Meeting The Challenges In Biomaterials Research Using Neutrons

Ian Anderson and J.K. Zhao
Spallation Neutron Source
Oak Ridge National Laboratory

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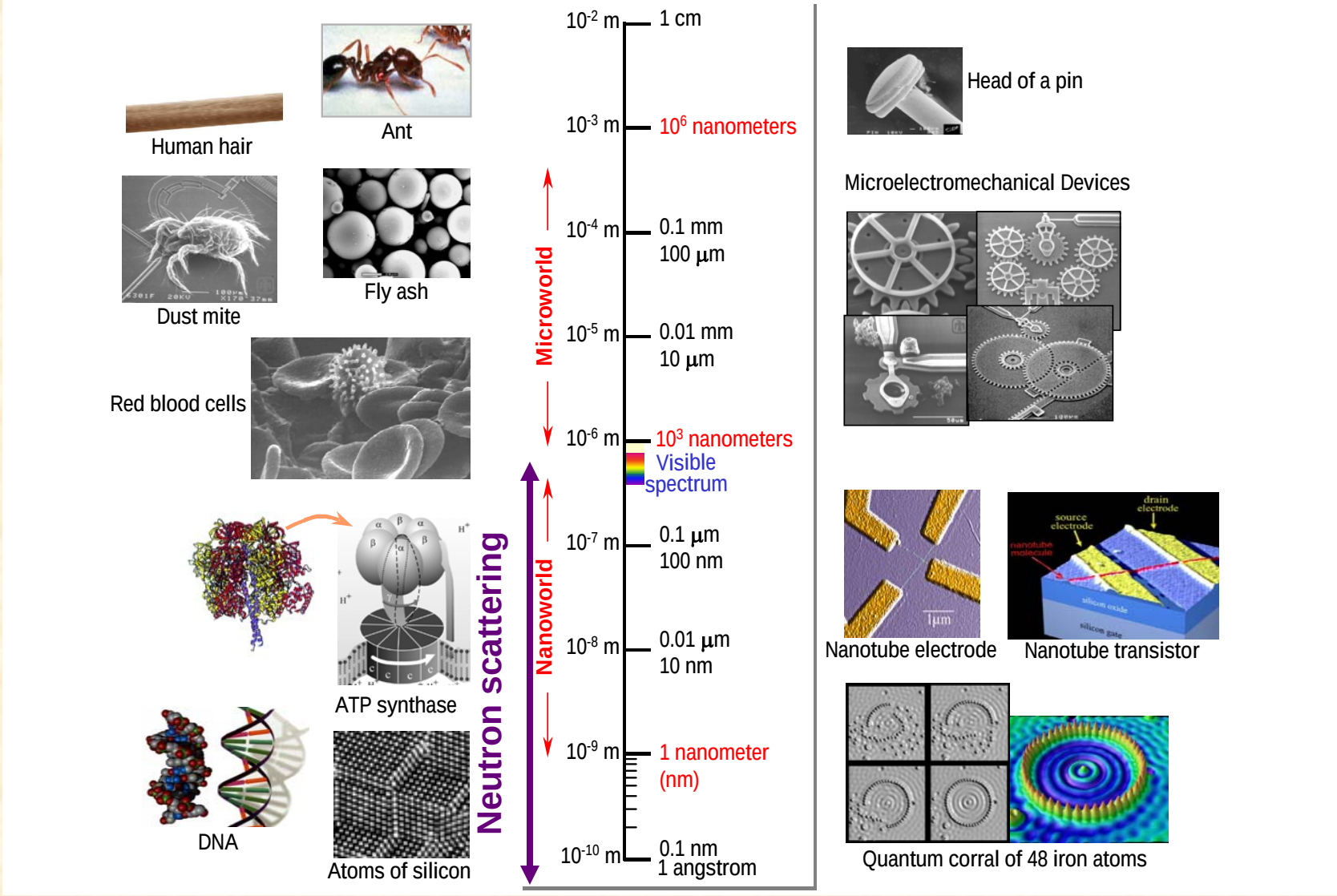
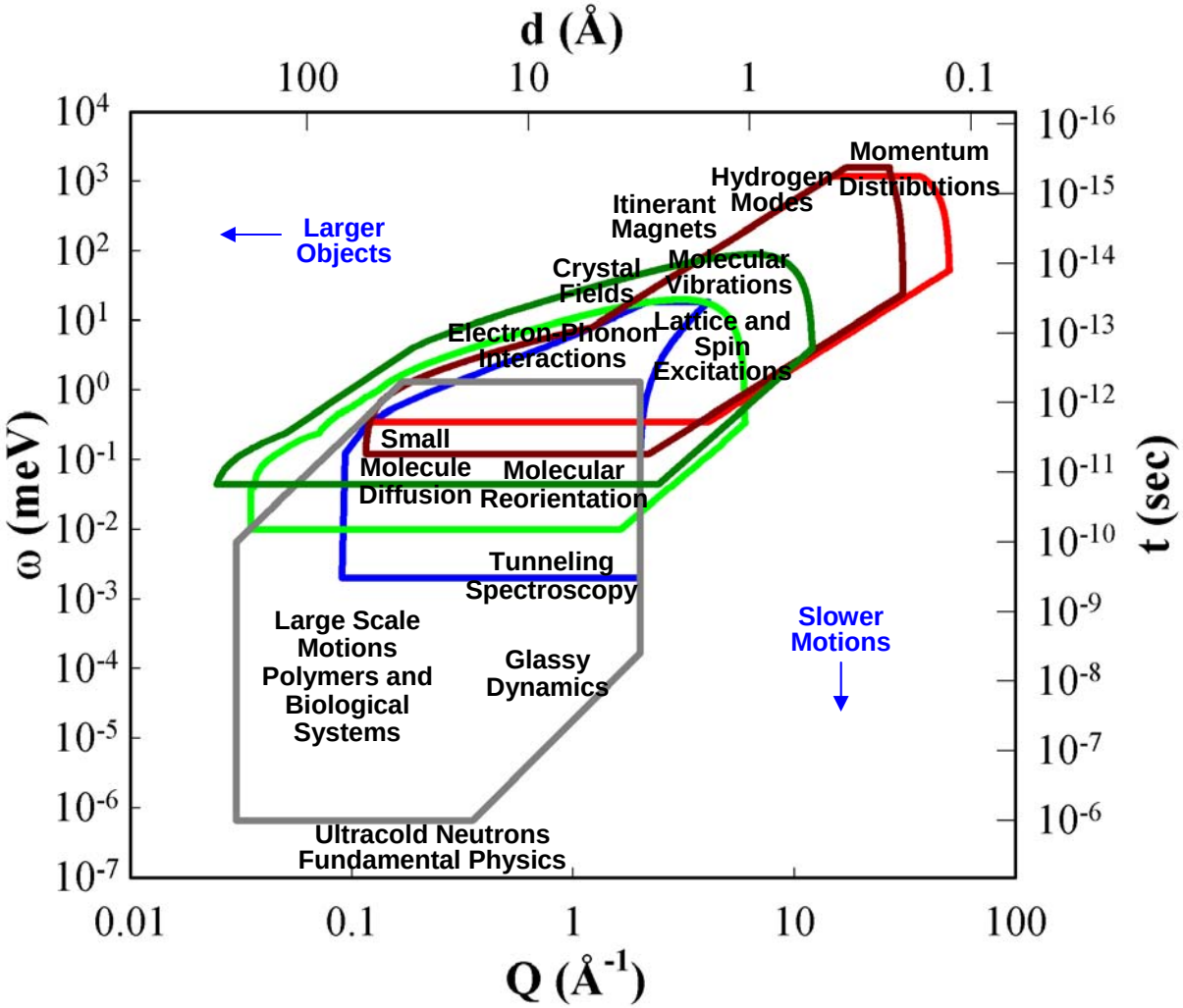
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Neutrons: microns to angstroms!



