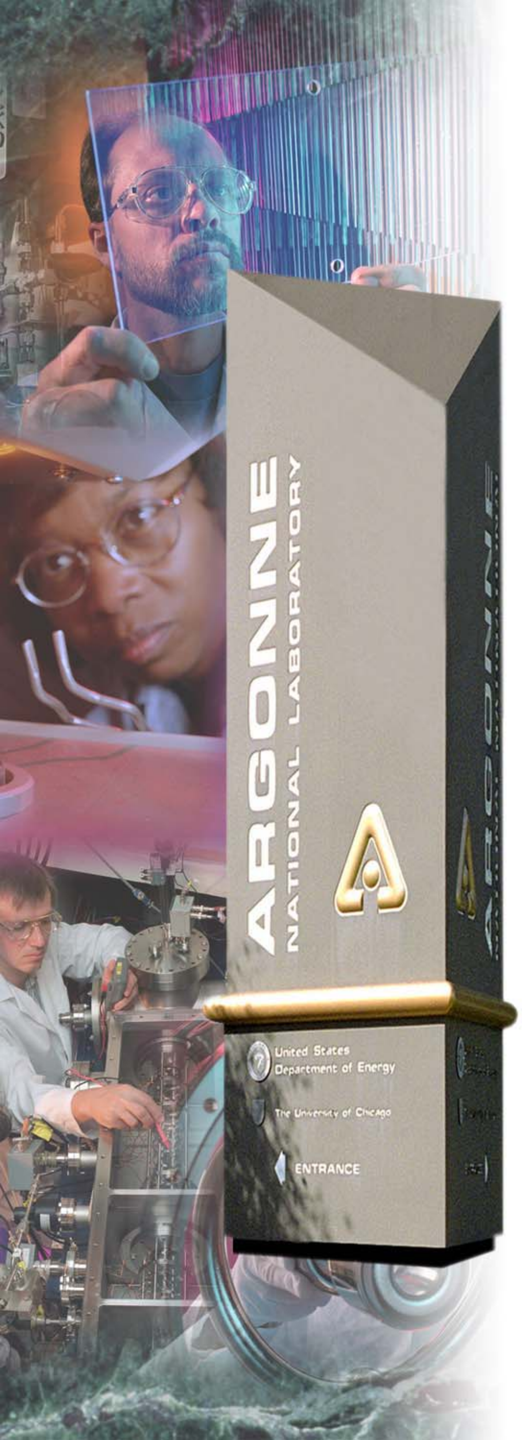


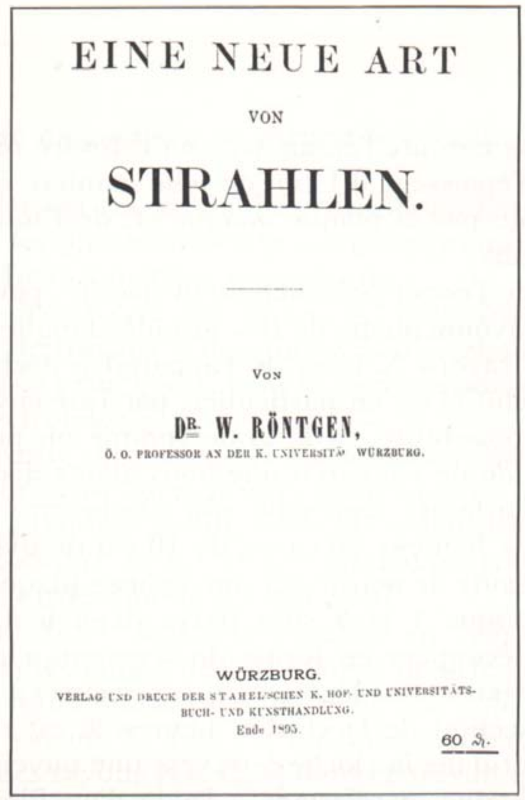
Opportunities for Nanoscience with Hard X-rays

Eric D. Isaacs
Center for Nanoscale Materials
http://nano.anl.gov
and
The James Franck Institute,
The University of Chicago

X-RAYS AND NEUTRONS
ESSENTIAL TOOLS FOR NANOSCIENCE RESEARCH
A Workshop of the National Nanotechnology Initiative

**Washington, D.C.,
June 16-18, 2005**

Wilhelm Conrad Röntgen 1845-1923



EINE NEUE ART

VON

STRAHLEN.

Von

DR. W. RÖNTGEN,

Ö. O. PROFESSOR AN DER K. UNIVERSITÄT WÜRZBURG.

WÜRZBURG.

VERLAG UND DRUCK DER STAHEL'SCHEN K. HOF- UND UNIVERSITÄTS-BUCH- UND KUNSTHANDLUNG.

Ende 1895.

60 ₰.

1895: Discovery of X-Rays

2005: X-ray phase contrast imaging

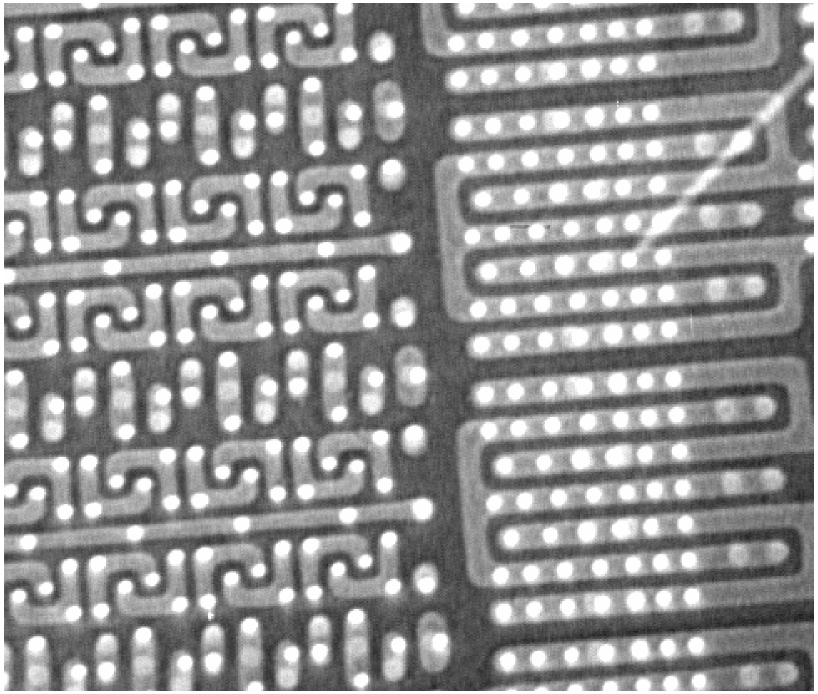
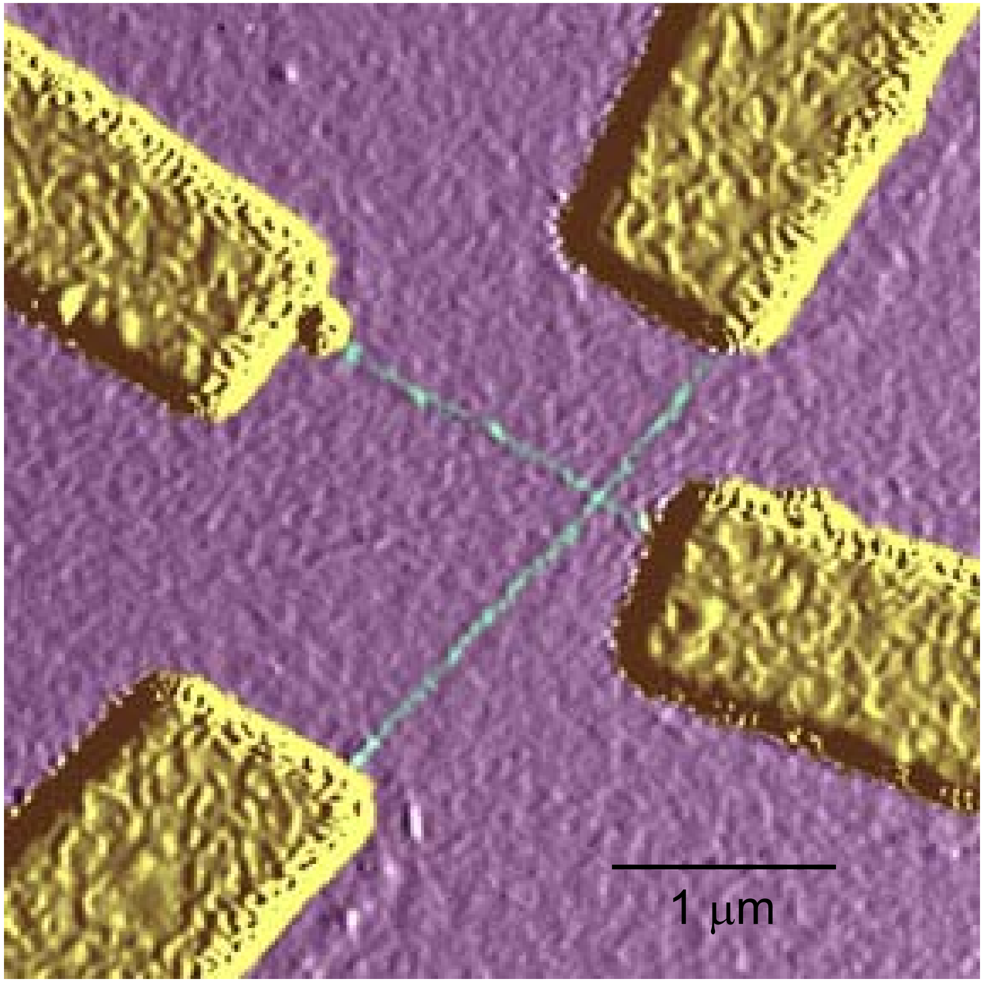


