Interfacial Science

Panel Members:

Paul Fenter (ANL, Chair)
Mike Bedzyk (Northwestern)
Joel Brock (Cornell)
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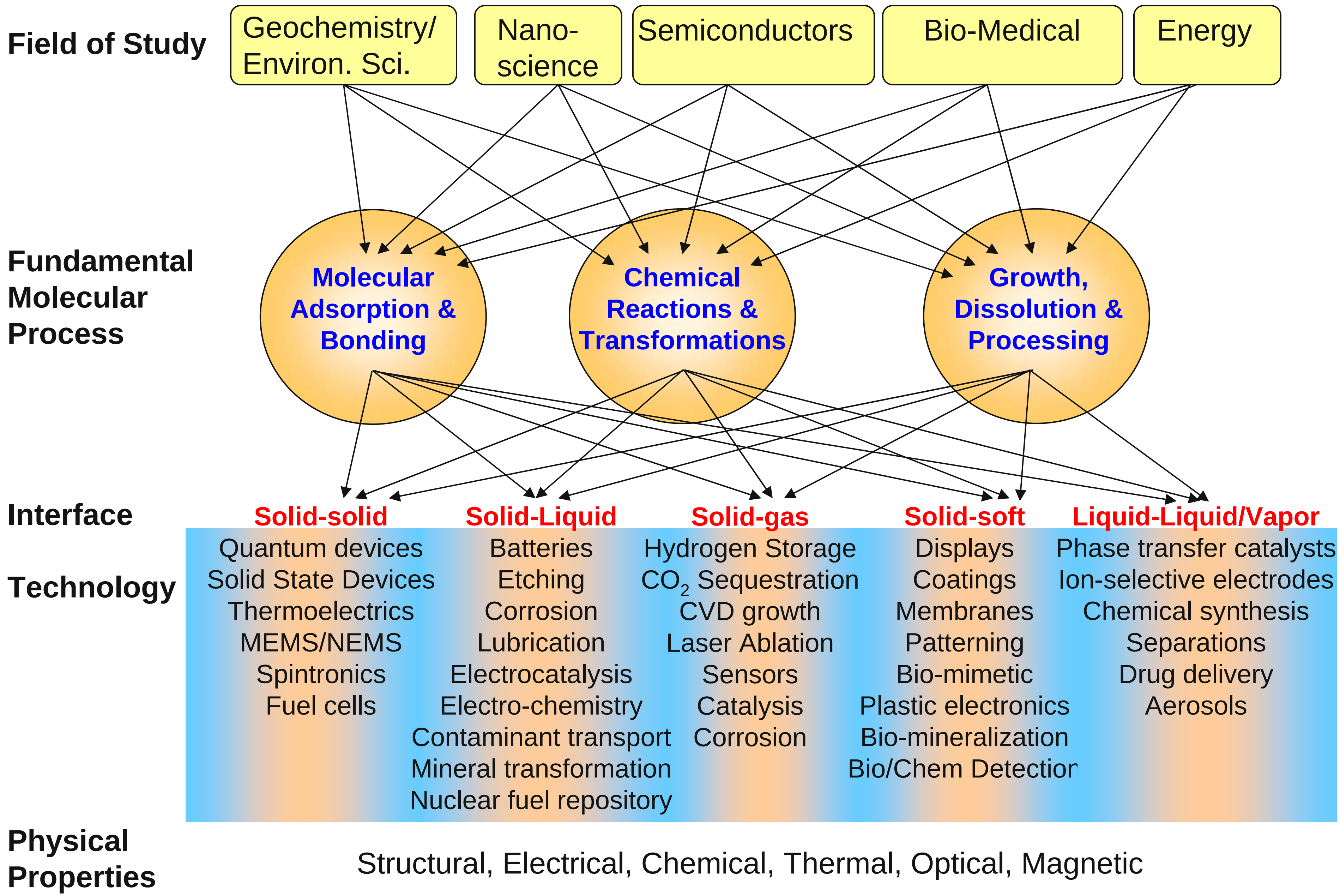
Hoydoo You (MSD/ANL)
Mike Toney (SSRL)
Ron Pindak (BNL)
Roy Clarke (Michigan)

Contributions from: Kent Blasie; Michael Pierce

Interfacial Science – From Processes to Properties



Interfacial Science: Challenges:

Small signal strength (R ~ 10^{-5} to 10^{-10})

Grazing angles of incidence (small effective sample area)

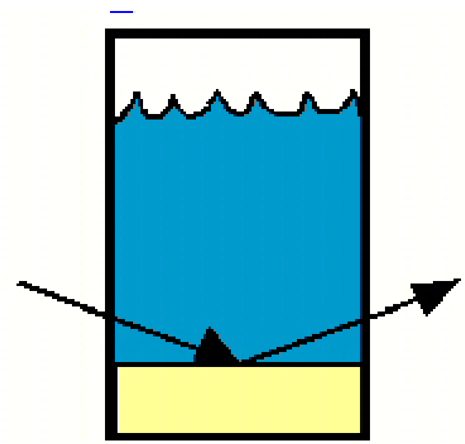
Lateral heterogeneity: structures, reactivity
averaging over large areas (mm's)