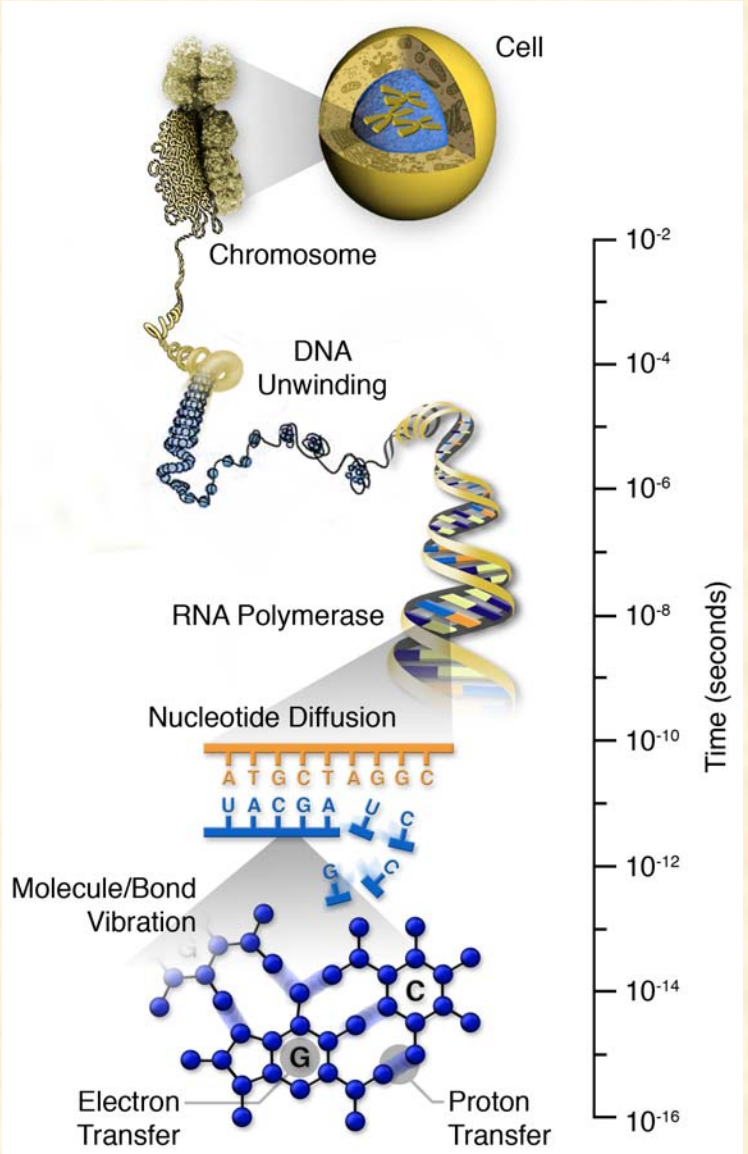
We get the dynamics too!



- ARCS Fermi Chopper
- SEQUOIA Fermi Chopper
- HYSPEC
- Cold Neutron Chopper Spectrometer
- Backscattering
- Neutron Spin Echo

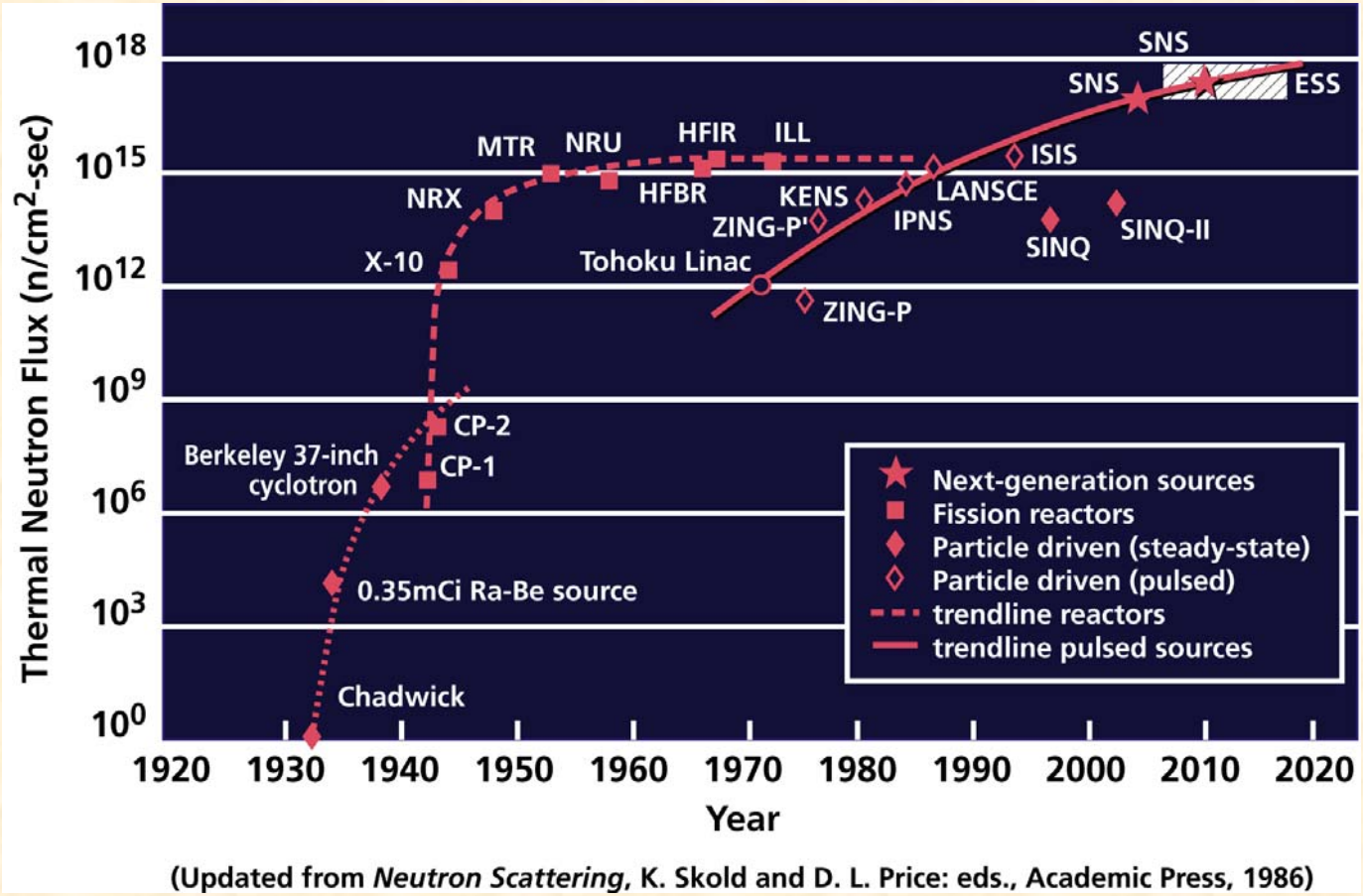
Time scales relevant to Biology

New instrumentation will allow us to access the time relevant time scales



We are often limited by neutron fluxes

Reactors have reached the limit at which heat can be removed from the core
Pulsed sources have not yet reached that limit and hold out the promise of higher intensities



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

The Spallation Neutron Source

- The SNS will begin operation in 2006
- At 1.4 MW it will be the world's leading pulsed spallation source
- The peak neutron flux will be ~20–100x ILL
- SNS will be the world's leading facility for neutron scattering
- It will be a short drive from HFIR, a reactor source with a flux comparable to the ILL

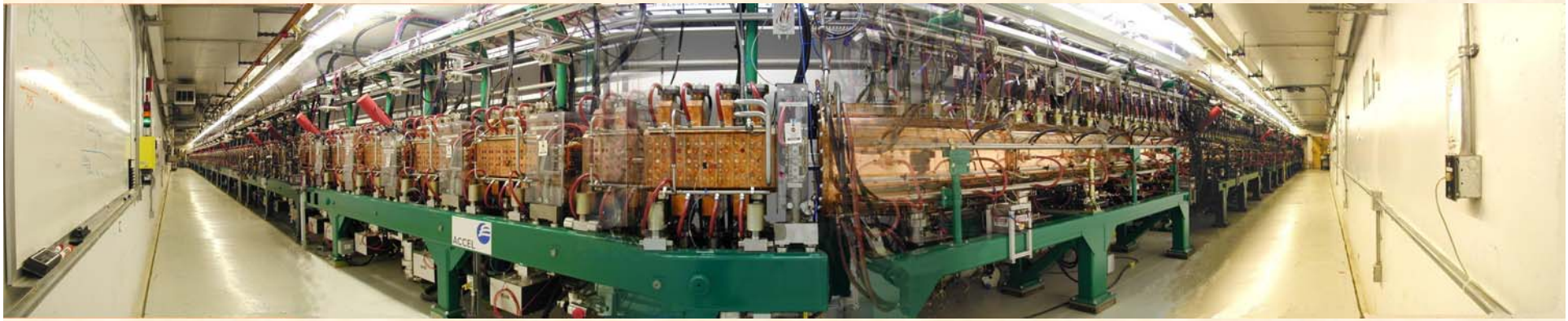
SNS - Guiding Principles

- **SNS will provide high availability, high reliability operation of the world's most powerful pulsed neutron source.**
- **It will operate as a User Facility to support peer reviewed research on a Best-in-Class suite of instruments**
  - **Research conducted at SNS will be at the forefront of biology, chemistry, physics, materials science and engineering**
- **SNS will have the capability to advance the state of the art in spallation neutron source technology. This includes:**
  - **R&D in accelerators, target, and instruments to keep SNS at the forefront**
  - **Planned enhancement of SNS performance through upgrades of the complex and ongoing instrument development as part of the normal operating life of the facility**

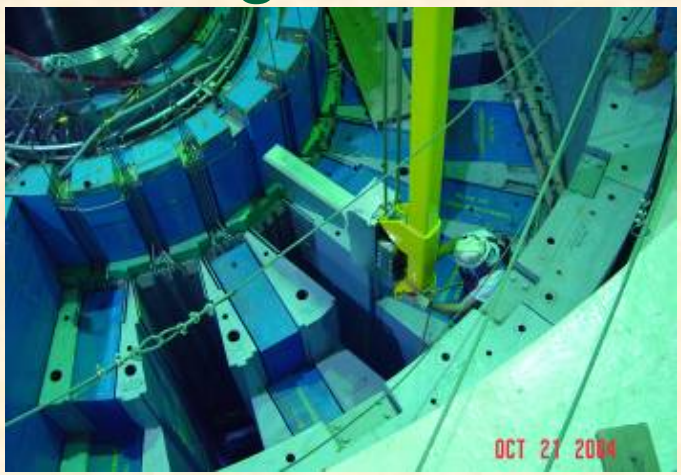
ORNL has a lot to offer....

