SAND2008-0977C

Modeling & Simulation Enabled Nano-Engineering:

Moving from Nanotechnologies to Emerging Applications

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VP Office of Science, Technology and Research Foundations

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National Nuclear Security Administration

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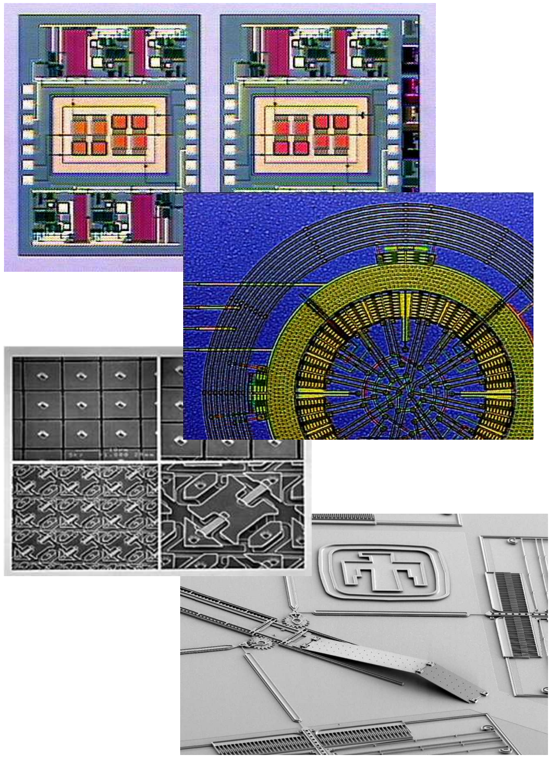
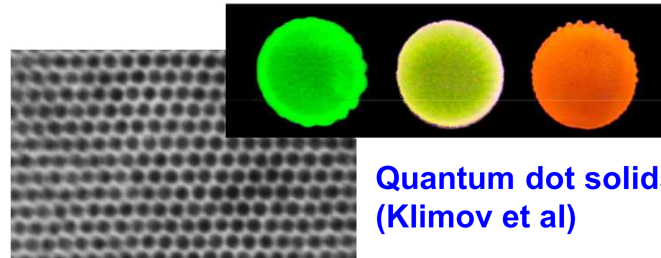
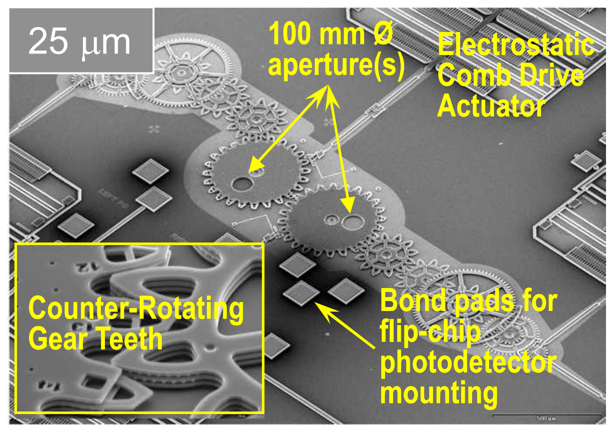
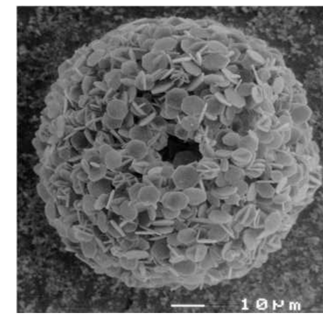
We want to take advantage on new functions from complex & hierarchical micro/nano materials





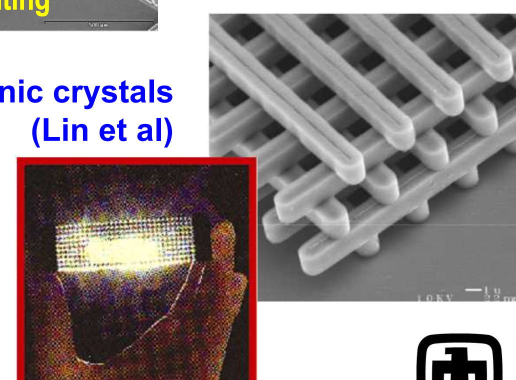
Quantum dot solids (Klimov et al)





Capillary induced aggregate formation (Bell and Adair)

Photonic crystals (Lin et al)



Future systems will be able to:

- ***Sense***
- ***Think***
- ***Act***
- ***Communicate***

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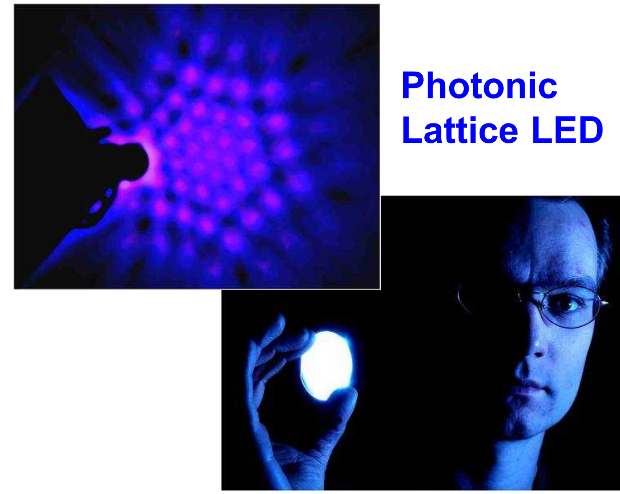
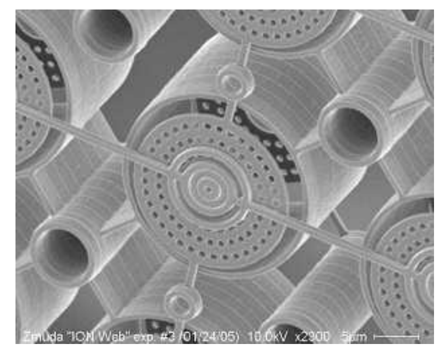
"There is plenty of room at the bottom."
– Nobel Laureate Richard P. Feynman

- Micro- and nano-scale devising will revolutionize engineering.
- Manufacturing micro- and nano-scale devices requires understanding phenomena over many length scales.
- But ... such small scales challenge conventional engineering approaches
  - Unexpected physical behaviors
  - Experiments are difficult
  - Intuition is suspect
  - Can't just scale down from macro-scale
    - » "Micro-sizing" doesn't work
- Profound implications for engineering education in the 21st century



Photonic Lattice LED



Micro-ion traps for quantum information processing

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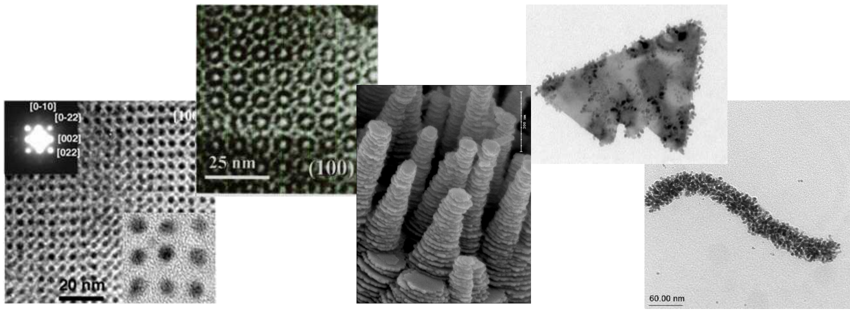
Nanotechnology is not a far-off, fuzzy, futuristic technology any more



Phase 1 (4-7 years ago)

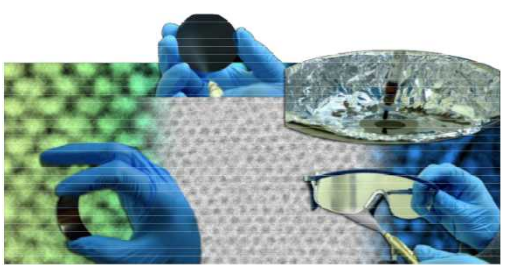
- Making building blocks
  - Quantum dots, nanotubes, nanoparticles, nanocrystalls, …

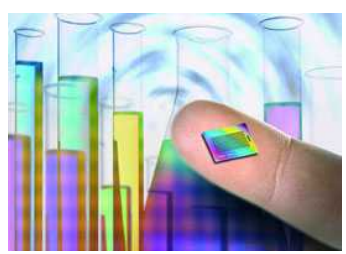
Phase 2 (2-3 years ago)

- Mixing building blocks into traditional bulk materials
  - Has already established a beachhead in the economy

Phase 3 (current)

- Building systems with carefully designed nanostructured materials





Silver Nano HEALTH SYSTEM

SAMSUNG

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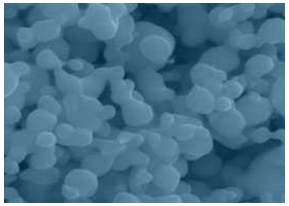
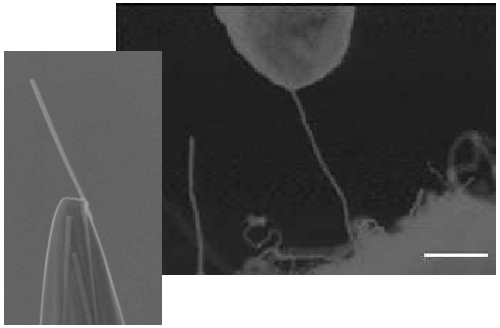
There are 3 enabling capabilities critical to the maturation of nano-engineering

Silver Nanoparticles



1. **Dimension Control for the Building Blocks**
   - Simple and cost effective processes to control the size and geometry of the building blocks precisely
     - Better understanding of the growth processes in controlled environments is needed.