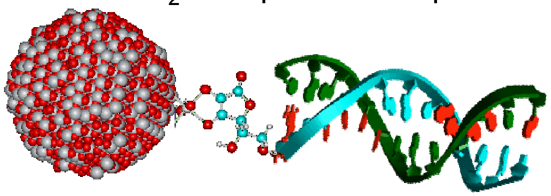
Image of buried structures in circuits with 60 nm resolution.
Courtesy W. Yun, Xradia.



Zettl, UCB

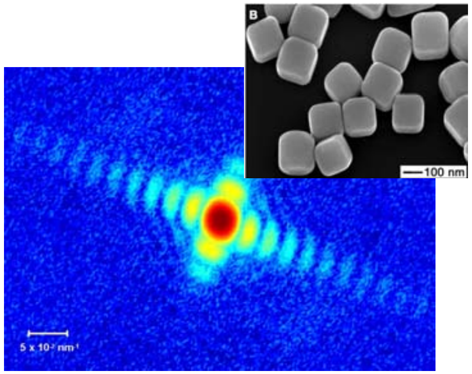
Opportunities for Nanoscience with X-rays

DNA-TiO_2 nanoparticle composite

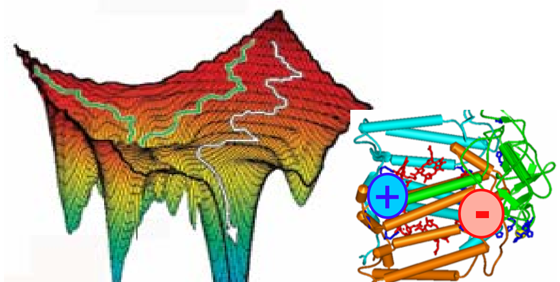


Spectroscopy of bonding/ surface states

Single particle diffraction



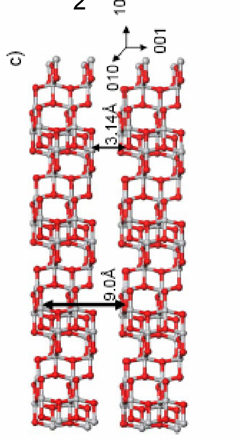
Coherent scattering e.g, dynamics w/XPCS



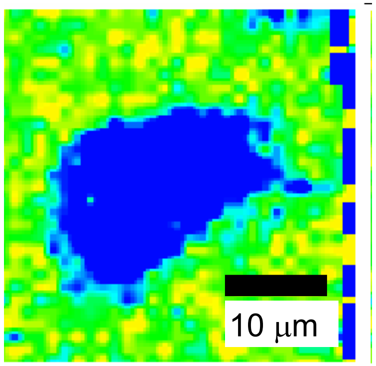
Photosynthetic proteins

Time-resolved, ultra-fast studies of excited states.

TiO_2 tubes

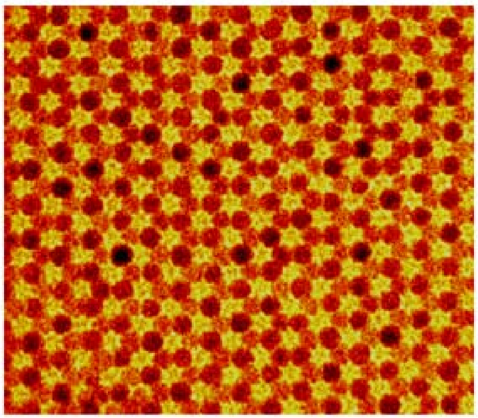


diffraction - structure



X-ray Nanoscope: imaging

Self-assembled Au nanoparticle array



In-situ techniques: growth; self-assembly

Five DOE Nanoscale Science Research Centers (NSRC) and Facilities integration

Opportunities for Nanoscience with X-rays

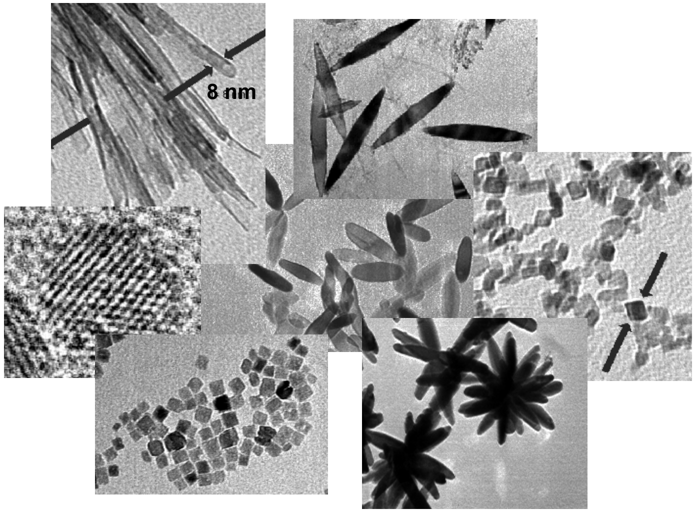
- Building blocks.
- Directed self-assembly.
- New properties.

Building Blocks

- Nanoparticle libraries.
- Bio-inorganic nanoparticle composites.
- Dynamic structure-function relationship.