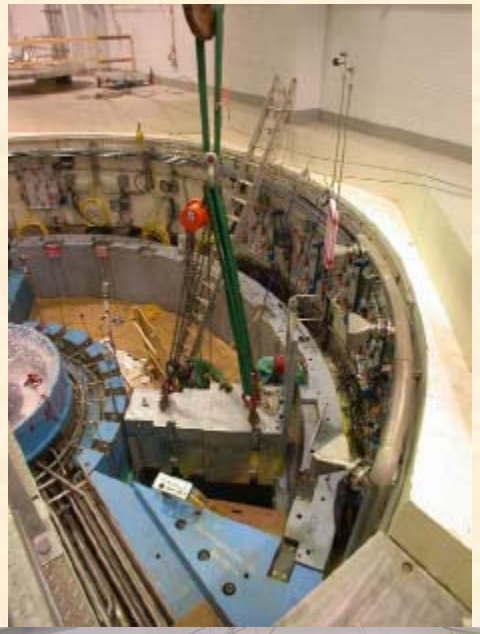
- **Neutron Scattering**
  - **HFIR**
  - **SNS**
  - **Joint Institute for Neutron Scattering**
- **Centre for Nanophase Materials Sciences**
- **Computational Resources**
  - **Center for Computational Sciences,**
  - **National Leadership Computing Facility**
- **Electron Microscopy**
  - **Shared Research Equipment (SHaRE) User Program**
  - **High Temperature Materials Laboratory**
  - **Condensed Matter Sciences Division electron microscopy program**