Complex environments
liquid-solid, vapor-solid, solid-solid, liquid-liquid

Structural/compositional evolution during reactions

Multi-element materials

Chemical state changes

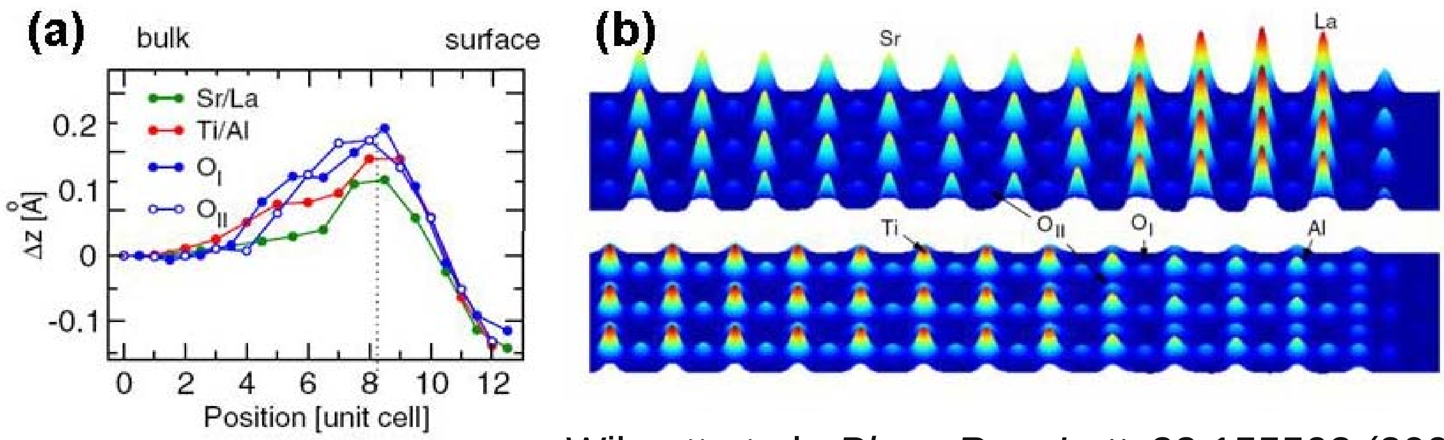


Major science themes:

Emergent Materials Behavior at Interfaces:

- metal insulator transition
- interface superconductivity
- 'colossal' magneto-resistance

Structure imaged using CoBRA algorithm: 4-layer film of $LaAlO_3/SrTiO_3$

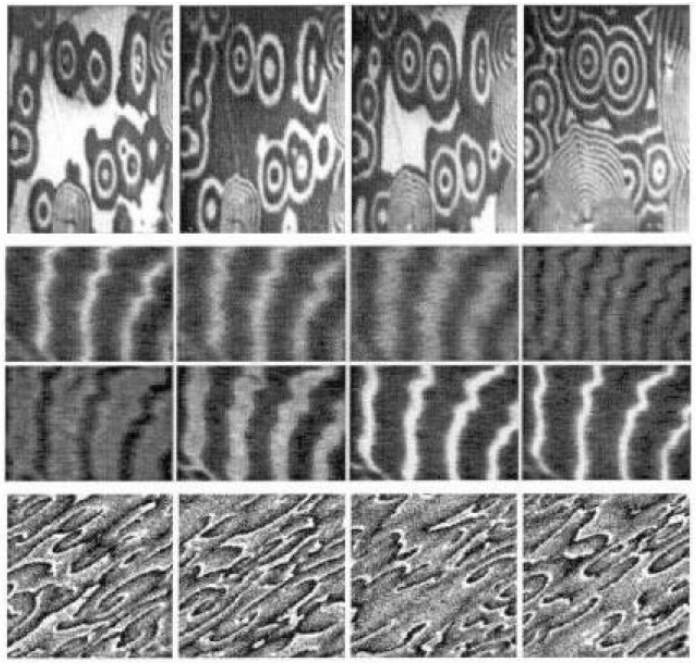


Wilmott et al., *Phys. Rev. Lett.* **99** 155502 (2007)

Currently: only understand laterally averaged static structure
→ Need to image structure and element-specific sub-structure
→ Real-time measurements during film growth