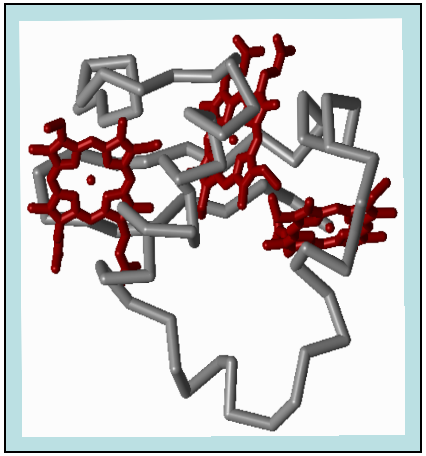
Building Blocks: Nanoparticle Libraries

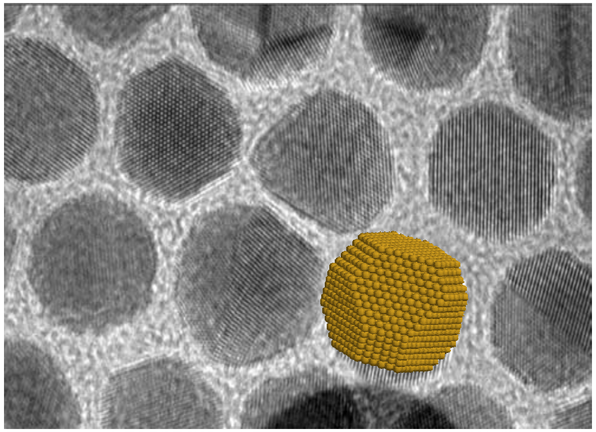
Rajh, et al



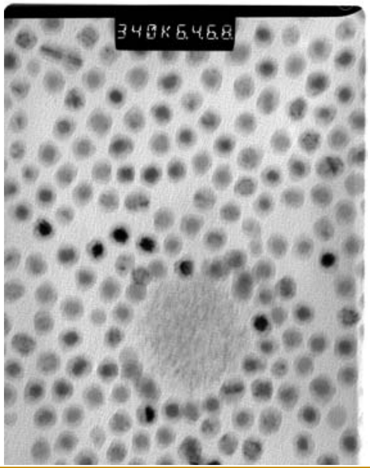
TiO_2 semiconductor

bio-molecules, eg.
cytrochrome c7

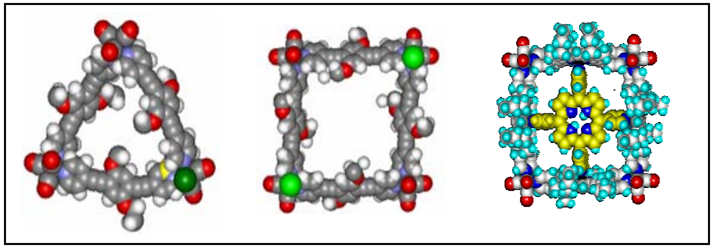




Au nanocrystals
X.-M. Lin, A. Samia



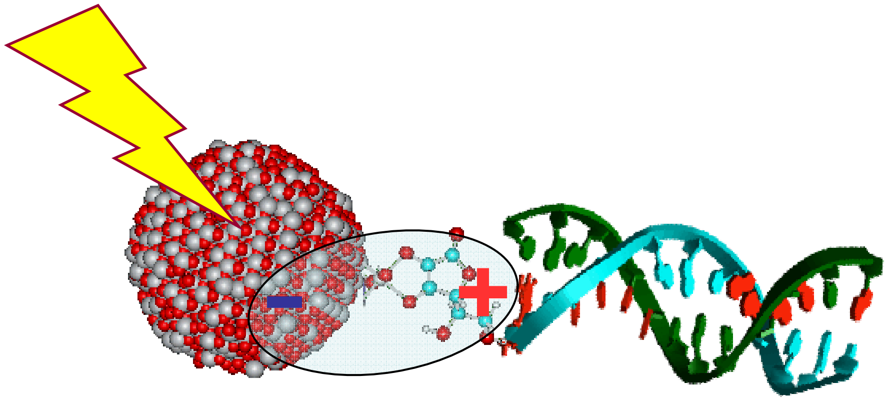
Co-CoPt
core-shell magnetic
nanoparticles
X.-M. Lin, S. Bader, et al



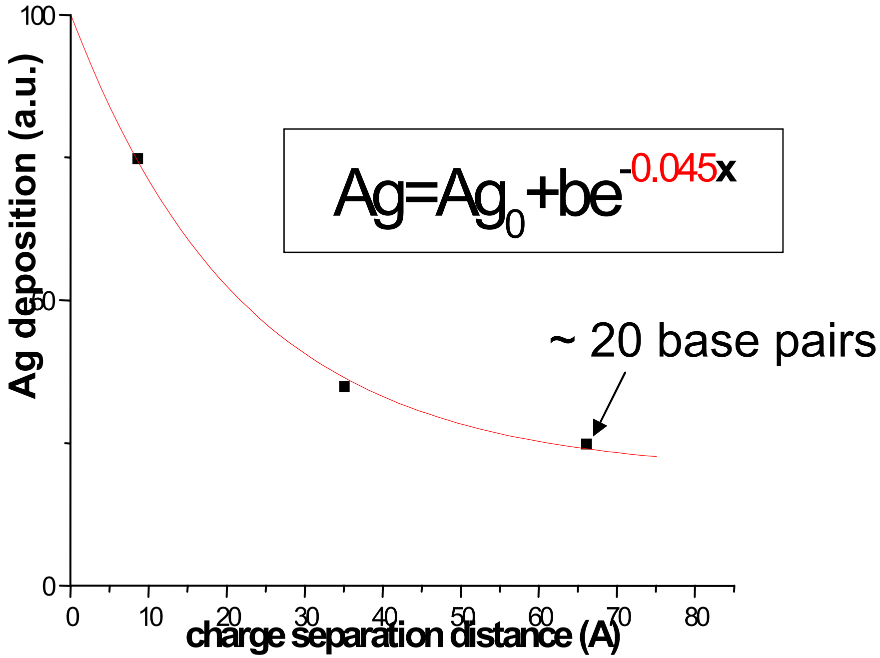
synthetic molecular assemblies
J. Hupp, et al.

Bio-inorganic Composites for Energy Conversion

T. Rajh, et al, ANL



DNA-TiO_2- nanoparticle assembly

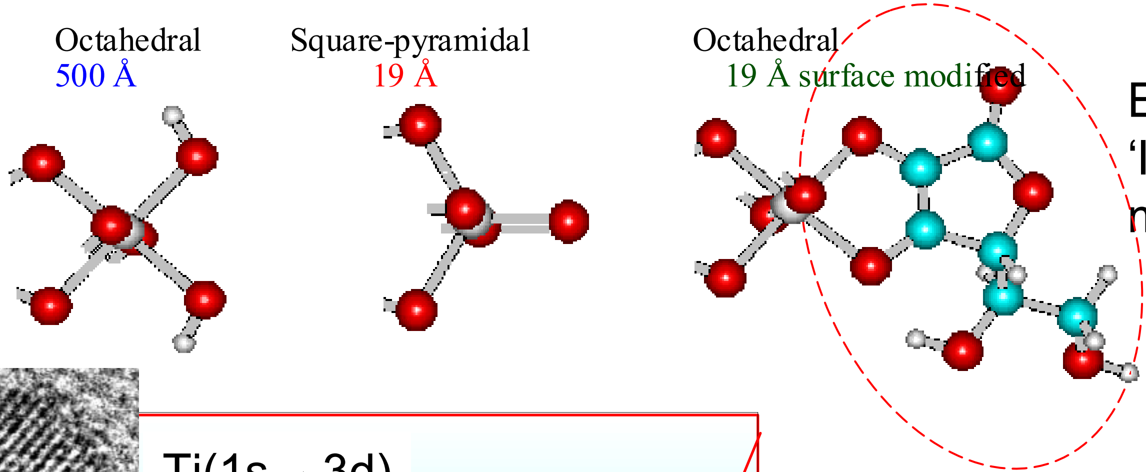


charge separation over large distances (~ 60 Å)

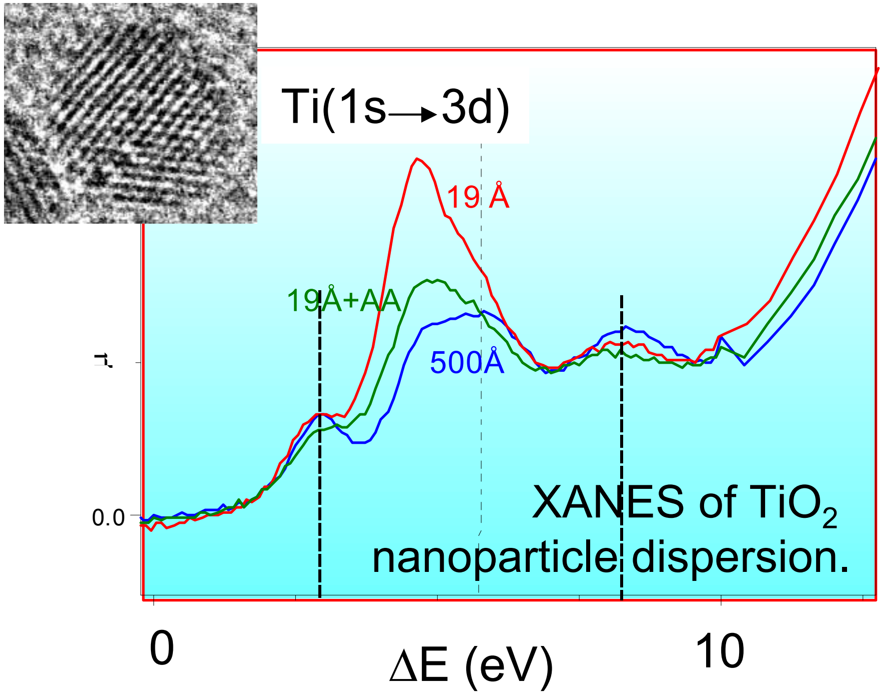
- photo-conversion
- in-vivo gene surgery
- …

