

# Neutron Generation and Detection Neutron Optics and Instrumentation

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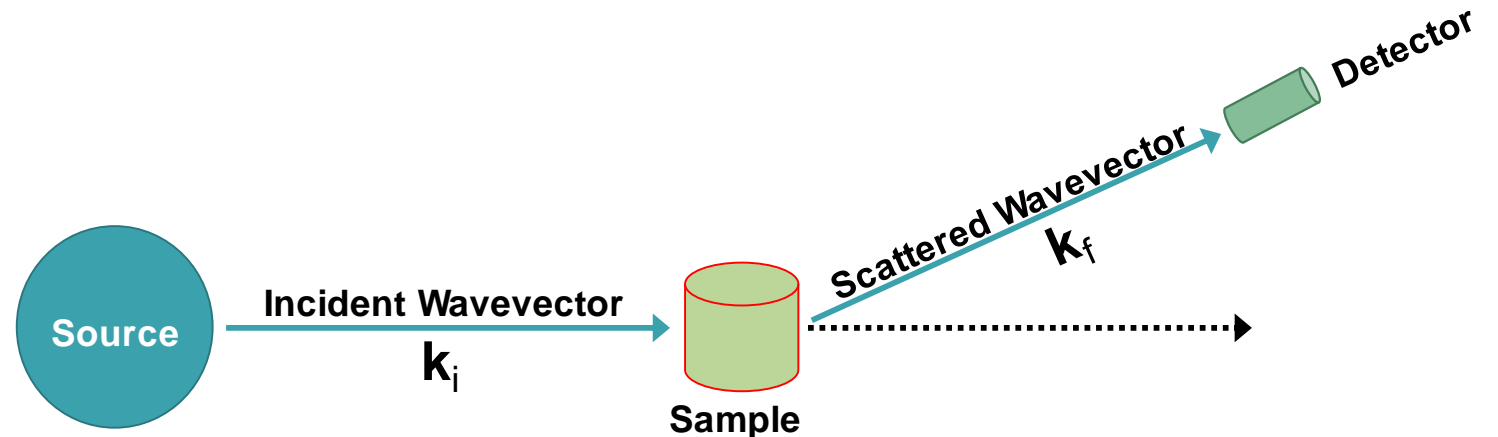
21st National School on Neutron and X-ray Scattering  
June 16-June 29, 2019

Sunday, June 16, 2019

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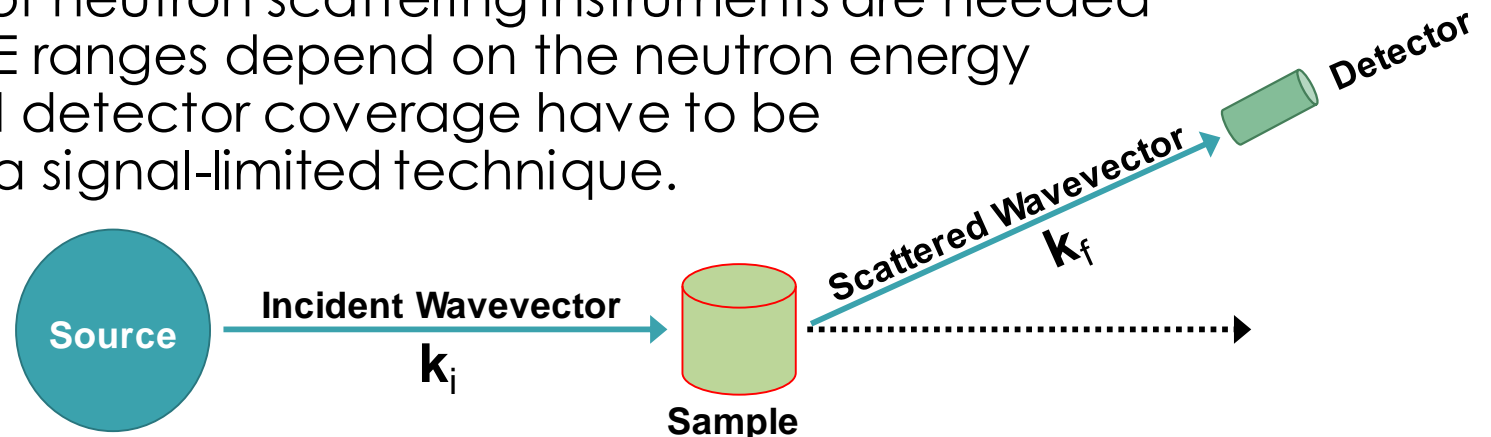
# What is a Neutron Scattering Instrument?

- Neutron scattering experiments measure the number of neutrons scattered by a sample as a function of the wavevector change ( $Q$ ) and the energy change ( $E$ ) of the neutron.
- What do we need to accomplish this?
  - 1) A source of neutrons
  - 2) A method for selecting the wavevector of the incident neutrons ( $k_i$ )
  - 3) A very interesting sample
  - 4) A method for determining the wavevector of the scattered neutrons ( $k_f$ )
  - 5) A neutron detector