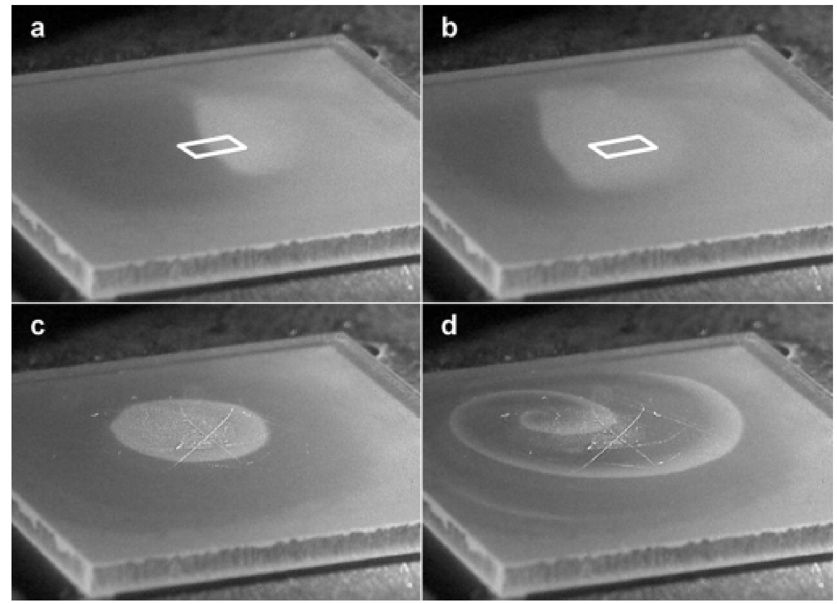
Major science themes:

Interfacial Chemistry: Spatio-temporal dynamics at interfaces



Progression of time => => => =>=> => => =>

www.fhi-berlin.mpg.de/surfimag
(Nobel Prize in Chemistry 2007)



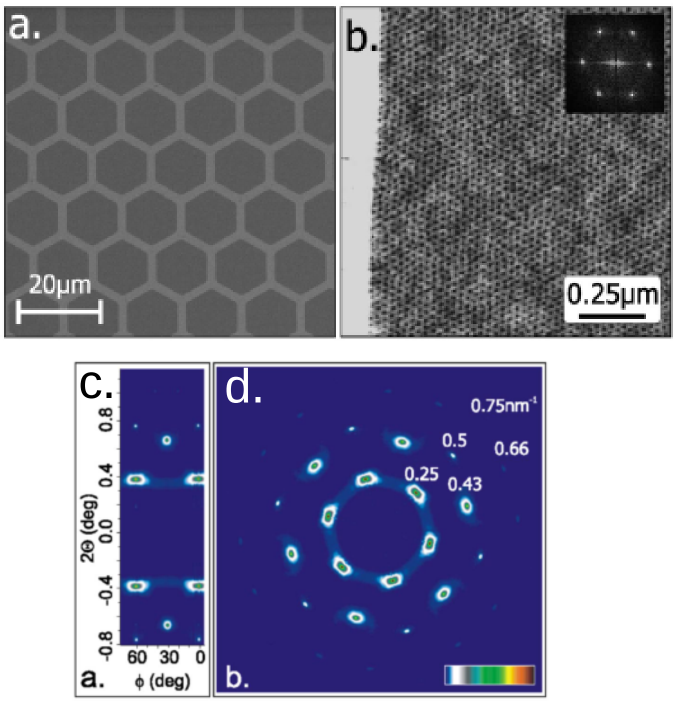
Jiang et al., *PRL* **101**, 086102, 2008

Interfacial reactivity is both spatially and temporally variable!!
Currently: only probe spatially averaged behavior vs. time
→ Need sensitivity to changes in oxidation states
→ Need to understand connection between molecular structure and transport

Major science themes:

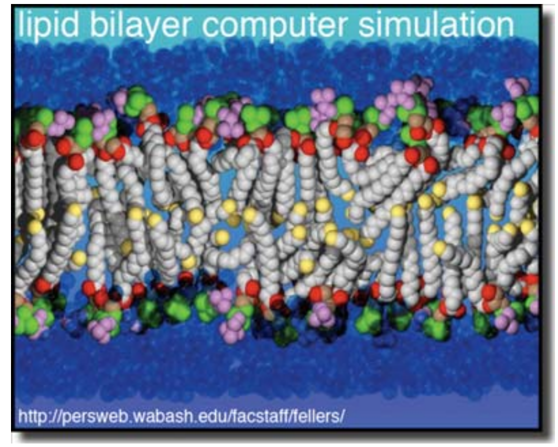
Soft-material interfaces: organization and complexity

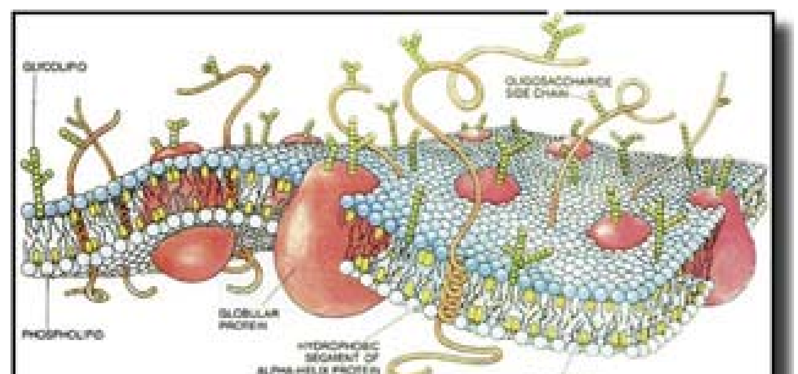
Control of long-ranged orientational and positional order in organic films:



Stein et al., *Phy. Rev. Lett*. **98**, 86101 (2007)

Membrane science: temporal/structural response of voltage-gated ion channels:





Cartoon of a biomembrane

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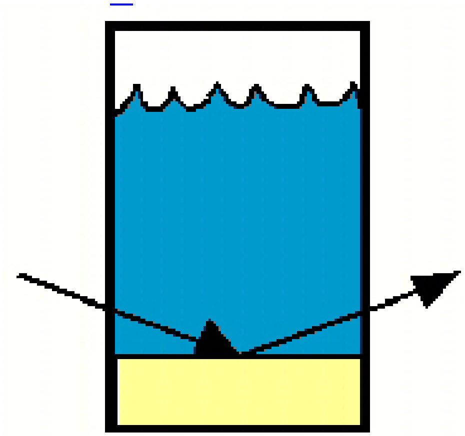


Interfacial Science: Current Opportunities:

High flux sources/advanced detectors

High brilliance source

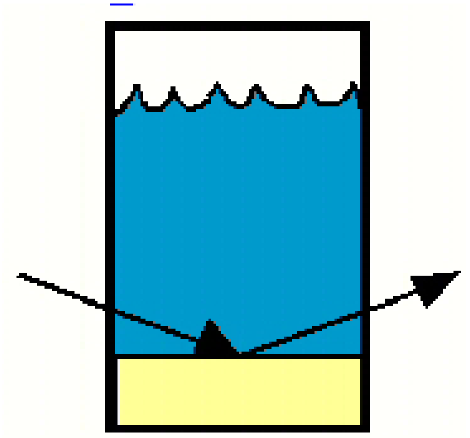
Real-space imaging (nm to mm)
laterally heterogeneous structure, reactivity

In-situ measurements
liquid-solid, vapor-solid, solid-solid, liquid-liquid

Temporal sensitivity (ps to hours)

Elemental sensitivity

Chemical sensitivity (e.g., oxidation states)



What we cannot do: multi-dimensional imaging

Observe elementary reactions in:

- real-space (nm → mm)

AND/OR

- real-time (ps → hours)

AND/OR

- in-situ (liquid-solid, solid-solid, solid-gas)

AND/OR

- elemental specificity/sensitivity

AND/OR

- chemical specificity/sensitivity

Requirements and Capabilities (short term):

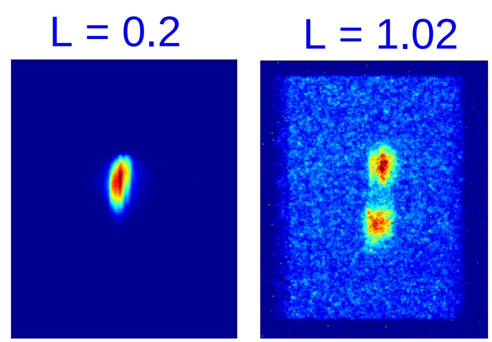
Detectors:

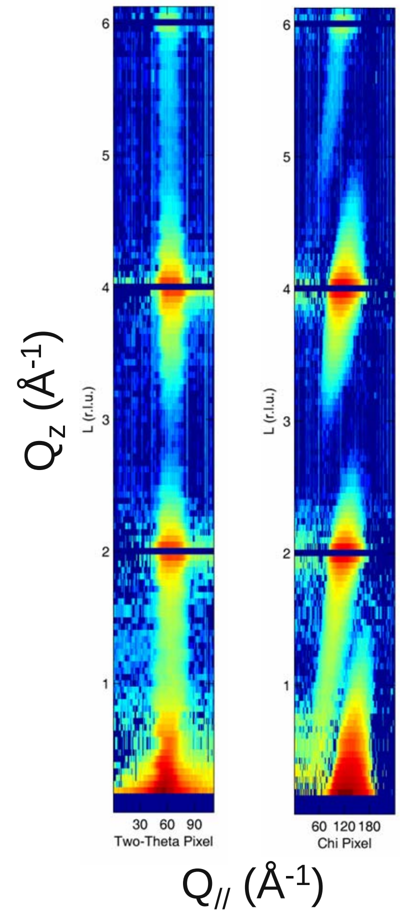
CCD area detectors

Pixel array detectors (e.g., pilatus)

Fluorescence detectors

Raw CCD images:





→ Make better use of existing sources

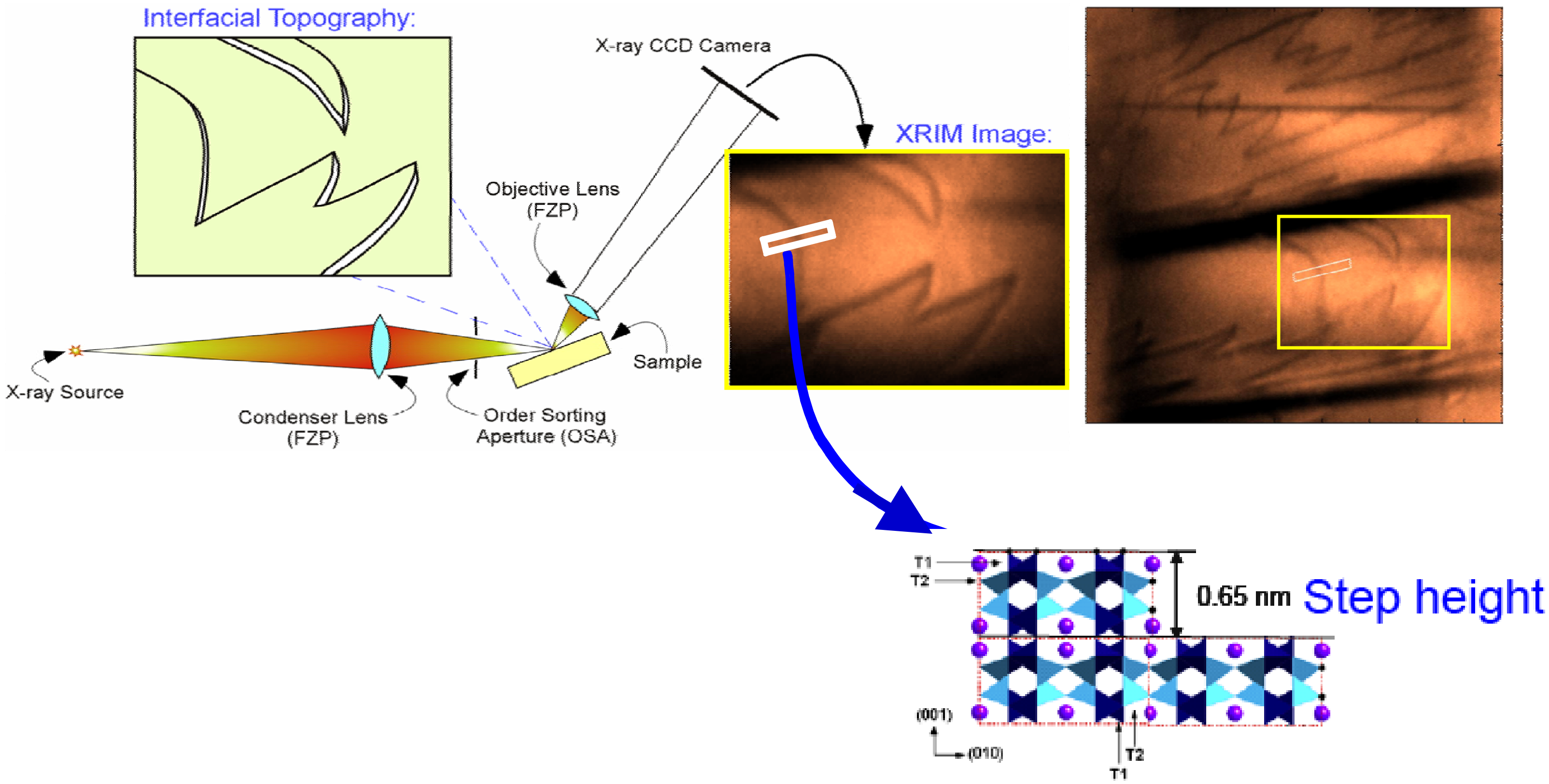
High energy:

E>40 keV

- penetration through complex environments
- large Ewald sphere: can probe relevant reciprocal space in single image

Requirements and Capabilities (long term):