Adsorption induced healing of metal-oxide nanoparticle surface

Lin Chen
Tijana Rajh
David Tiede



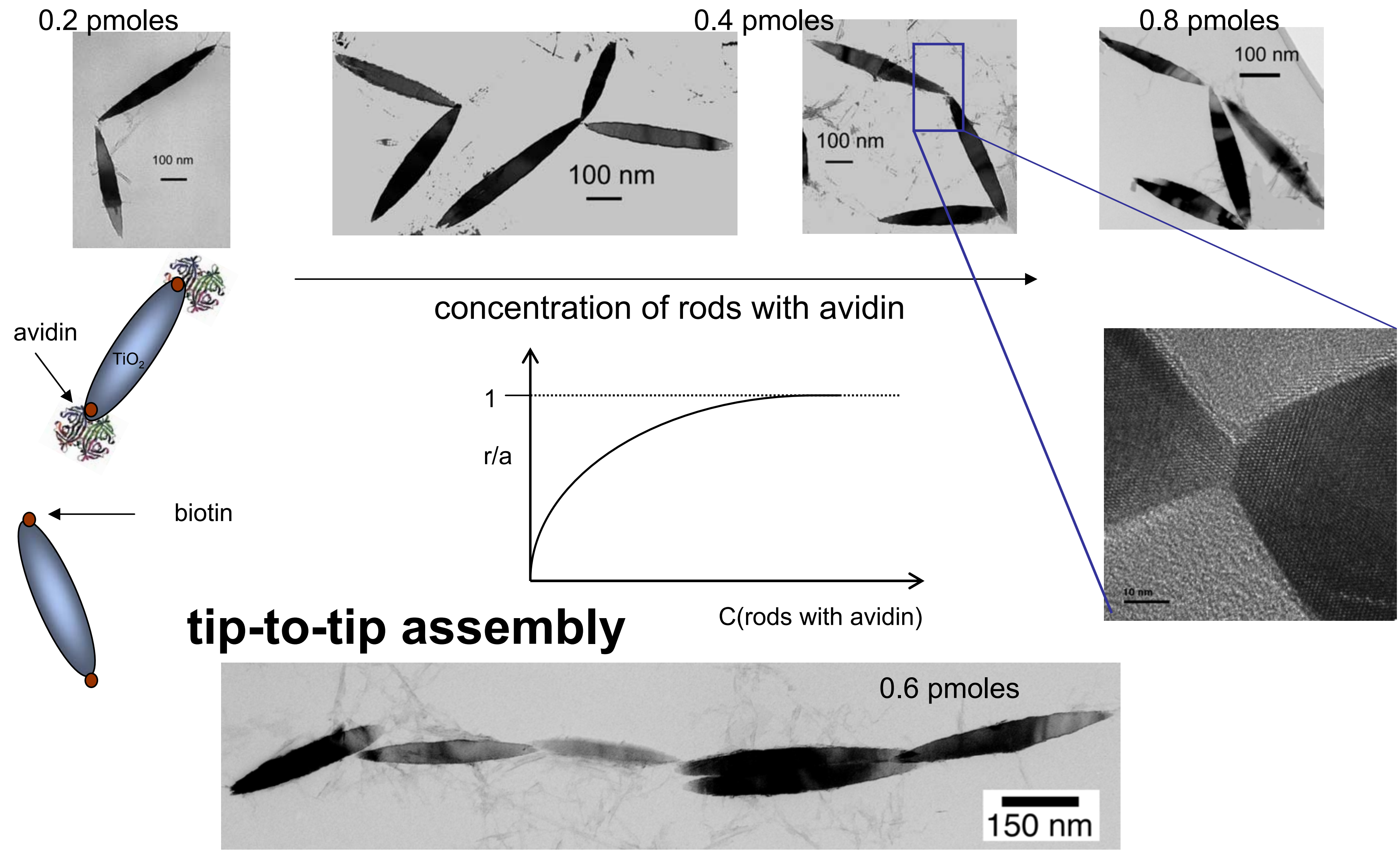
Enediol 'linker' molecule



Interior vs. surface sites of metal-oxide crystalline nanoparticle

Future: Measure the surface states in single nanoparticles.

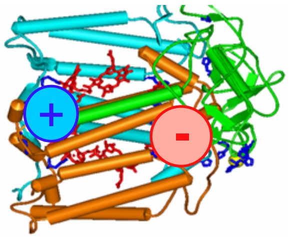
Shape Matters:
Bio-scaffolding of TiO_2 anisotropic nanoparticles



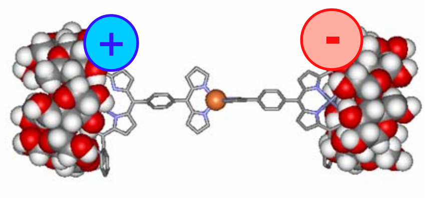
Structural Landscapes Underlying Function: towards ps time-resolved x-ray scattering

D. Tiede

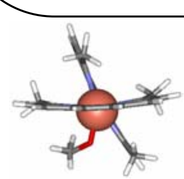
Observation of Ground and Excited-State Structural Landscapes Underlying Function



photosynthesis



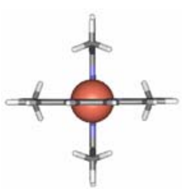
Molecular electronics



Model (*ps* TR-XAFS)