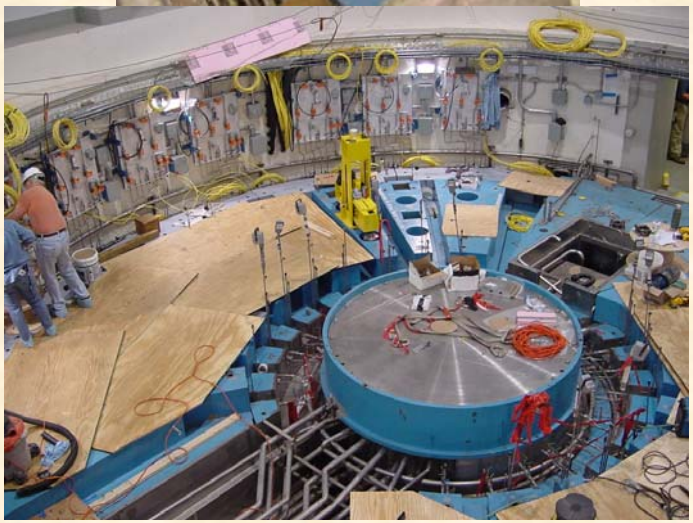
Linear Accelerator

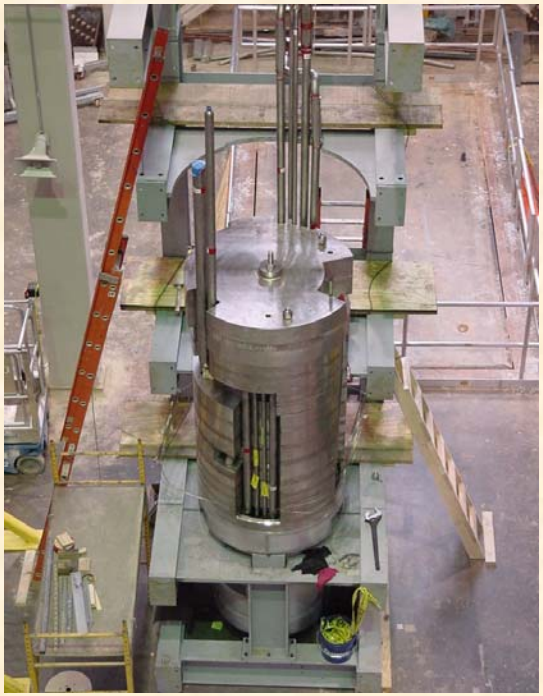


Target installation

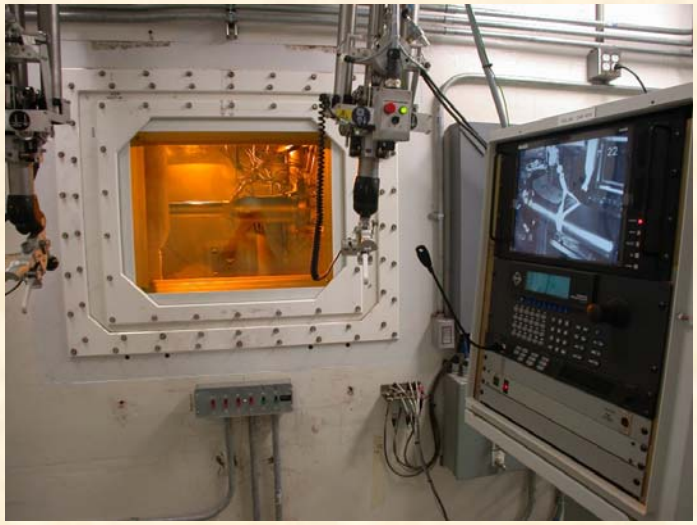




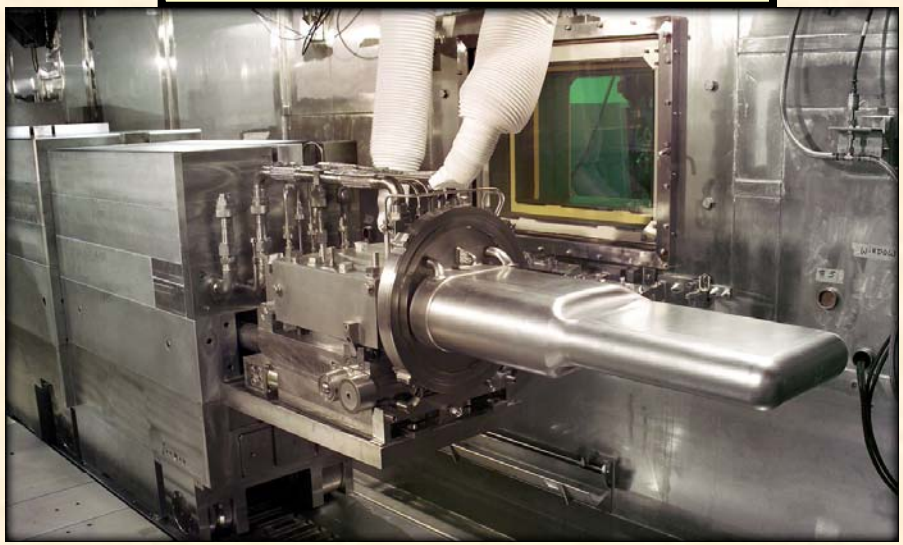




Mercury Target



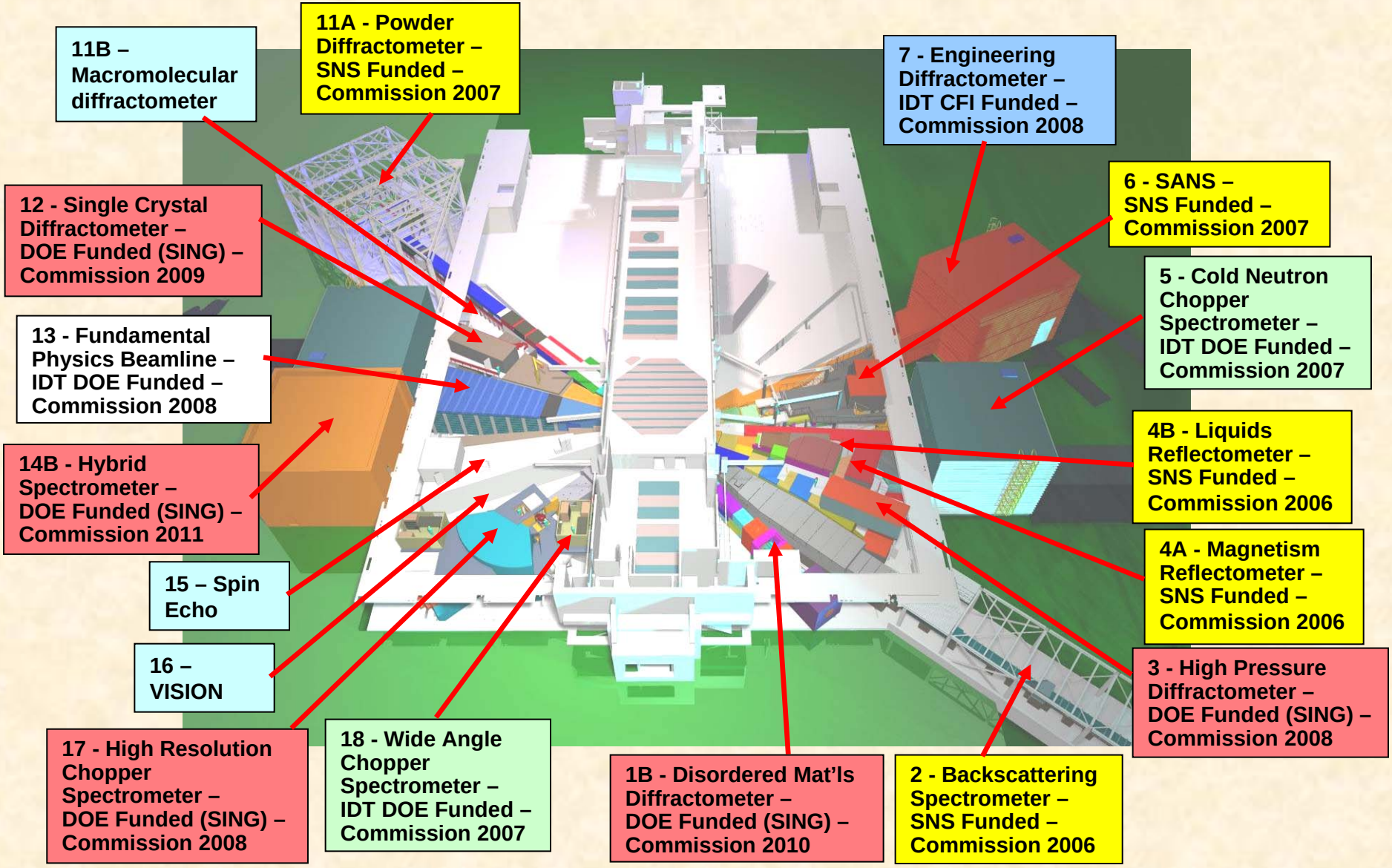
Target installed on Carriage



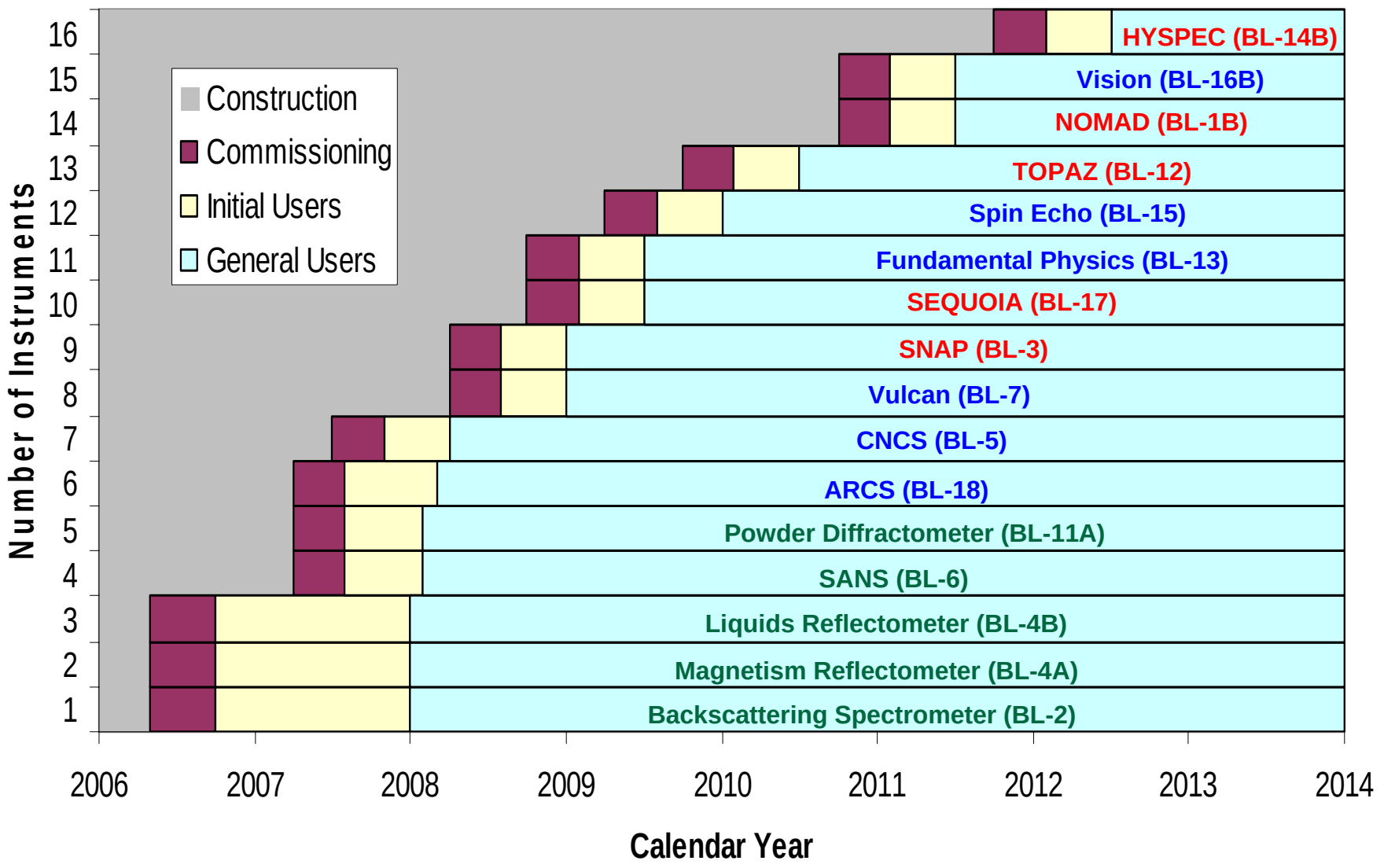
Remote Handling

You can teach the robots anything....

17 Approved Instruments and more to come



Schedule for Funded Instruments



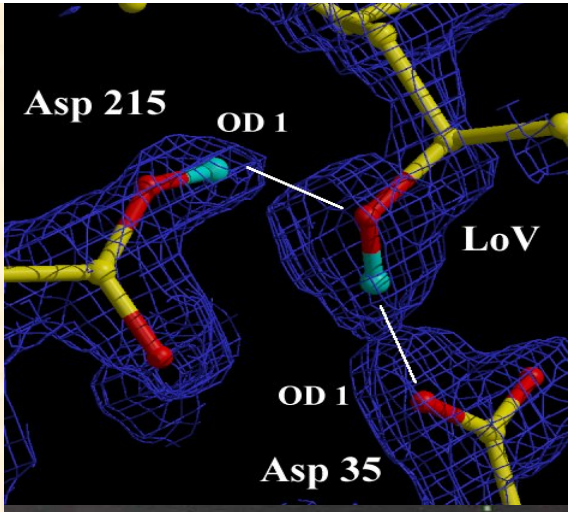
Neutrons and Structural Biology

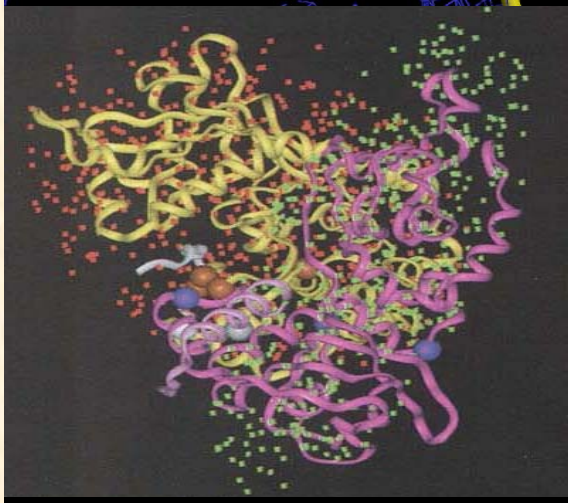
Neutrons are excellent probes for hydrogen

