Argonne NATIONAL LABORATORY

… for a brighter future

U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by The University of Chicago

Neutron and synchrotron radiaiton studies for designer materials, sustainable energy and healthy lives

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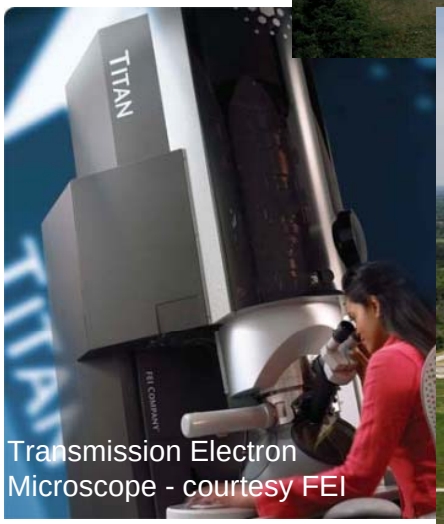
Denver Meeting May 2nd 2009

Three major useful types of radiation for materials study

- Electrons, neutron and x-rays are complementary
  - All are forms of diffracting radiation with $\lambda < 0.1$nm (interatomic separations in materials)
- All can be produced by accelerators - only neutrons and x-rays are large-scale

Spallation Neutron Source
Oak Ridge National Laboratory



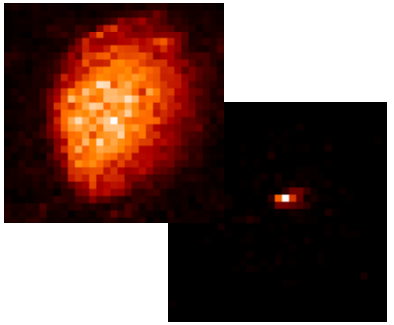
Transmission Electron Microscope - courtesy FEI

Advanced Photon Source
Argonne National Laboratory

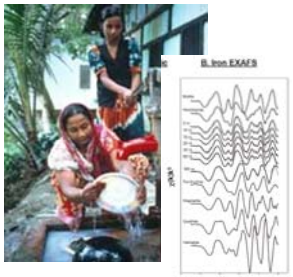
Key uses of x-rays (or neutrons or electrons)

- Imaging

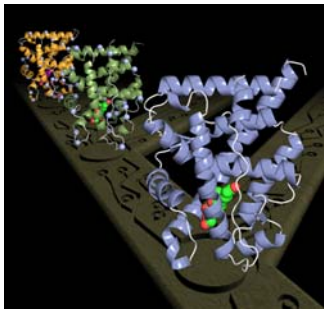
110 years



- Spectroscopy

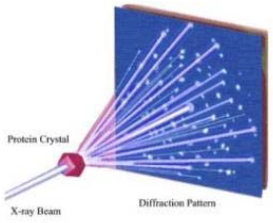


Preventing mass As poisoning, Polizzotto et al., Chem. Geol. **228**, 97 (2006)

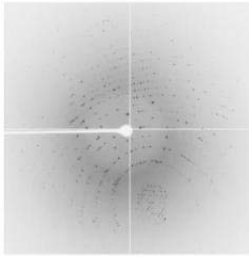


Evolution seen in proteins
Ortlund et. al. SER-CAT

- Diffraction (Scattering)



Diffraction Process

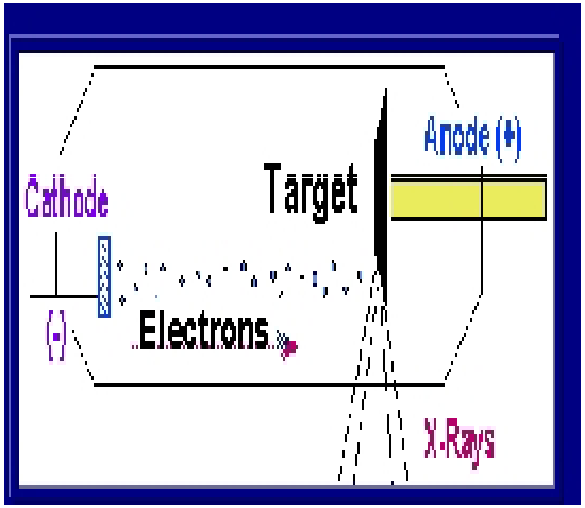


Diffraction Pattern from NSLS

- All three are greatly improved by “brilliant” sources, such as third-generation x-ray sources and spallation neutron sources

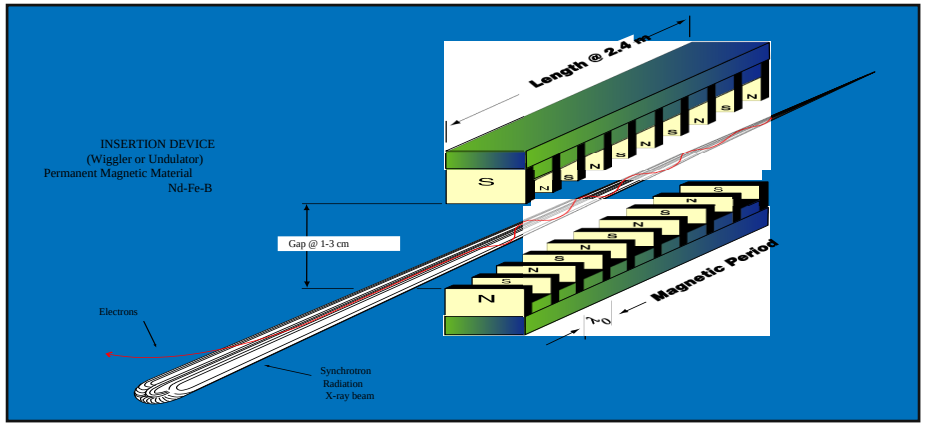
How are x-rays produced?

- Charged particles (electrons) are accelerated or deccelerated

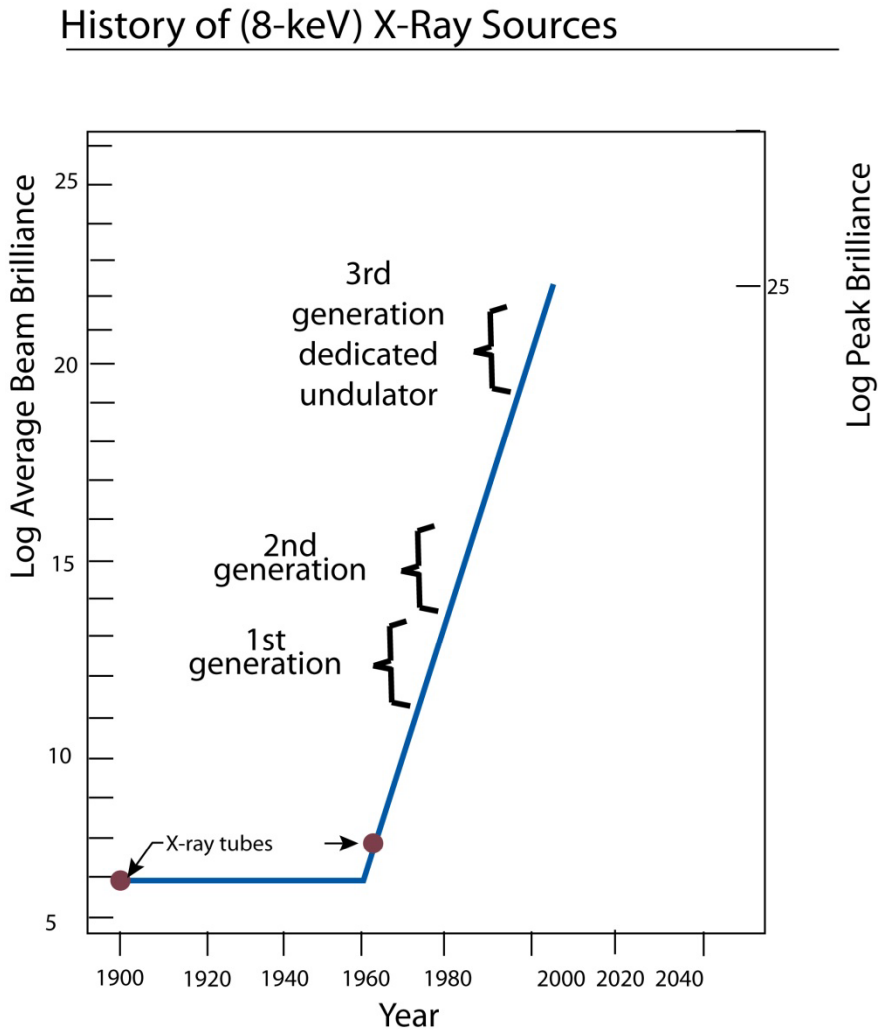


Laboratory x-ray tube
- not efficient but cheap

Synchrotrons use very fast electron beams, and “undulators”:
Tunable and many, many orders of magnitude more brilliant



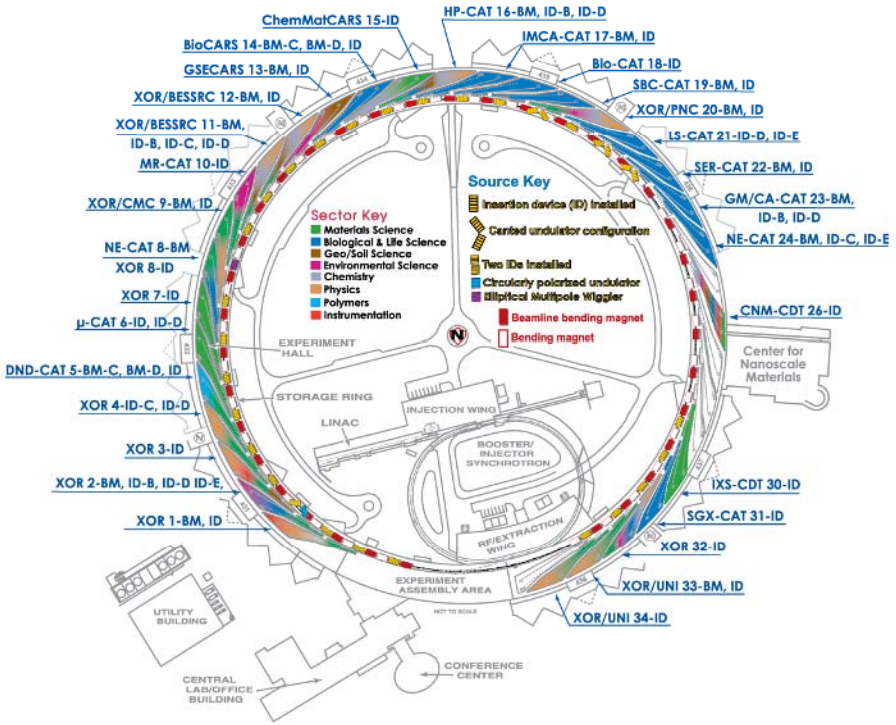
Brilliance available from x-ray sources today



