NATIONAL NANOTECHNOLOGY INITIATIVE

Scientific/Technology Challenges for the Nanotechnology Community

E. Clayton Teague
Director
National Nanotechnology Coordination Office
Nanoscale Science, Engineering, and Technology Subcommittee
Committee on Technology
National Science and Technology Council

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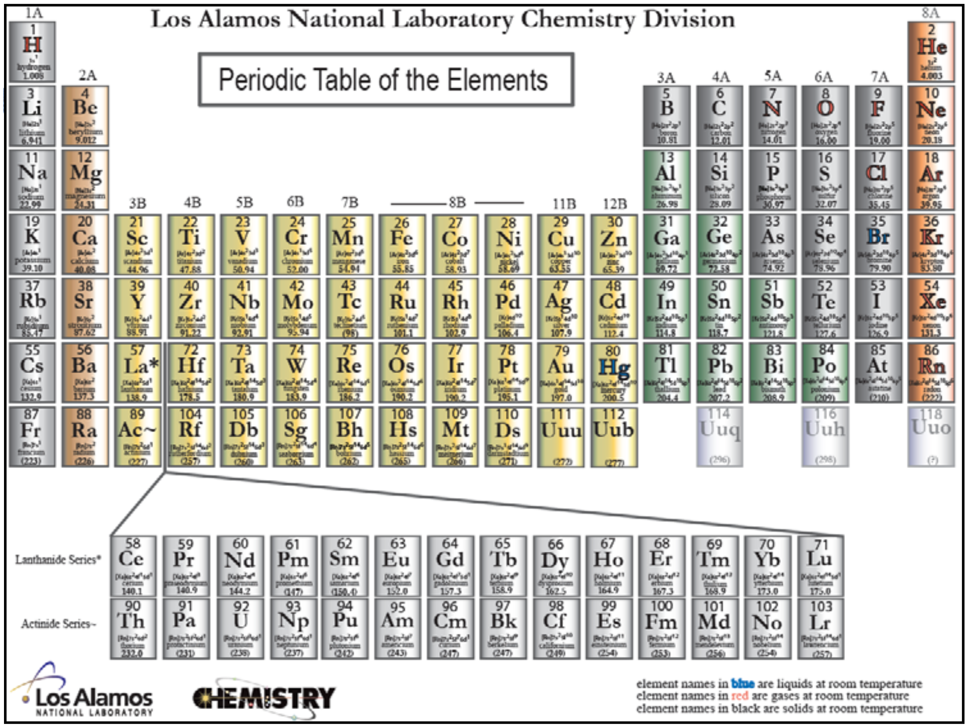
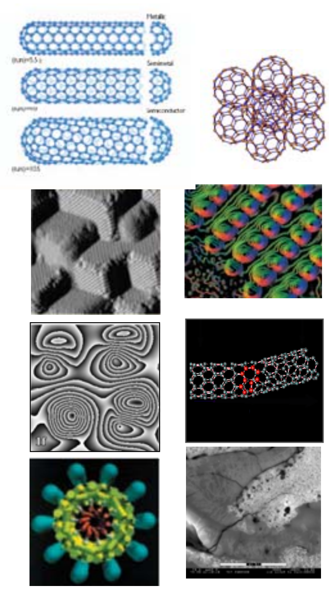
Challenges for Moving Nanotechnology Forward