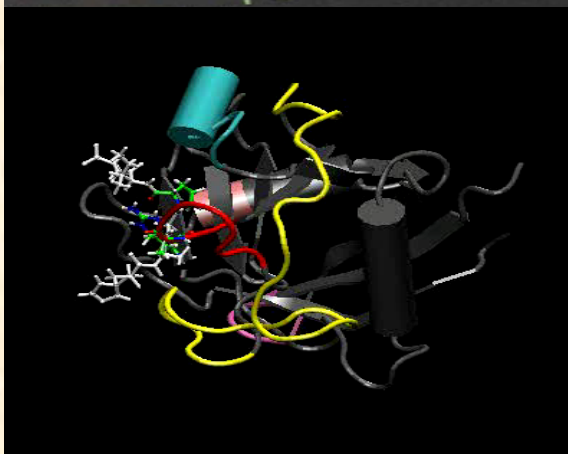
- **Function:** enzyme mechanism; drug binding, proton shuttling & transfer

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

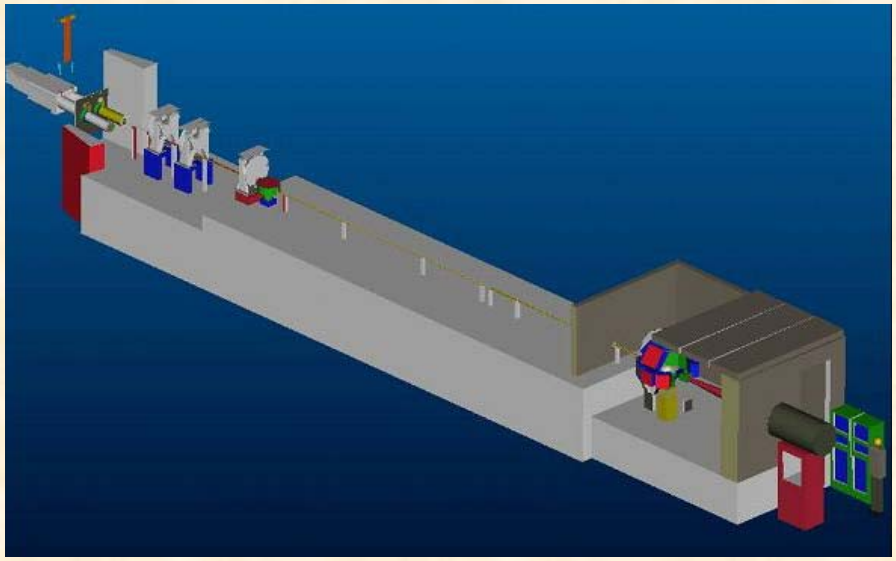
- **Dynamics:** Mapping the molecular motions of life







Mandi – Neutron Macromolecular Crystallography



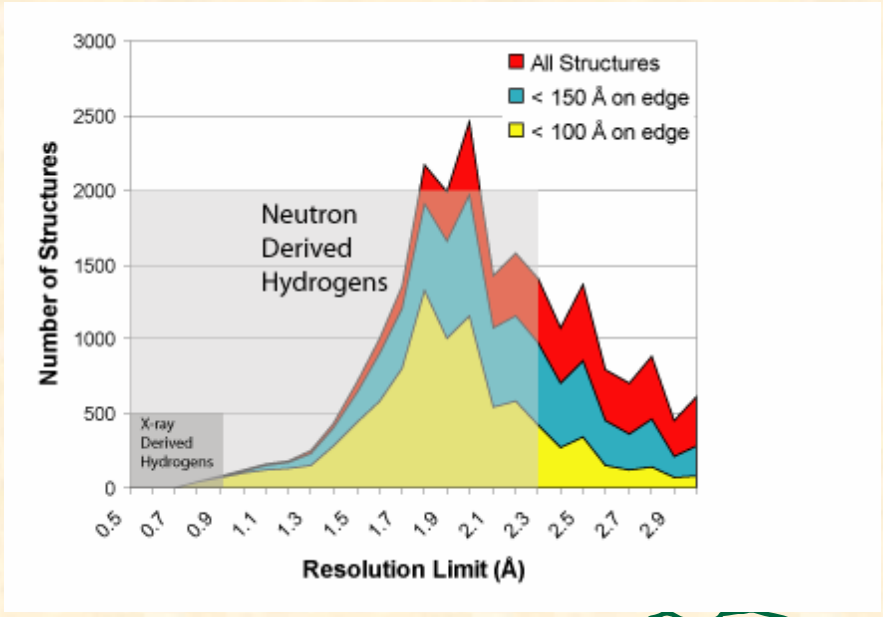
Design Criteria

d_{min} = 1.5 to 2.0 Å for crystals with a lattice constant *a* up to 150 Å

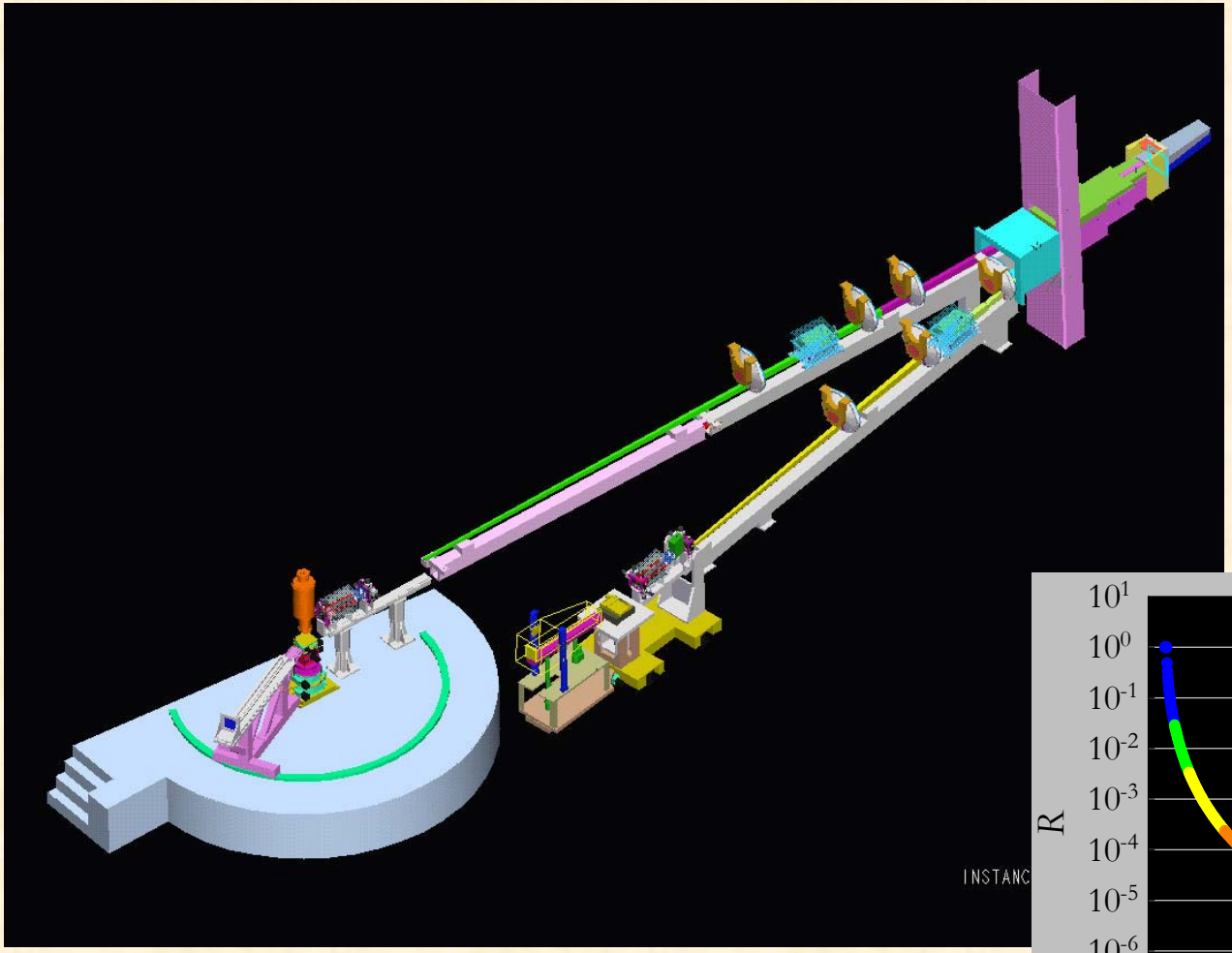
d_{min} = 2.5 to 3 Å for a lattice constant *a* = 150 -300 Å