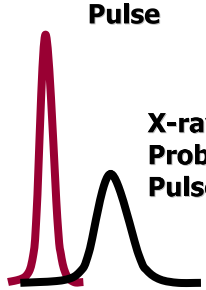
Cu(II) ligand^{1-}

hv



Cu(I) ligand

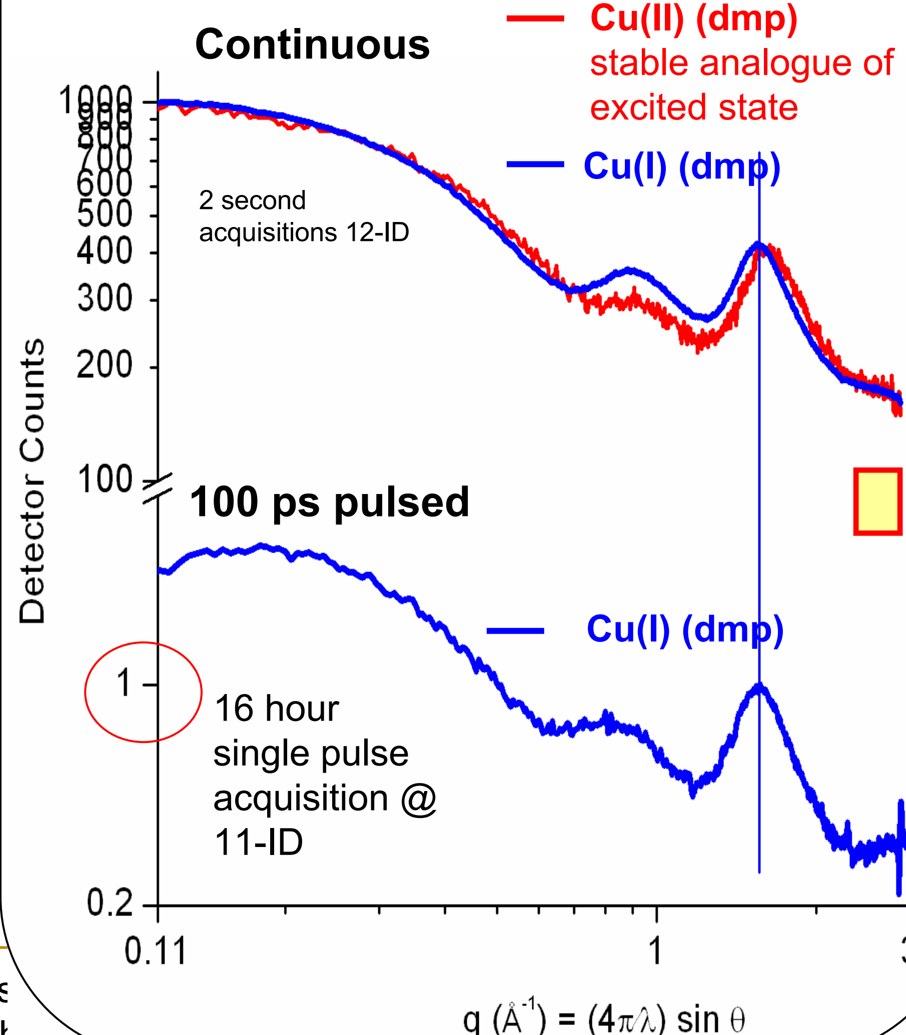
L. Chen



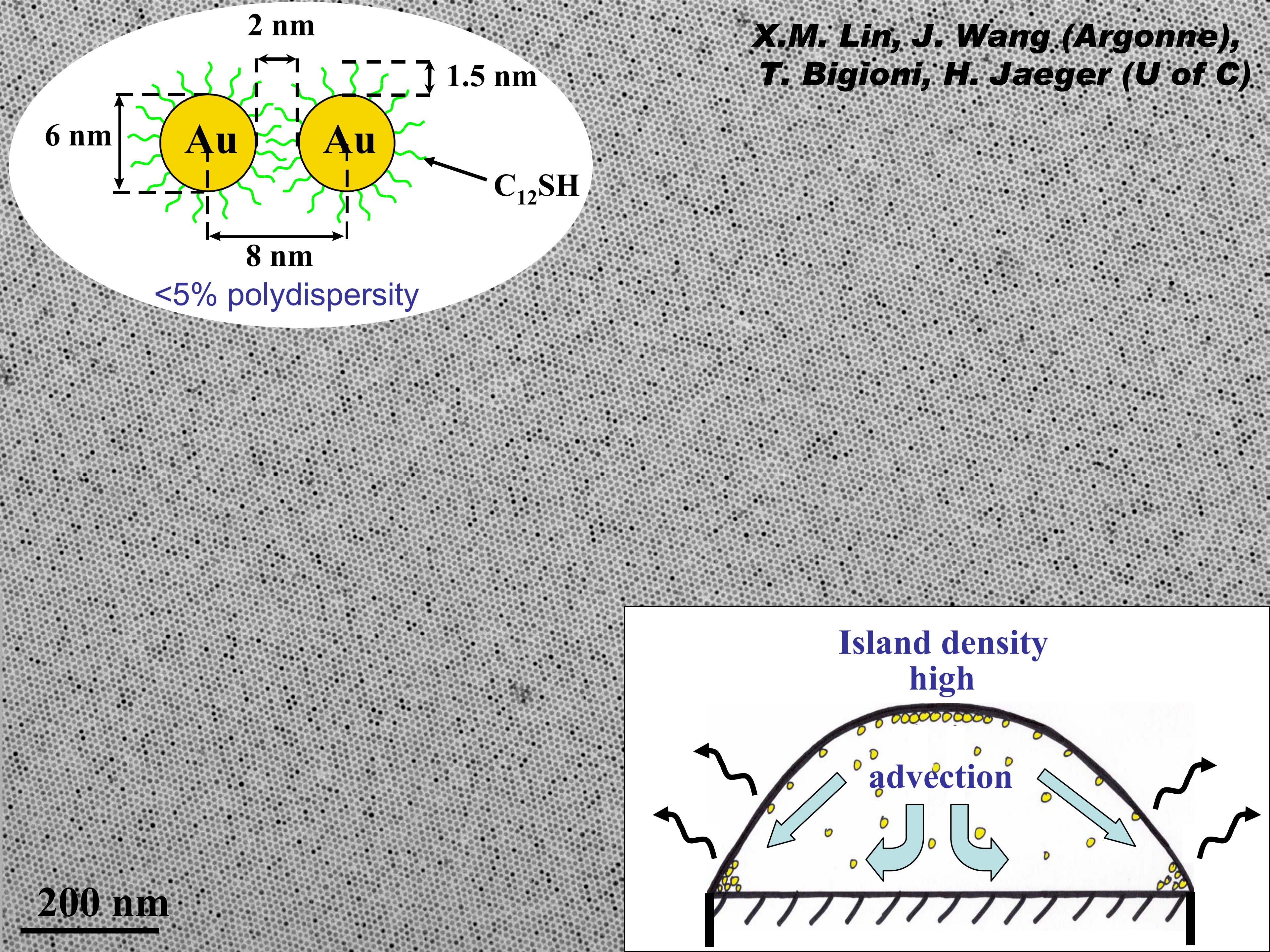
copper dimethyl-phenanthroline (dmp)

1st single bunch SAXS image !!!

April 2005 (2 Å spatial resolution)



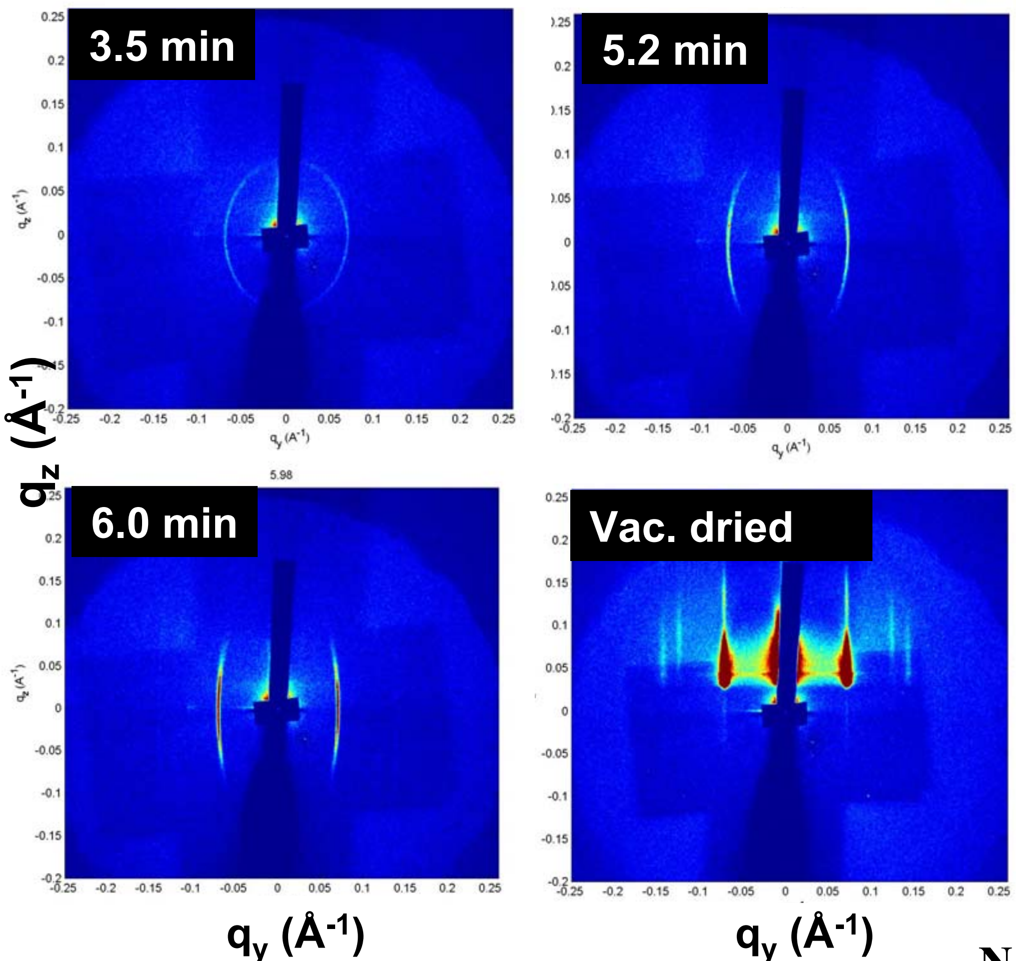
Directed Self-assembly

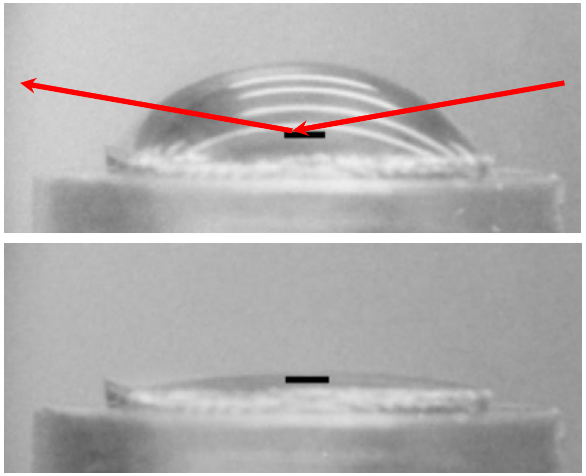

X.M. Lin, J. Wang (Argonne),
T. Bigioni, H. Jaeger (U of C)
2 nm
1.5 nm
6 nm
Au
Au
$C_{12}SH$
8 nm
<5% polydispersity
Island density
high
advection
200 nm