2. **Nanomanipulation**
   - Distribute and/or arrange the building blocks into a desired pattern
     - A great challenge when dealing with a system including many dissimilar materials
     - We are still in the early stage of R&D.

3. **Modeling and Simulation**
   - Although many challenges exist, it is a highly promising tool.

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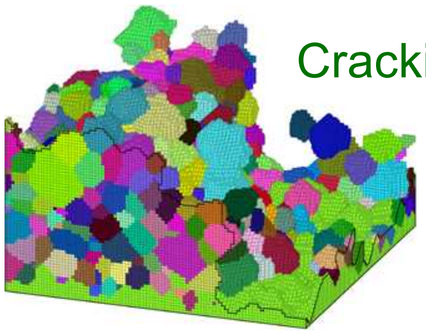
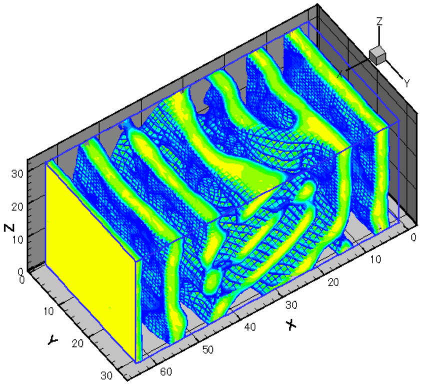
Modeling & simulation has an essential role

Integrate ***state-of-the-art modeling techniques*** and ***high performance computing*** to:

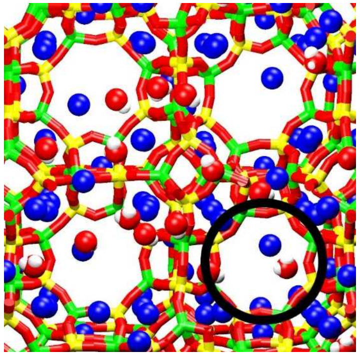
- Elucidate mechanisms of materials behaviors
- Describe details in materials processing
- Predict material properties
- Design material substructure for desired performance



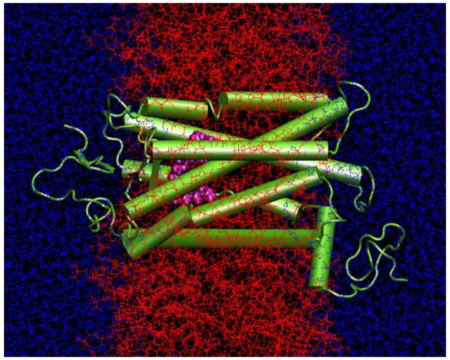
Cracking



Self-assembly of nanostructure



Chemistry in nanoporous materials



Molecular physics in bio-materials

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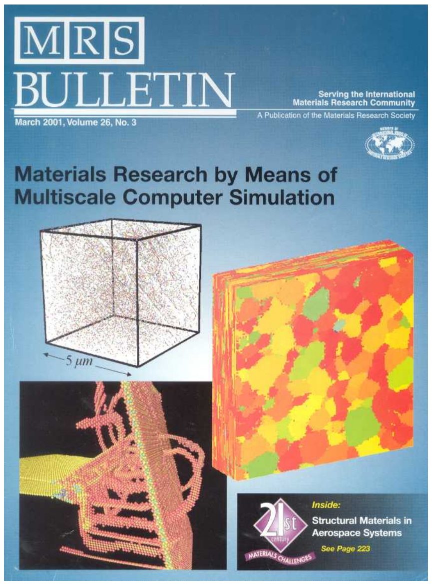
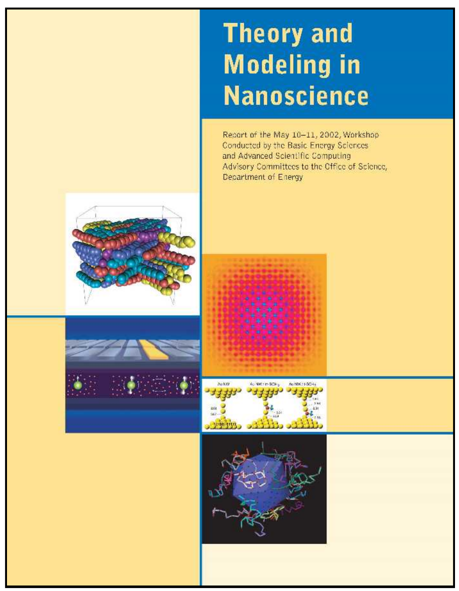
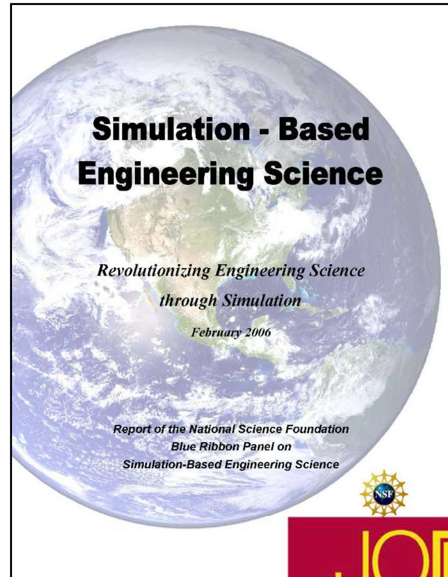
Computational materials & nanosciences are young, but steady progress is being made



R. Phillips, *"Crystals, Defects, and Microstructures – Modeling Across Scales."* MRS Bulletin v.26 #3, March 2001

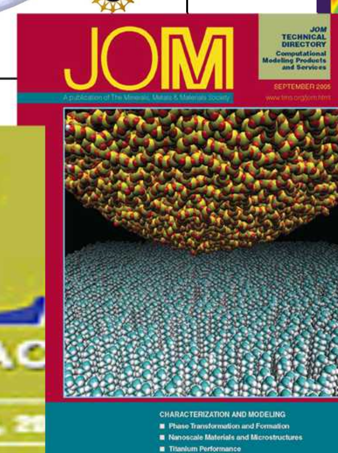
Report from a workshop, hosted by Basic Energy Sciences and Advanced Scientific Computing Advisory Committees, on May 10-11, 2002 in San Francisco, CA.





Report of the NSF Blue Ribbon Panel on Simulation-Based Engineering Science (2006)

(Aug 2005)



(Sep 2005)

(Sep 2006)

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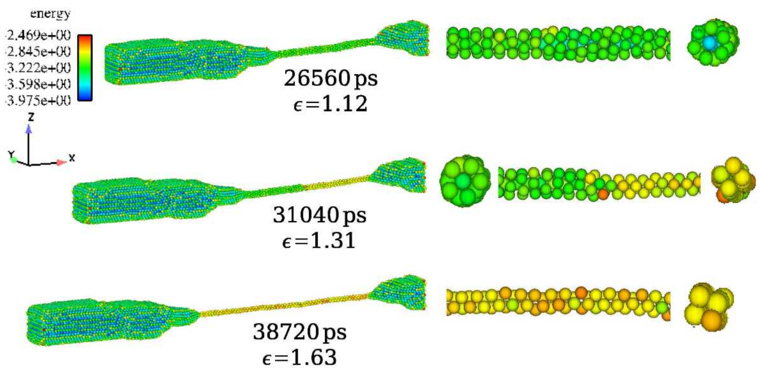
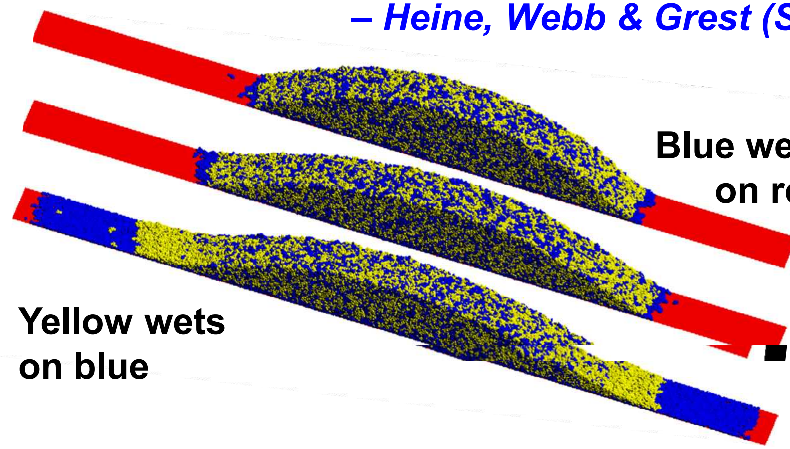
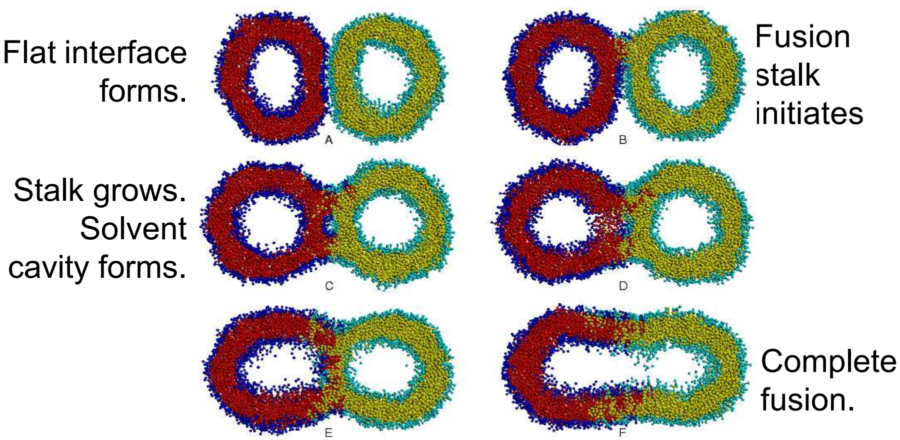
Examples of Recent Accomplishments on Atomistic Modeling of Nanomaterials