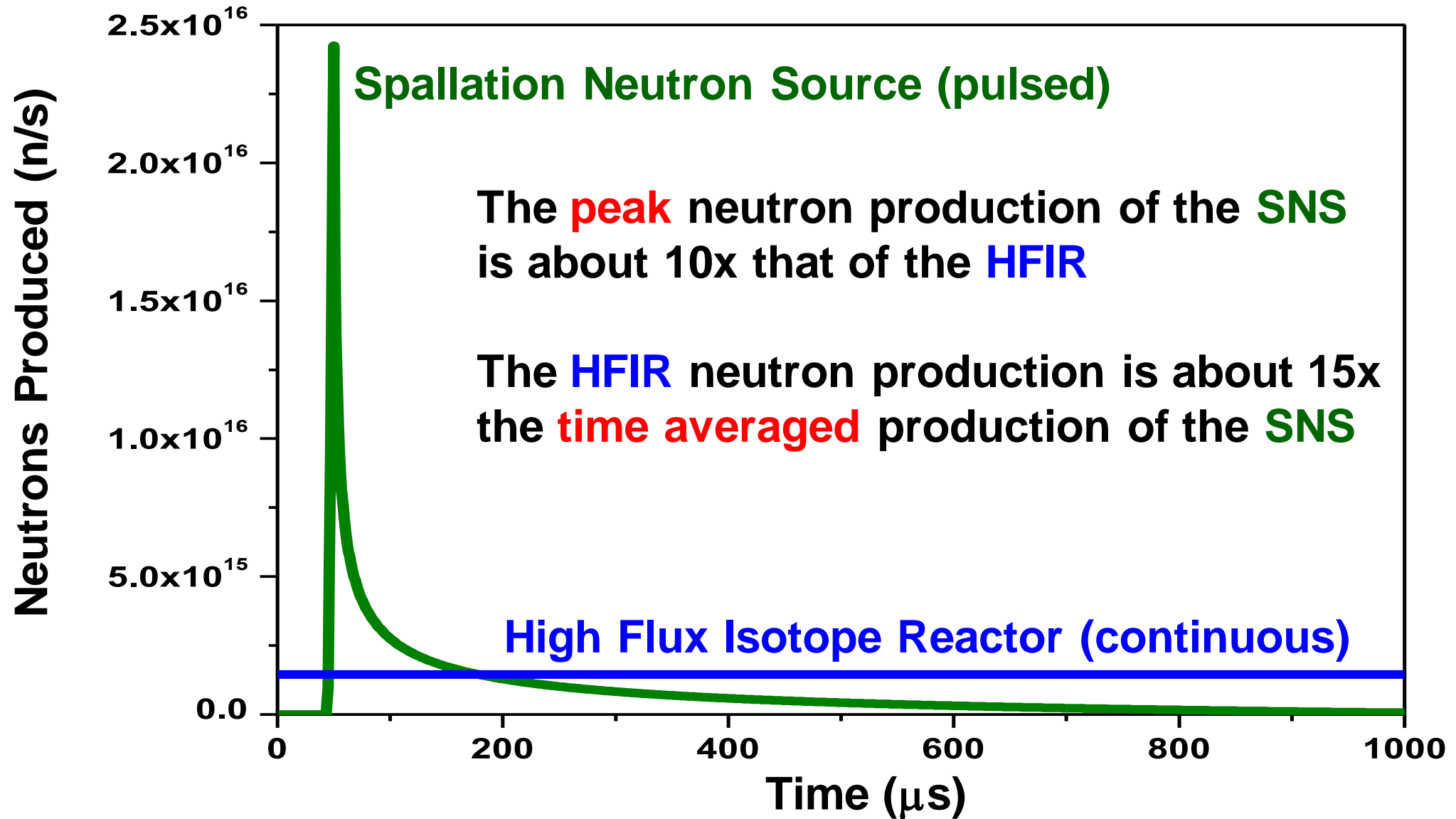


# Why Not Just Build a Universal Neutron Scattering Instrument That Can Do Everything We Need?

- Two types of sources (continuous and pulsed)
- Two methods for determining the neutron wavevector,  $k$  (time-of-flight and diffraction)
- Two types of scattered neutrons (elastic and inelastic)
- Two types of interactions between the neutrons and the sample (nuclear and magnetic)
- Wide range of length scales driven by the science
- The energy of the neutron is coupled to its wavelength and velocity:  
 $\lambda^2(\text{\AA}^2) \sim 81.81/E(\text{meV})$  and  $v^2(\text{m}^2/\text{s}^2) \sim 191313 \times E(\text{meV})$
- $S(Q,E)$  the scattering properties of the sample depend only on  $Q$  and  $E$ , not on the neutron wavelength ( $\lambda$ )
- **Message:** Many different types of neutron scattering instruments are needed because the accessible  $Q$  and  $E$  ranges depend on the neutron energy and because the resolution and detector coverage have to be tailored to the science for such a signal-limited technique.