Brilliance – flux in photons/sec/cm^2/mrad^2/0.1%bandwidth

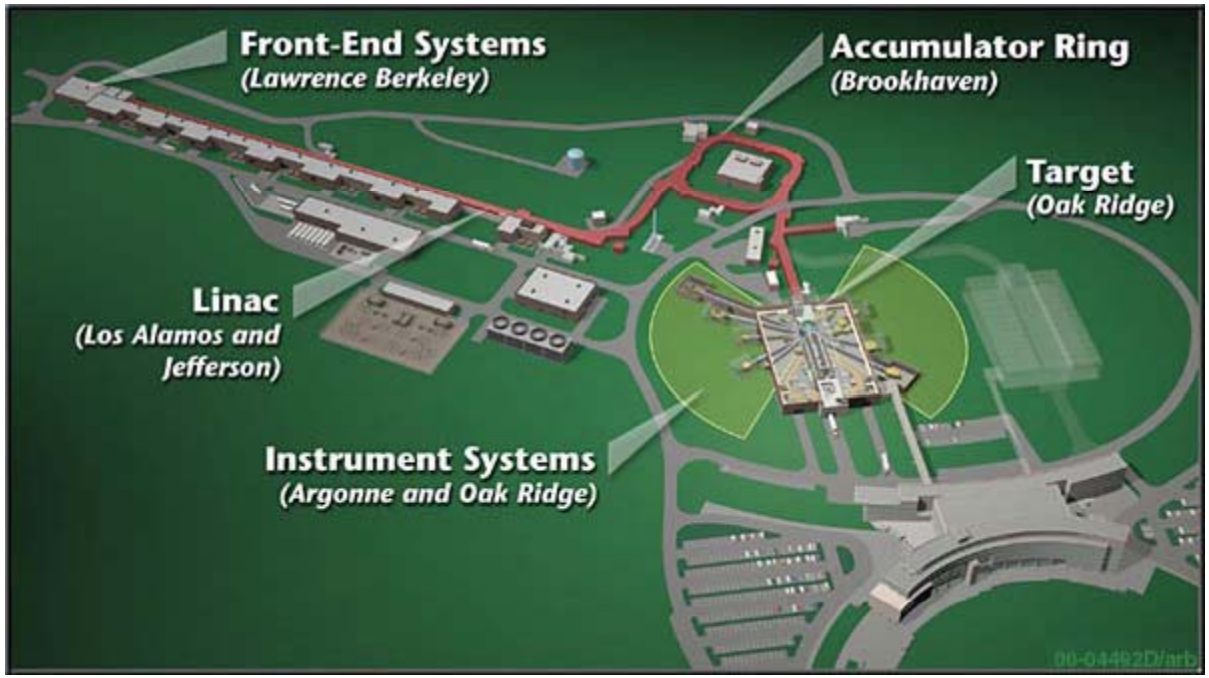
What does a third-generation x-ray source look like?

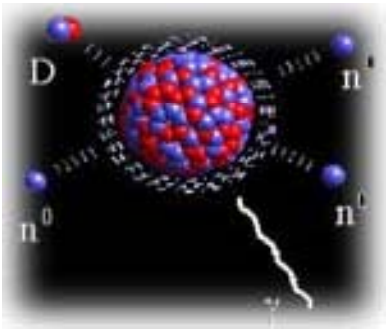
QuickTime™ and a
Cinepak decompressor
are needed to see this picture.



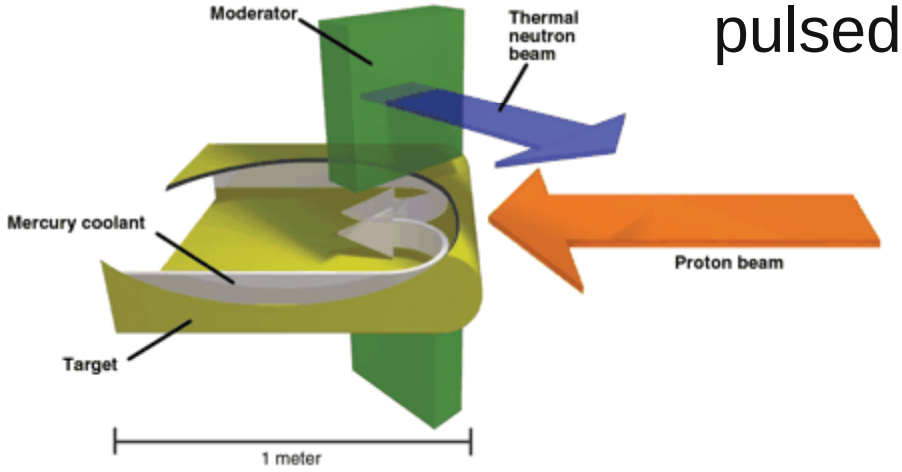
3500 users per year -
massively parallel

How are neutrons produced by accelerators?

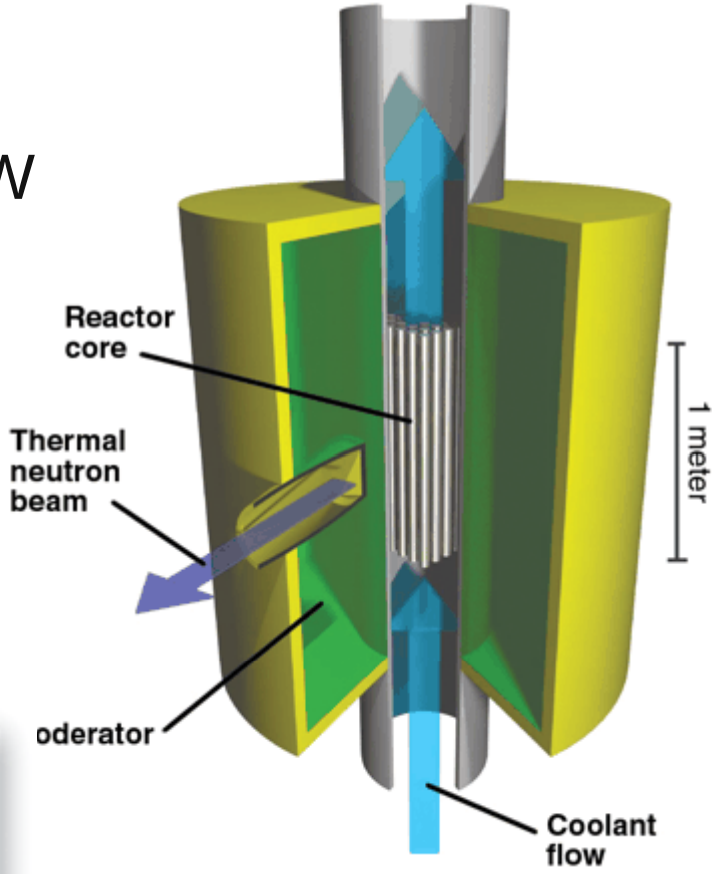




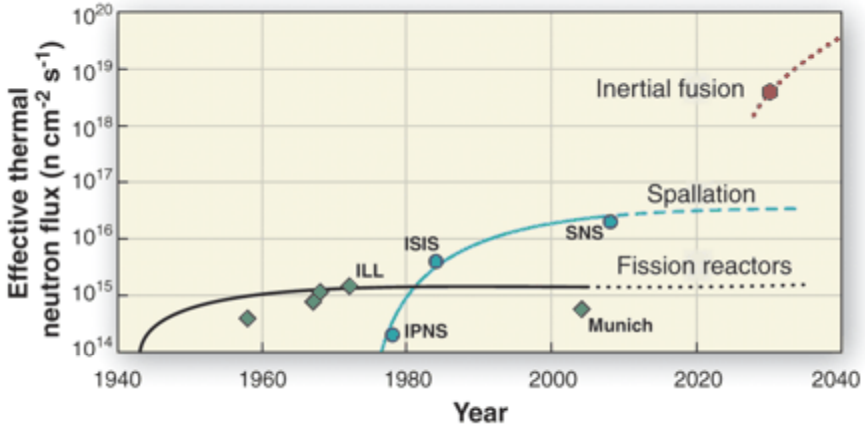
How do spallation sources compare with reactors?



pulsed vs CW



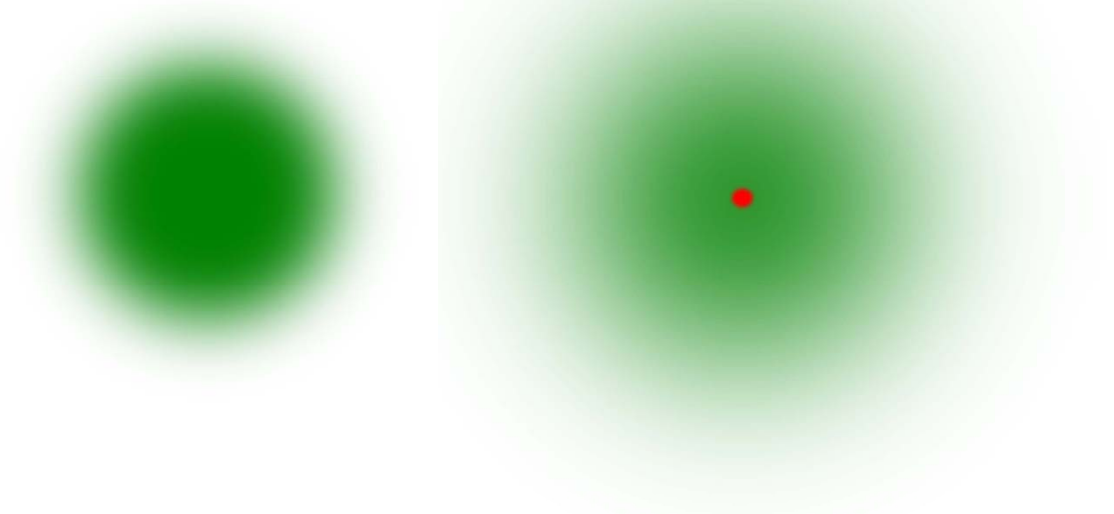
courtesy Andrew Taylor ISIS



reactor source - ILL

What the particle sees….