Deformation of Gold Nanowire – Zimmerman (SNL) & Park (CU-Boulder)



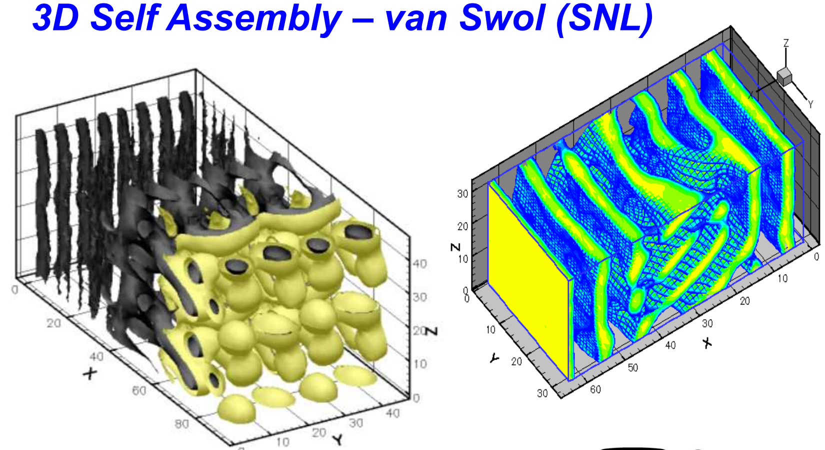
Wetting & Spreading of polymer droplets – Heine, Webb & Grest (SNL)





Coarse-Grained Model of Membrane Fusion – Stevens (SNL)

3D Self Assembly – van Swol (SNL)



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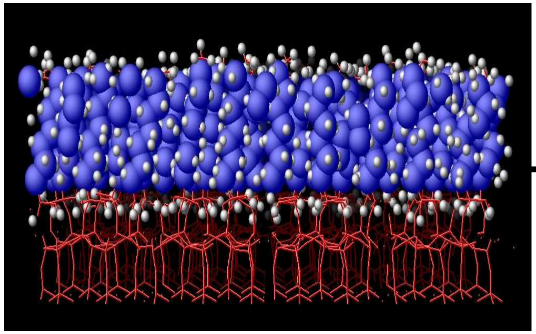
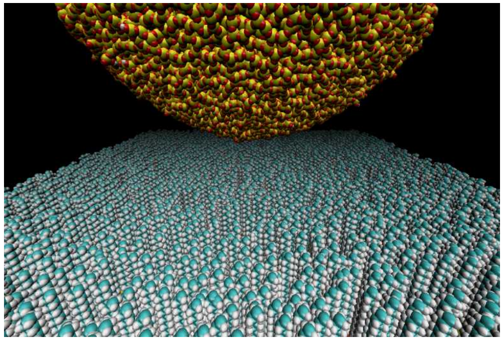
Direct comparison between simulation and experiment is becoming achievable.

MD Simulation of Experimental AFM Study on the Reliability of MEMS Coating

M. Chandross, SNL (2005)

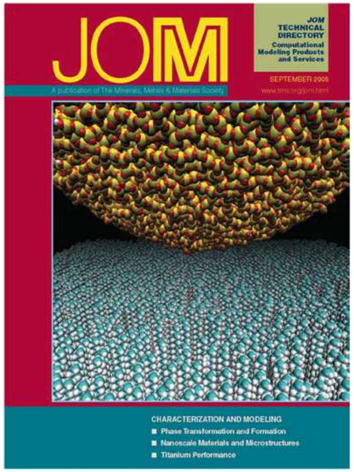


Polymer coating (blue) on polysilicon surface (red)

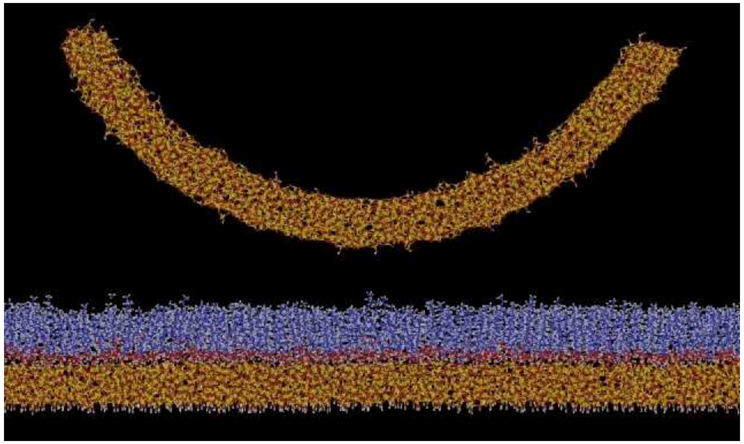


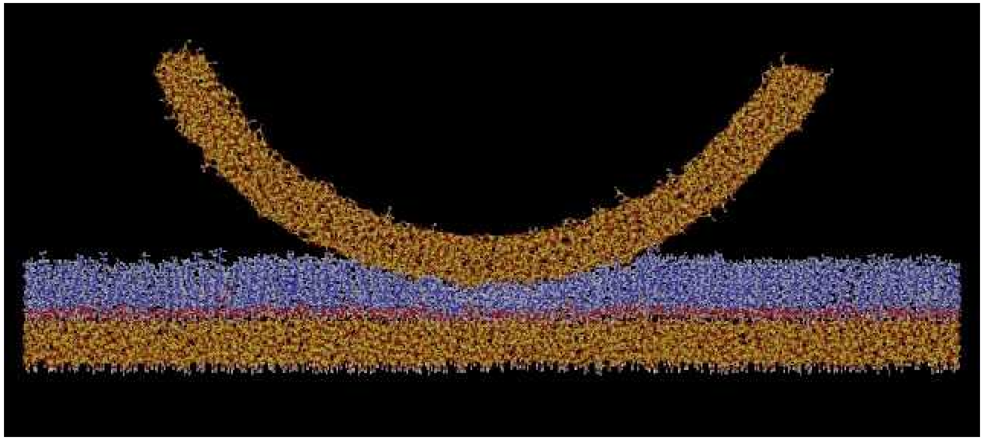
Over 200,000 atoms in the model
Radius of the tip = 10 nm

Curved tips mimic AFM and single asperity contacts



Vol. 57, Issue 9, 2005





- Coated & uncoated tips
- Amorphous & crystalline substrates

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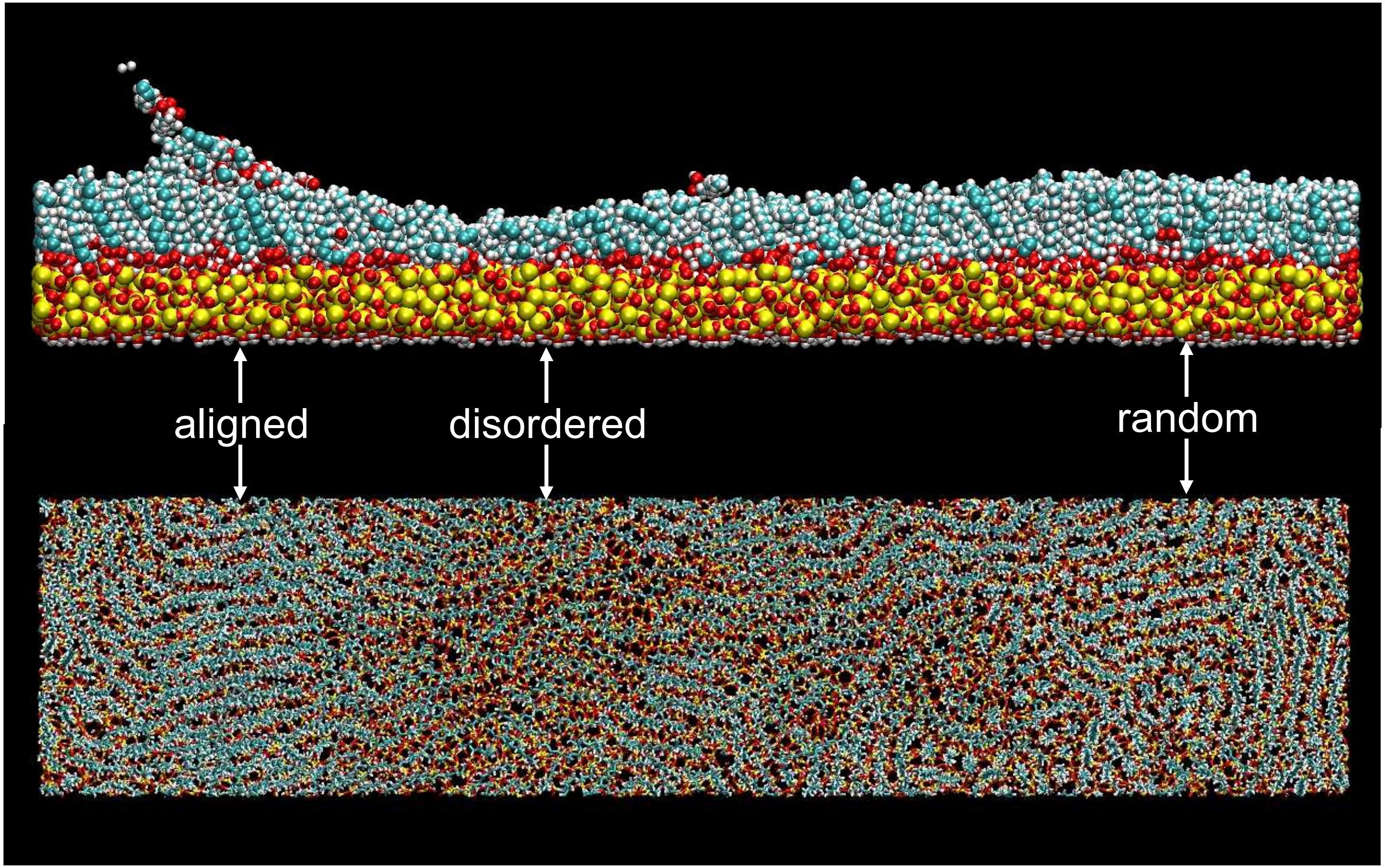
Chain Alignment with Shear