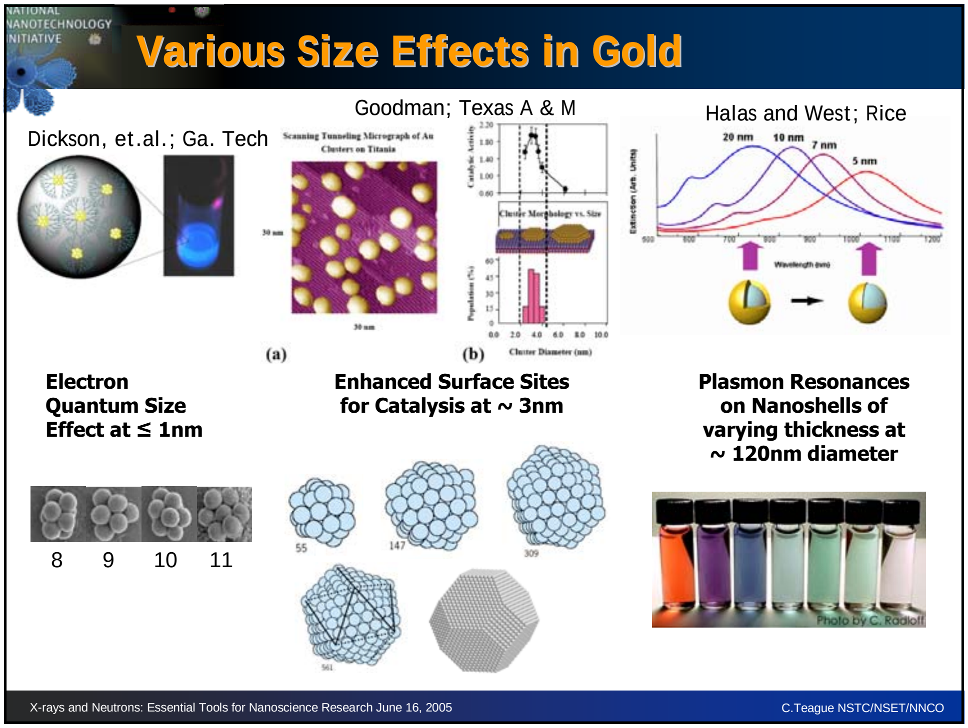
- Exploring the vast “nanomaterials” space
- Developing and implementing highly controlled, cost-effective processes for nanomanufacturing
- Advancing state-of-the-art for measurement and characterization of matter at the nanoscale



Functional Properties

- High strength, toughness
- Corrosion resistance
- Superhardness and wear resistance
- Catalytic
- Conducting
- Semiconducting
- Superconducting
- Magnetic
- Photovoltaic
- Fluorescent
- Piezoelectric
- Thermoelectric

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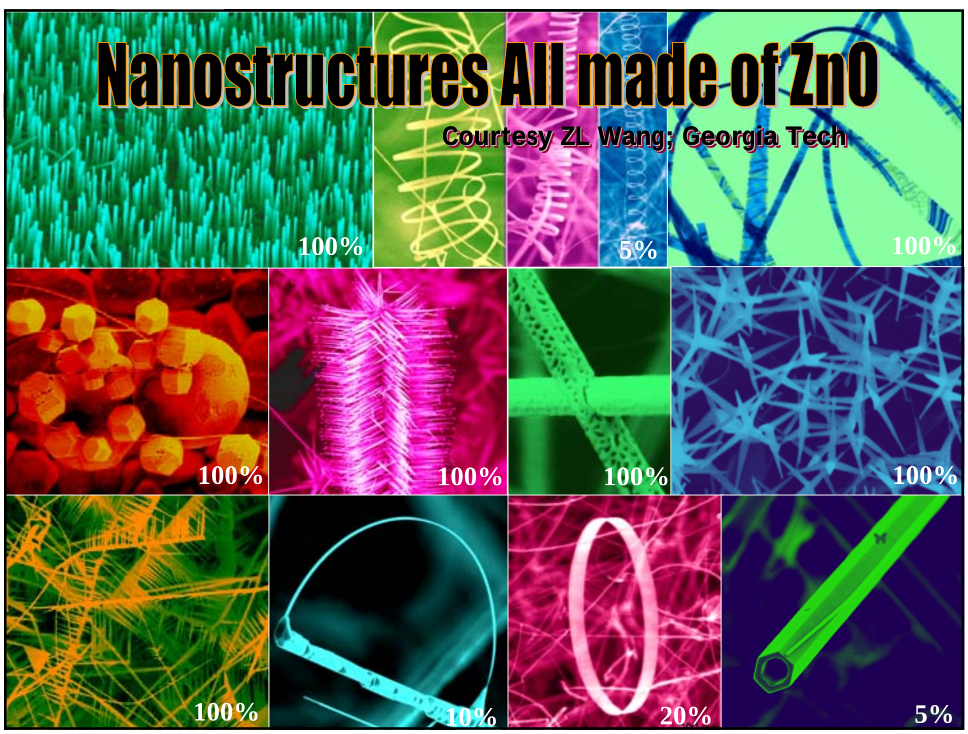
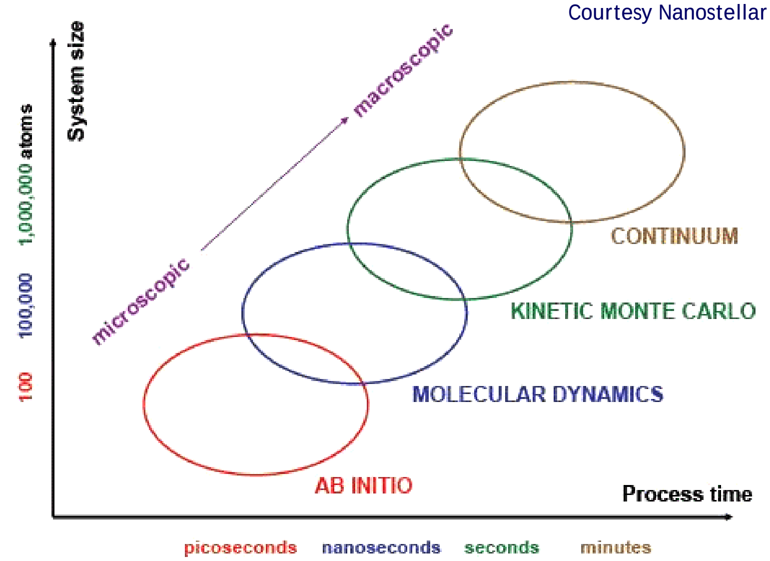
Various Size Effects in Gold
Dickson, et.al.; Ga. Tech
Goodman; Texas A & M
Halas and West; Rice
Electron Quantum Size Effect at ≤ 1nm
8 9 10 11
Enhanced Surface Sites for Catalysis at ~ 3nm
Plasmon Resonances on Nanoshells of varying thickness at ~ 120nm diameter
Photo by C. Radloff
X-rays and Neutrons: Essential Tools for Nanoscience Research June 16, 2005
C.Teague NSTC/NSET/NNCO