# Pulsed vs Continuous Neutron Sources



# Neutron Scattering Instruments at Continuous Sources Are Typically Based on Diffraction Techniques

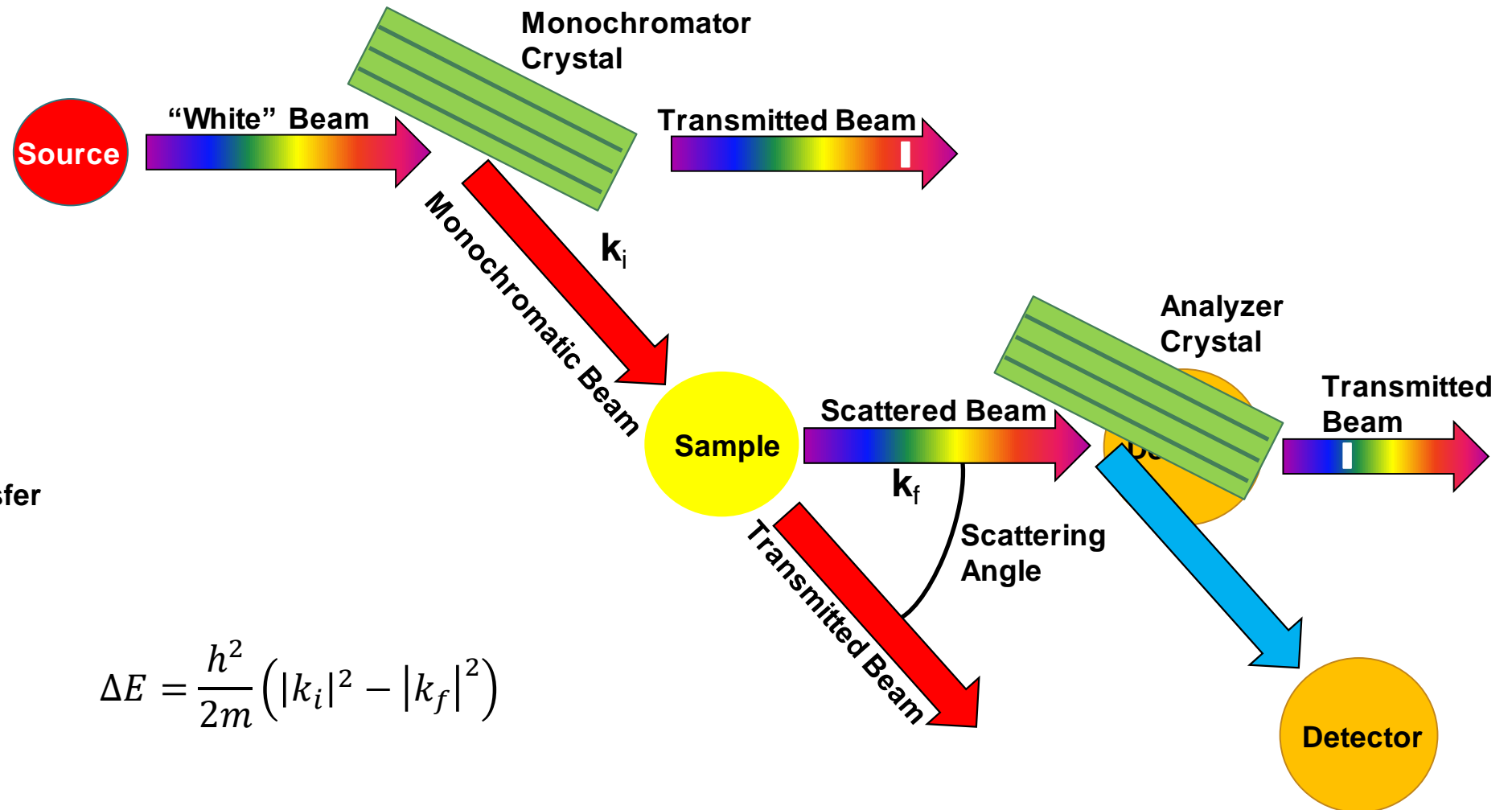
Bragg's Law

$$n\lambda = 2d \sin \theta$$

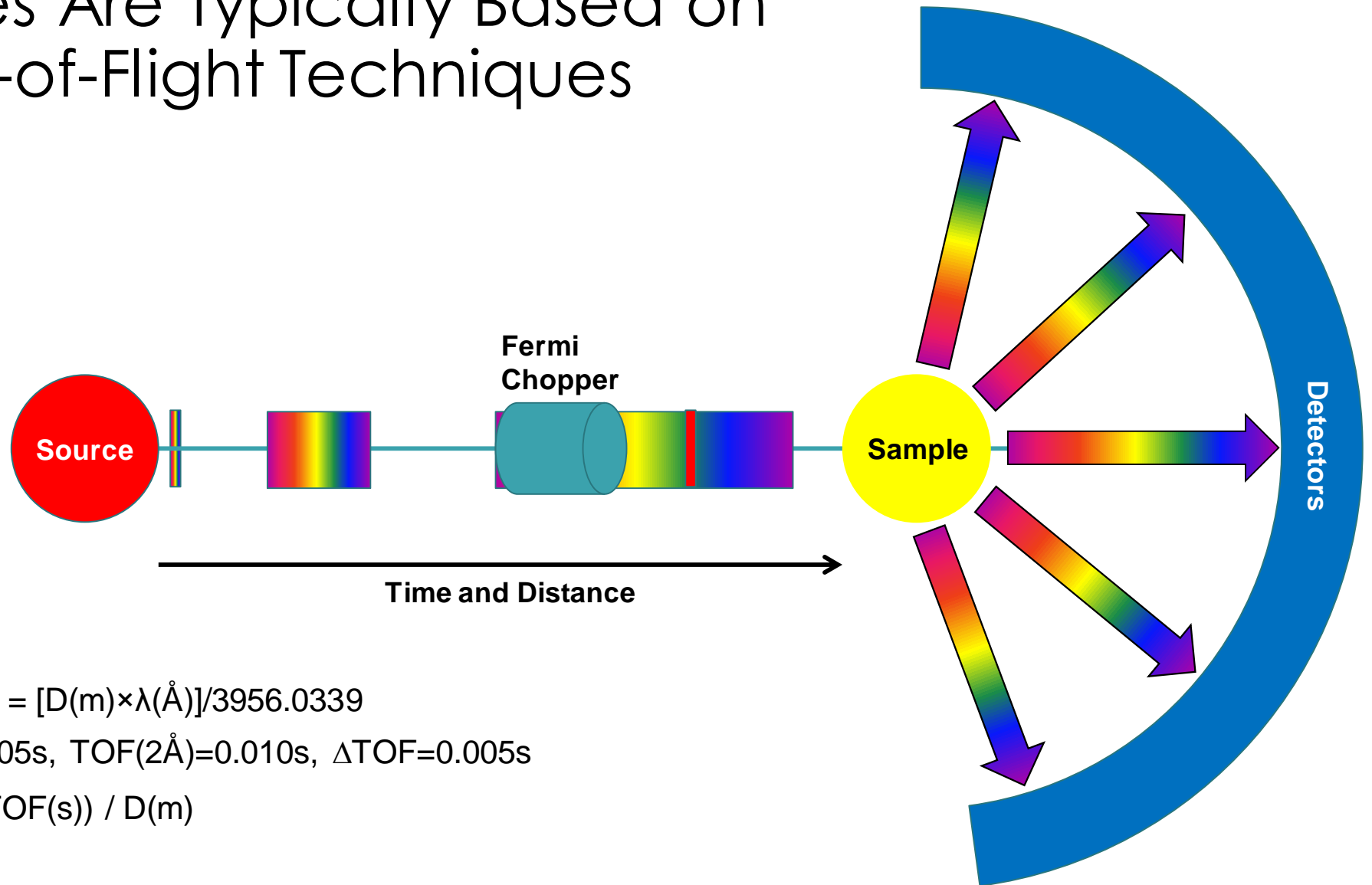
Momentum Transfer

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

$$\Delta E = \frac{h^2}{2m} (|k_i|^2 - |k_f|^2)$$



# Neutron Scattering Instruments at Pulsed Sources Are Typically Based on Neutron Time-of-Flight Techniques



$$v(1.8\text{\AA}) = 2187\text{m/s}$$

$$\text{TOF(s)} = D(\text{m})/v(\text{m/s}) = [D(\text{m}) \times \lambda(\text{\AA})] / 3956.0339$$

$$D=20\text{m}, \text{TOF}(1\text{\AA})=0.005\text{s}, \text{TOF}(2\text{\AA})=0.010\text{s}, \Delta\text{TOF}=0.005\text{s}$$

$$\lambda(\text{\AA}) = (3956.0339 * \text{TOF(s)}) / D(\text{m})$$

# Neutron Optics

The following neutron optical components are typically used to construct a neutron scattering instrument

- **Monochromators / Analyzers:** Monochromate or analyze the energy of a neutron beam using Bragg's law
- **Choppers:** Define a short pulse of neutrons or select a small band of neutron energies
- **Guides / Mirrors:** Allow neutrons to travel large distances without suffering intensity loss
- **Polarizers / Spin Manipulators:** Filter and manipulate the neutron spin
- **Collimators:** Define the direction of travel of the neutrons
- **Detectors:** Neutron position (and arrival time for TOF) is recorded. Neutrons are typically detected via secondary ionization effects.

# Instrument Resolution

- Uncertainty in the neutron wavelength and direction limit the precision that  $Q$  and  $E$  can be determined
- For scattering, the uncertainty comes from how well  $k_i$  and  $k_f$  can be determined
- For TOF, the uncertainty primarily comes from not knowing the exact start time for each neutron
- The total signal observed in a scattering experiment is proportional to the phase space volume within the elliptical resolution volume – the better the resolution, the lower the count rate

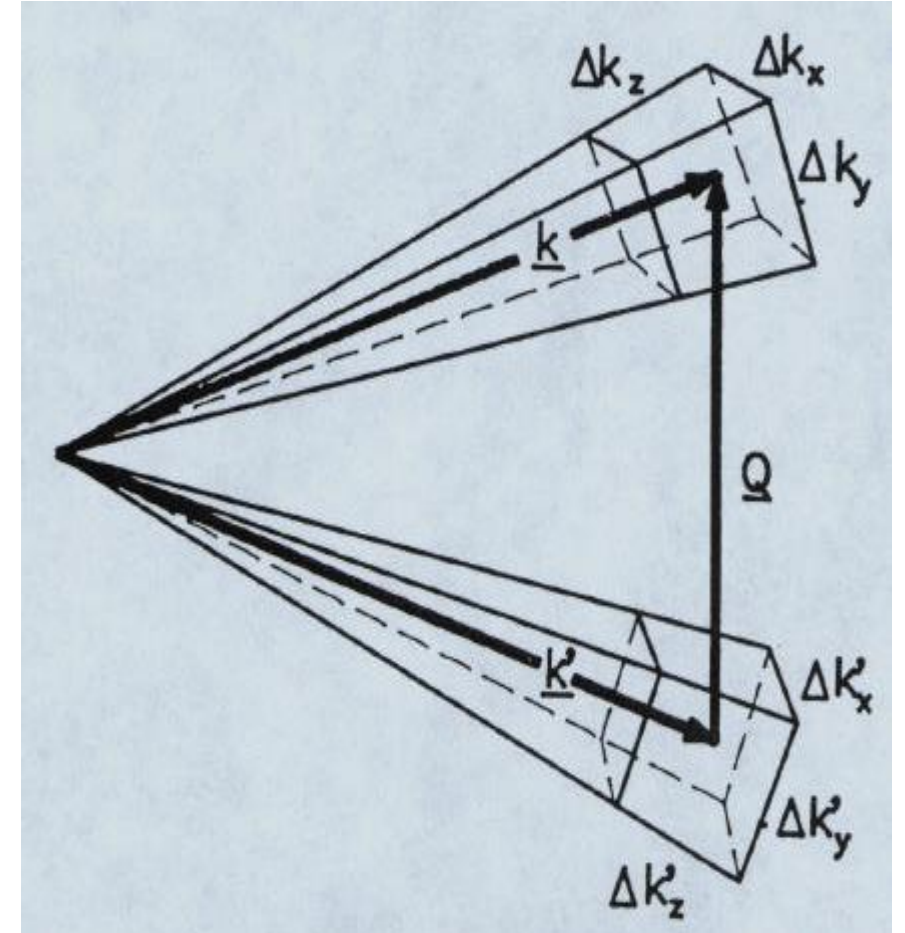
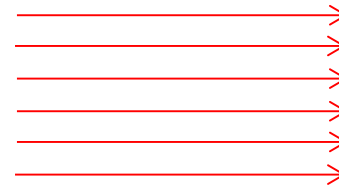
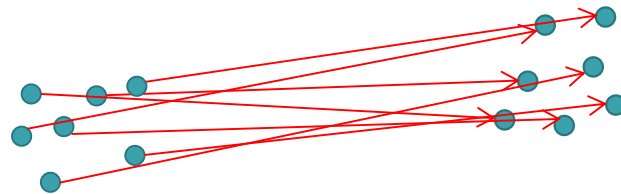


Figure borrowed from Roger Pynn

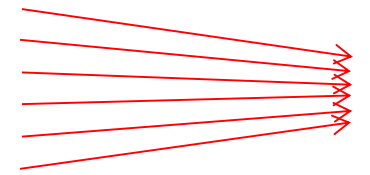


# Liouville's Theorem

- In the geometrical-optics the propagation of neutrons can be represented as trajectories in a six-dimensional **phase space**  $(p, q)$ , where the components of  $q$  are the generalized coordinates and the components of  $p$  are the conjugate momenta.
- Simply stated, Liouville's Theorem says that phase space volume is conserved.
- Translation: It costs flux to increase resolution and it costs resolution to increase flux.
- There is no way to win!