Fully optimized for high resolution and throughput

Data collection rates 50 times higher than current capabilities

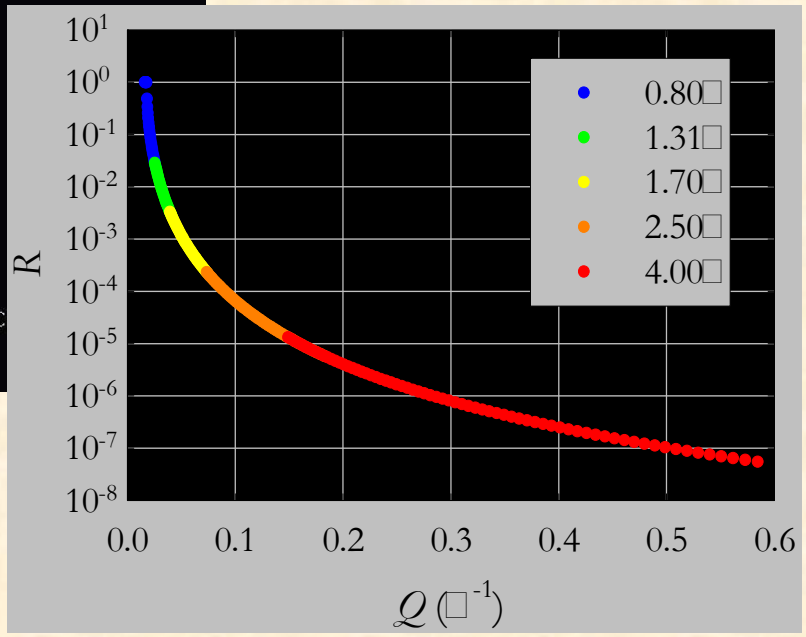


Reflectometry Beamlines



Magnetism:
vertical sample
Liquids:
horizontal sample

$R_{min} < 5\times10^{-10}$
$Q_{max} \sim 1.5$ Å^{-1}
$d_{min} \sim 7$ Å



5 mins to measure D_2O surface

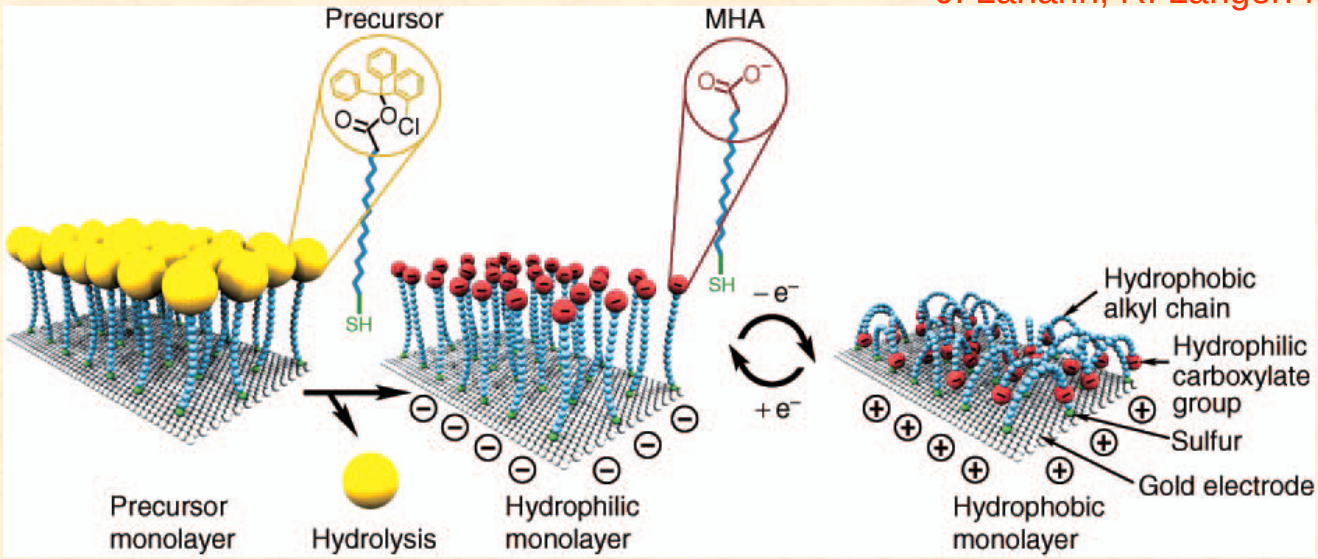
Liquids Reflectometer Science

- **Phase separation in polymer films**
- **Inorganic templating at air/water interfaces**
- **Complex fluids under flow**
- **Vesicles and gels**
- **Reaction kinetics**
- **Surfactants at interfaces**
- **Interfacial structure in drug delivery systems**
- **Membranes and their intermolecular interaction**
- **Protein adsorption**
- **Critical phenomena in fluid systems**
- **Biocompatibility and sensors**

Biomimetics – functional surfaces

Dynamically Controlled Surface Properties (T, pH, Light, V, etc.)

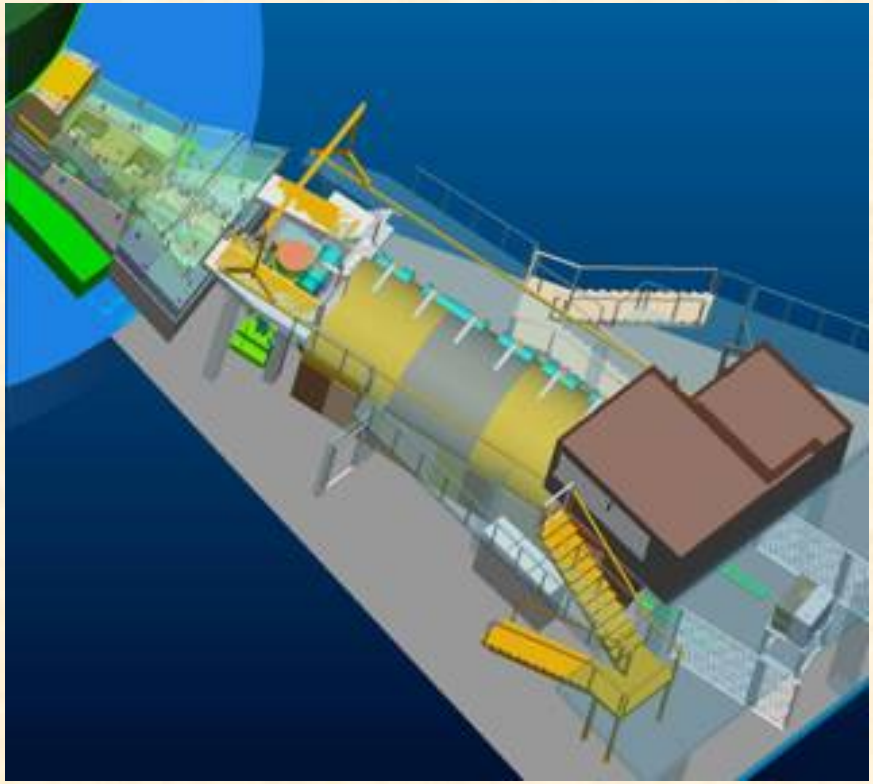
J. Lahann, R. Langer: MRS Bulletin

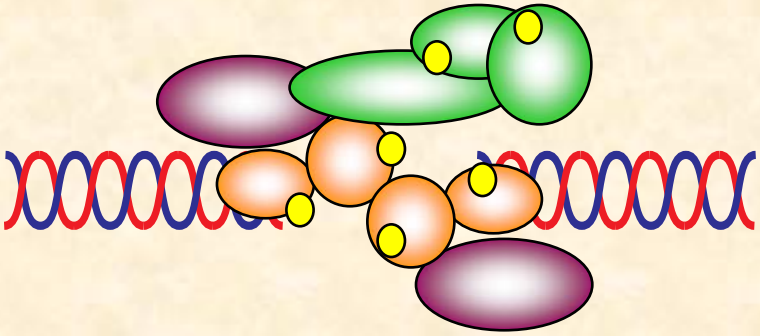


Applications:

- Biosensors
- Microfluidic devices (valves, reservoirs)
- Structural templates for tissue engineering
- Drug delivery
- Study of cell/cell and cell/protein interactions