Nanostructures All made of ZnO
Courtesy ZL Wang; Georgia Tech
100%
5%
100%
100%
100%
100%
100%
100%
10%
20%
5%

Simulation Tools for Material Modeling

Courtesy Nanostellar



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High-throughput Screening w/*ab initio* Methods

- ***Ab initio*** **methods defined as those that accurately solve the fundamental quantum mechanical equations for states of the electrons of a system**
- **Enabled by major advances in algorithm development and in computing power**
- **Examples:**
  - Predicted band gaps in semiconductors and simulated annealing methods to find phase of largest band gap of $Al_{0.25}$ $Ga_{0.75}As$ (Franceschetti and Zunger –1999)
  - Calculated formation energies of 200 transition metal hydrides (Smithson –2002)
  - Formation energies and structural parameters for 80 binary alloys in 176 different structures – 14,000 alloy structures (Morgan, et.al. 2004)

X-rays and Neutrons: Essential Tools for Nanoscience Research June 16, 2005 C.Teague NSTC/NSET/NNCO

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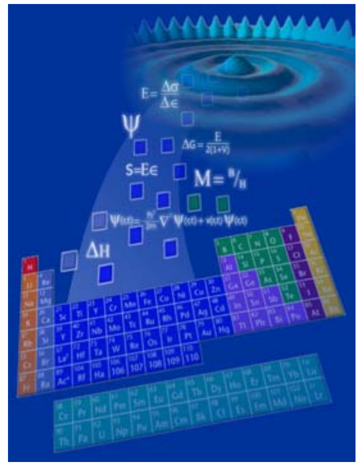
Nanomaterials By Design

The ability to employ scientific principles in deliberately creating structures with nano-scale features (e.g., size, architecture) that deliver unique functionality and utility for target applications



Based on Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

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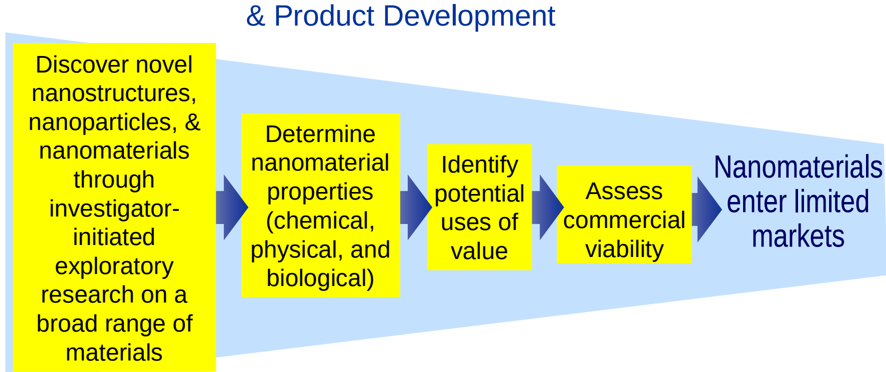
Nanomaterial Development: Today

