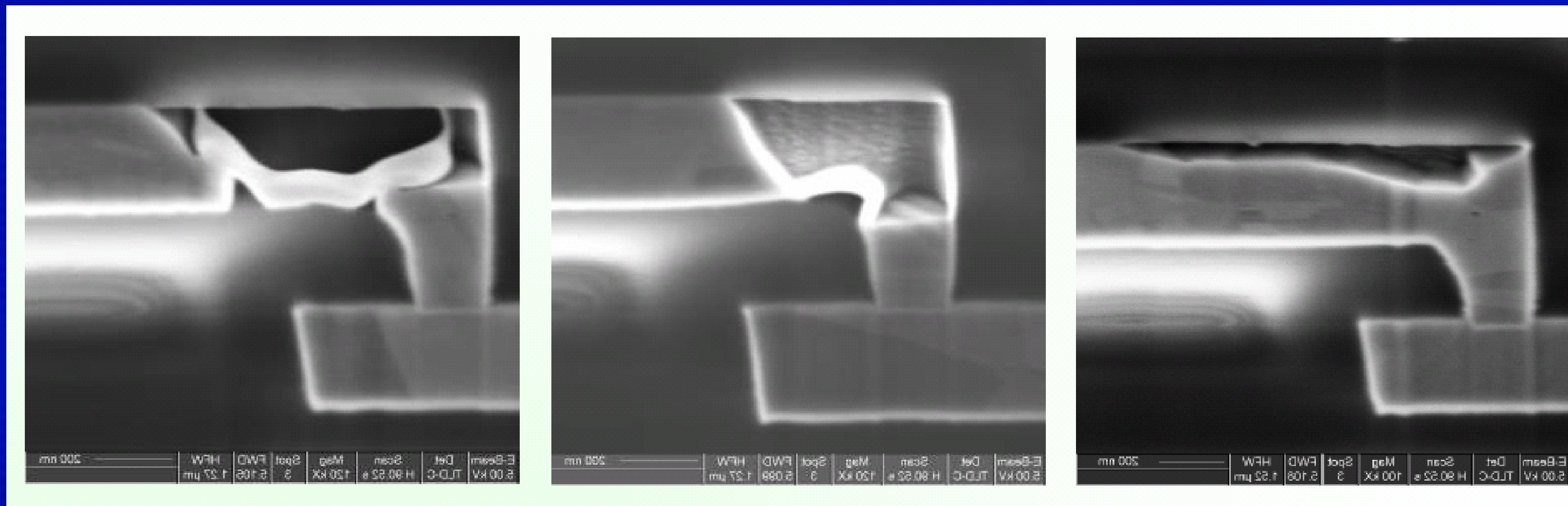


Animation showing entire structure
Contours show vertical stress



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

Comparison with experiments



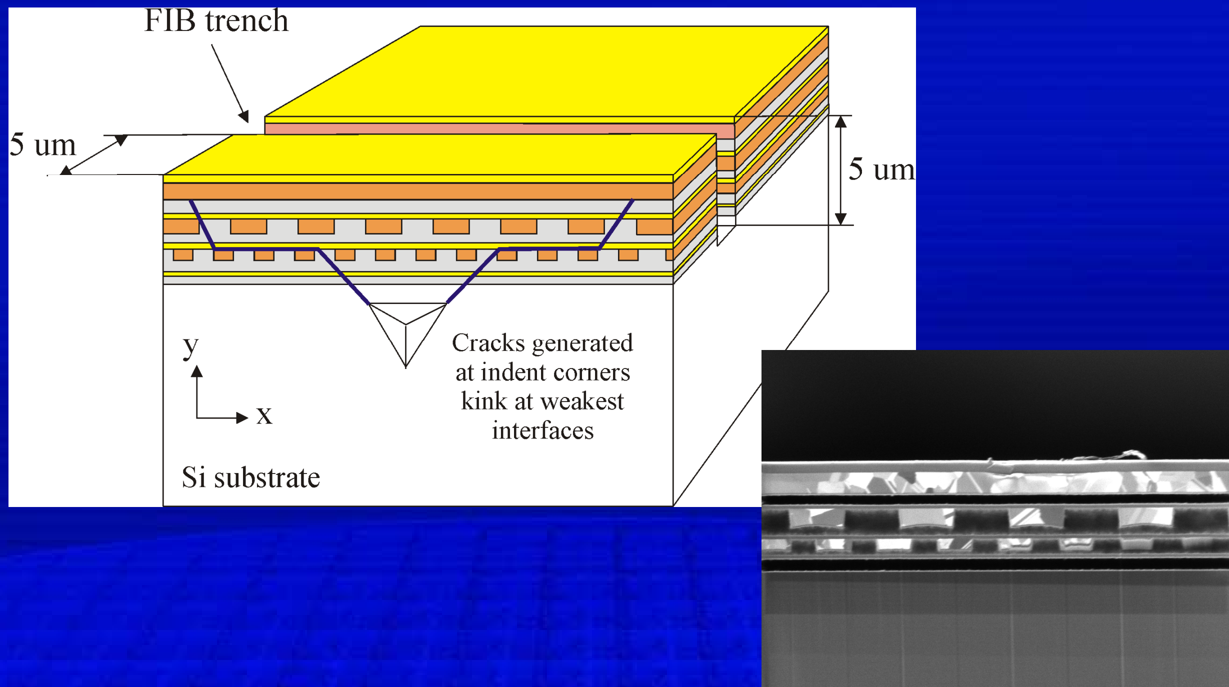
Hauschild *et al* (Proc AIP stress workshop, 2004)