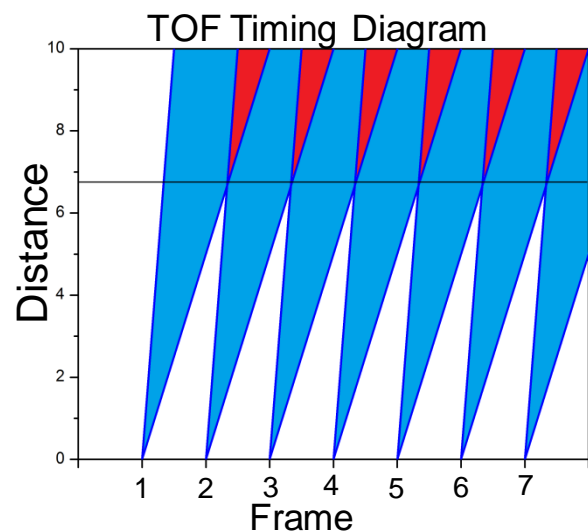
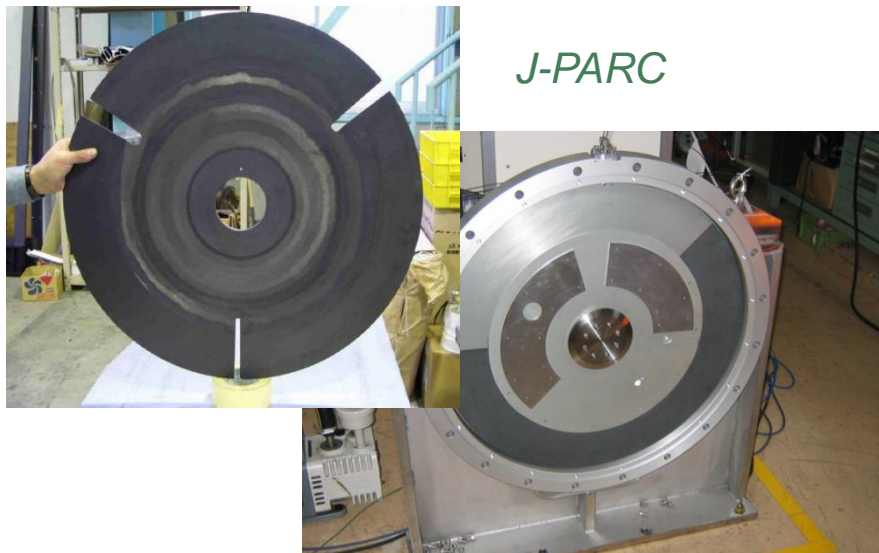
Parallel



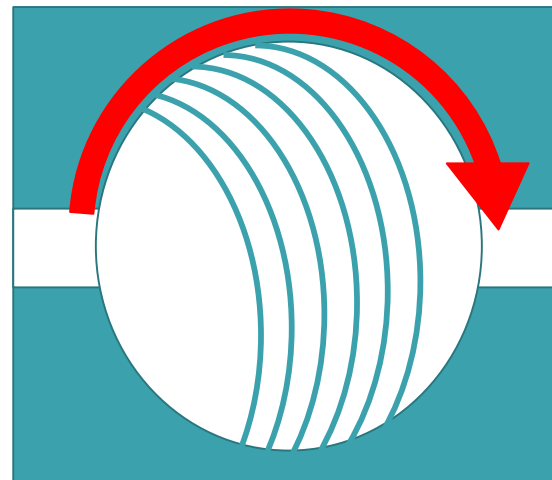
Converging

# Choppers and Velocity Selectors

## Disk Chopper



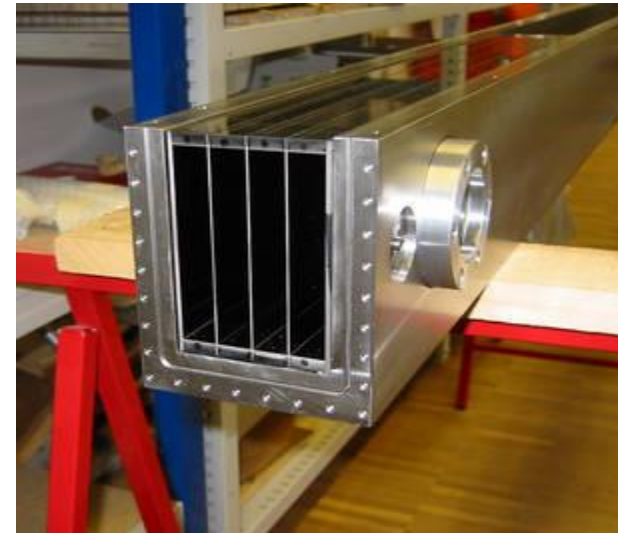
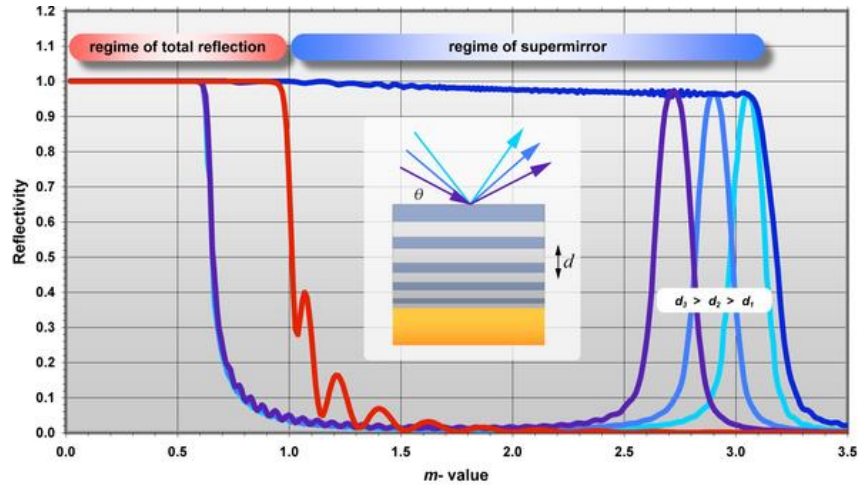
## Fermi Chopper



## Velocity Selector



# Neutron Mirrors and Supermirrors / Neutron Guides



Multichannel Curved Guide  
*Fabricated by Swiss Neutronics*



80m Guide for HRPD at J-PARC  
*Fabricated by Swiss Neutronics*



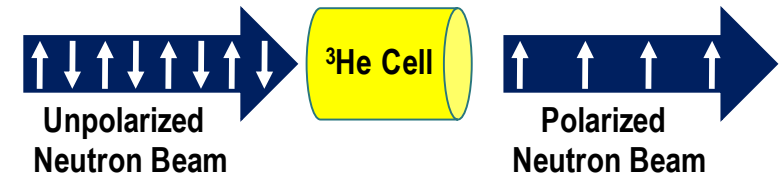
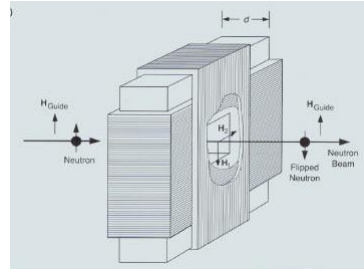
Guide  
Installation  
at ISIS