TODAY: Discovery-based Science & Product Development



Based on Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

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Nanomaterial Development: Future

FUTURE: Application-based Problem Solving

Start with existing needs, problems, or challenges in end-uses → Design, produce, and scale up nano-based materials with the exact properties needed* → Large numbers of diverse products based on Nanomaterials By Design rapidly enter and succeed in multiple markets

* Based on established understanding and methods

Based on Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

Developing and Implementing Nanomanufacturing Processes

Nanomanufacturing includes:

- All means that have the capability to

  reproducibly transform matter — from a bulk form or from individual atoms, molecules, and supramolecular structures — into nanoscale or nanostructured materials, devices, or systems

  with desired properties and performance characteristics

  typically in large quantities
- Design, simulation, and implementation that enable cost-effective synthesis and production of nanomaterials - nanostructures
- Assembly methods and technologies

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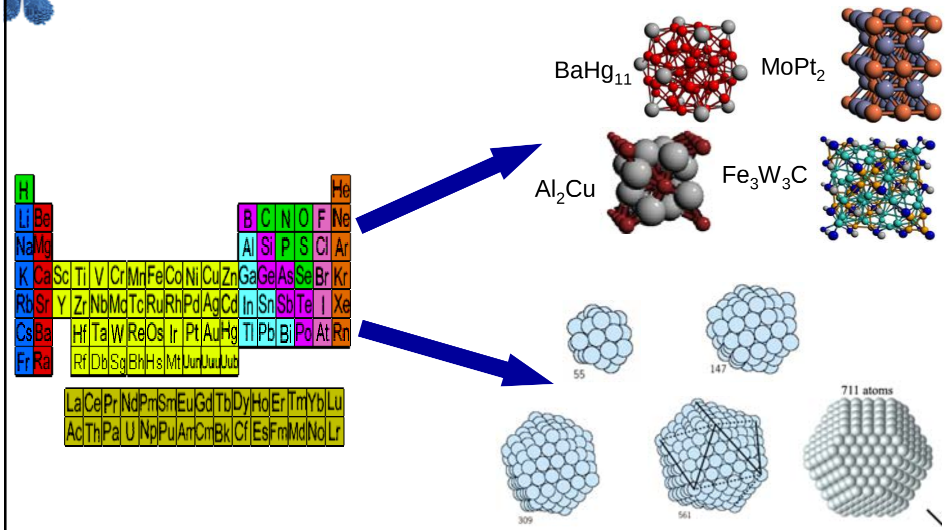
Nanomanufacturing: Building Blocks

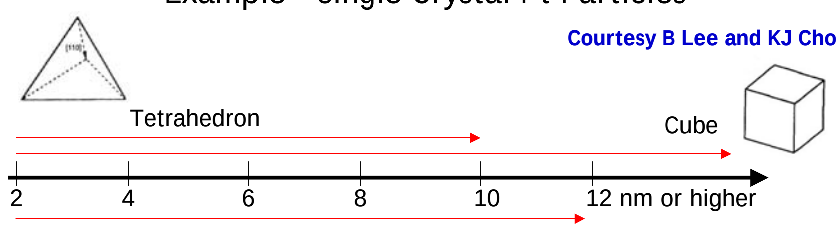


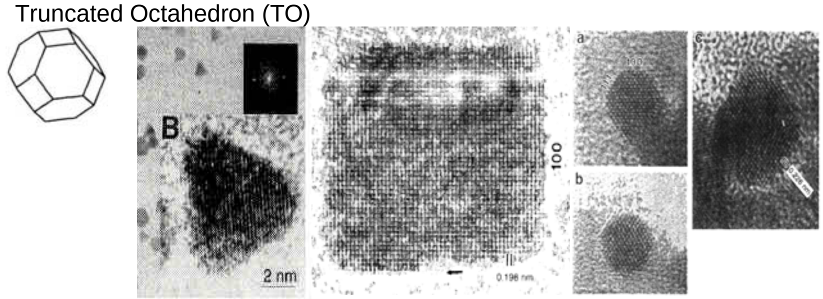
NRL Center for Computational Materials Science