$\rho_e(\underline{r})$ $V(\underline{r})$ $m_n, \underline{J}$



x-ray electron neutron

Advantages/Disadvantages

Thermal Neutrons

$\lambda \sim d_{hkl}$
penetrates
strong contrast possible (e.g. H/D)
E~elementary excitations
strong magnetic scattering

low brilliance
some elements absorb strongly
restrictions on Q for large ΔE
excitations < 100meV

Synchrotron X-rays

$\lambda \sim d_{hkl}$
high brilliance
no kinematic restrictions
no ΔE restriction

strong absorption at low E
little contrast e.g. H-C
weak scattering
from light elements
radiation damage

Fast Electrons

$\lambda << d_{hkl}$
high brilliance, nanoprobes
no kinematic restrictions
no ΔE or ΔQ restriction
charge sensitive

thin samples (or surfaces)
dynamical scattering
little contrast e.g. hydrocarbons
weak scattering from light elements
radiation damage

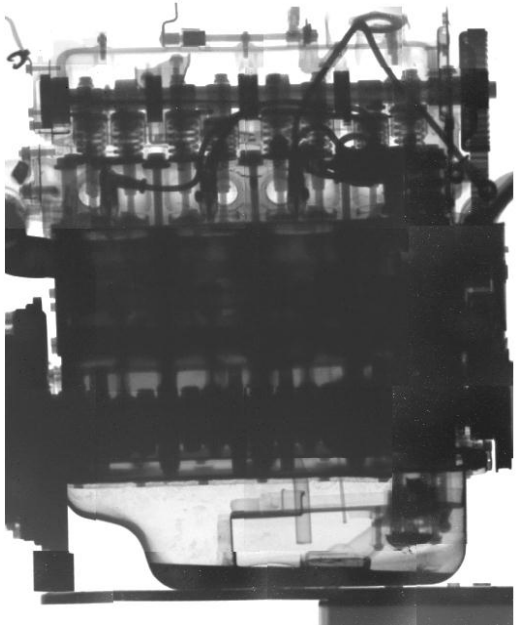
The facts of life

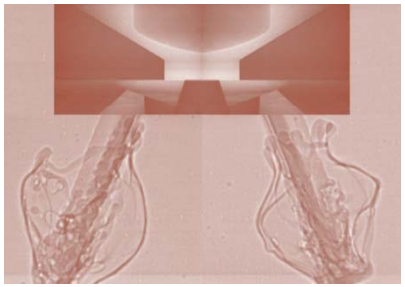
- Penetration increases
- As sensitivity decreases
- And spatial resolution decreases

- But so does source brilliance

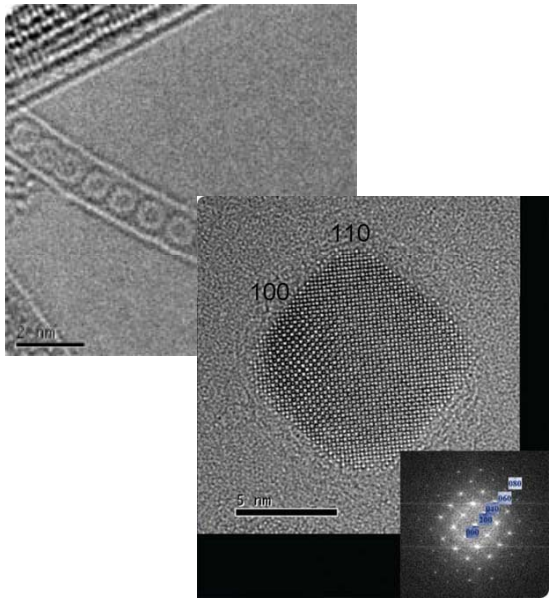
What are the properties of neutrons and x-rays for study of materials?

- Neutrons penetrate furthest through materials



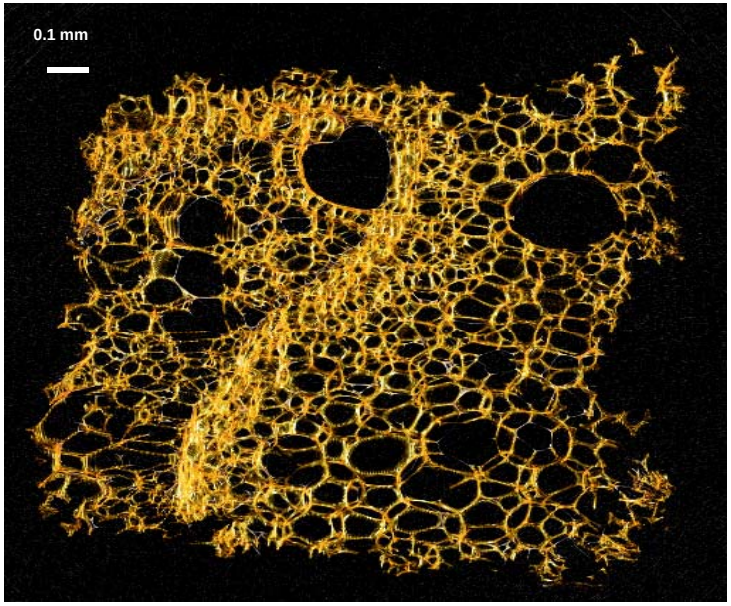


Hard x-rays do well
but have higher spatial and
temporal resolution



Electrons have the highest spatial resolution, least penetration

X-ray CAT scanning at very high spatial resolution



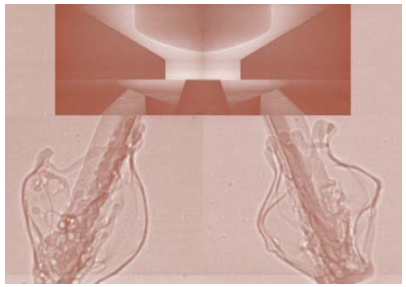
Space shuttle foam
(real time under deformation)

Can do this with a special lab source,
but very slow - synchrotrons necessary for dynamics

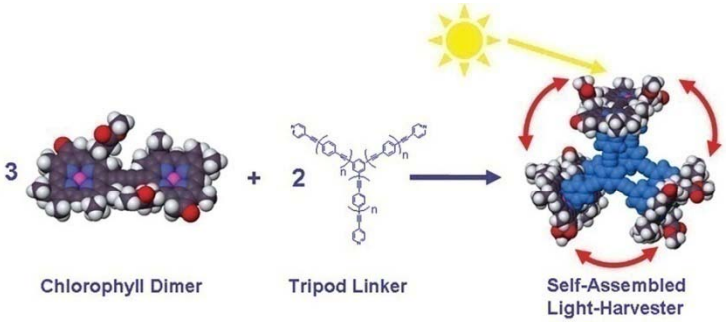
Comparative uses of neutrons and x-rays

- Magnetism
  - Very important in information technology
  - Both neutrons and x-rays are powerful and complementary
    - *Neutron signal stronger, but orbital only and not element specific*
- Spectroscopy
  - Neutrons excellent for atomic dynamics
  - X-rays for electronic (and atomic) dynamics and structure