SANS





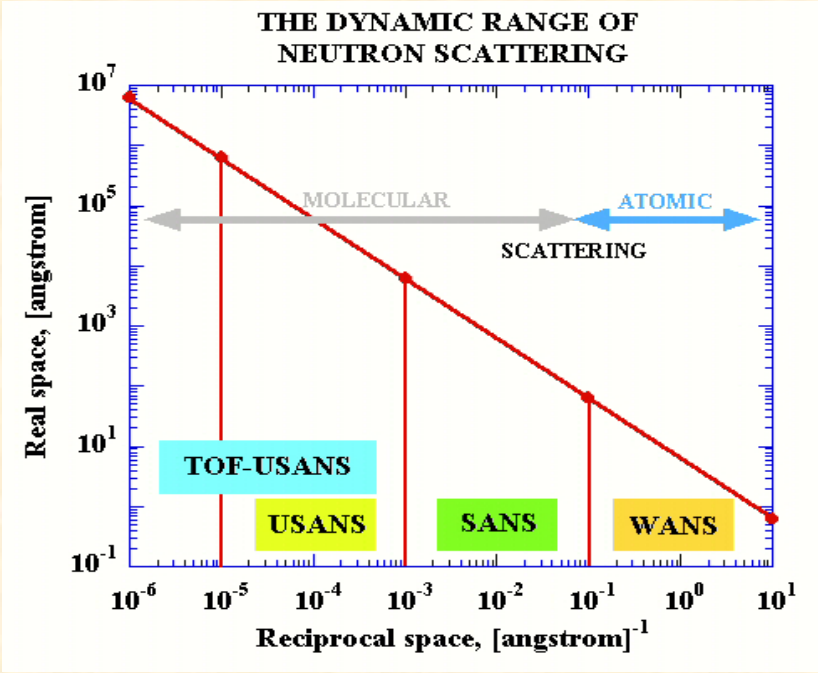
EQ-SANS Features:

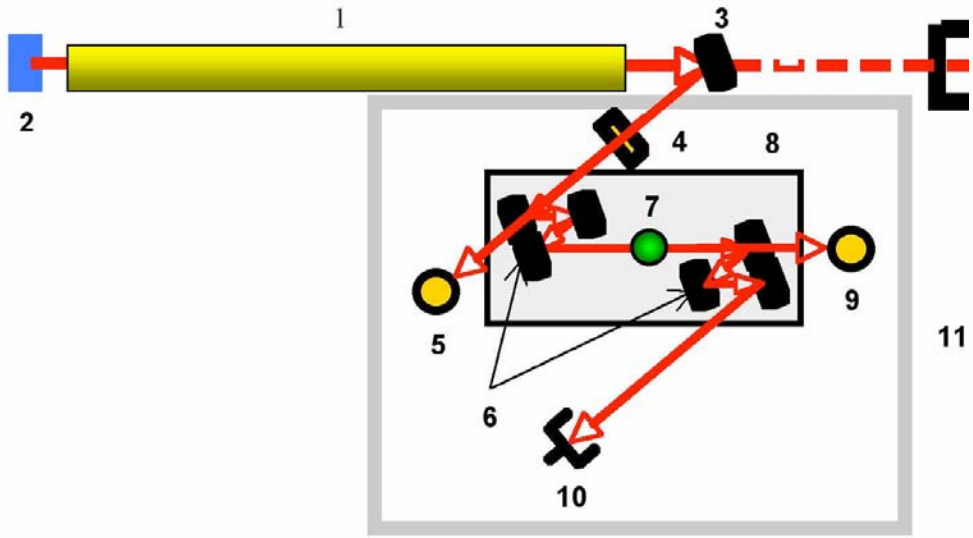
- Covers multiple length scales
- High intensity
- Very high wavelength-resolution

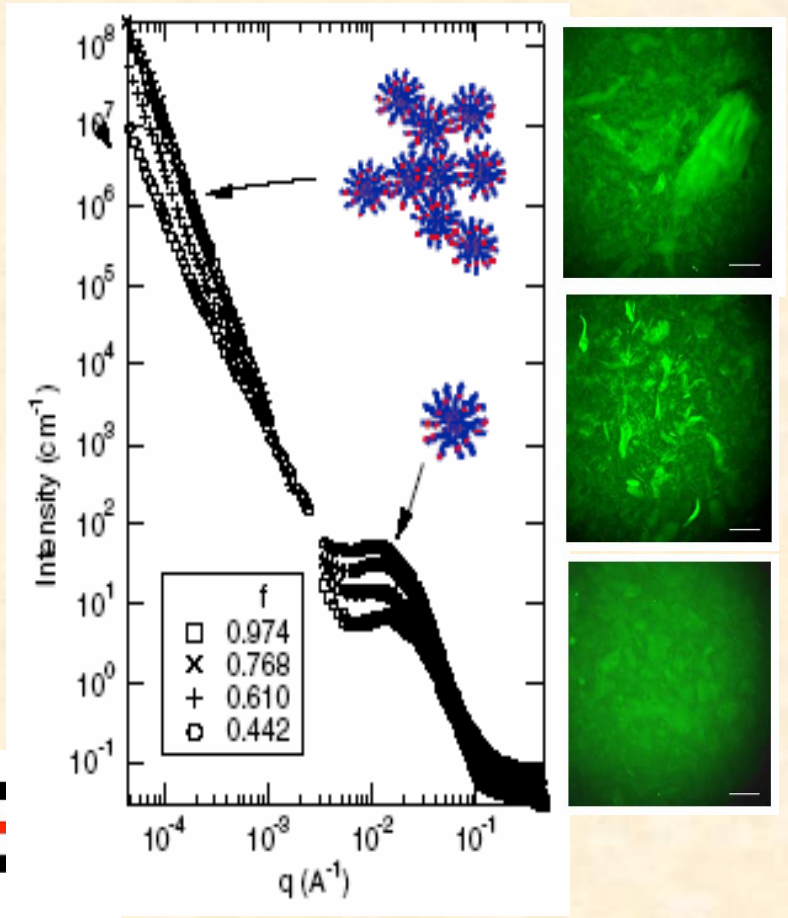
Example Applications:

- Protein/DNA, protein-membrane structures, functions and interactions
- Vesicles for drug delivery
- Complex fluid, polymers, aerosols, micelles etc.