Forms of Nanostructures - Size Dependent

Example - Single Crystal Pt Particles

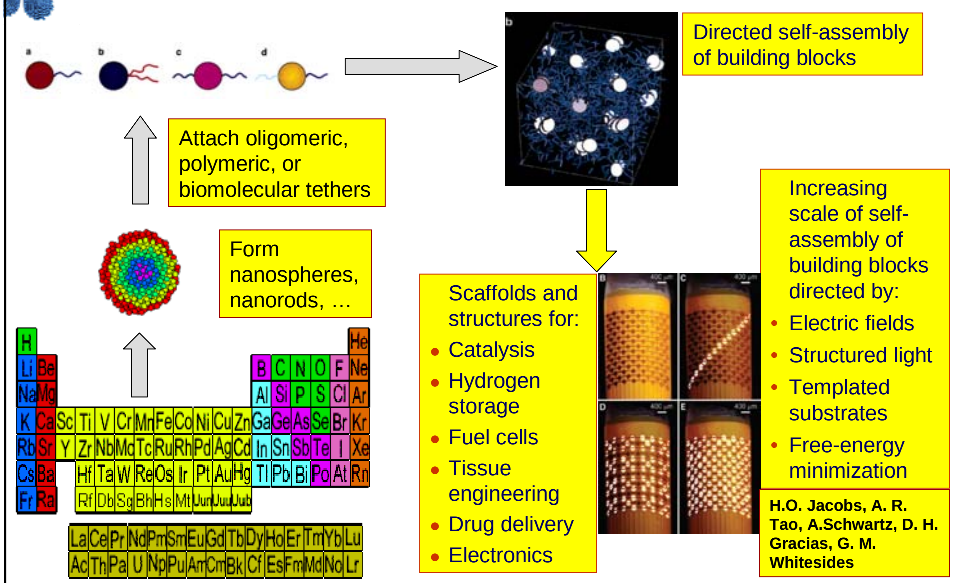
Courtesy B Lee and KJ Cho





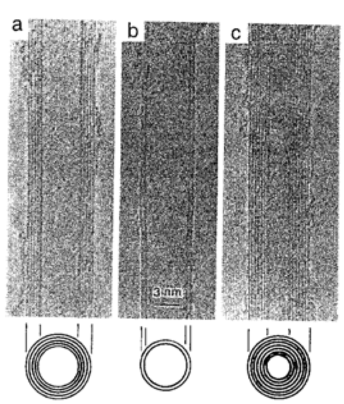
Z.L. Wang et al., Science 272, 5270 (1996); Surf. Sci. 380, 302 (1997); J. Phys. Chem B 102, 3316 (1998); J. Phys. Chem B 102, 6145 (1998)

Possible Nanomanufacturing Steps Based on Directed Self-Assembly



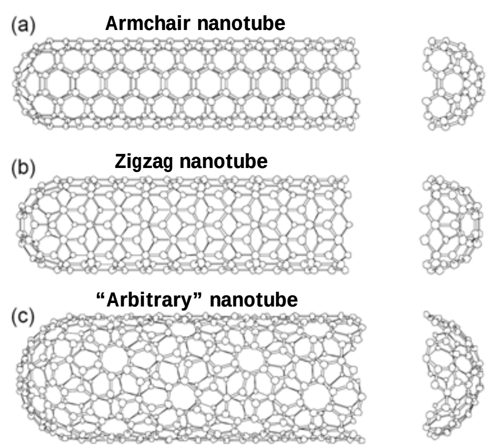
H.O. Jacobs, A. R. Tao, A.Schwartz, D. H. Gracias, G. M. Whitesides

A Sampling of Carbon Nanotube Forms



S. Iijima in *Nature* 1991

Observation by TEM of multi-wall coaxial nanotubes with various inner and outer diameters, di and do, and numbers of cylindrical shells N: (a) N = 5. do=6.7 nm, (b) N = 2, do=5.5 nm, and (c) N = 7, di =2.3 nm, do=6.5 nm



From Dresselhaus, Dresselhaus, and Sato *Carbon* 1995

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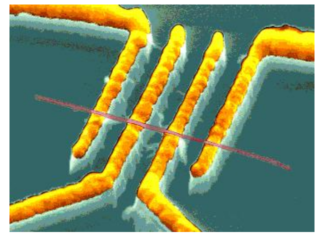
Electronic Applications of Nanotubes

"It takes about 0.1 g of CNTs per TV"



"For nanotubes to be useful in nanoelectronics, one would need 10^8 to 10^9 nearly identical nanotube segments"

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Potential Commodity Markets for CNTs

Worldwide annual production of automobiles is about 50 million

5 kg of CNT per automobile
=> 250 million kg market

The challenge:
MWCNT in ton qtys. ⇒ \$250 - \$1250/kg
To be considered for light weighting automobiles, need \$5/kg

1 billion kg of copper produced annually in U.S. for home wiring

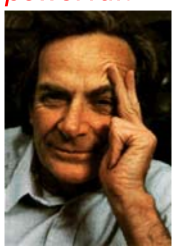
Cost of copper is ~\$3.30 per kg

Need to reduce cost of commodity levels of production by factor of ~ 50 – 250

Feynman's Measurement Challenge

"It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are. The only trouble is that the electron microscope is one hundred times too poor … I put this out as a challenge: Is there no way to make ~~the electron microscope~~ more powerful?"