- 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

Metrology Examples

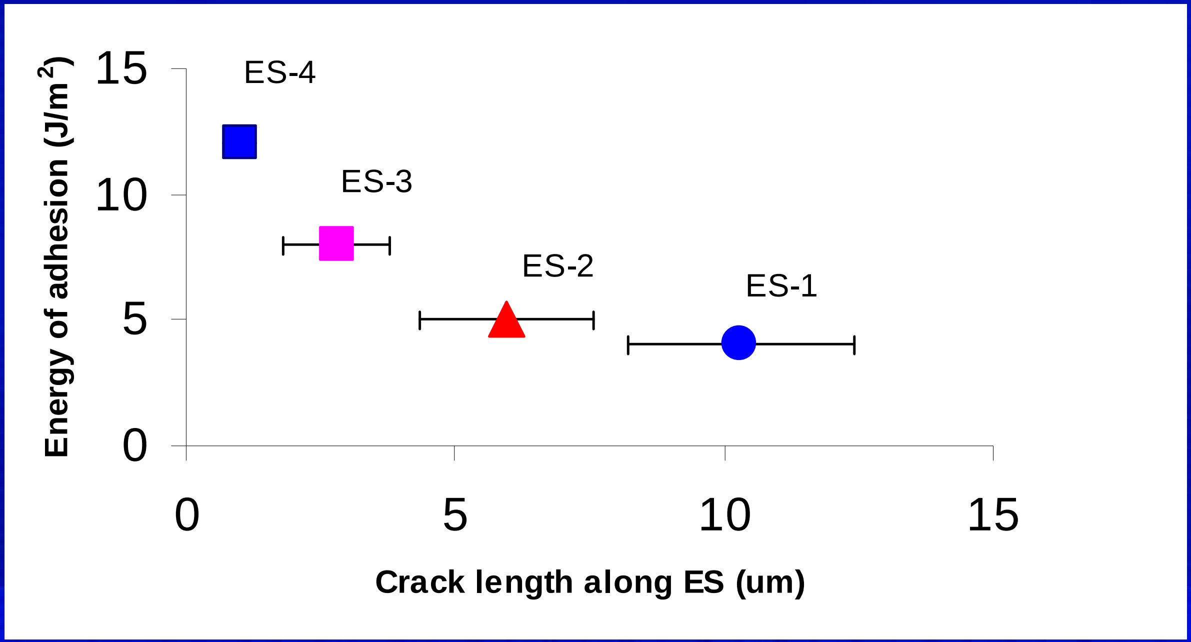
Modified cross-sectional nano-indentation



Schematic of the indentation procedure. The SEM picture at the bottom shows the arrangement of the stack with three levels of metallization.