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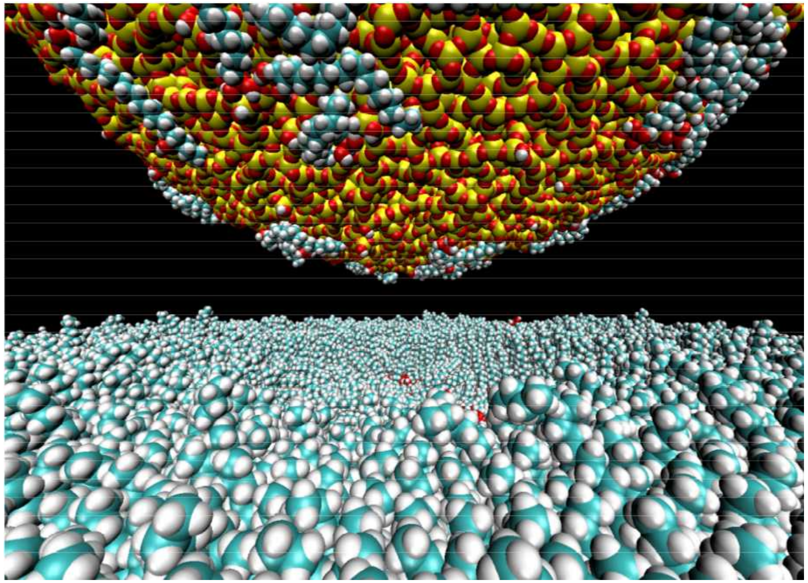
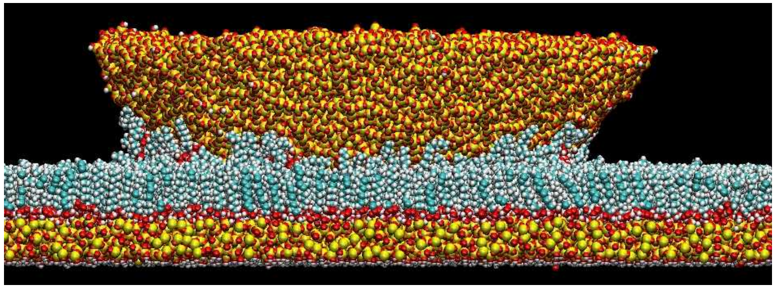
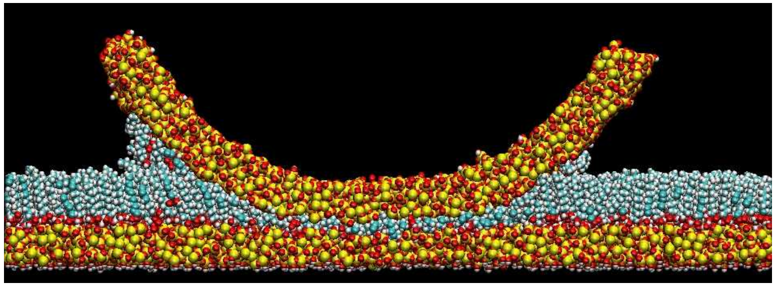
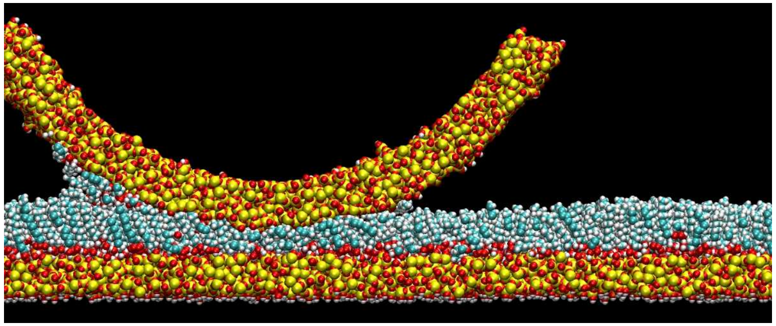
Simulated Results of the AFM Experiment



Rendering of simulations demonstrates, even with very low loads (<15 nN), coating material is transferred from the substrate to the AFM probe tip during shear.







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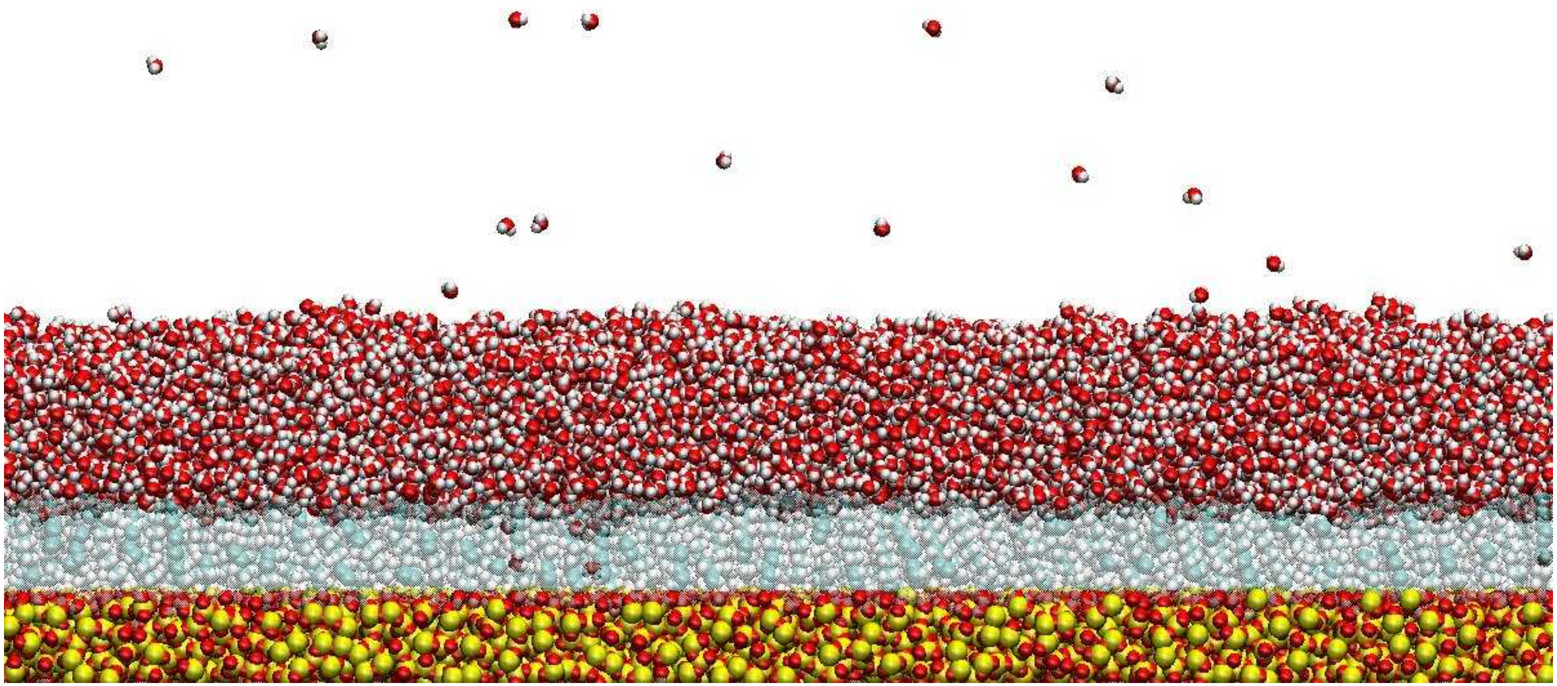
Water Penetration – Undamaged SAM