APS research addresses key challenges in energy…

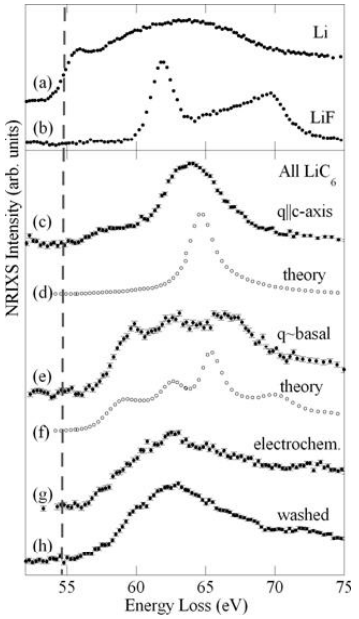


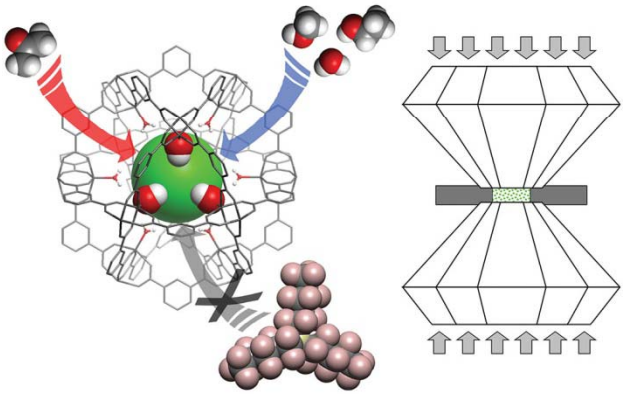
Better burning



Natural solar cells

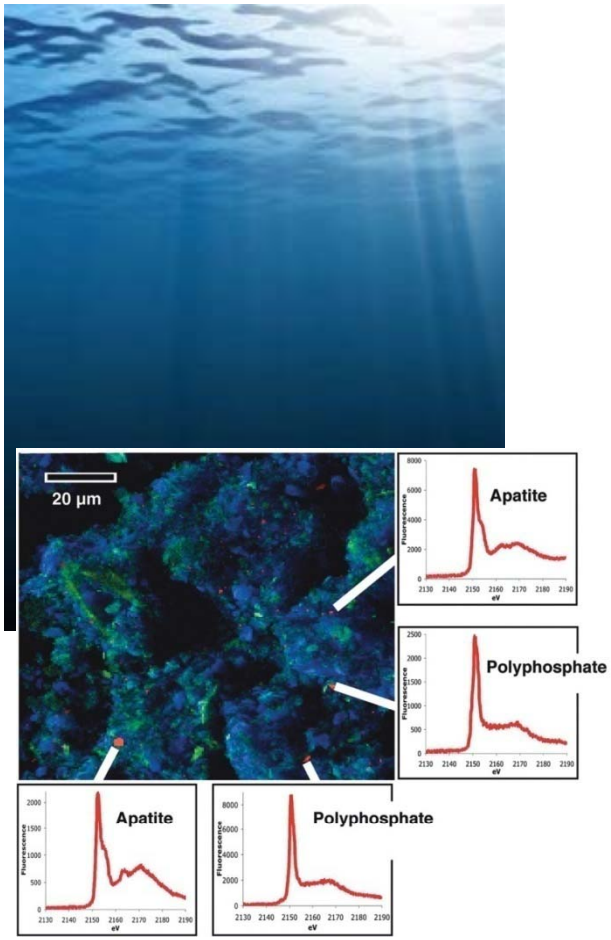
Better batteries



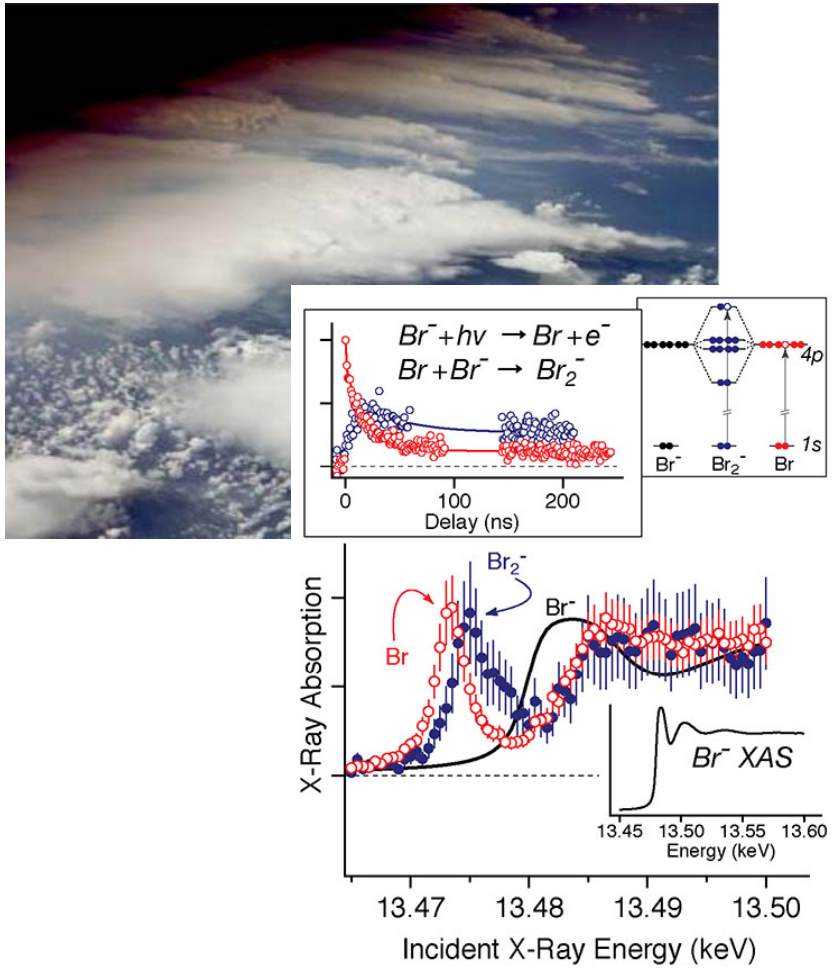


Storing hydrogen

and climate change…

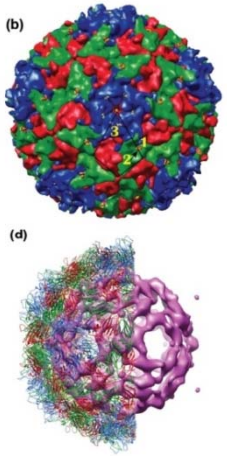


how sea animals capture carbon

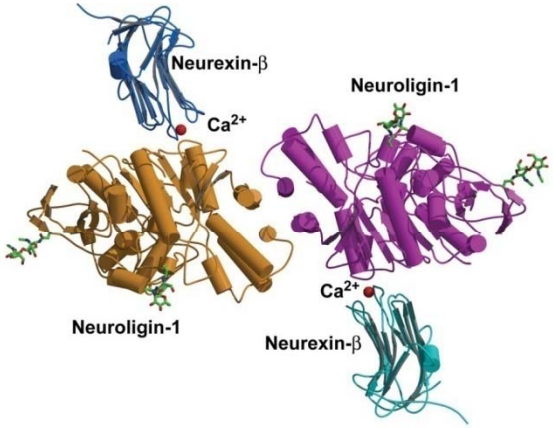


understanding free radicals in the atmosphere

human health…

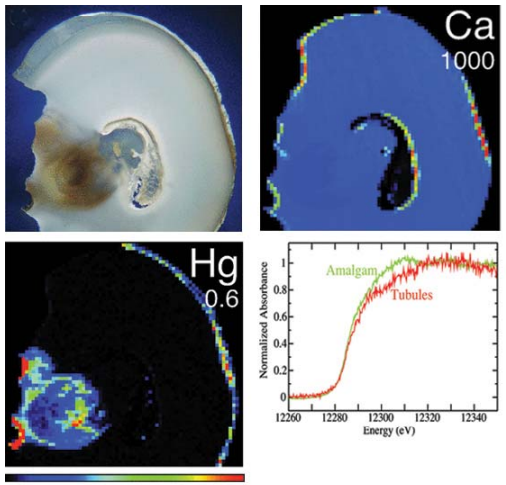


viruses that attack cancer

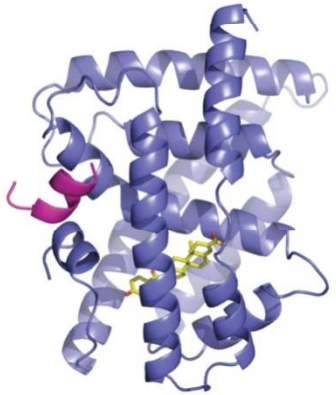


understanding autism

taming a killer

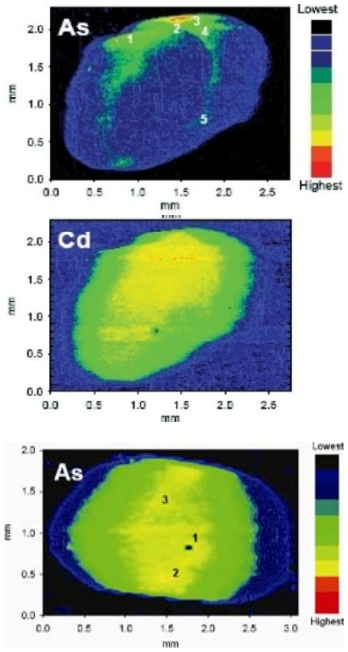


does your tooth hurt?

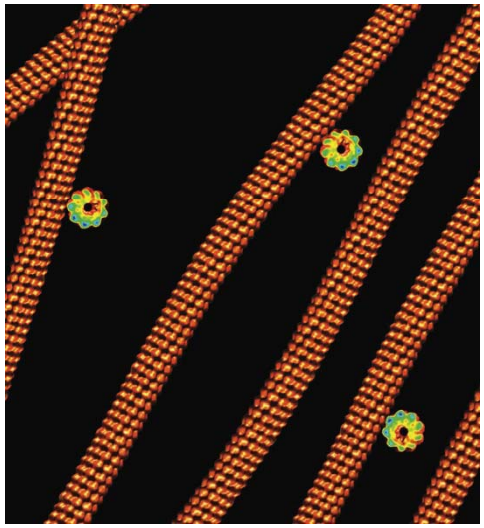


living with obesity

food and water…



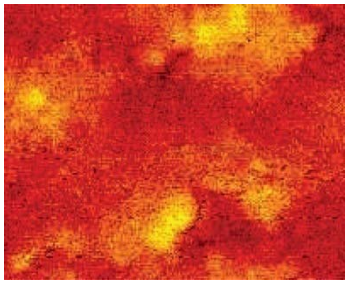
is brown rice good for you?

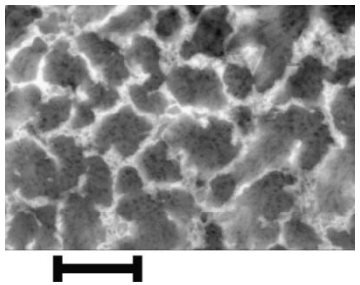


understanding plant viruses

jets and aerosols

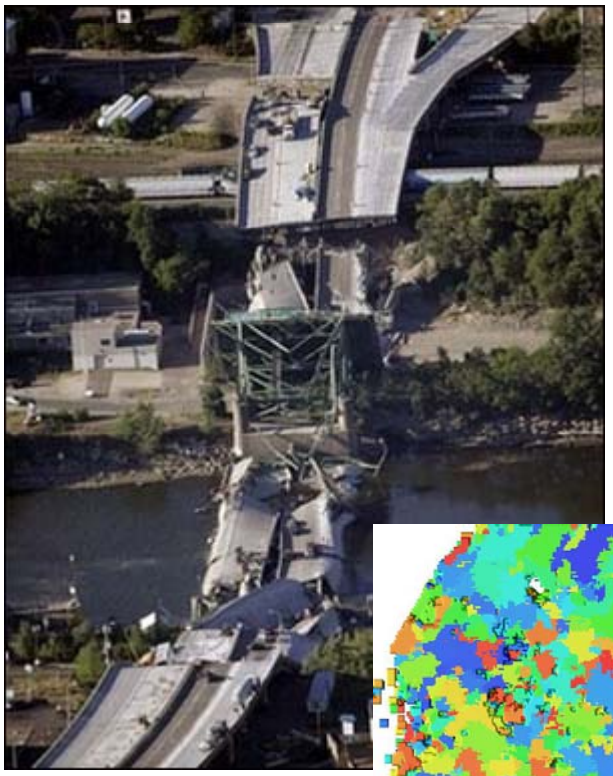
better infrastructure…

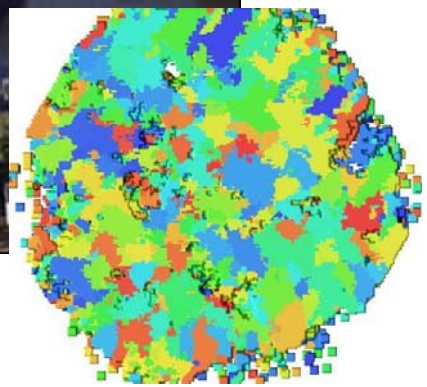




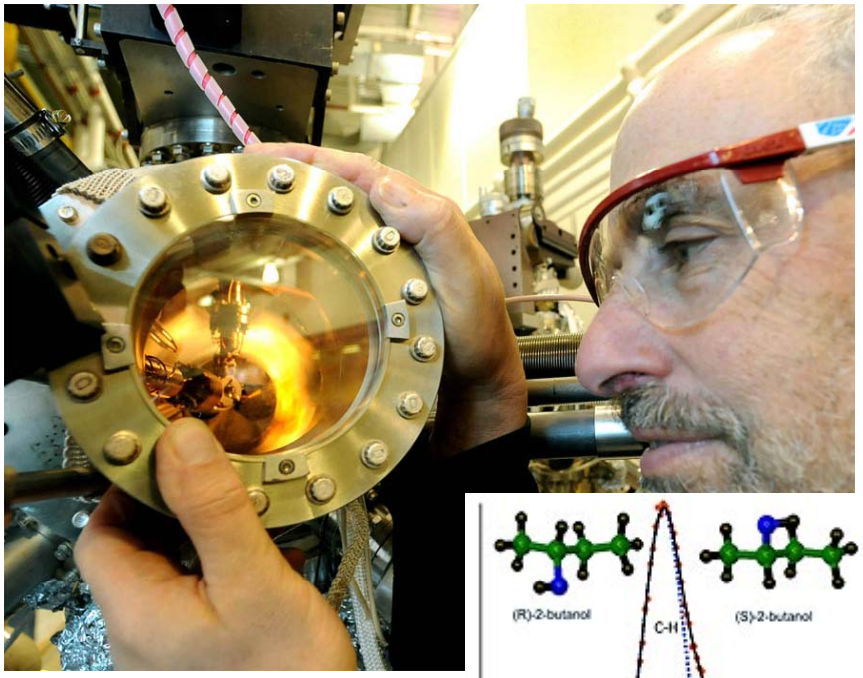
oxide scales
could save $1B for
US hydrogen industry

understanding metal fatigue
could save lives and money

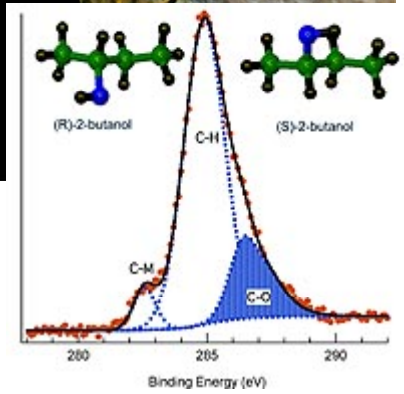




ancient history...