J. Molina1, I. Ocana1, D. Gonzalez1, M.R. Elizalde1, J.M. Sanchez1. J.M. Martinez-Esnaola1, J. Gil-Sevillano1, T. Scherban2, D. Pantuso2, B. Sun3, G. Xu2, B. Miner2, J. He2, J. Maiz2

Modified cross-sectional nano-indentation



Correlation between the energy of adhesion for the interface ES/Cu measured by 4 point bending and the crack length along the same interface measured by MCSN for the case of ILD-2 (ES/ILD-2 adhesion energy is about 3 J/m^2 in all cases). Error bars represent the standard deviation for the mean value for 5-7 indentations. Typical standard deviation for four-point bending is 10%

J. Molina1, I. Ocana1, D. Gonzalez1, M.R. Elizalde1, J.M. Sanchez1. J.M. Martinez-Esnaola1, J. Gil-Sevillano1, T. Scherban2, D. Pantuso2, B. Sun3, G. Xu2, B. Miner2, J. He2, J. Maiz2

Modified cross-sectional nano-indentation

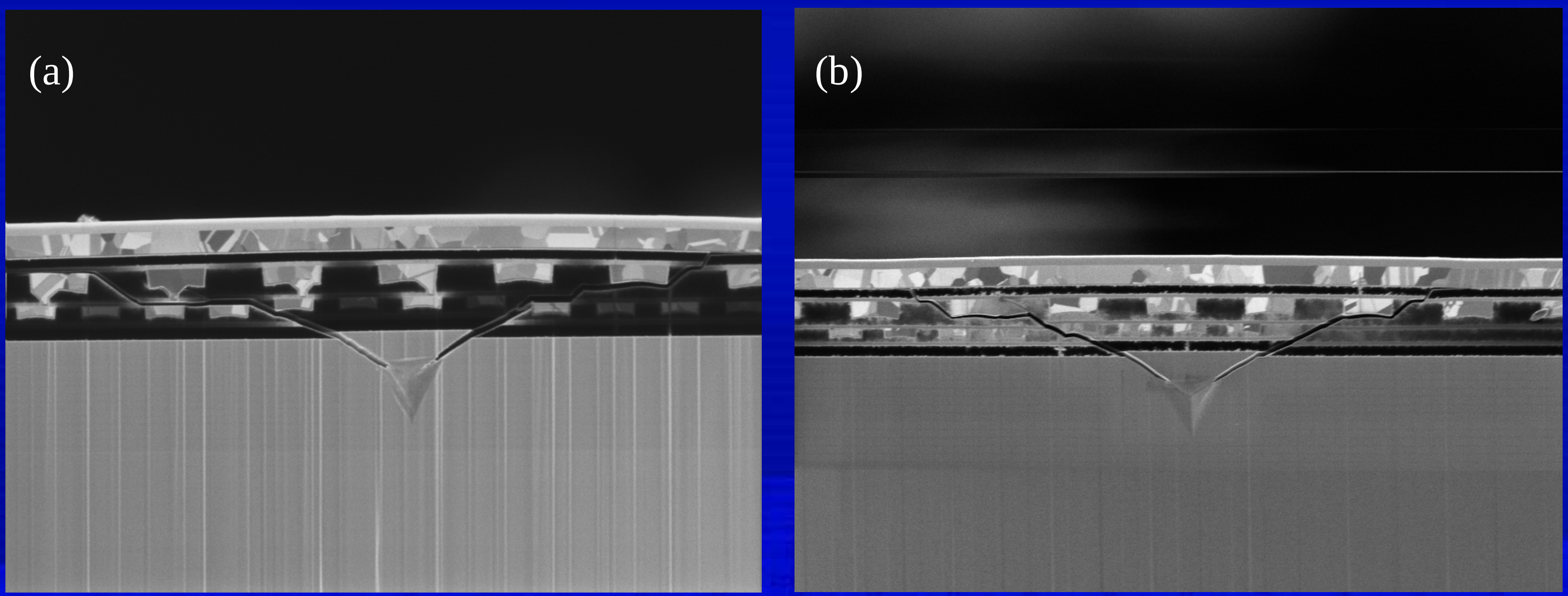


Figure 6: SEM images of the crack path in two different samples. (a) ES-1 (poor adhesion). The crack kinks into the interface; (b) ES-4 (good adhesion). Almost all the cracking occurs through the ILD.