25 Å thick slab with 40K molecules in liquid

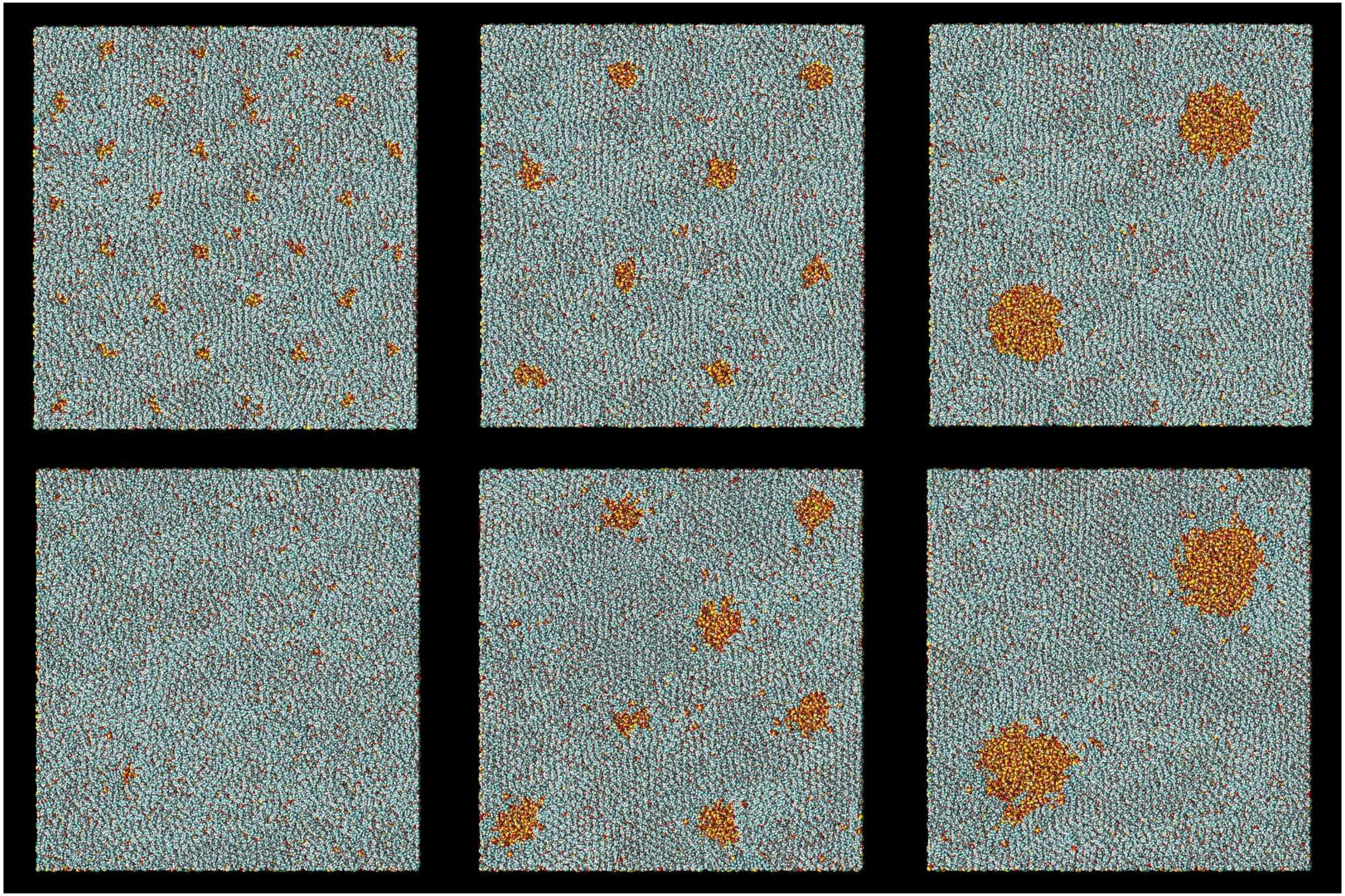
Minor penetration at defect sites



Water Penetration – Damaged SAMs

0 ns

1.8 ns



32 holes @ 5 Å

8 holes @ 10 Å

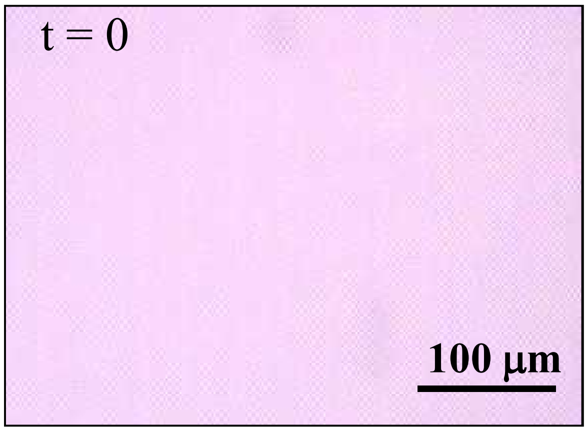
2 holes @ 25 Å

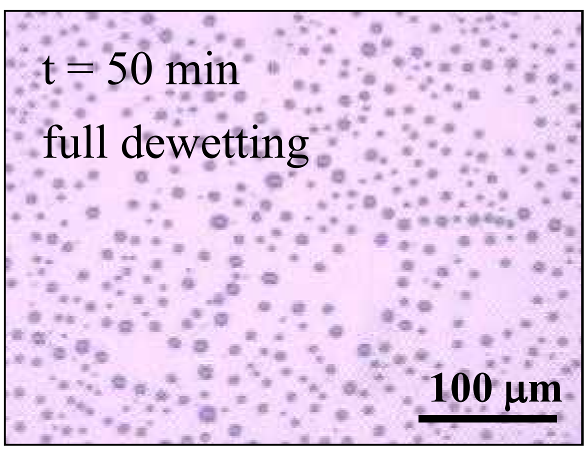
Running bigger simulations

is not always the right way to go!

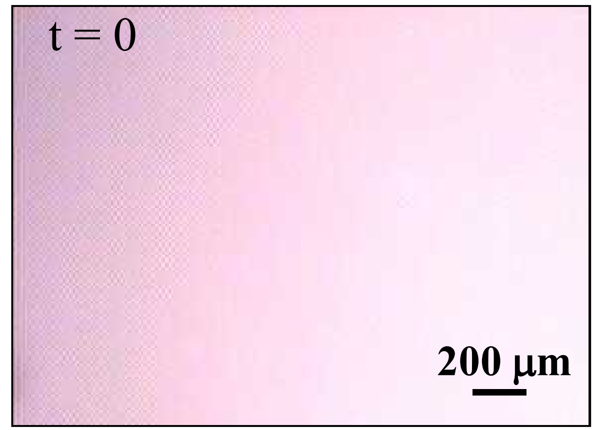
Prevention of Dewetting in Polymer Films

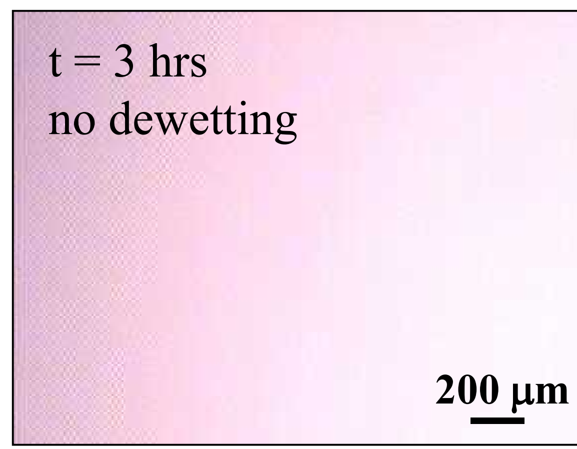
33 nm polystyrene film on "piranha" cleaned Si wafer





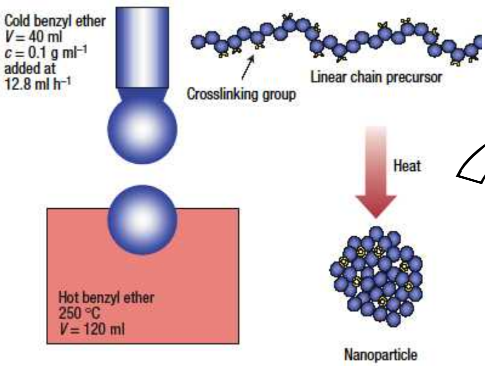
33 nm polystyrene film with 3 weight % fullerenes on "piranha" cleaned Si wafer

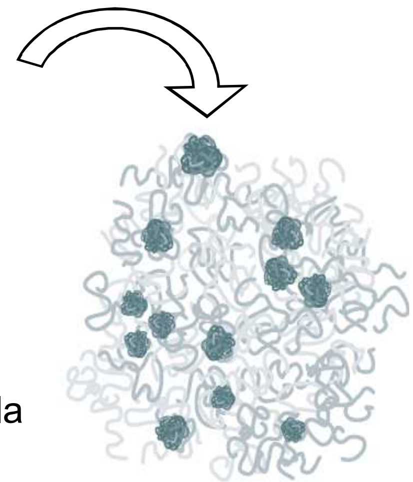




Mackay et al (Michigan State University)

Modeling Polymer Nanocomposites





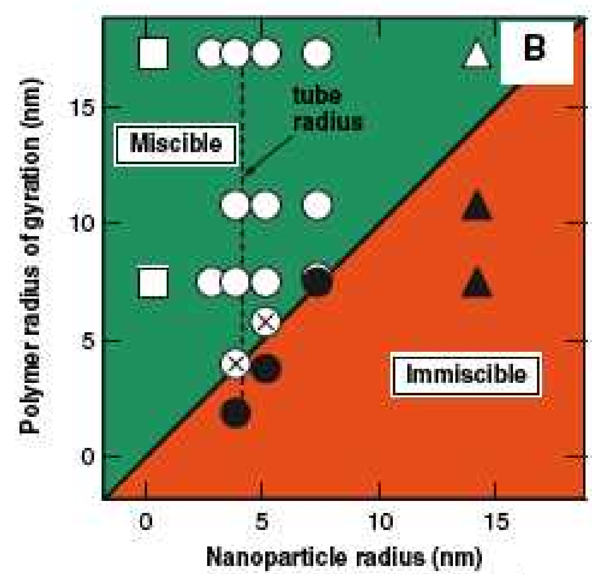
Craig Hawker (UCSB)

R_{NP} – size of nanoparticla
R_g – radius of gyration

An "ideal" system:

Hard-sphere like PS nanoparticles mixed with linear PS

- Nanoparticle radii R_{NP}: 2.5nm - 14nm
- Polymer R_g: 4nm - 14nm
- Monomer size: ≈ 1 nm



Nanoscale phenomena:

- Gap between particles ≈ R_{NP}
- Chains stretch when add particles.
- NPs disperse well for $R_{NP} < R_g$ (but not if too small).