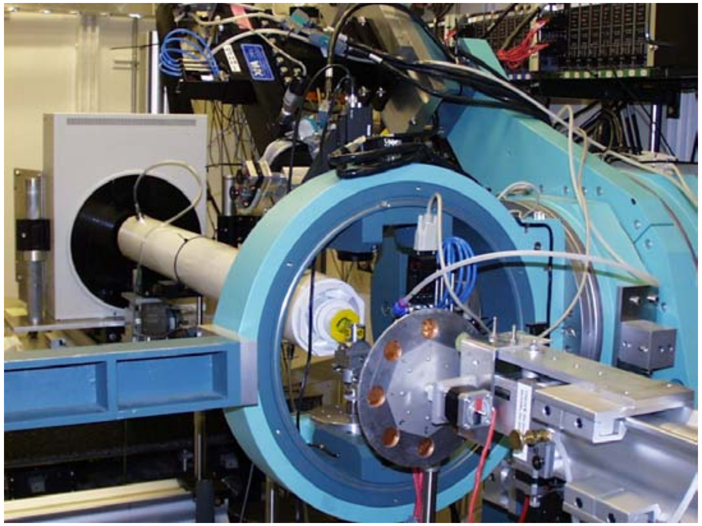
Kinetics of self-assembly

Jin Wang

Key result: lattice assembles at droplet's *top surface*





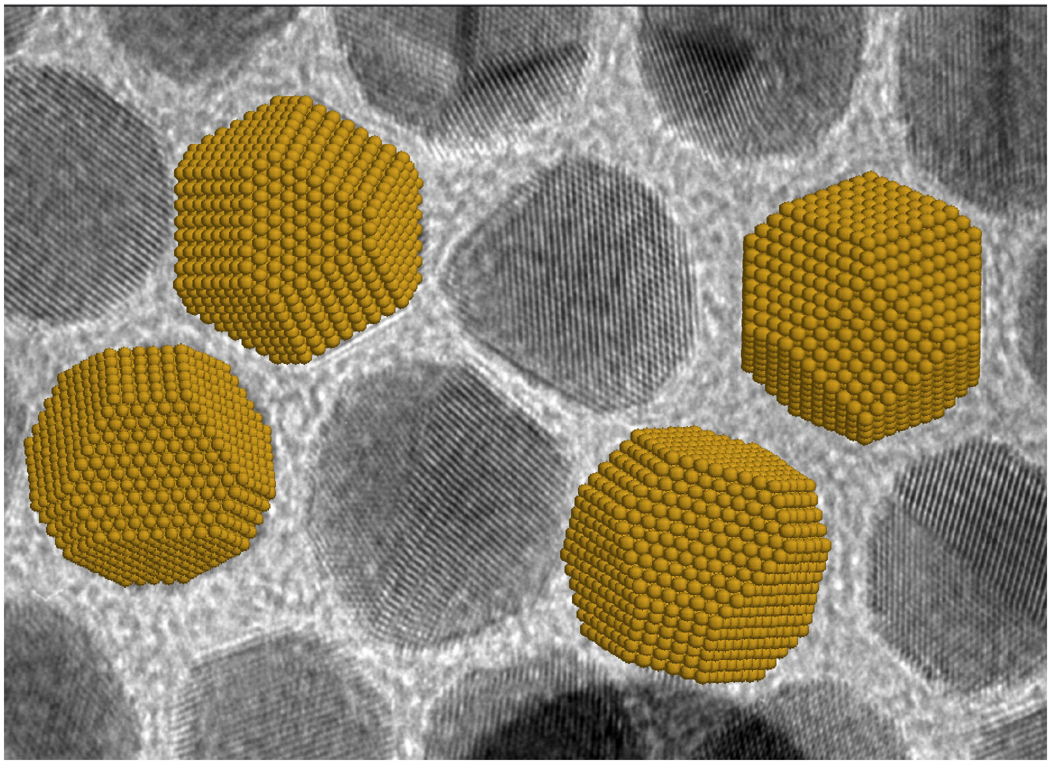


Narayanan, Wang & Lin, PRL (2004)

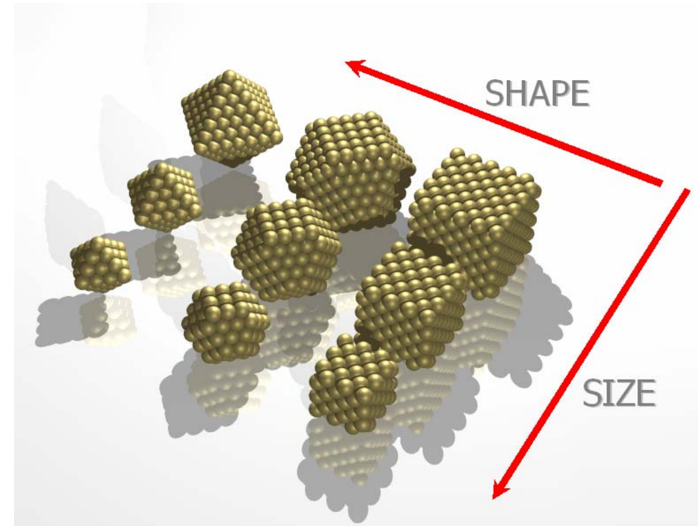
Exp't /theory/simulations: Kinetics versus Energetics

Computational Experiments - ‘Virtual Fab Lab’

Shape matters: plasmonics, photo-conversion, catalysis, etc..



Au nanocrystals with dodecanethiol ligand



Using theoretical methods the factors affecting nanocrystal shape my be investigated and then used predict conditions required to grow desired shapes