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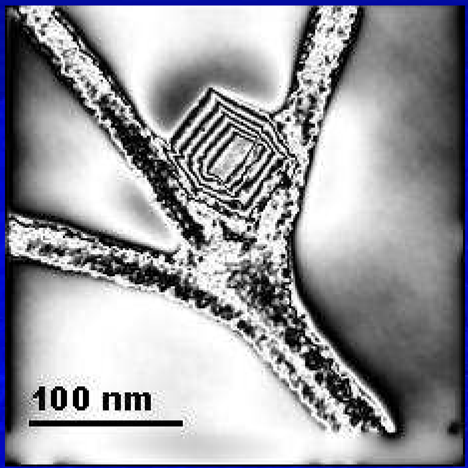
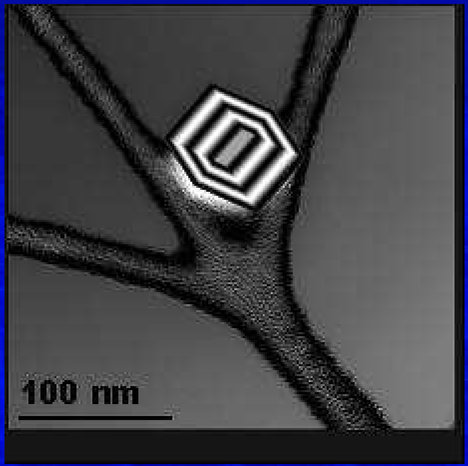
Phase Retrieval Approach

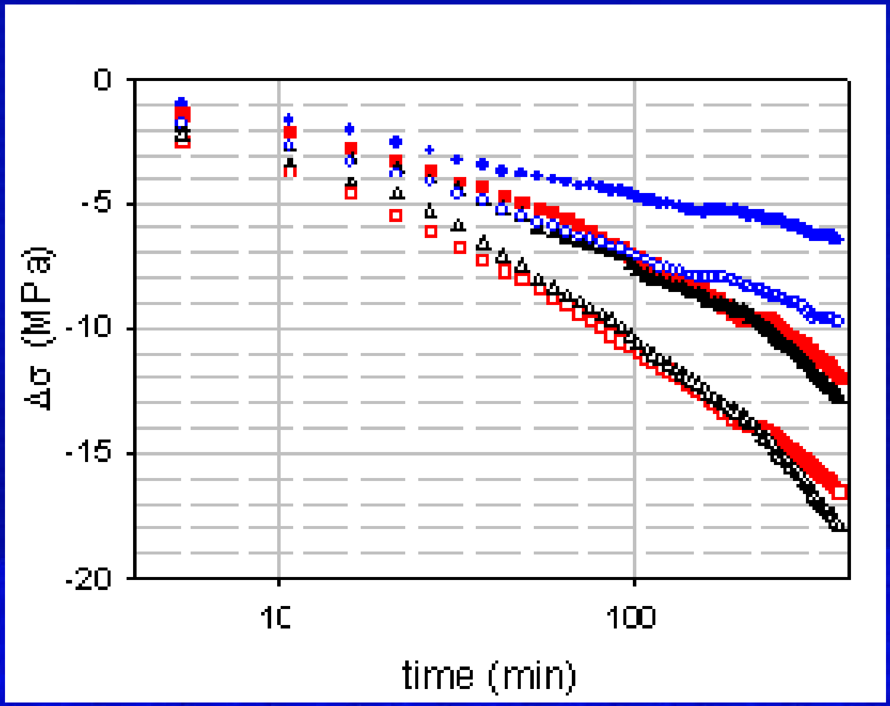
- Quantitative phase imaging is one method for extracting geometric information from TEM images.
- At below left, the transport of intensity equation was solved for a stack of TEM images to extract the geometry of an MgO particle. The result compares well to the modeled image at right.