Mackay et al, Science 311, 1740 (2006)

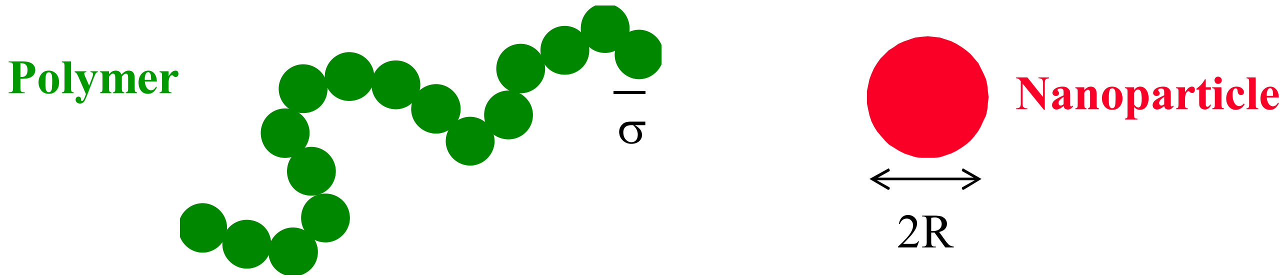
How do we model / simulate this?

Atomistically? No!!! System is too big (even bulk PS is hard).

Important length scales:
- Size of monomers, size of particles, & chains from 1 nm to 10's of nm

Coarse-Grained (CG) Model:

Repulsive LJ spheres



Length where PS is a random walk: 1.26 nm

$1\sigma = 1.26$ nm

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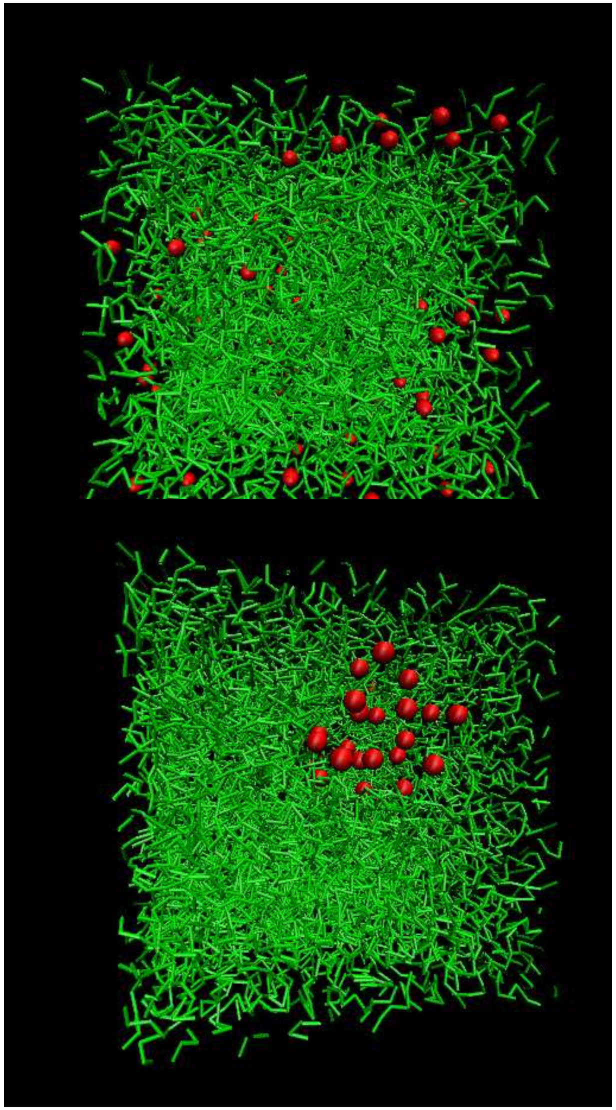
Result of MD Simulations



- 30 nanoparticles
- R_{NP} = 2.2 nm
- 145 polymer chains, 80 monomers/chain
- R_g = 4.7 nm
- NP volume fraction 10%
- Repulsive LJ interactions

Aggregated! But not in experiments...

Problem: CG model not quite right!

A more accurate model …

Need:

- Longer chains: 150 monomers/chain
- Bigger particles: R_{NP} = 4 x monomer size
- Attractions: Range of 2.2 x monomer size

“Small” Simulation

10 NPs, 10% volume fraction, 46060 monomers
Run on 32 processors

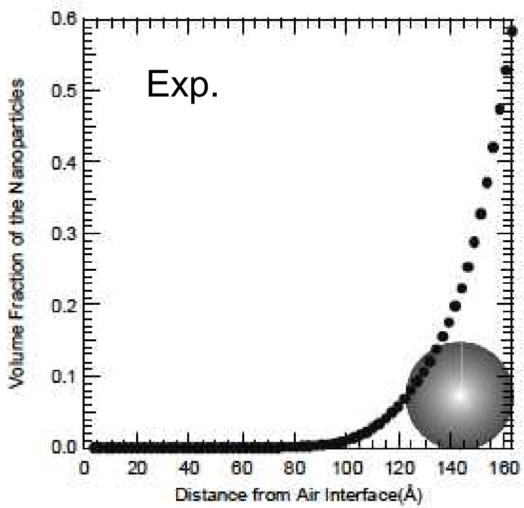
For particle to move its own size: 8960 CPU days

MD simulation not practical!

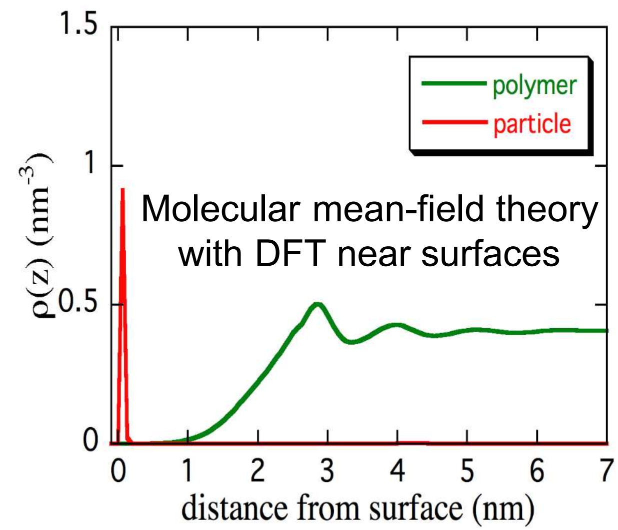
So, try theory instead....

Coupled experiment & theory study has explained the phenomenon, but more can be done

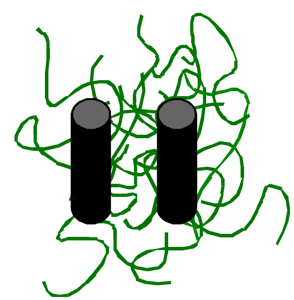
PS NPs/PS thin films
particles go to surface



80 monomers/chain
R_{NP} = 3.5 x monomer size

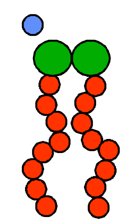


- How about different sizes and shapes of nanoparticle?
- How about different materials for nanoparticle?
- How about mix of different nanoparticles?
- How nanoparticles disperse or aggregate in different materials?



nanorods in
polymer melt

inclusions in
lipid bilayers



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Linking length and time scales is still a grand challenge

"Materials modeling is like an onion!"