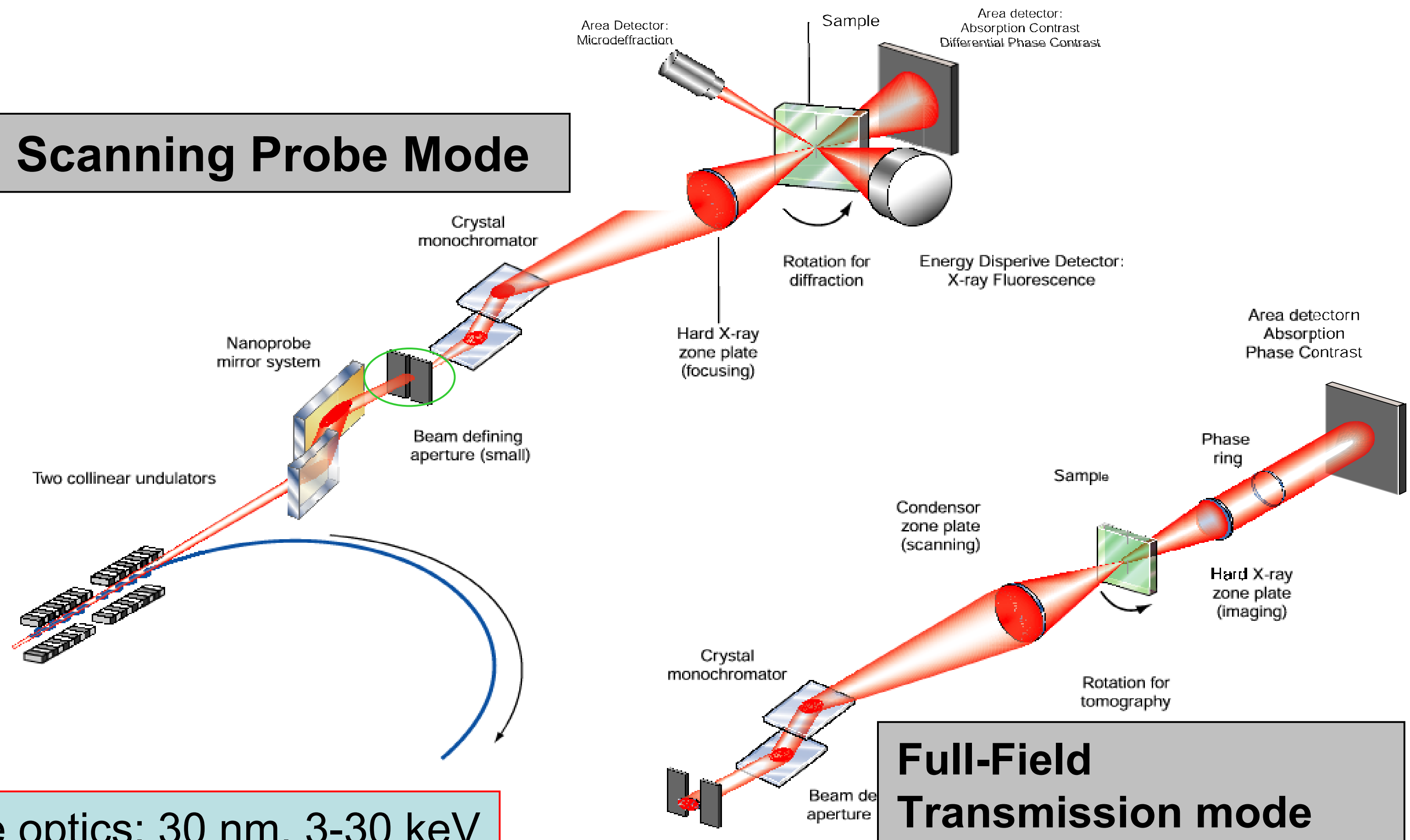
$$G_x = G_x^{bulk} + G_x^{surface} + G_x^{edge} + G_x^{corner}$$

$$G_x = \Delta_f G_x^o + \frac{M}{\rho_x}(1-e)\left[q\sum_i f_i \gamma_{xi} + p\sum_j g_j \lambda_{xj} + w\sum_k h_k \varepsilon_{xk} \right]$$

Amanda Barnard, Larry Curtiss, Xiao-Min Lin, to be published

X-ray Imaging

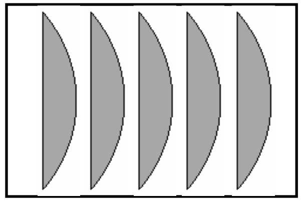
Center for Nanoscale Materials X-ray Nanoprobe at the Advanced Photon Source



Zone-plate optics: 30 nm, 3-30 keV

High Numerical Aperture Optics for Hard X-ray Focusing

- Refractive:

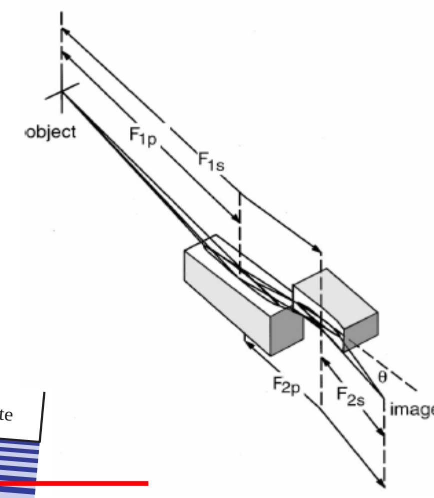


> 100 nm

Compound refractive lens

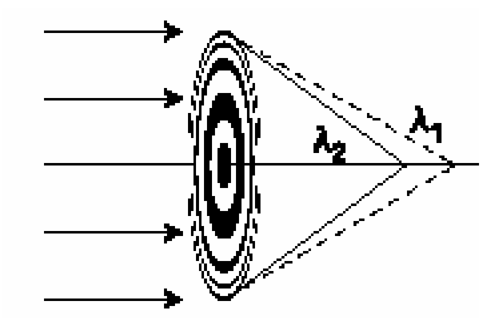
- Reflective: Kirkpatrick-Baez Mirrors

Figure by differential deposition, multilayer coated for high NA

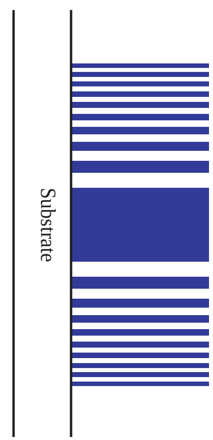


- Diffractive: Zone Plates - 40 nm

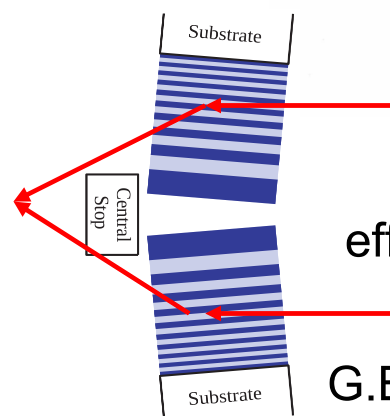
High aspect ratio, tilted zones for high NA



Fresnel zone plate



Lithographic zone plate



Transmission multilayer

30 nm w/46 % efficiency @ 19.5 keV (6/5/05).

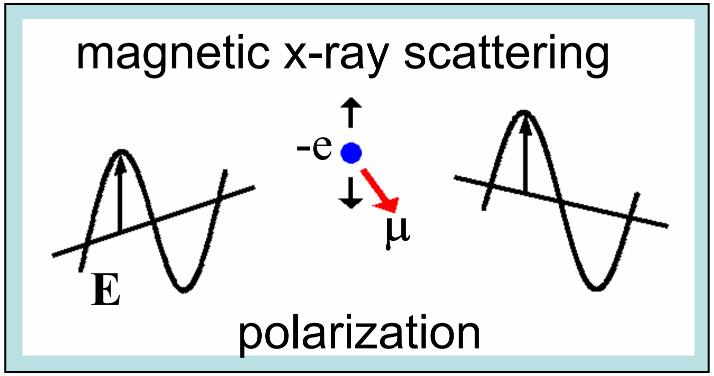
G.B. Stephenson, et al

Materials Physics Example: Antiferromagnetic Domain Evolution

10 μm

Challenge: Measure structure and dynamics of antiferromagnetic domains.

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.



(0,0,1-δ) SDW Bragg peak in Cr with 1 μm resolution.

Magnetic diffraction contrast allows imaging of regions with different magnetic order.