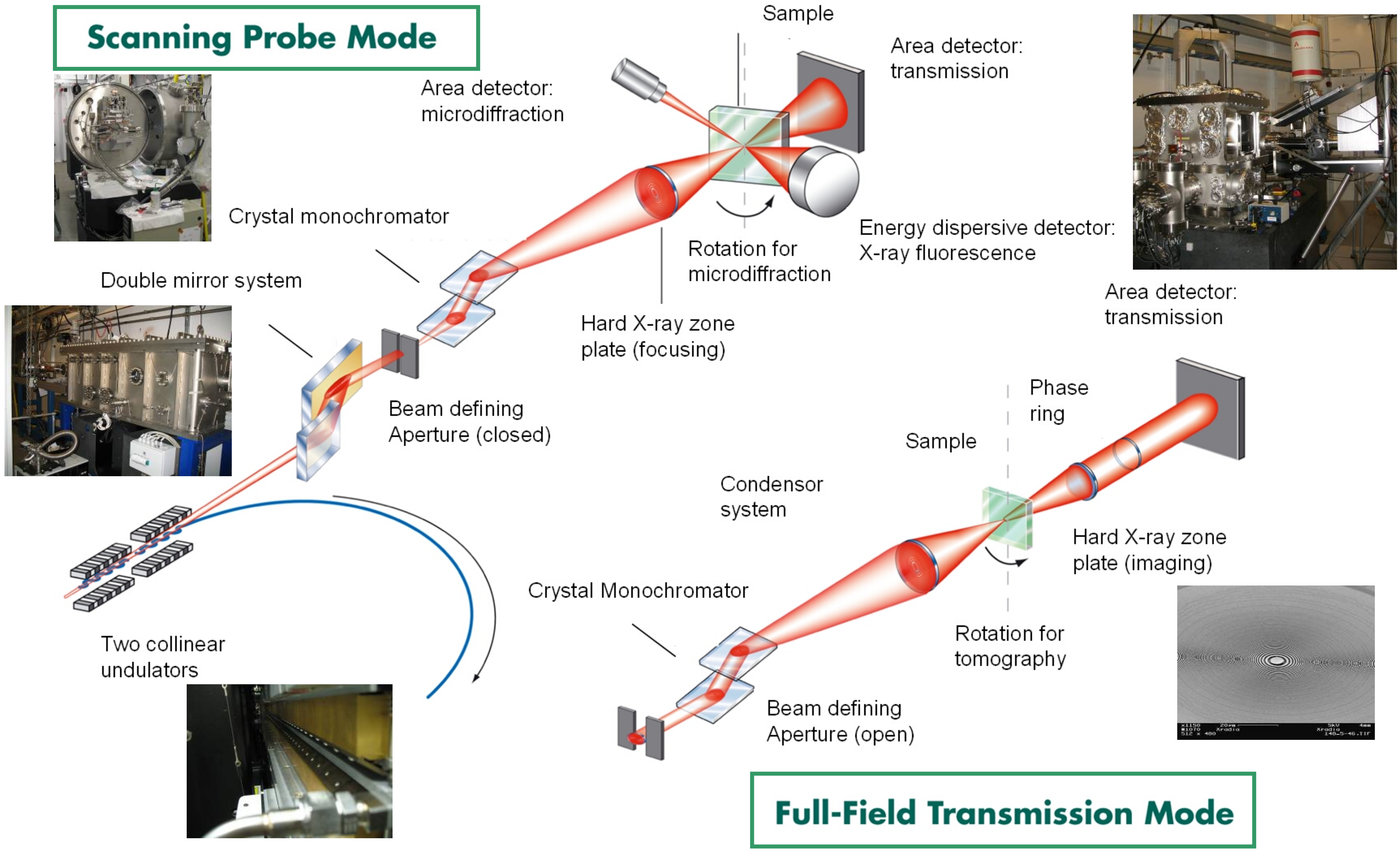
Imaging: Full field X-ray microscopy



→ Implement as a general capability
→ Significant improvements possible with new optics/detectors:
- resolution (~5x better to ~ 30nm)
- image rate (>100x better to < 1 sec)

Fenter et al., *Nature Physics*, **2** 700-704 (2006)

Hard X-ray Nanoprobe: Combined Analytic and Imaging Mode



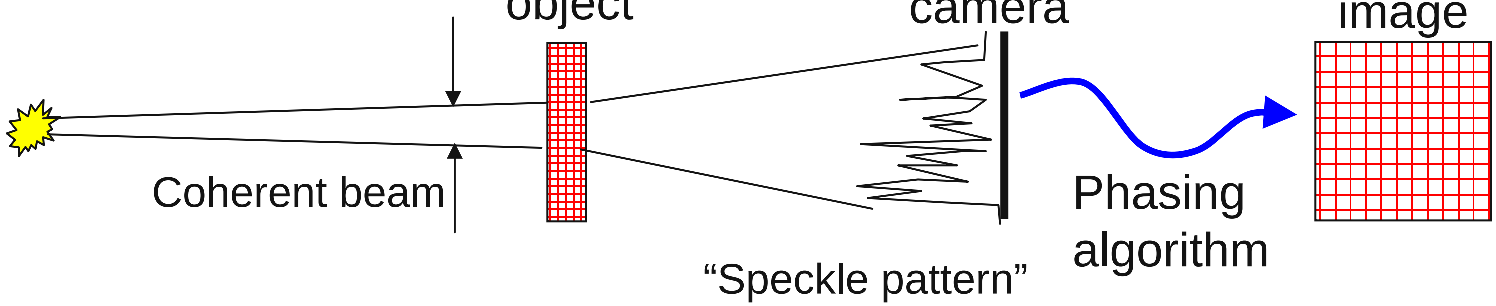
→ Imaging fast-dynamics of individual nano-particles

Courtesy of Maser, Winarski, Holt, Rose, Stephenson, (CNM, APS, MSD)

Requirements and Capabilities (long term):