--- an anonymous SHREK lover

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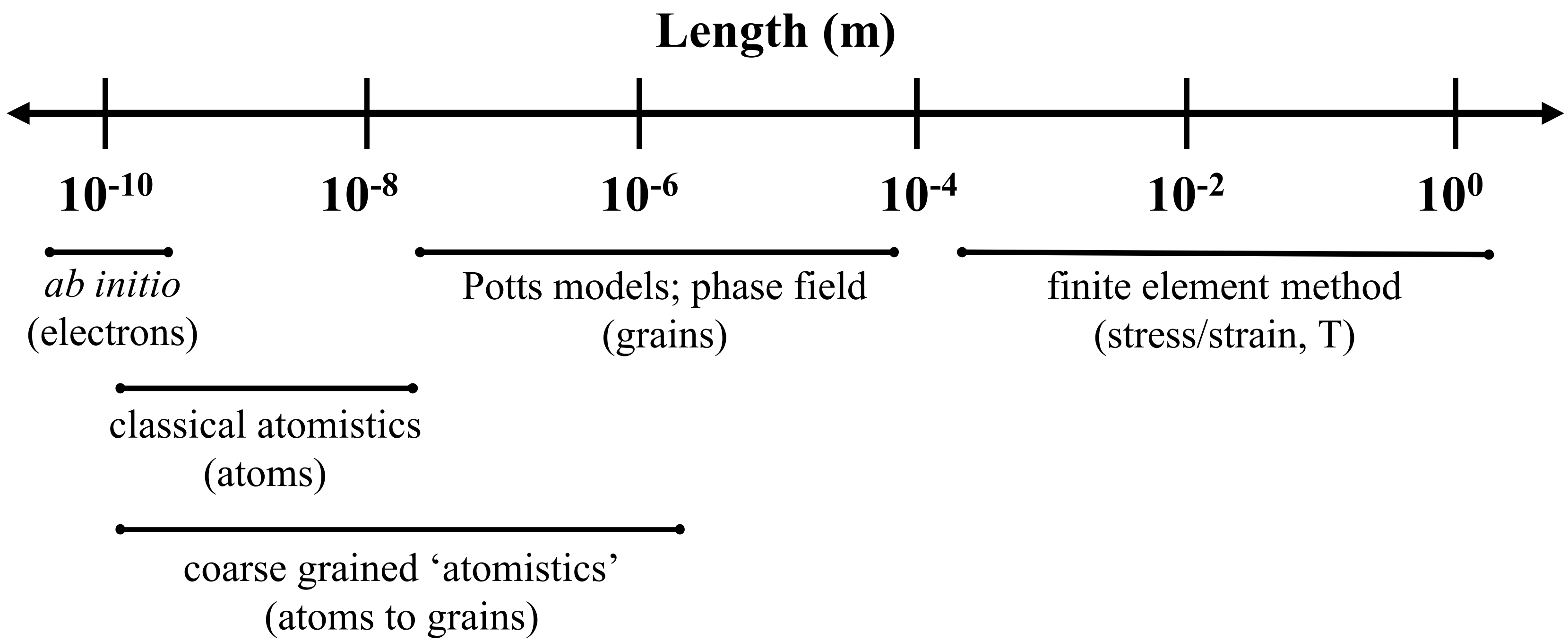
Materials Modeling Across Length Scales



10 orders of magnitude!!

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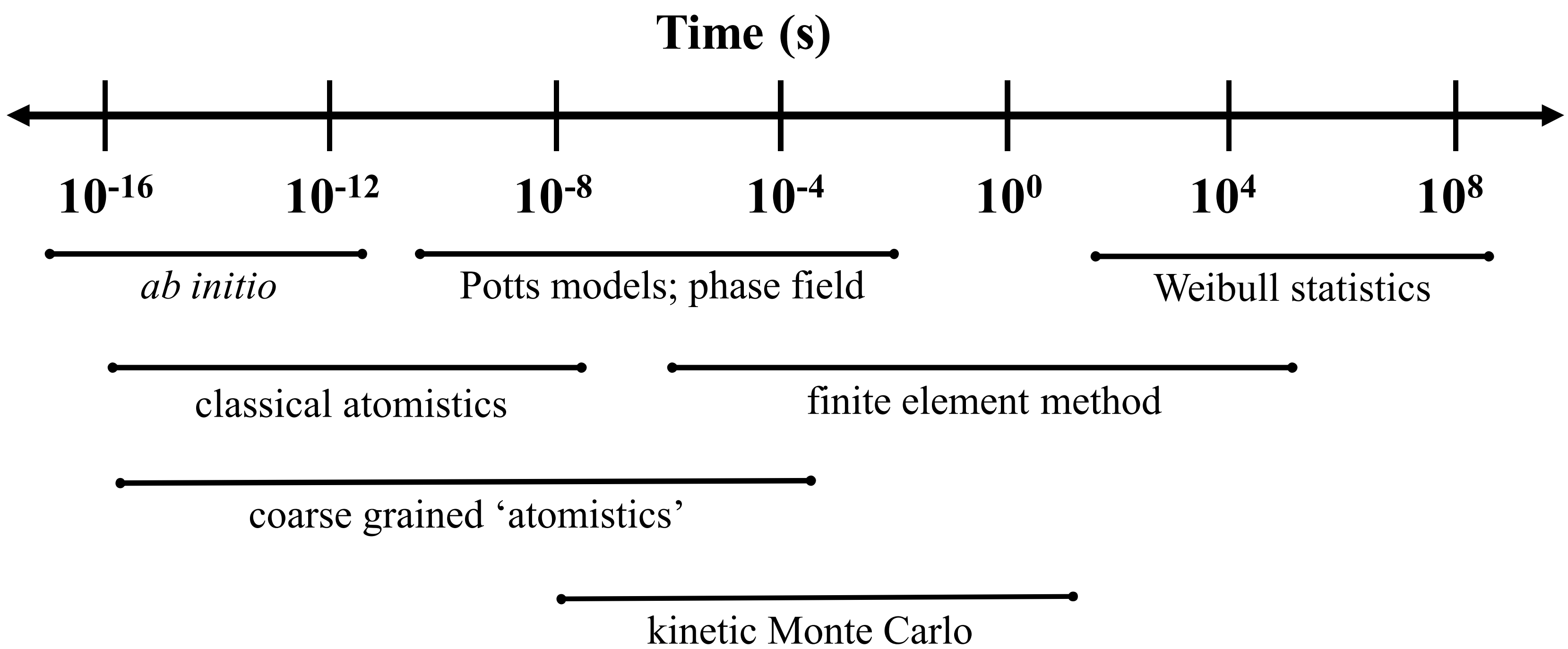
Materials Modeling Across Time Scales



24 orders of magnitude!!

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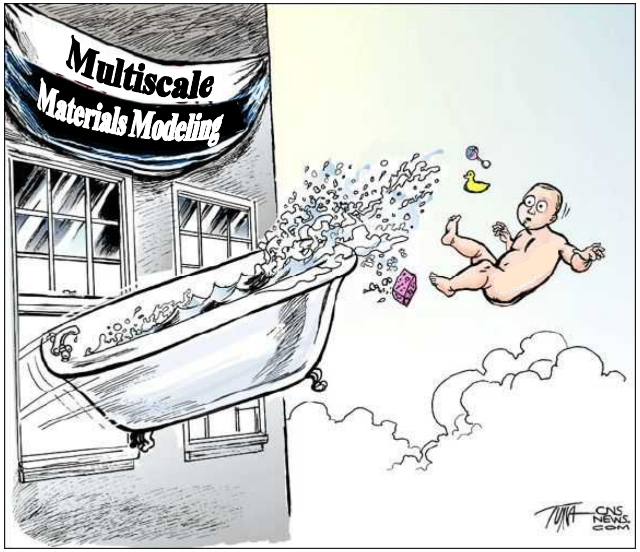
Linking length and time scales is still a grand challenge

"Materials modeling is like an onion!"

--- an anonymous SHREK lover

How to throw out the bathwater and still save the baby?



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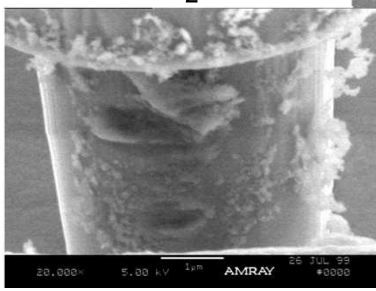
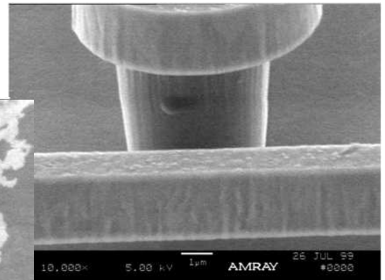
Challenges is not on modeling the geometry, but on simulating the real performance