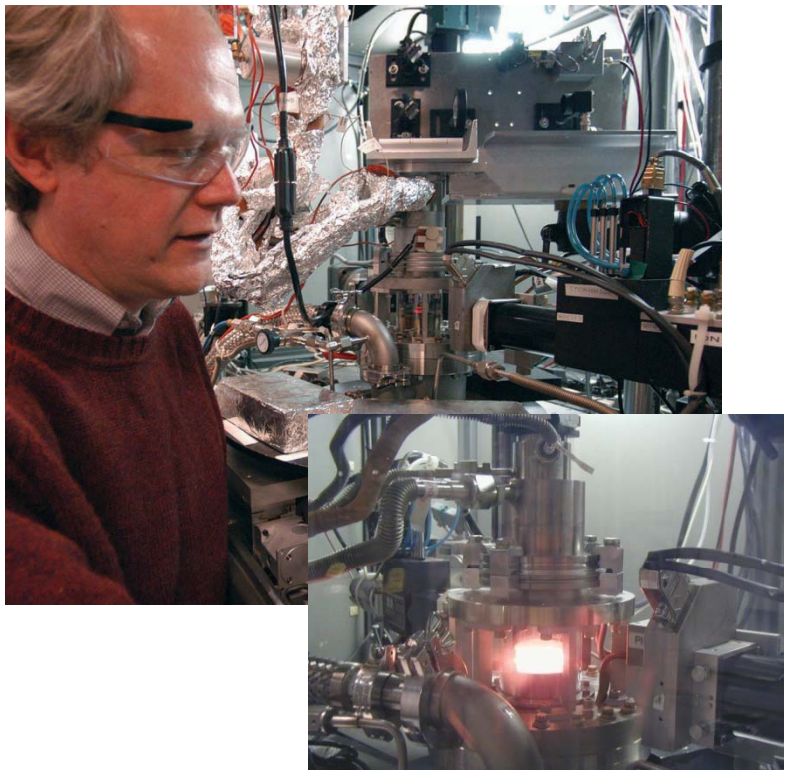


life began with
a twist

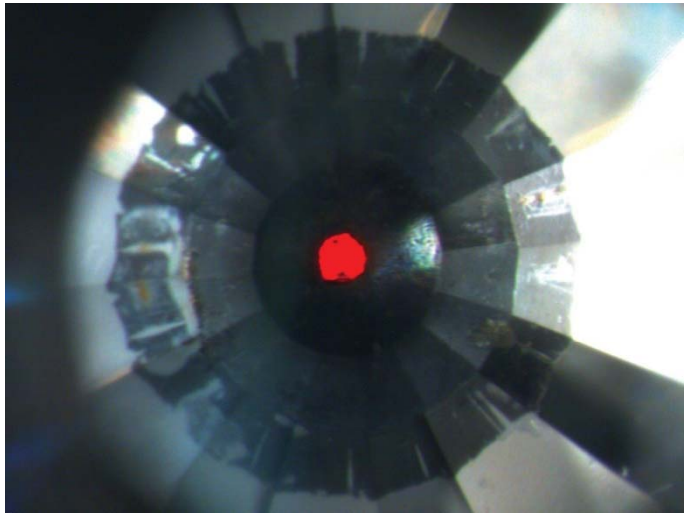


trading with the
enemy in 1000BC

and some very basic science that will enable new technology…

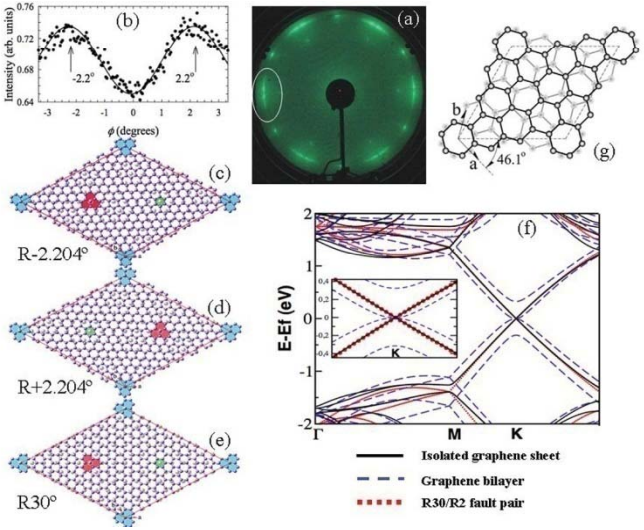


making waves for efficient lighting

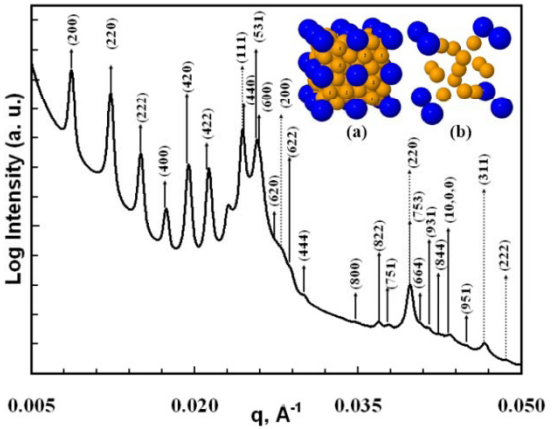


solid oxygen holds surprise at HP

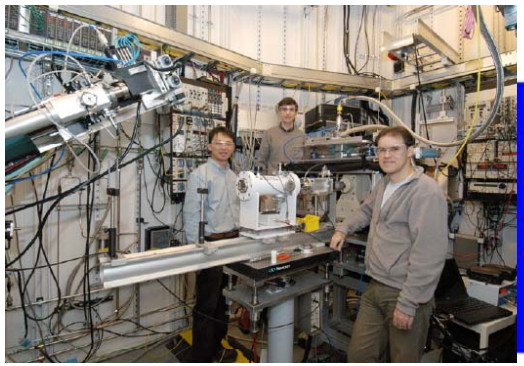
and economic competitiveness

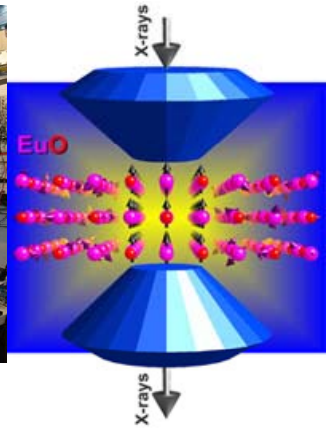


the road to "graphene" electronics



self-assembly of polymers

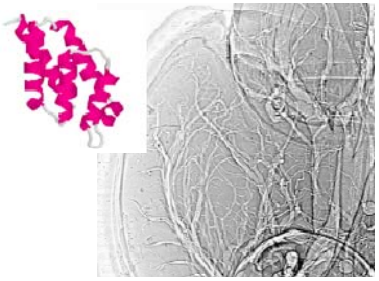




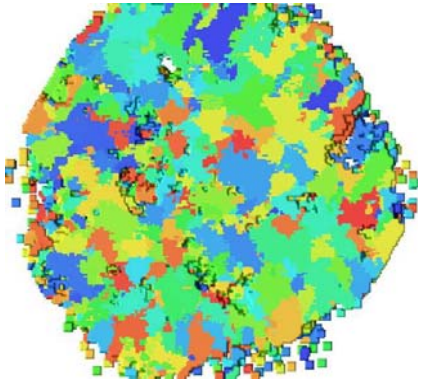
better magnetic materials

We have developed a medium term APS Renewal plan:

- Mastering hierarchical structures through x-ray imaging

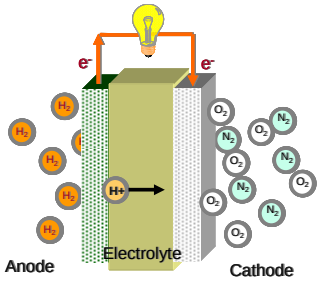


Images from proteins to living organisms will help connect the dots in understanding how genetics controls health and disease (image courtesy W.K. Lee)

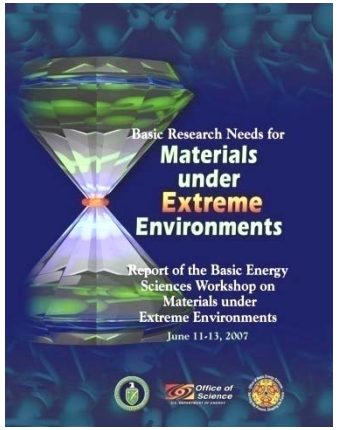


3-D distribution of grains in a 1 mm cube of Al (courtesy R. Suter)