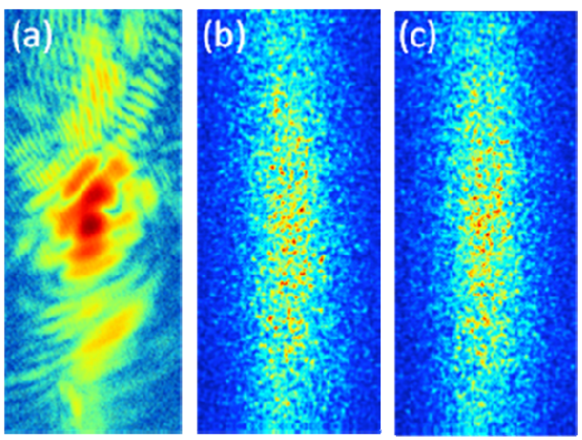
Coherence:

Coherent Diffraction Imaging:

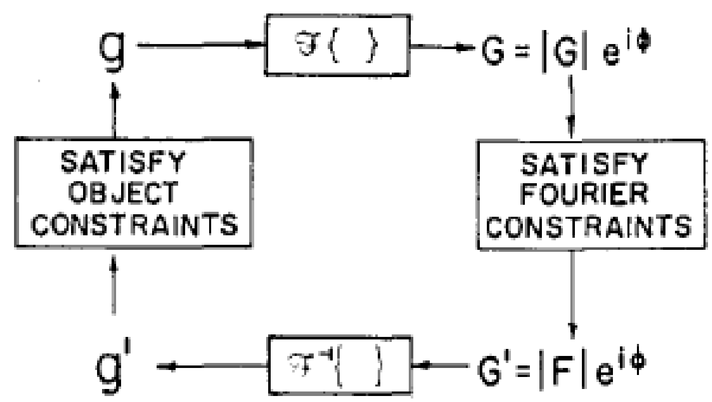


- photon correlation spectroscopy
- coherent diffraction imaging

-robust phasing transforms scattering data to microscopic images



Au(001) Hexagonal reconstruction peak:
Pierce et al., unpublished results (2008)



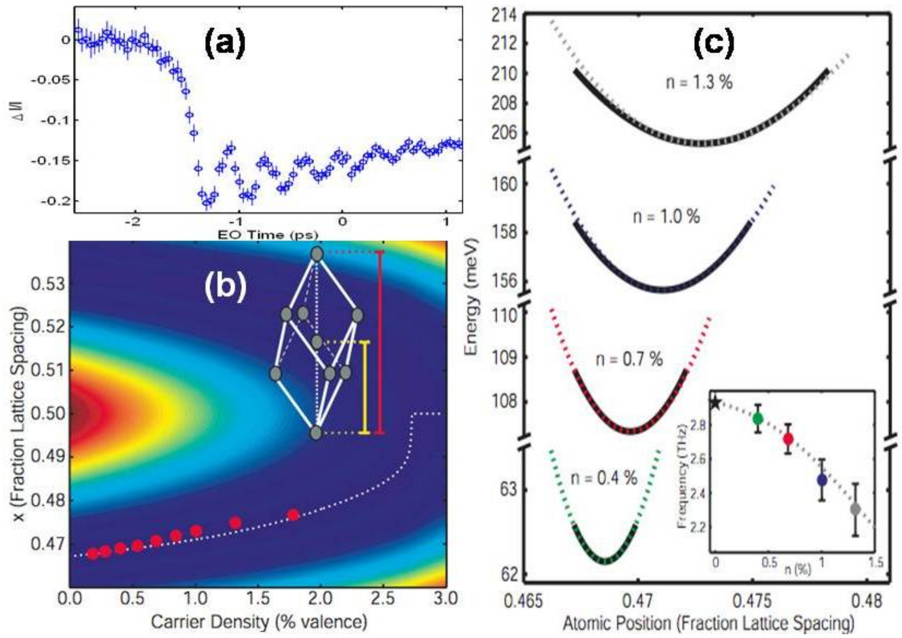
Fienup, Opt. Lett. 3, 27 (1978)

Requirements and Capabilities (long term):

Temporal resolution: Short Pulse X-ray facility:

~1 ps time resolution (pump-probe; photo-excited processes)

Lattice excitations:



Ultrafast measurement of lattice potentials of (111) Bismuth [Fritz et al., *Science*, **315**, 633-636 (2007)]

→ Application to interfaces opens up new dimension in temporal sensitivity

Needs for Interfacial Science:

Implementing new or anticipated capabilities:

- ~10’s of nm spatial resolution
  - new *interfacial* microscopes; nanoprobe
- ps temporal resolution (SPS facility)
- imaging elemental/chemical sub-structures
- detectors (rapid data acquisition)
- software (phasing algorithms and visualization)

New Beamlines:

- Proposed X-ray Interfacial Science sector (Bedzk, PI)
  - new capabilities
  - increase in capacity
  - a home-base for interfacial science

Complex instruments (PLD, MOCVD, MBE…)