# Polarizers and Spin Manipulators

Heussler Monochromator  
AlCuMn



Larmor Precession  
Flipper



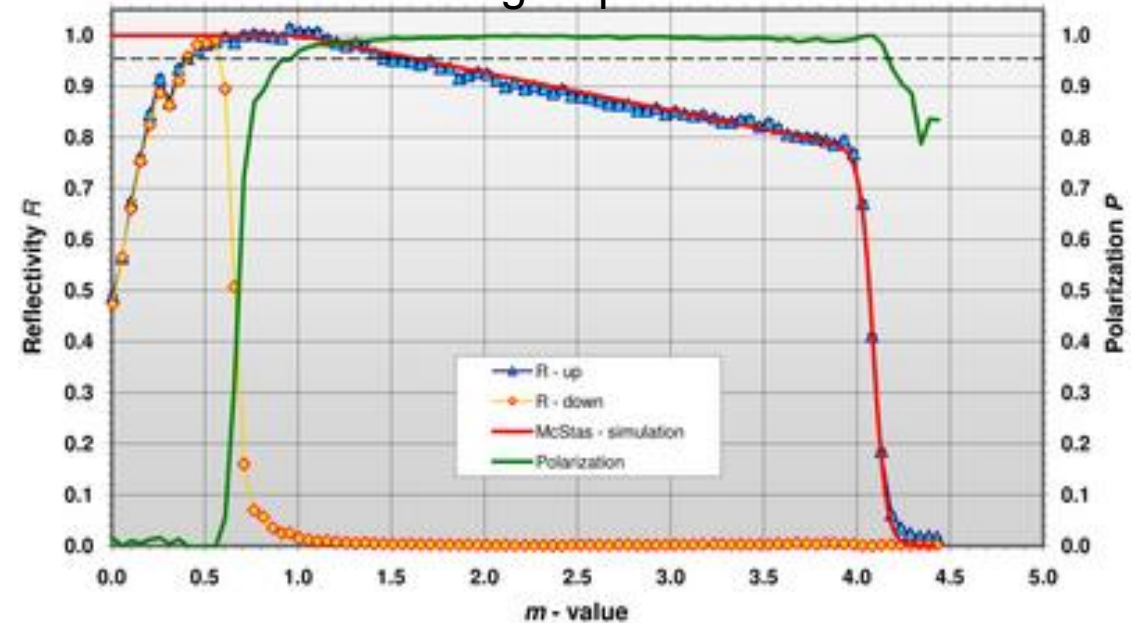
<sup>3</sup>He Spin  
Filters

Spherical Neutron Polarimetry



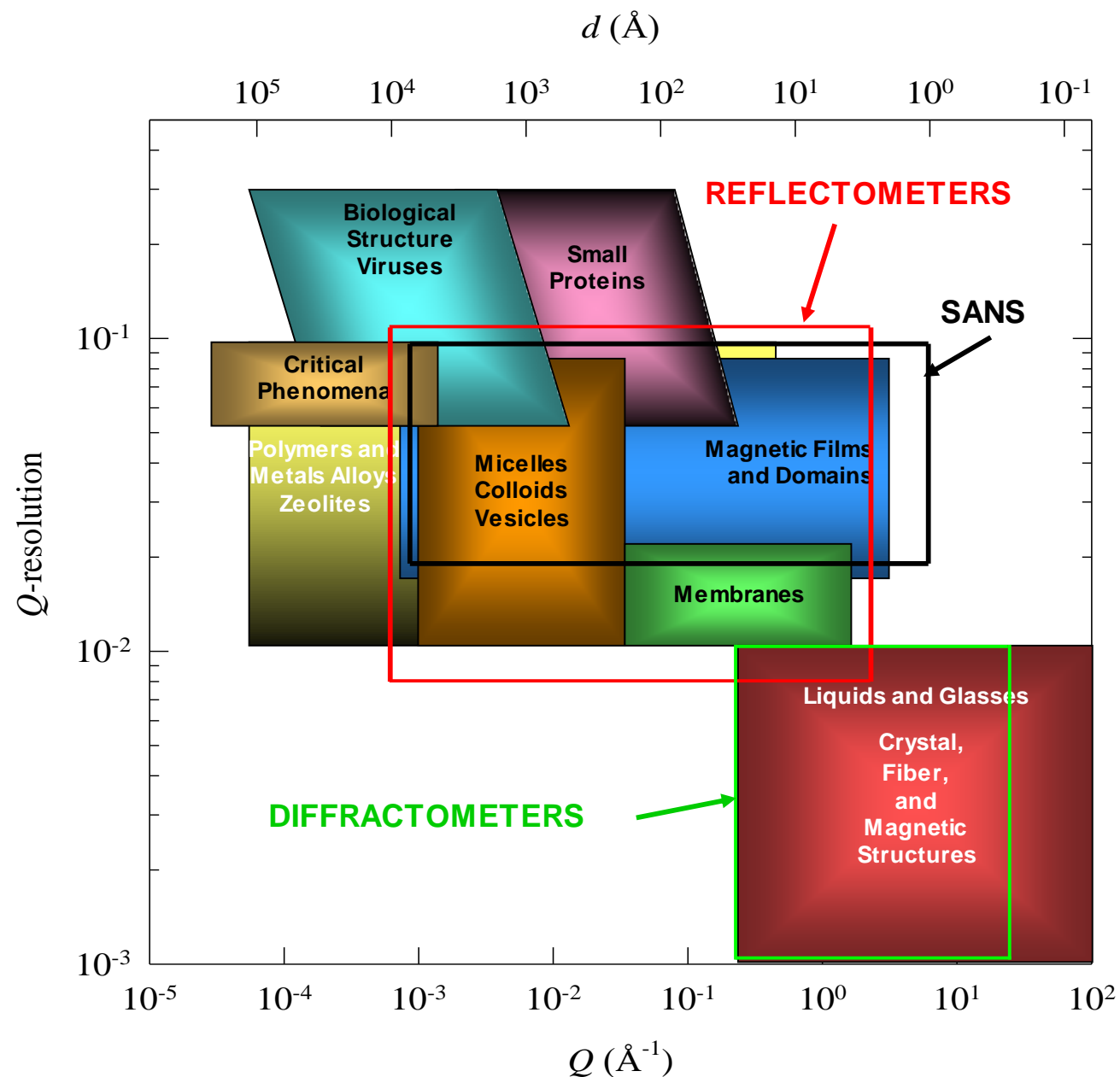
POLI-HEiDi at FRMII

Polarizing Supermirrors

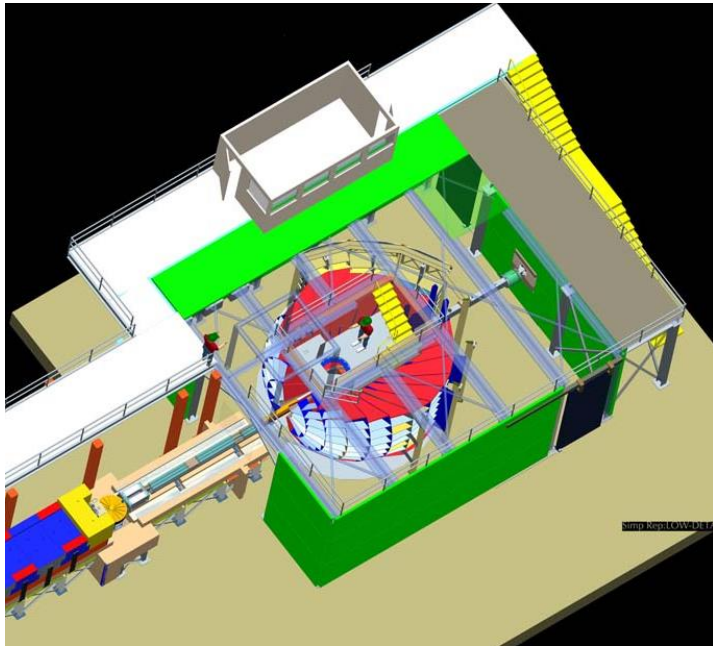


# Elastic Neutron Scattering Instruments

- Elastic instruments include:
  - Powder diffraction
  - Single Crystal diffraction
  - SANS (typical)
  - Reflectometry
- Used to determine the average structure of materials (i.e. how the atoms are arranged)