MicroSANS





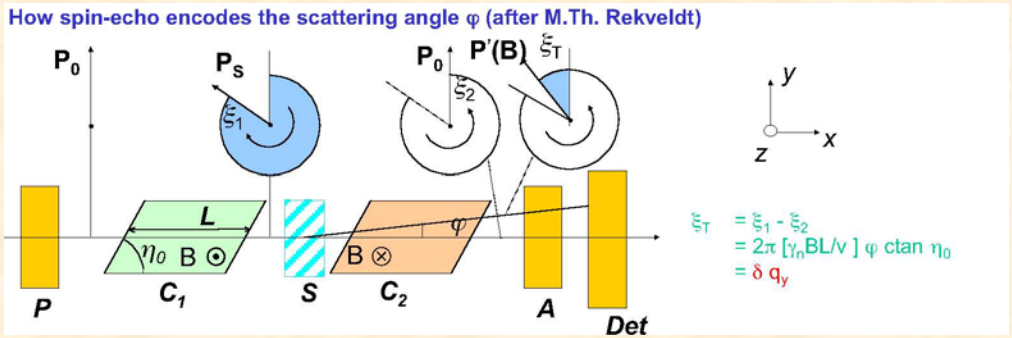


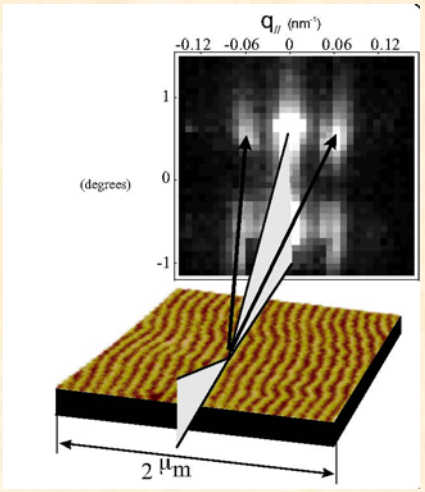
– Q ~ 2 . 10-6 Å-1

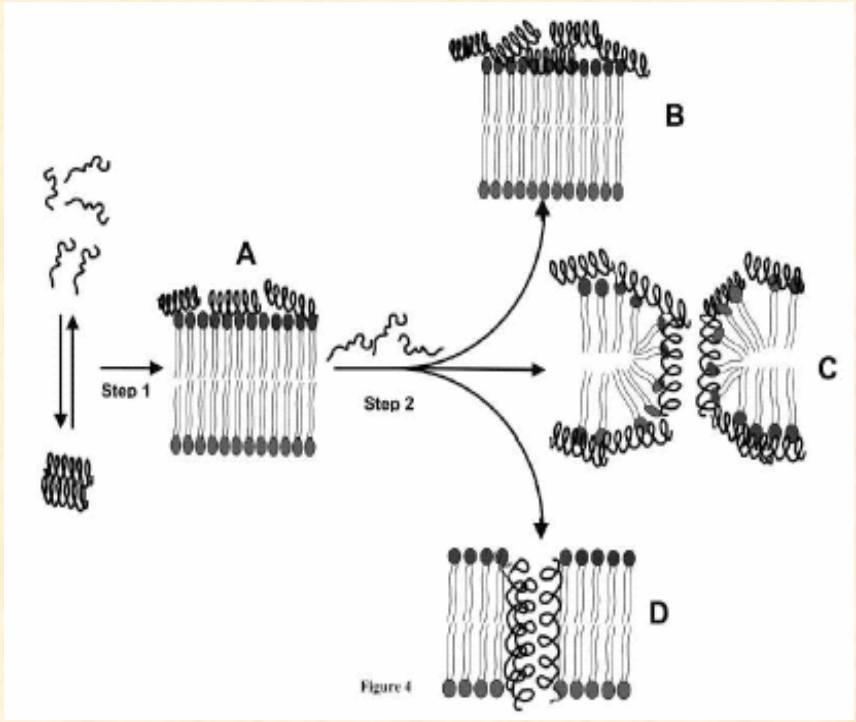
UT-BATTELLE

Spin Echo to probe space and time correlations

- **In plane structures 10nm to 1000nm**
- **Correlation times from ps to μs**



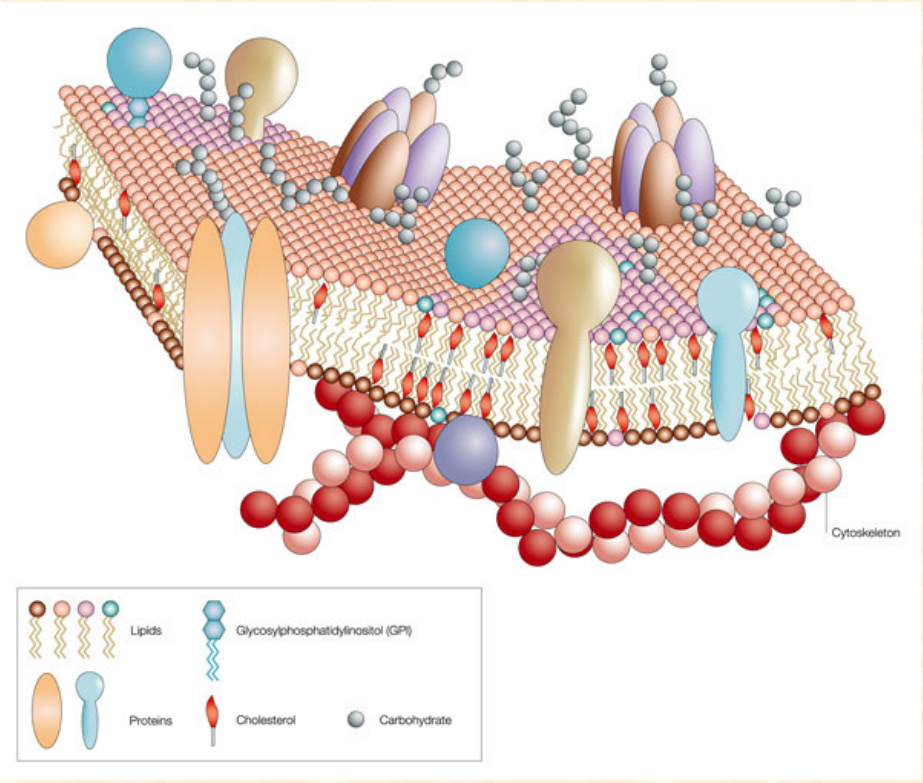


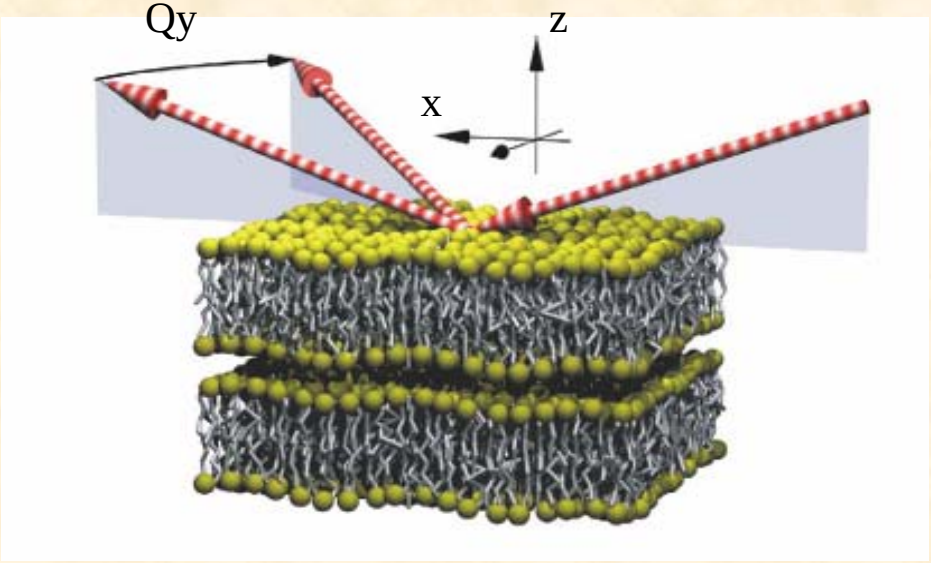


- Artificial Bio membranes
- Block copolymers
- Lubricating or adhesive layers
- Wetting phenomena
- Liquid crystals

R. Pynn
G. Felcher

Understanding Structure formation in Membranes…





…and the dynamics

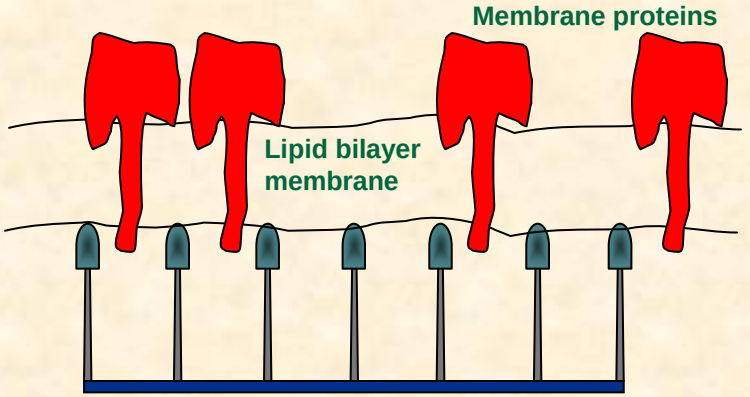
- Local
  - Diffusion
  - Rotation
  - Chain defect motion
  - Flip flop modes
  - Vibrations
- Collective
  - Membrane undulations

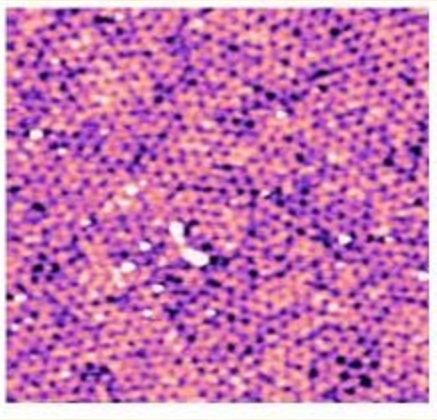
Looking to the future

Understanding and control of:

- Membrane fusion
- Transport phenomena across membranes
- Artificial Bio membranes
- Block copolymers
- Lubricating or adhesive layers
- Wetting phenomena
- Liquid crystals
- and more…

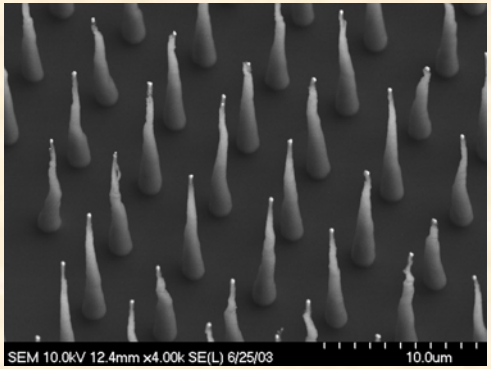
Synthesis of unique functionalized nanofiber scaffolds for membranes





Neutron reflection of single bilayer membranes on hexagonally patterned silicon oxide surfaces

Baker S.M., Kolthammer W.S., Tan J.B., and Smith G.S., ZEITSCHRIFT FUR KRISTALLOGRAPHIE **219** (3): 179-185 (2004)



Melechko AV, Merkulov VI, McKnight TE, Guillorn MA, Klein KL, Lowndes DH, and Simpson ML, "Vertically aligned carbon nanofibers and related structures: Controlled synthesis and directed assembly," J. Appl. Phys., 97 (4), 041301(2005).

SNS 20-Year Plan

The SNS is designed to allow operations with two target stations

- **Phase 1 – Power Upgrade**
  - **3-4 MW**
  - **Completion FY10**
- **Phase 2 - Long Wavelength Target Station (LWTS)**
  - **22 Instruments**
  - **440 – 880 kW**
  - **20 Hz**
  - **Completion FY13**