The Case for Interfacial Science:

Multi-dimensional, multi-scale imaging:

- an “interfacial observatory”

$$\rho(x, y, z, t, Z, \text{oxidation state})$$

The Case for Interfacial Science:

Energy Storage (stability of interfaces):
- more stored energy, longer lifetime, safer batteries

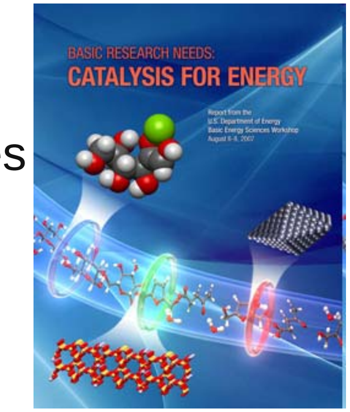
Catalysis:
-observe the reactivity of supported nano-particles

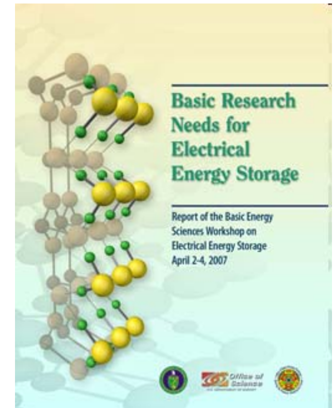
Materials Growth:
- create novel materials
    - electronic materials
- solid-state lighting

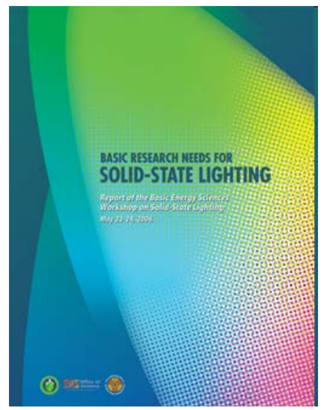
Materials Chemistry:
- corrosion

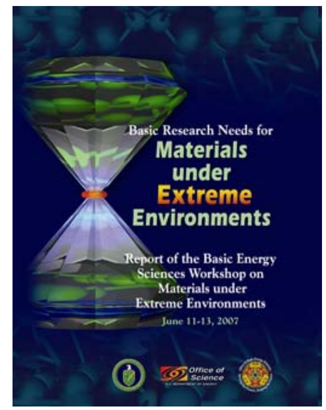
Geochemistry:
- sequestration of energy by-products:
    - spent nuclear fuel, CO_2
- transport of contaminants in the environment

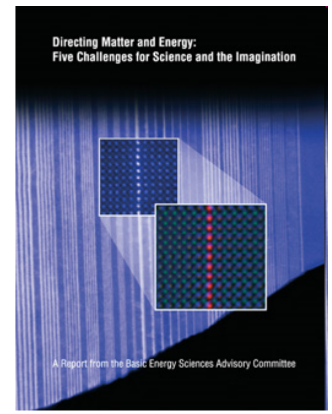
Actinide Science
- reprocessing nuclear fuel

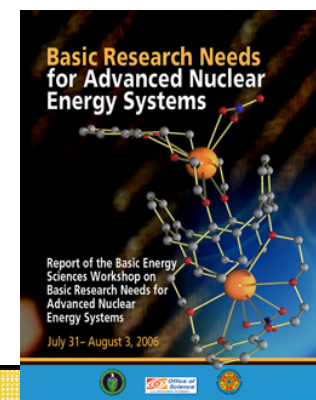








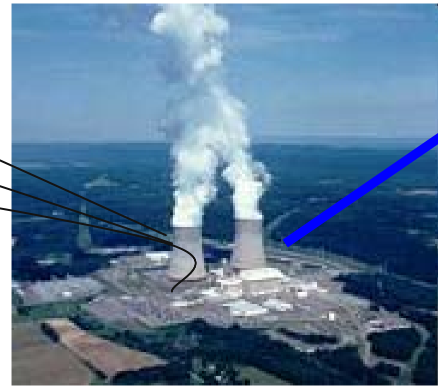




The Case for Interfacial Science:

The Chevy Volt:

The Case for Interfacial Science:



High T/P corrosion
in nuclear reactors

Nuclear repository
(geological sequestration)
and reprocessing (separations)

On-board computer
(electronic materials)

The Chevy Volt:

Energy Storage
- interfacial stability
- safe operation

Solid-state
lighting (??)
(materials
growth)

CO_2 repository
(carbonate nucleation
and growth)

Catalytic converter
(supported catalysts)

Corrosion

Agenda For Breakout Session:

1:00 Introduction/Charge (Fenter)
- feedback on report

Technical Frontiers and Discussion
1:15 Phasing Scattering Intensities (Pindak)
1:30 Coherent surface diffraction (You)
1:45 Interfacial microscopy (Fenter)
2:00 Scanning Probes/X-ray science (Rose)
2:10 Membranes (Blasie)

2:20 General Discussion

3:30 Preparation for Summary