# TOF Powder Diffractometer: POWGEN (SNS)

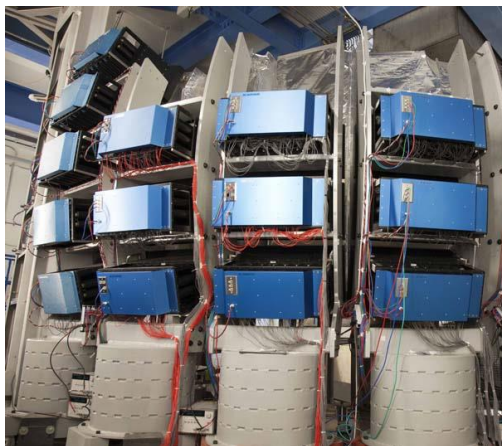
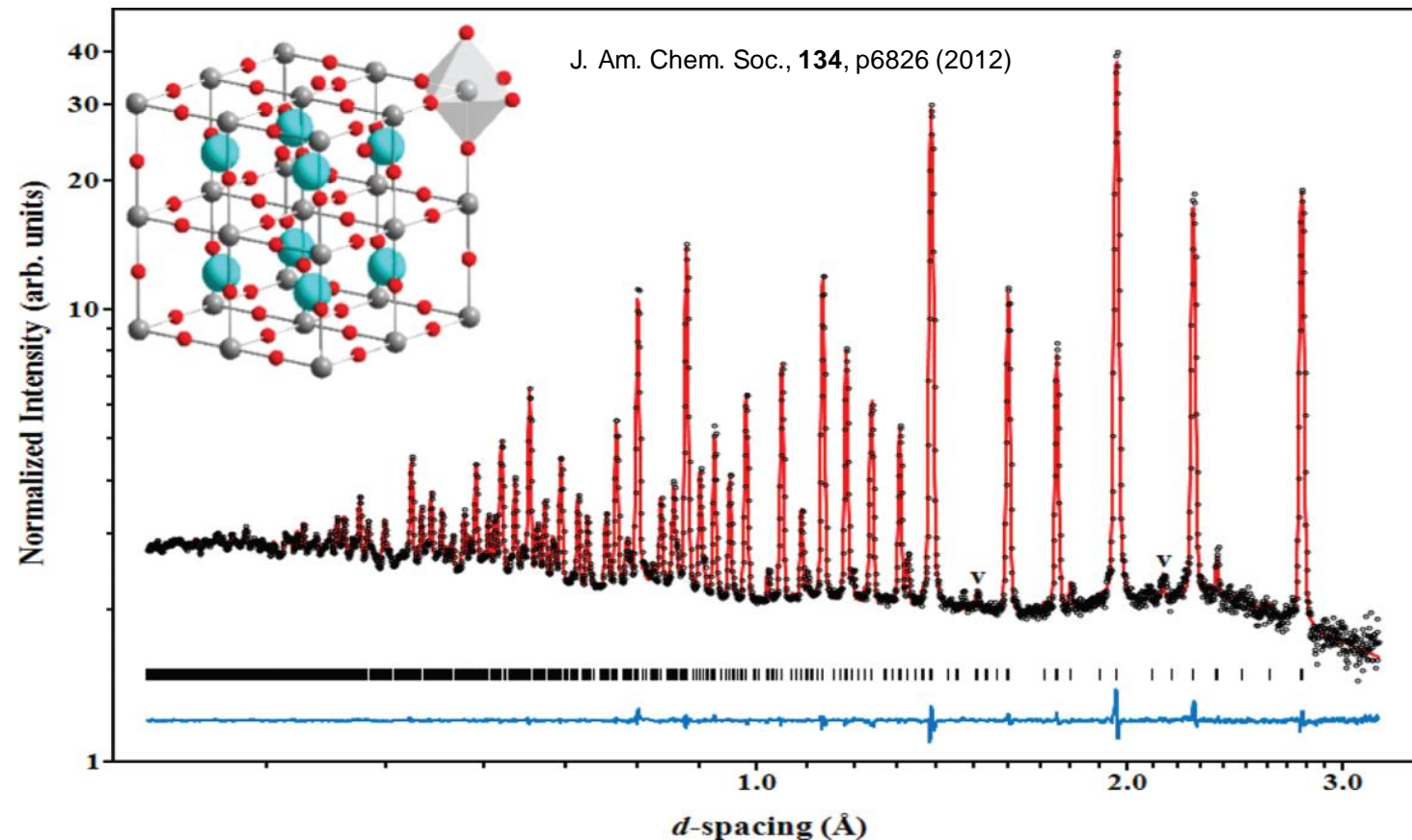


$$d = \frac{\lambda}{2 \sin \theta} = \frac{2\pi}{Q}$$

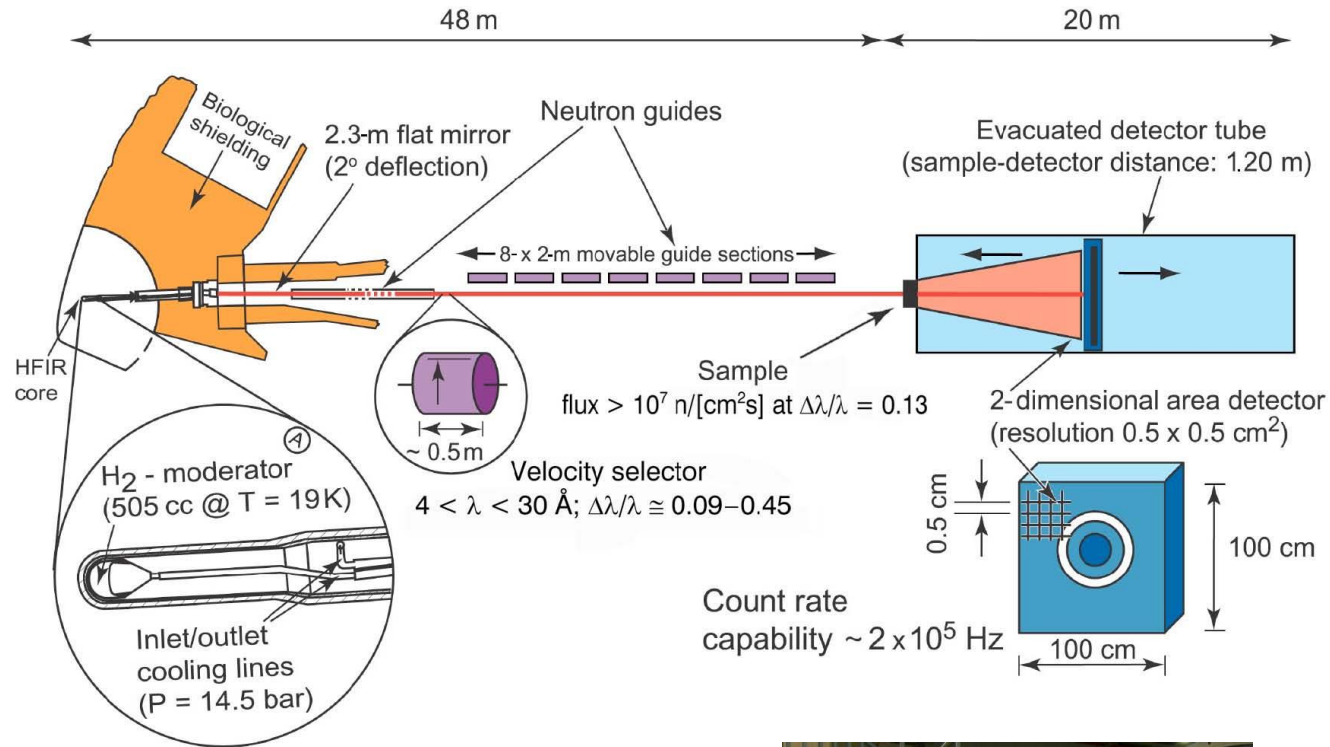
$$d = \frac{(3956.0339 * \text{TOF}) / D}{2 \sin \theta}$$

$$\lambda(\text{\AA}) = (3956.0339 * \text{TOF}(\text{s}) / D(\text{m})) \quad \text{For POWGEN } D = 64.5\text{m}$$