- Real materials in real conditions in real time



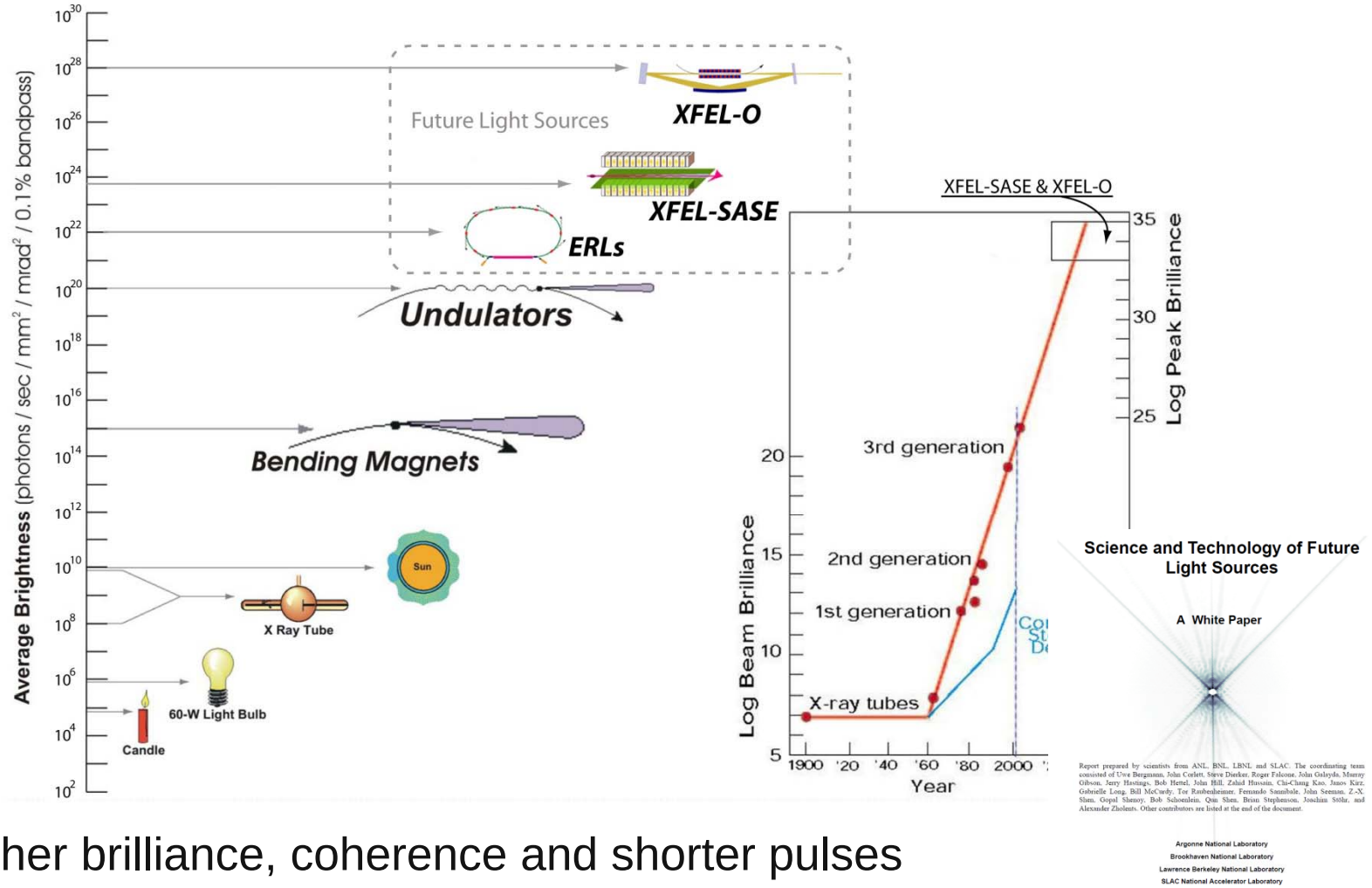
Schematic of an H_2 fuel cell



The cover of this BESAC report shows a diamond anvil cell. APS has been the most prolific source of high pressure science.

Scientific themes for renewal (aim for CD0 this summer)

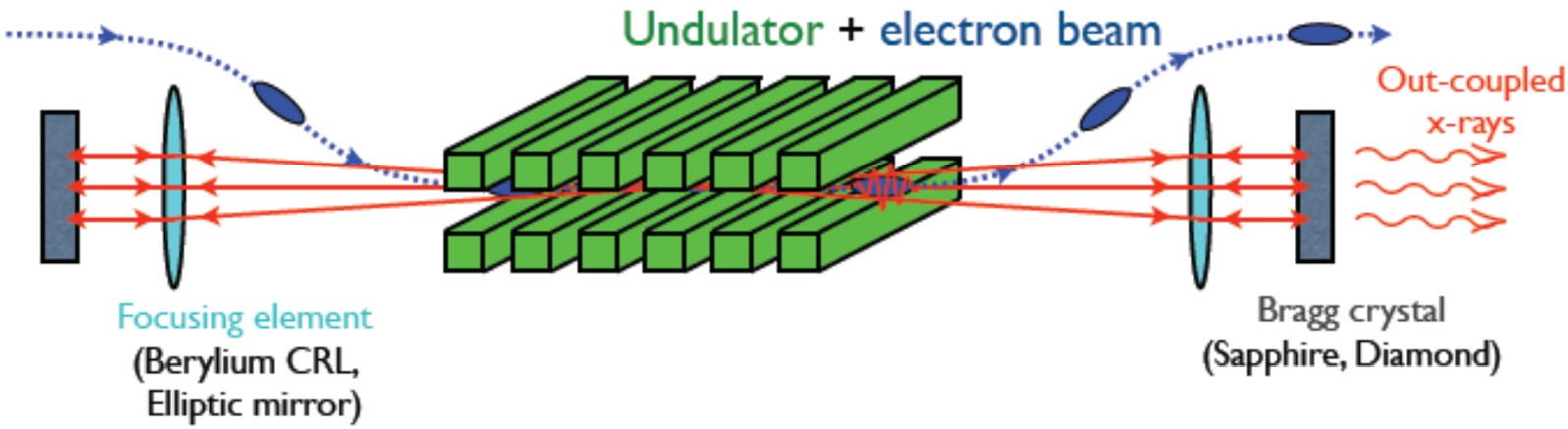
Longer term we are also evaluating future hard x-ray sources



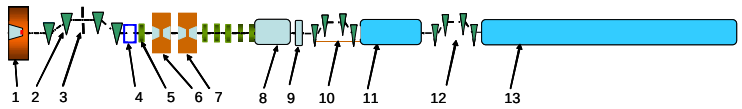
Offer far higher brilliance, coherence and shorter pulses

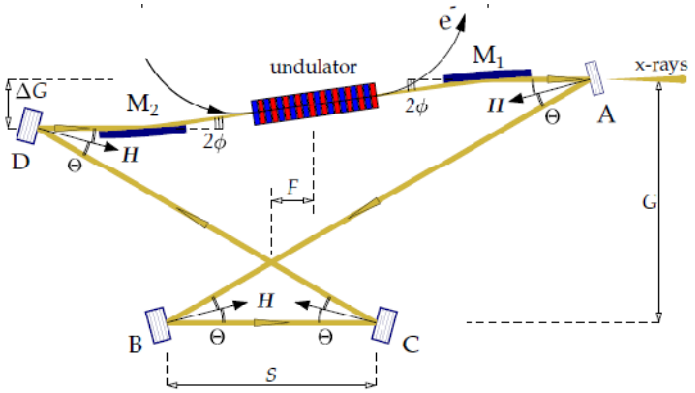
Complementary to storage ring sources

An X-Ray FEL Oscillator (XFELO) looks very promising



- Concept developed by Kwang-Je Kim and Yuri Shvyd'ko
- Active R&D program addressing feasibility is going on with very promising results

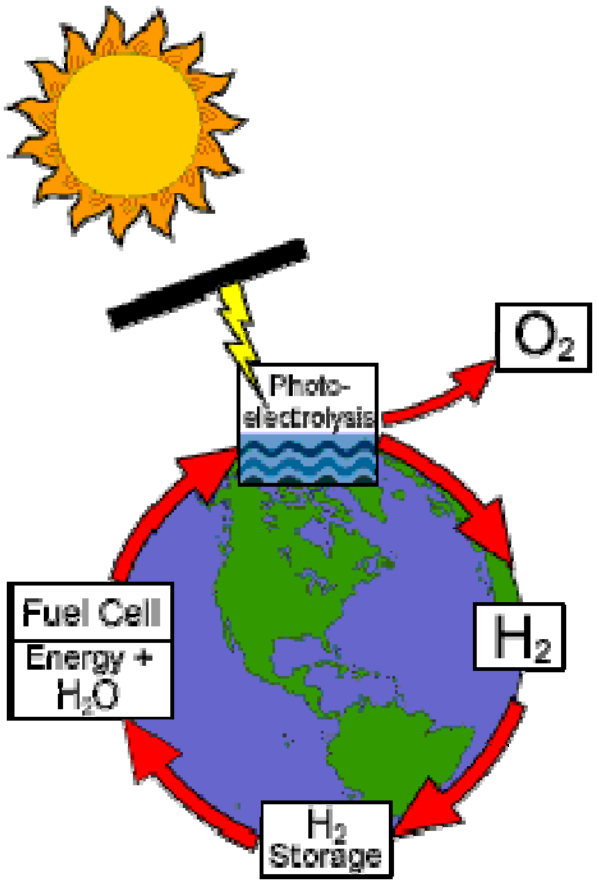


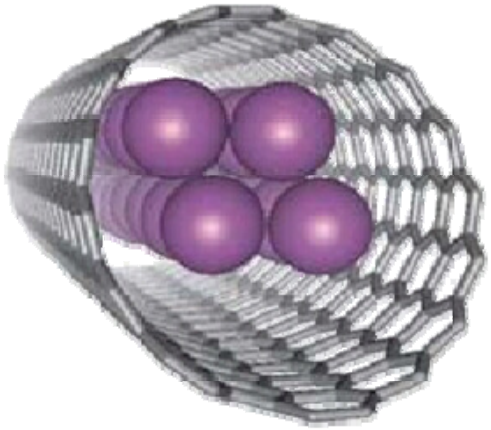


Neutron Applications to Materials

courtesy Ian Anderson, SNS

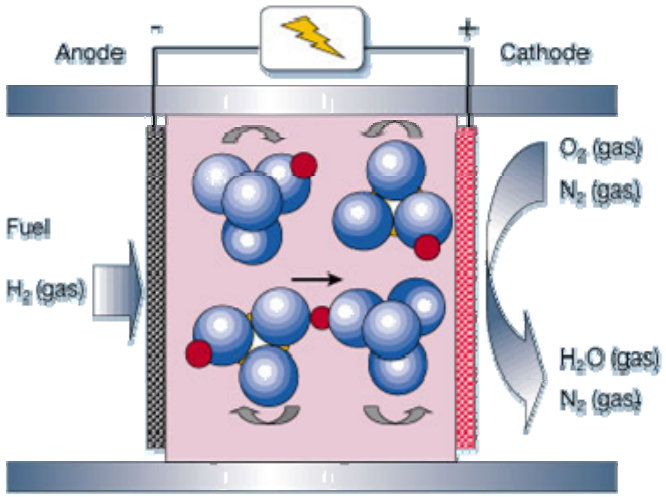
Neutrons are good for seeing hydrogen





H-storage

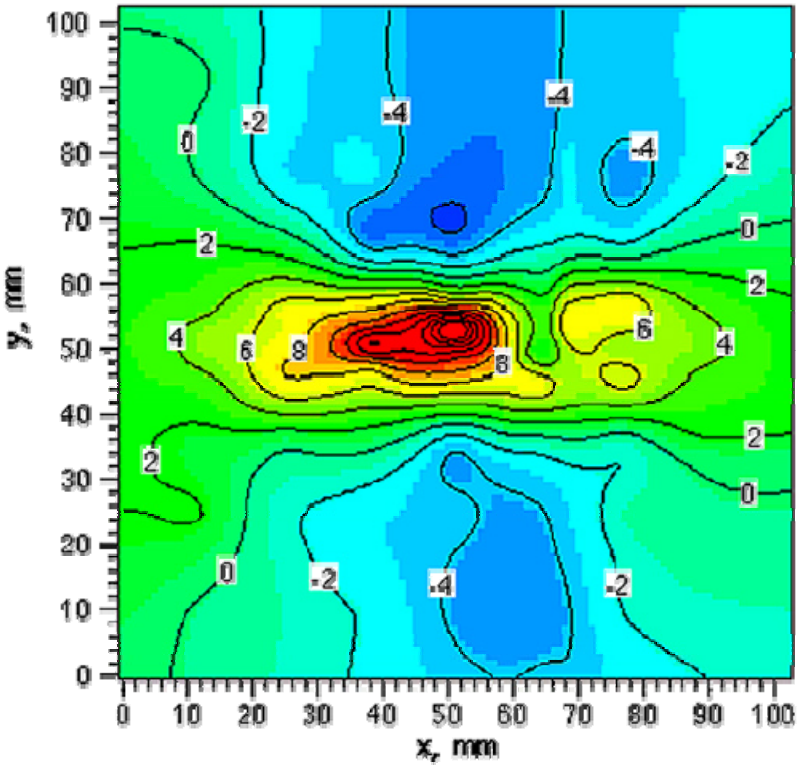
- **Structure**
- **Diffusion**
- **Aging**