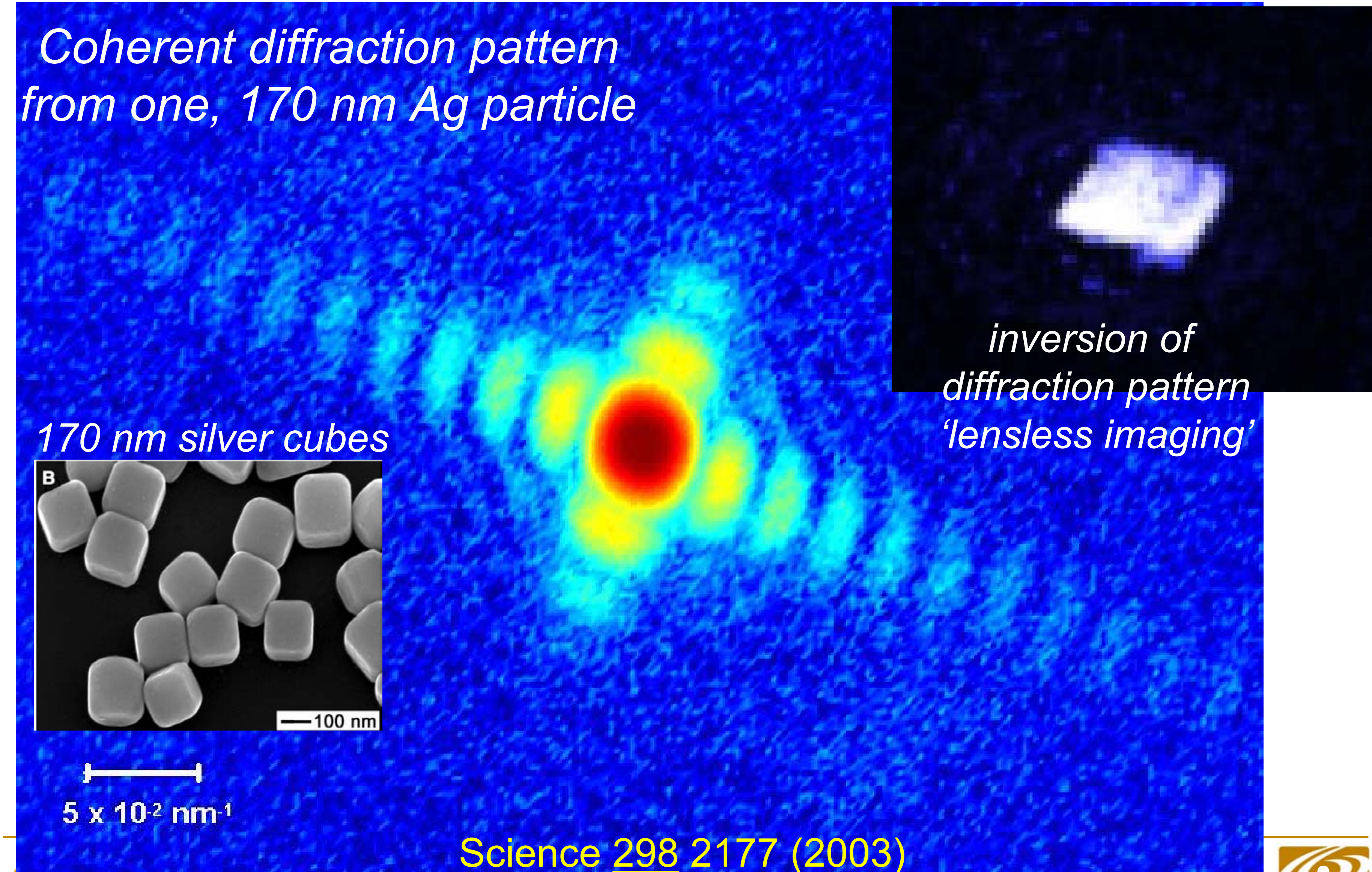
Evans, Isaacs, et al., *Science* 295, **1042 (2002).**

Dynamics on the Nanoscale

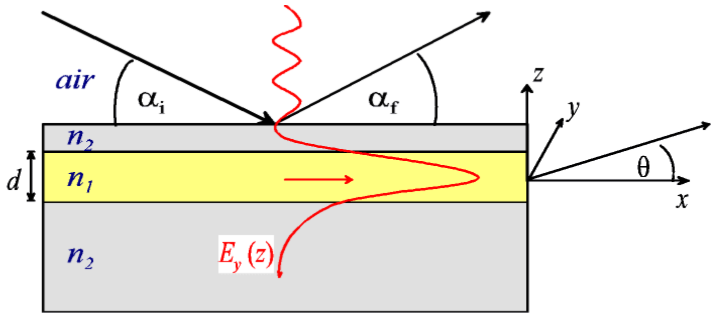
- Speed of sound 1 nm/psec sets natural length and time scales.
  - Pulse length at APS is 100 psec ⟺ 100 nm.
  - 10^7 photons/sec/pulse @ the APS.
  - e.g., can do ferroelectric and magnet domain dynamics.
- Future: LCLS
  - 100 fsec pulses ⟺ 1 Å
  - 10^{12} photons/pulse

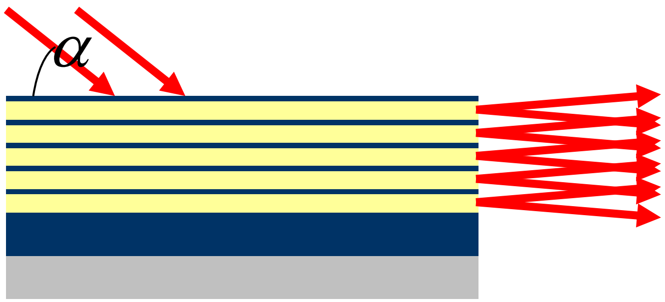
‘Lens-less’ Imaging of individual nanoparticles

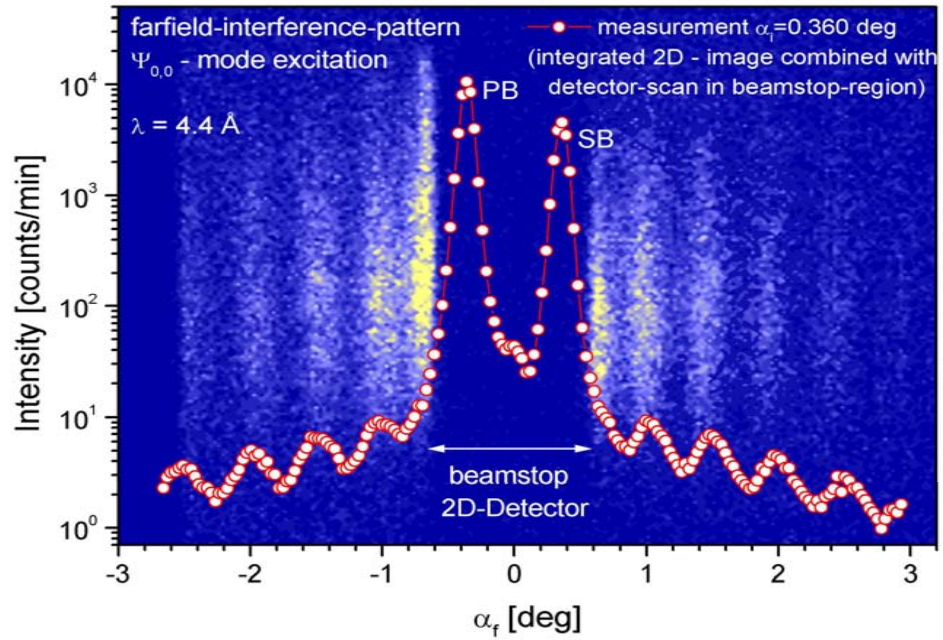
Ian Robinson, UIUC

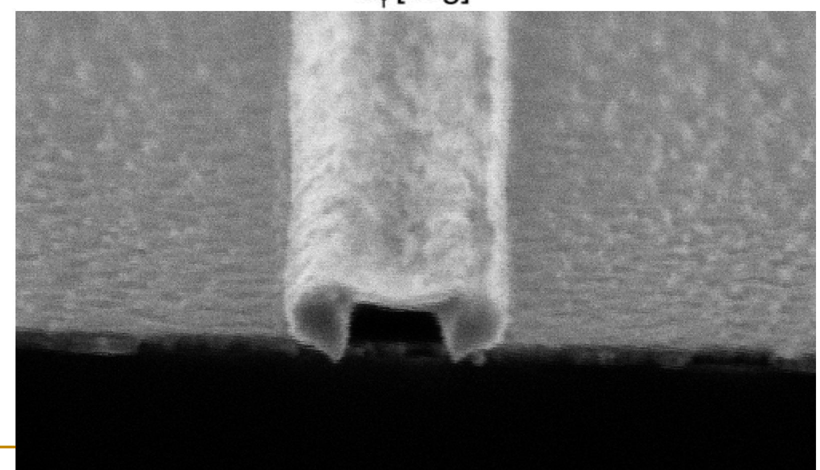


Neutron Wave guides
– coherent nanometer beams!









The future (after the slide rule)
- 2D neutron nano-guides?

I.S. Anderson, et al

Global Research Challenges for Nanoscience with X-rays

- Imaging with 1 nm resolution.
  - How do we get there?
- 3D structure and dynamics of individual (and ensembles of) nanoparticle(s).
  - Crystalline or non-crystalline.
  - Will require complement of tools, not just scattering.
- All of the above in-situ.
- Two comments:
  - Develop capabilities with nanoscience community (non-expert x-ray Users) and make them widely available.
  - Develop capabilities that complement and don't compete with other tools.