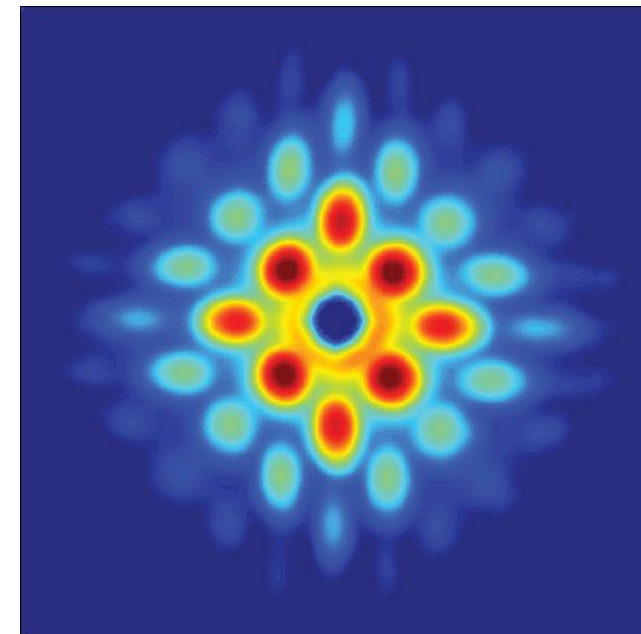
**Sr<sub>2</sub>Fe<sub>1.5</sub>Mo<sub>0.5</sub>O<sub>6</sub>, Electrode Material for Solid Oxide Fuel Cells**



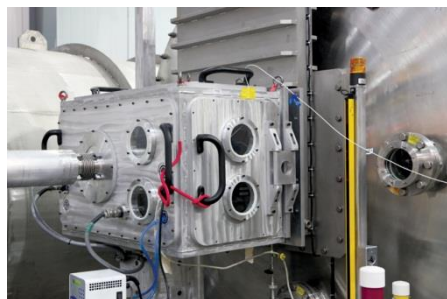
# Small Angle Neutron Scattering (SANS)



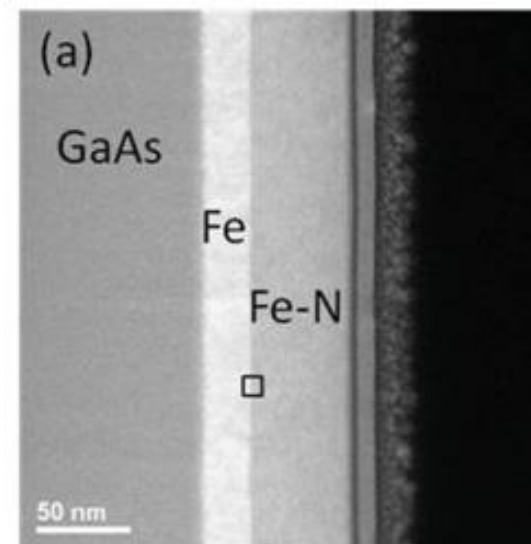
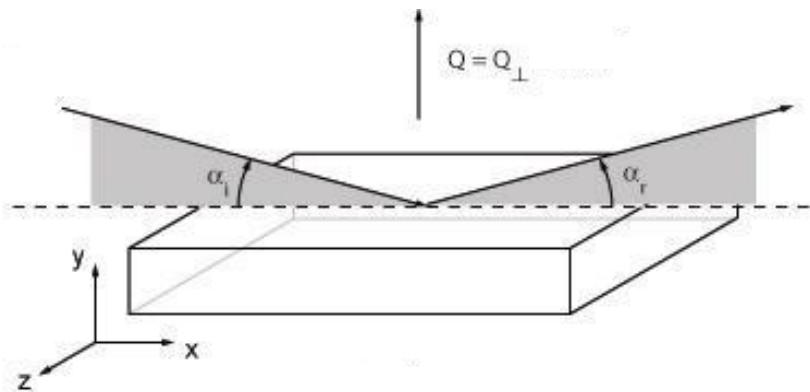
TmNi<sub>2</sub>B<sub>2</sub>C Vortex Lattice



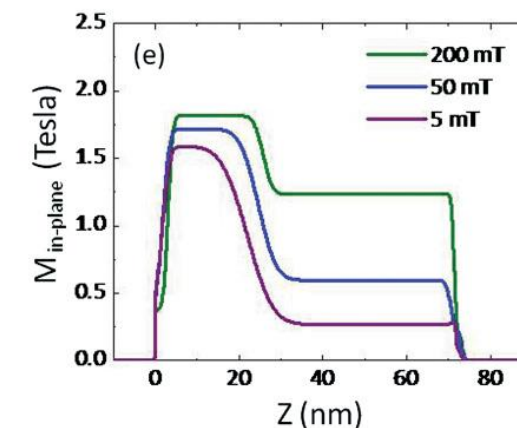
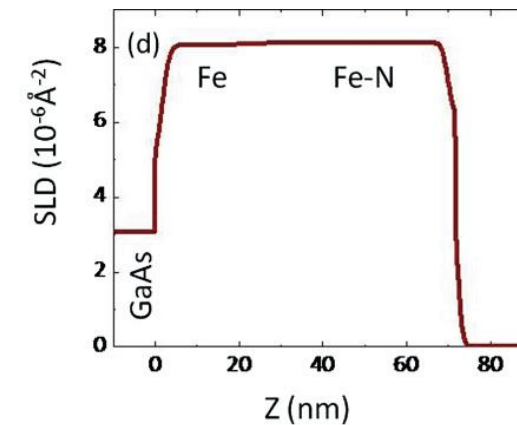
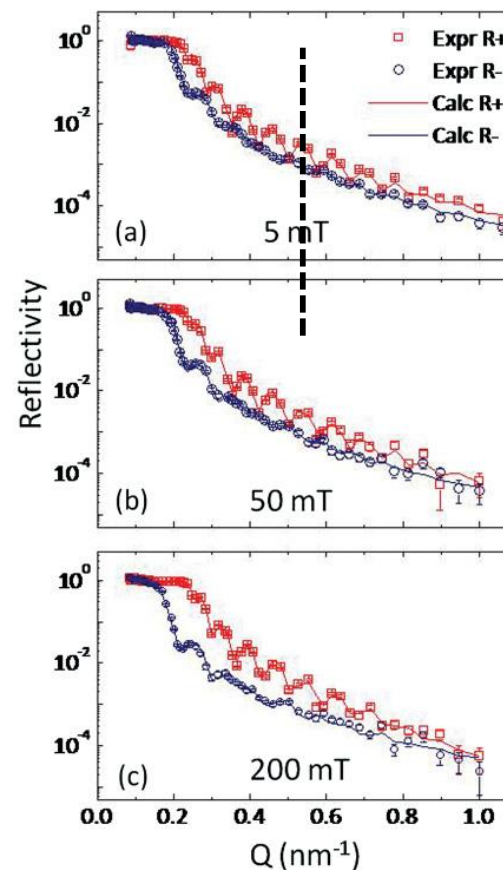
PHYS REV B **86**, 144501 (2012)