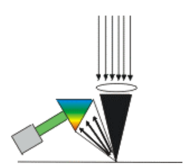
X-ray and Neutron Scattering and Spectroscopies



– *Richard P. Feynman, 1959, "There's Plenty of Room at the Bottom"*

Imaging and Chemical Information

- Atomic scale imaging
  - Approaches:
    - Field Ion Microscope (Atom Probe)
    - Scanned Probes (STM, AFM)
    - High Resolution Transmission Electron Microscopy
  - Takes advantage of broad spectrum "interaction"
  - Lacks specificity or requires specific sample
- Chemical Information
  - Requires spectroscopy
  - Inherently poorer signal to noise
    - Selective interaction with very low cross section
- Chemical Imaging is MOST challenging

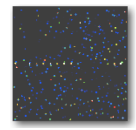


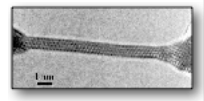
Extraordinary Scientific Opportunities

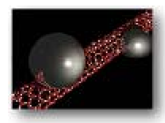
by direct observation of individual nanostructures

Key challenges identified in several TEAM workshops

- **three-dimensional atomic-scale structure, shape, and defect distribution**
- **spectroscopic identification and location of individual dopant atoms**
- **direct imaging of the atomic-scale structure of glasses**
- **electronic structure of individual point defects**
- **non-spherical charge density and valence electron distribution**
- **in-situ observation of properties and response to external variables**
  - temperature, stress, chemical activity, and applied electric and magnetic fields…







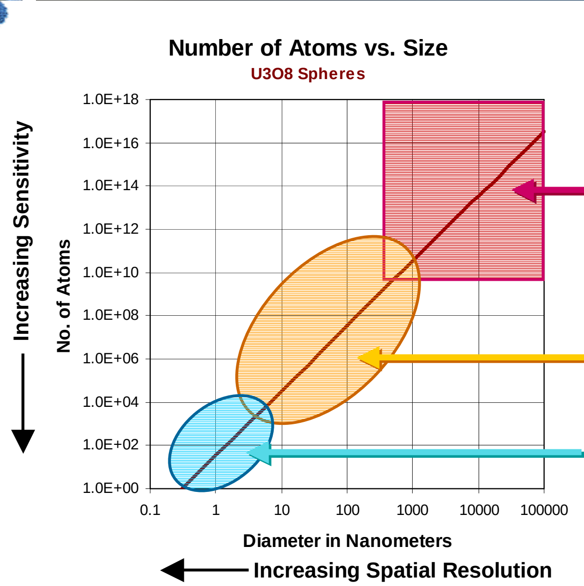
… all with unprecedented spatial, spectral & temporal resolution

Courtesy U. Dahmen, DOE

Where to go in the future of characterization?

Still need dramatically improved sensitivity

Courtesy E. Steel, NIST



Comfort zone for most analytical laboratories

Current research

New technology needed

Nanoscale Material Characterization

Improve Sensitivity ⟷ Increase Spatial Resolution

These two needs are often incompatible

- **Improve probe**
  - Increase Intensity
- **Improve detectors**
  - Change detector efficiency
- **Increase interaction with specimen**

- **Improve Probe**
  - Reduce size
- **Reduce interaction volume**
  - Change probe physics

New technology is needed to break through this incompatibility

Chemical Characterization

- Higher Speed –
  - At nm sized pixels a 1 X 1 mm area would take 1000 pixels x 1000 pixels x ~1 sec = 12 days
- Higher Sensitivity
  - From 100's of atoms to single atom
  - Zeptogram analysis
- Move from 1D and 2D to 3D
  - Spectroscopic tomography
  - Know each atom and relationship to all others

Summary

- **Three major challenges for moving nanotechnology forward**
  - Exploring the vast "nanomaterials" space
  - Developing and implementing highly controlled, cost-effective processes for nanomanufacturing
  - Advancing state-of-the-art for measurement and characterization of matter at the nanoscale