Fuel cells

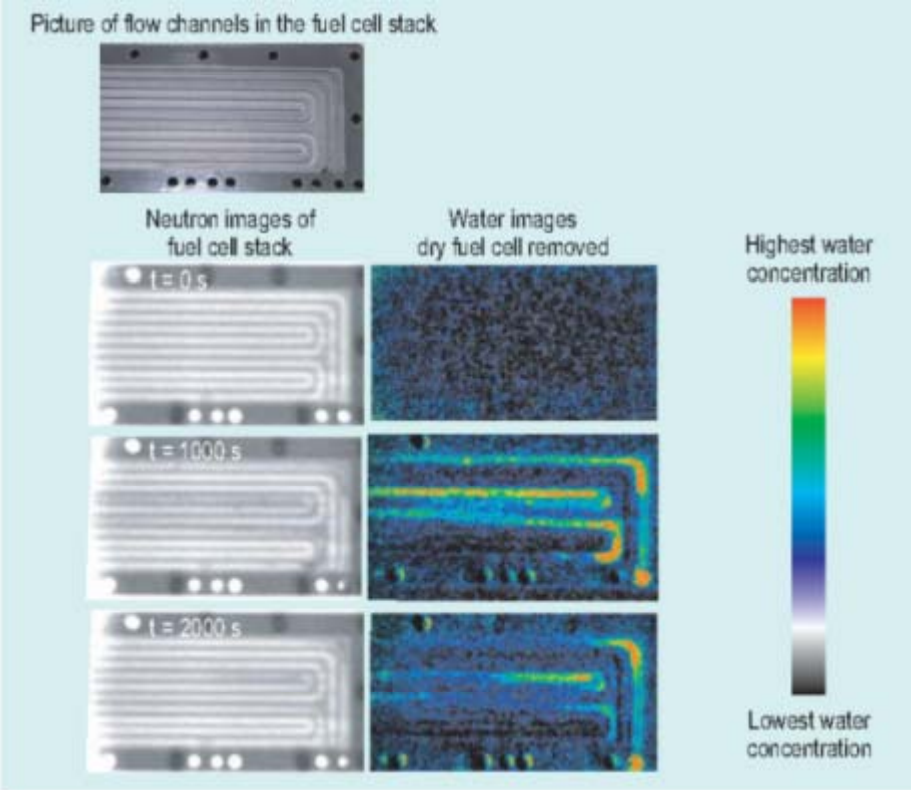
- **Electrochemistry**
- **Hydrogen transport**

A good problem for neutrons

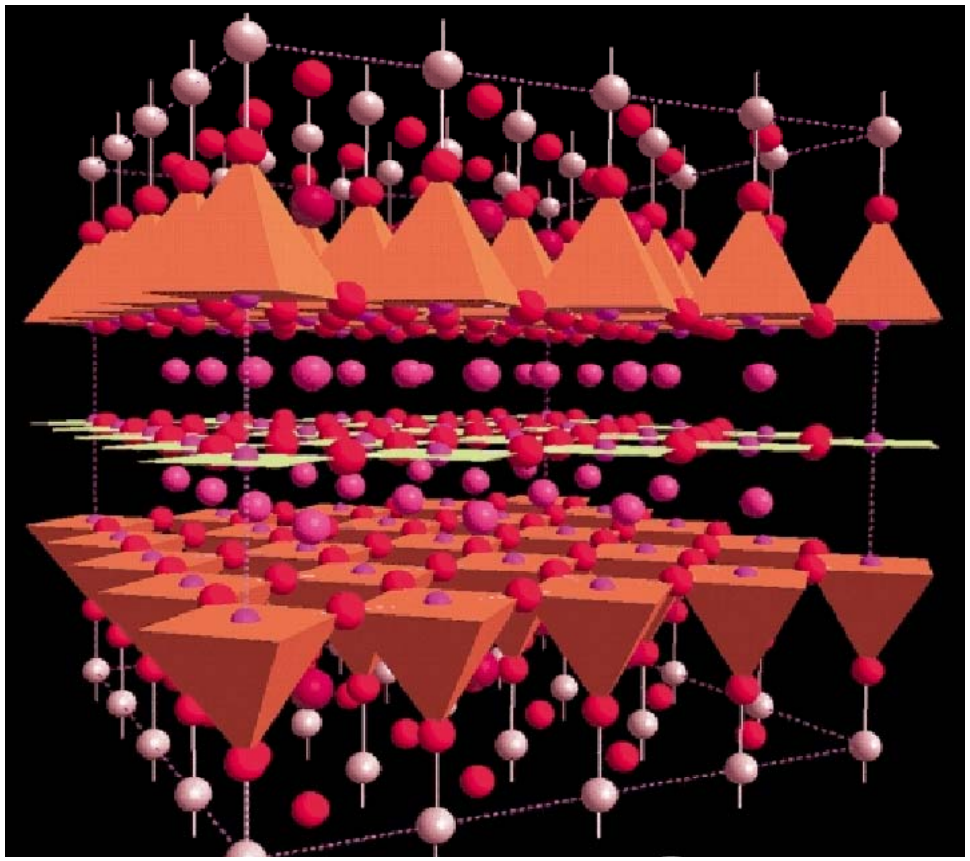


The aircraft of tomorrow: welding instead of rivets

Looking inside fuel cells



Water build up in the channels limits operation



Crucial oxygen positions revealed by neutrons

High temperature superconductors for the technology of tomorrow.

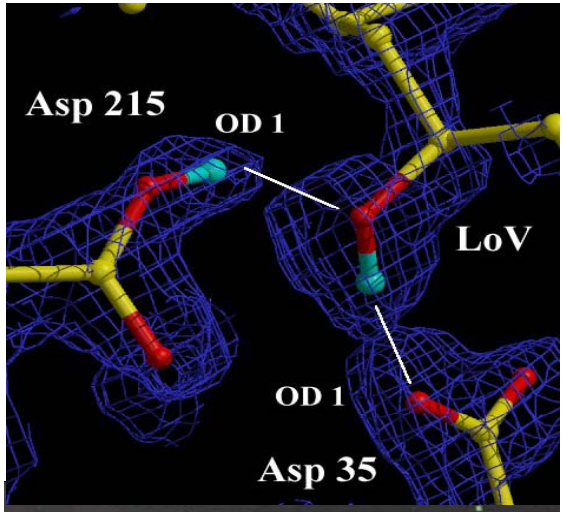
Neutrons and Structural Biology

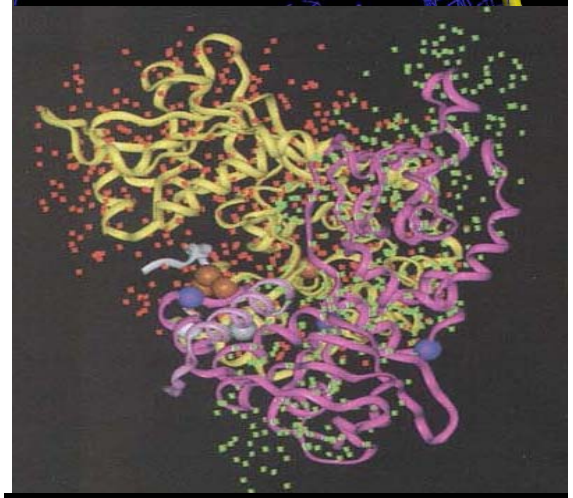
Neutrons are excellent probes for hydrogen

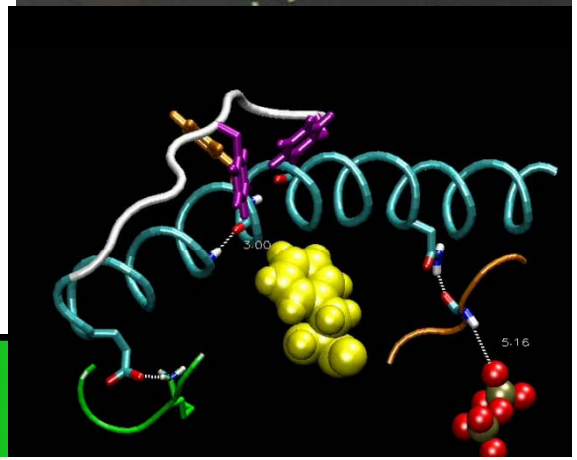
Function: enzyme mechanism; drug binding, proton shuttling & transfer

Structure: H/D labeled components in protein complexes and assemblies

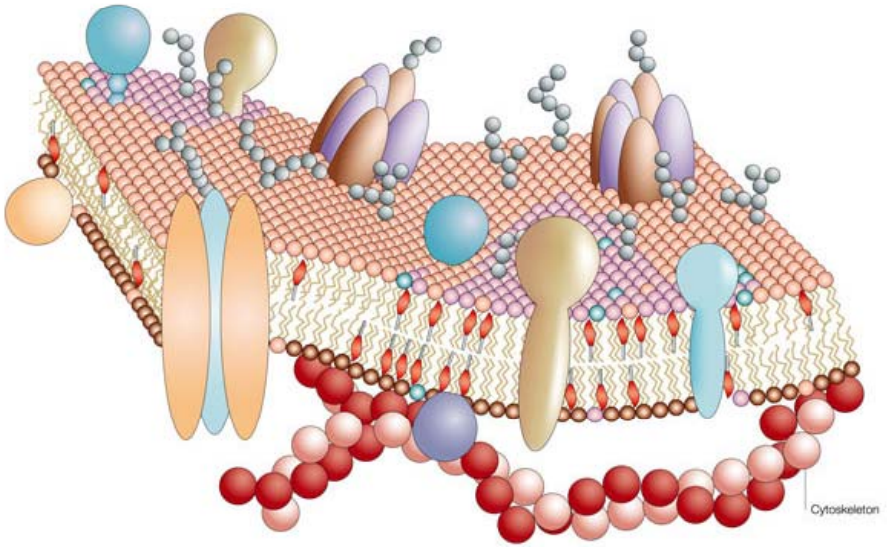
Dynamics: Mapping the molecular motions of life