T. Pedersen et al University of Sydney

Metrology Modeling



Ack: Ho, IITC, 2003

- **Stress relaxation with modeling used to assess Cu interconnect reliability with different passivation layers**

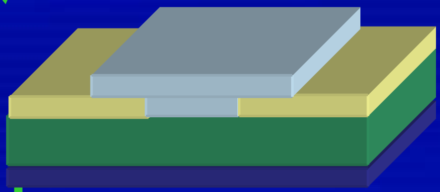
Challenges

Complexity of Multi-scale Systems

Technology performance is determined by the behavior of materials at the integrated level

Mesoscale

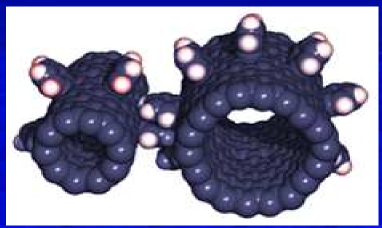
Thin Film Or Macrostructure



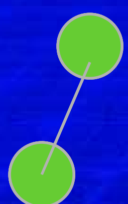
Quantum and Atomistic

Quantum Mechanics

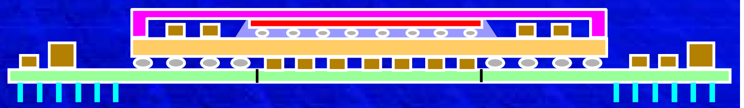
Nanostructure



Molecule



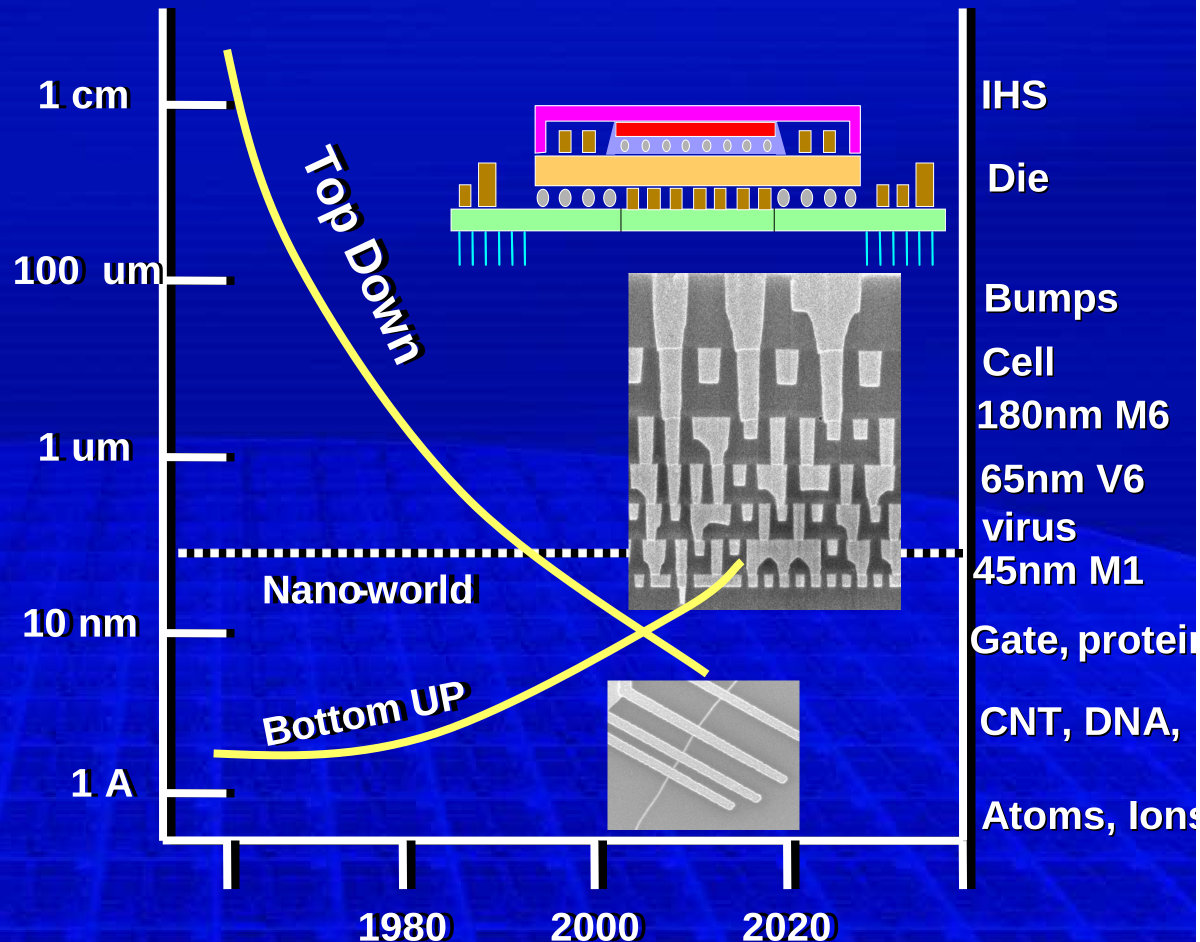
Circuit



Integrated Device

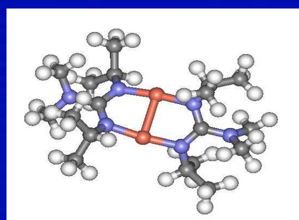
Material Dimensions falls between Molecules and Structures

The Frontier



Modeling & Simulation Requirements

Synthesis: Precursor



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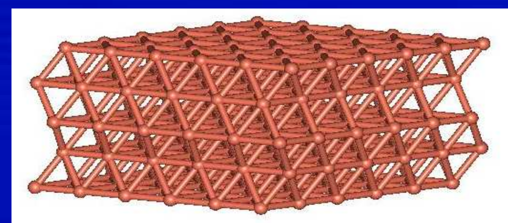
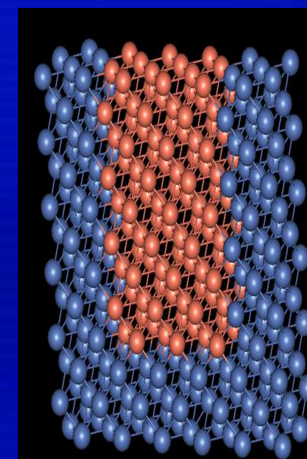
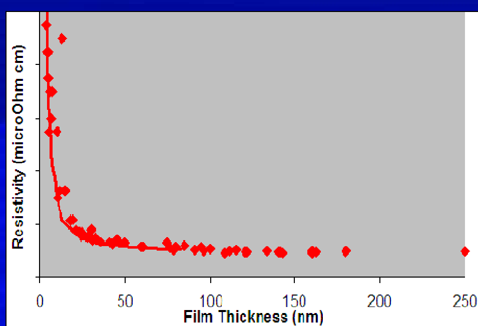
Synthesis: Substrate



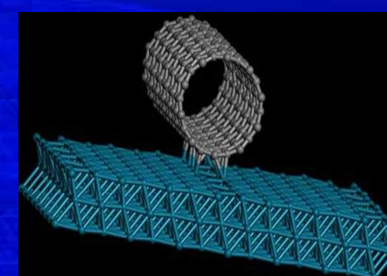
Structures and Composition



Properties



Atomic Scale Probes



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

Summary

- "Nanotechnology" needs new levels of understanding
- Demonstrated successful applications of modeling & metrology
- Needs in modeling
  - Theory Development
    - Examples: Density Functional Theory, low concentration defects
  - Algorithm Development
    - Bridging length scales for integrated systems
  - Software Development
    - Scalability and Productization
- Needs in metrology
  - Characterize different properties
    - Electronic structure, transport, optical properties
  - Classes of Materials
    - Semiconductors (III-V, IV), Graphene, CNT, Complex Oxides and Nitrides
- The convergence of today's difficult challenges, emerging market drivers, and recent breakthroughs in materials technology represents a rare opportunity for chemists, chemical engineers, materials scientists, and others to develop breakthrough material and process application options

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