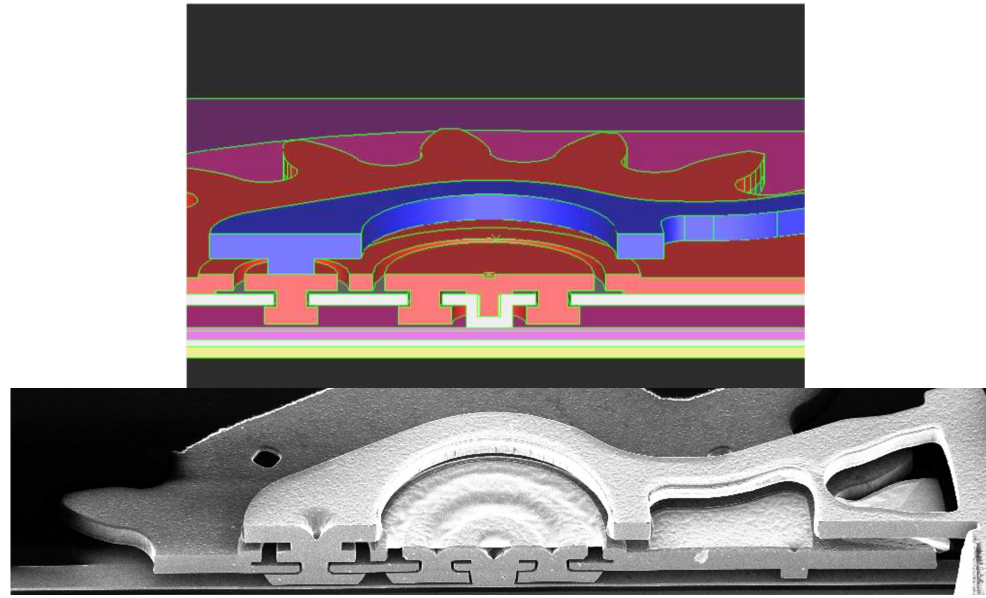
100,000 cycles
1.5 vol% H_2O

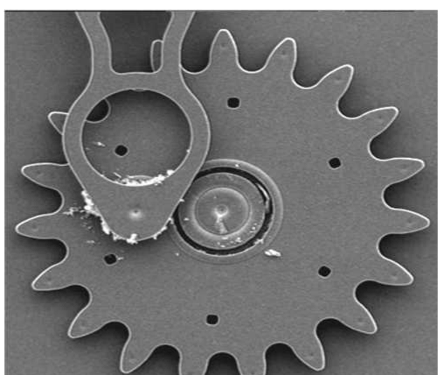




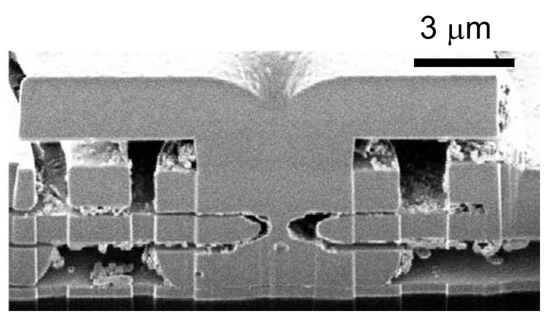
500,000 cycles
Dry air

Breakdown of SAM coatings with time and environment





1 million cycles



607,000 cycles

Abrasive wear limits life

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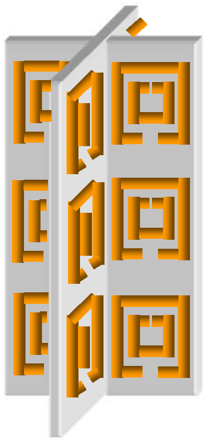
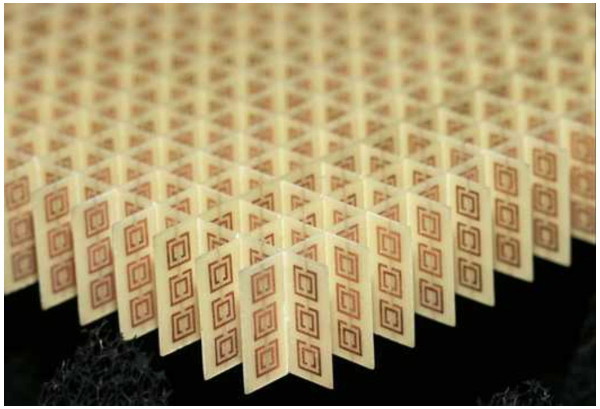
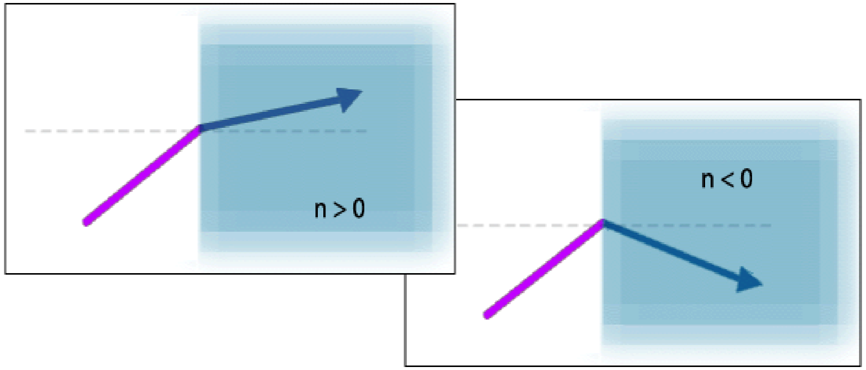
Metamaterials make light waves flow backward and behave in many counterintuitive ways

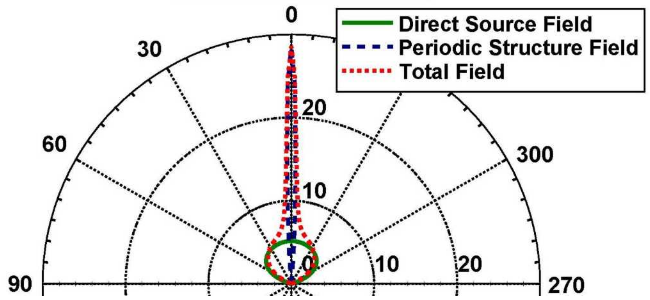
- Metamaterials are artificial electromagnetic materials that comprise an array of subwavelength unit cell structures periodically arranged in space
  - very small relative to their resonant wavelength
  - can be used to exhibit both a negative permittivity and negative permeability near its resonance frequency





Split-ring resonator based unit cell forming a metamaterial structure





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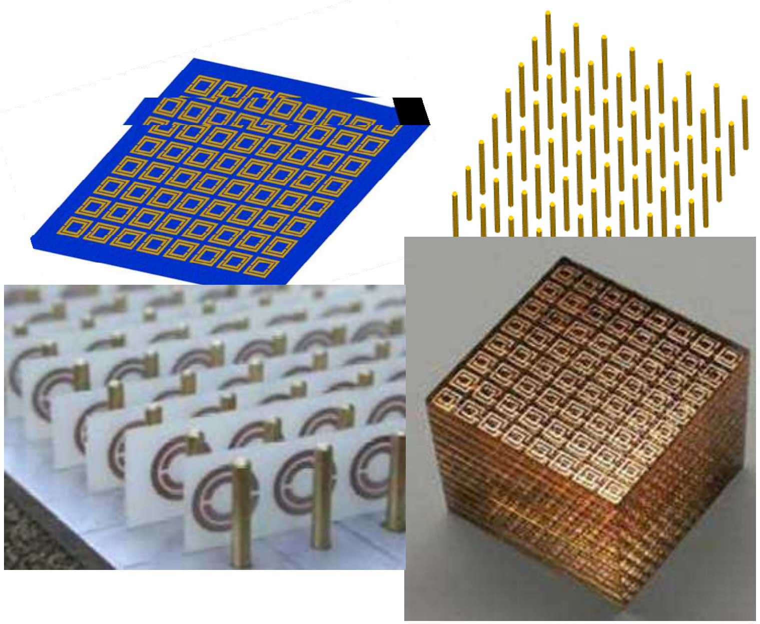
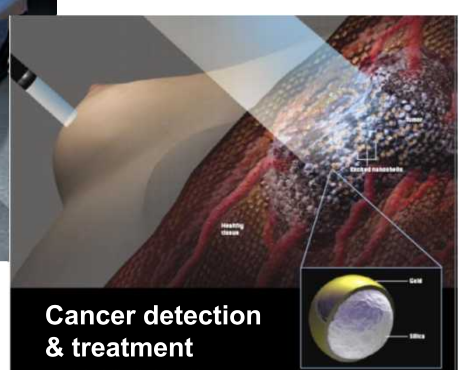
Study on metamaterials asks more work to correlate structure and properties



- Optical transmission enhancement
  - Design of miniaturized devices
  - Optical lithography
  - High-density optical storage
  - Biological and chemical sensors
  - Superlens
- Cloaking – making objects nearly “invisible” or “transparent”
- Reflect or transmit electromagnetic waves with frequency discrimination
- Improve radiation pattern performance

Cloaking



Cancer detection & treatment

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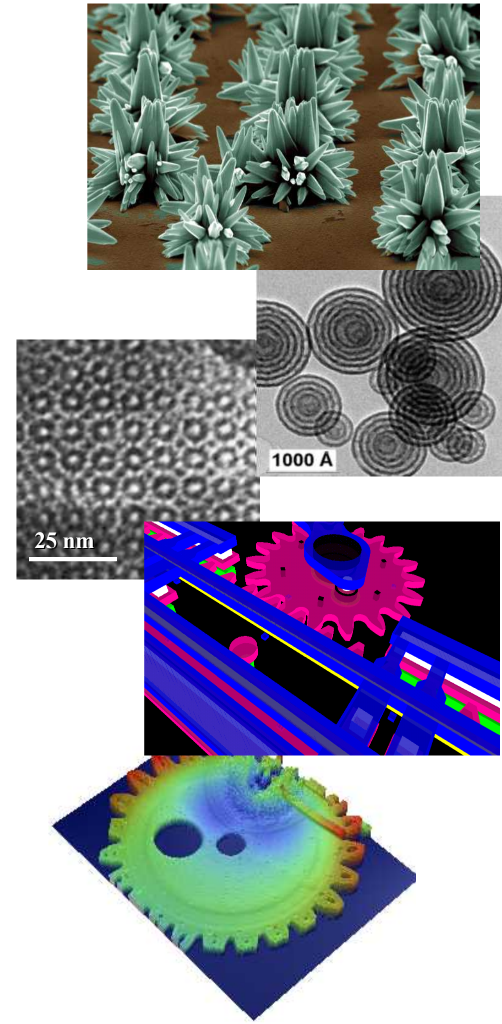
The journey is not impossible, but we still have a long way to go

- Nano-engineering in the future will involve simulations at different levels (quantum, atomistic, coarse-grained, modified-continuum) that probe different phenomena much like different experimental techniques measure different aspects of a system.
- We need to encourage out-of-box thinking to address issues in modeling integrated science (i.e. multi-scale in length & time; multi-physics; multi-functionality; …)
  - Don't get spoiled by supercomputers.
- There is no single solution or approach for bridging between all scales of length and time, or even for bridging between a pair of neighboring scale.
  - Solutions are material and application specific.
- Transition between scales is the essential challenge. It is not an engineering or algorithm issue but a science issue.
  - A model should be as simple as possible but not any simpler.



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