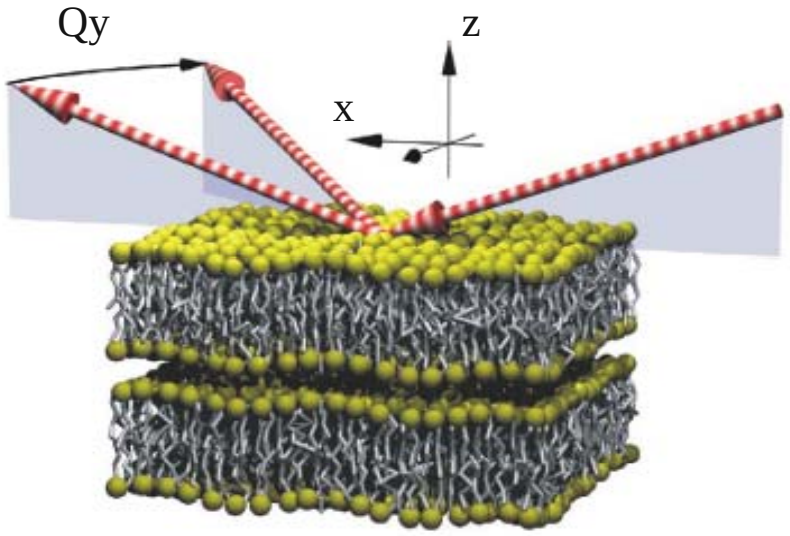






Understanding structure formation in membranes…





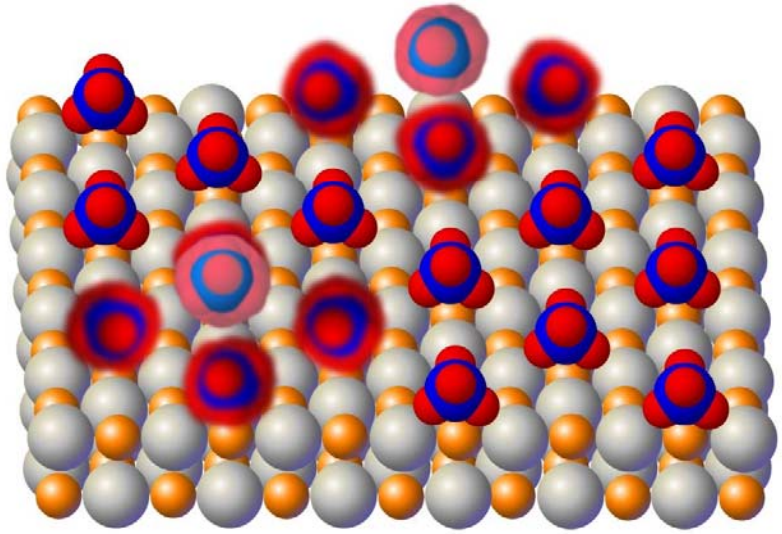
…and the dynamics

Local
- **Diffusion**
- **Rotation**
- **Chain defect motion**
- **Flip flop modes**
- **Vibrations**

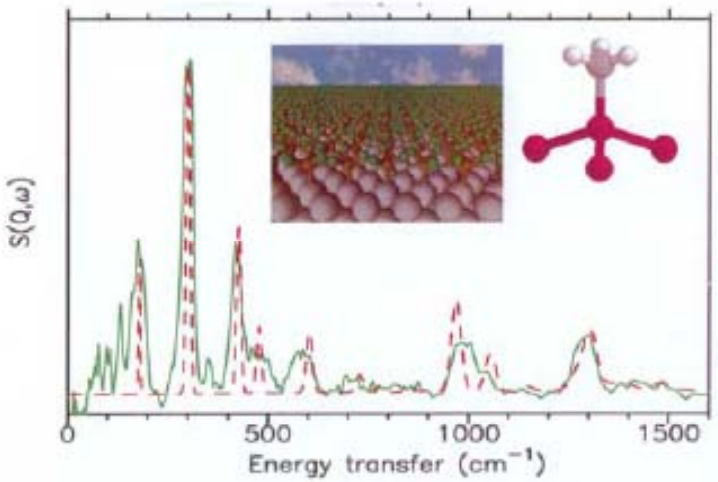
Collective
- **Membrane undulations**

Dynamics too!
Adsorbed Films on Nanoparticles

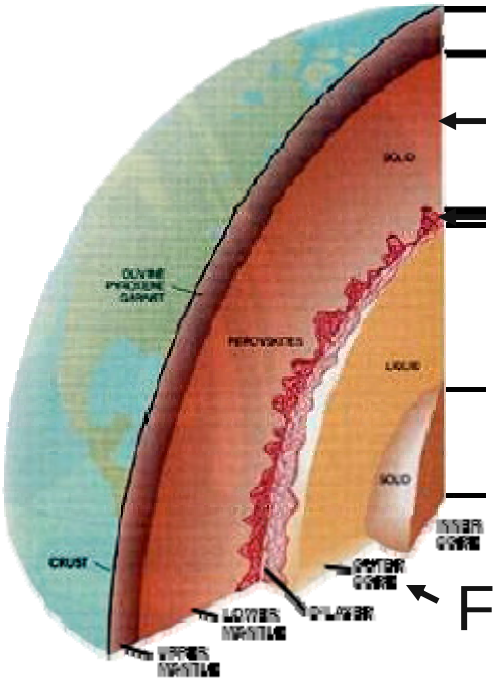
Neutrons are powerful probes of the structure and dynamics of adsorbed molecular films on nanoparticle surfaces and interfaces



Deactivation of an Industrial Pd catalyst



Studying the Earth

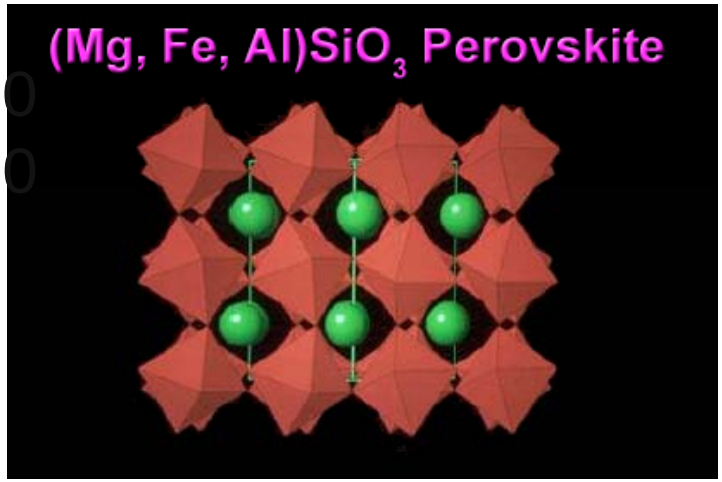


GPa **K**

25 2000

100 4000

Most abundant mineral in the planet



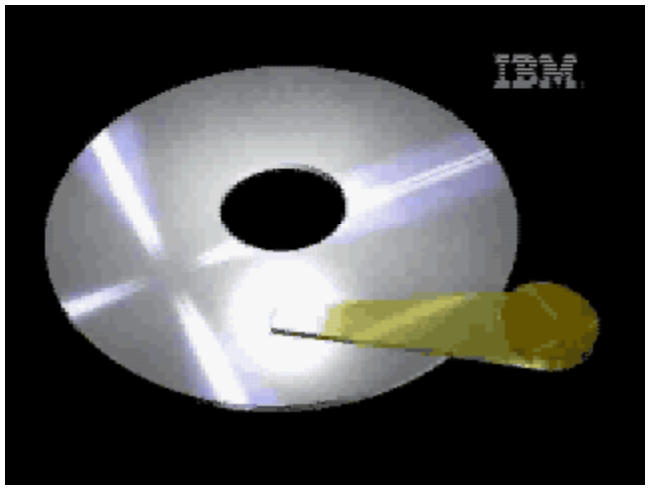
FeO, FeS, H

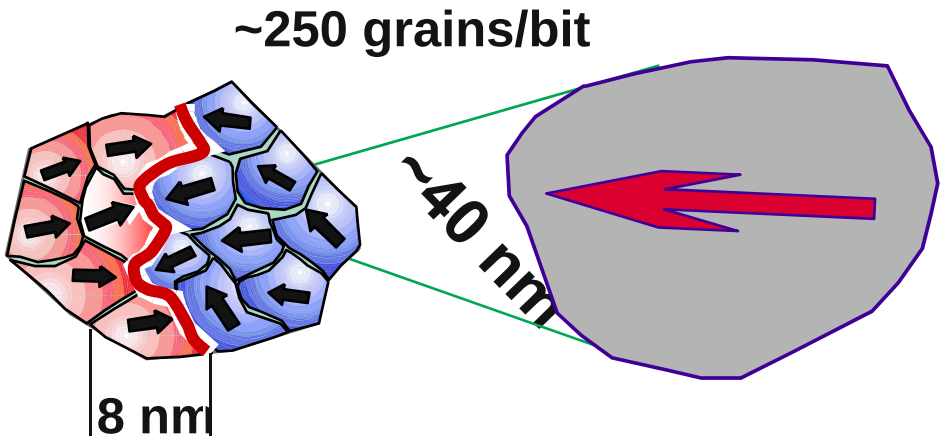
In situ melting temperatures?

Phase transitions?

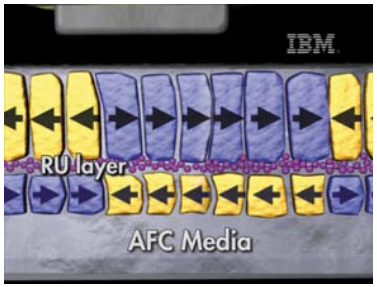
Pressure cell of the type to be employed on SNAP (Spallation Neutrons and Pressure) beamline

Hard Disk Technology





$$E = K_U V > 55\ k_B T \text{ (for 10 y stability)}$$



35 Gb/in^2

>100 Gb/in^2

Conclusions

- Accelerator-based sources of neutrons and x-rays have many uses
- Major impacts on society
  - Energy, environment, health, economy…
- These sources benefit from world-wide accelerator technology development, including nuclear and high-energy physics
- The techniques are complementary
  - Neutrons suited to larger samples
  - Good for very light elements
  - X-rays have higher spatial and temporal resolution
- Demand for ***more*** and ***better*** capabilities strong worldwide
- Dramatic improvements in x-ray production with next generation and improved sources offer major impacts