# Magnetism Reflectometer (SNS)

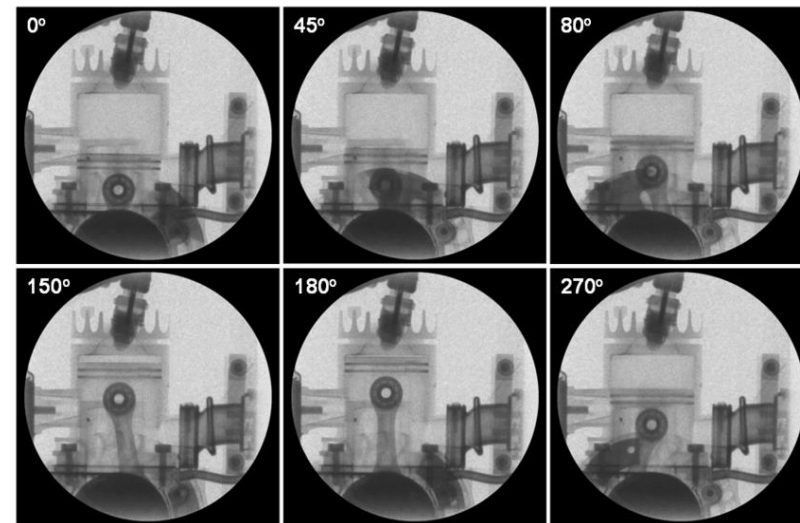
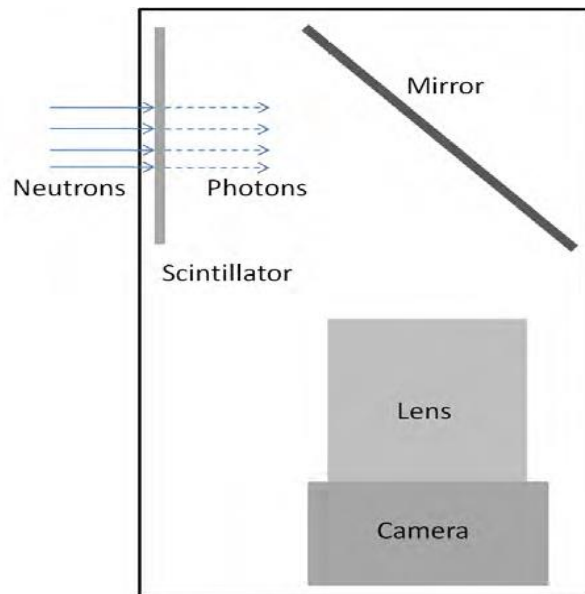


PHY REV B **84**,  
245310 (2011)

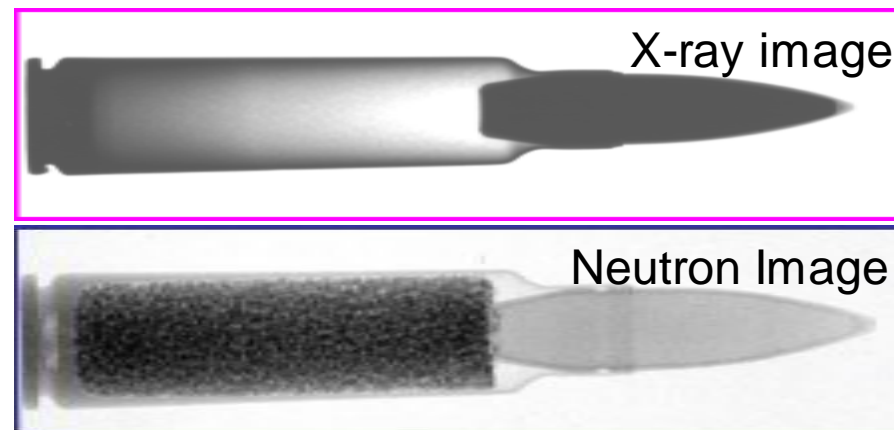
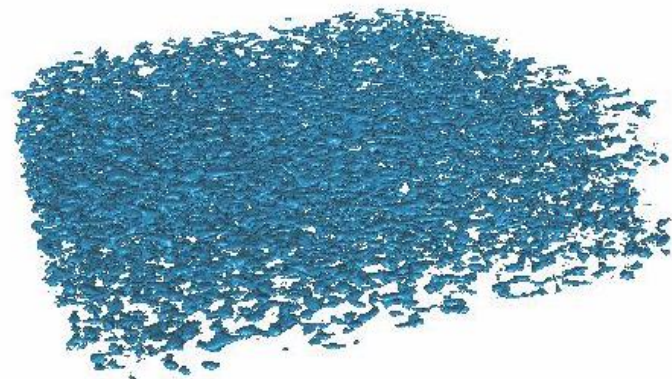




# Neutron Imaging

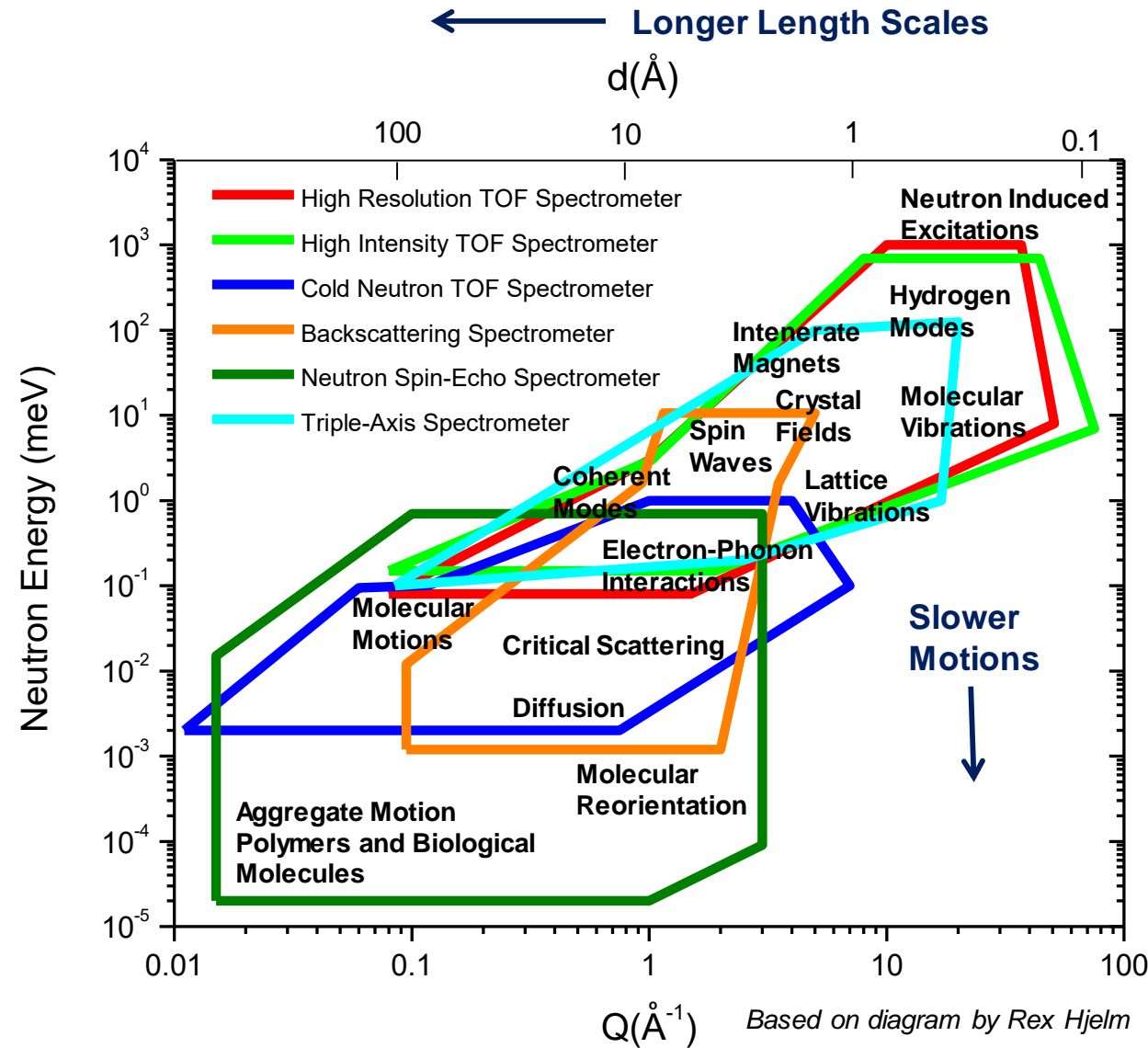


**Carbon foam matrix in a Li battery  
(H. Bilheux and S. Voisin)**

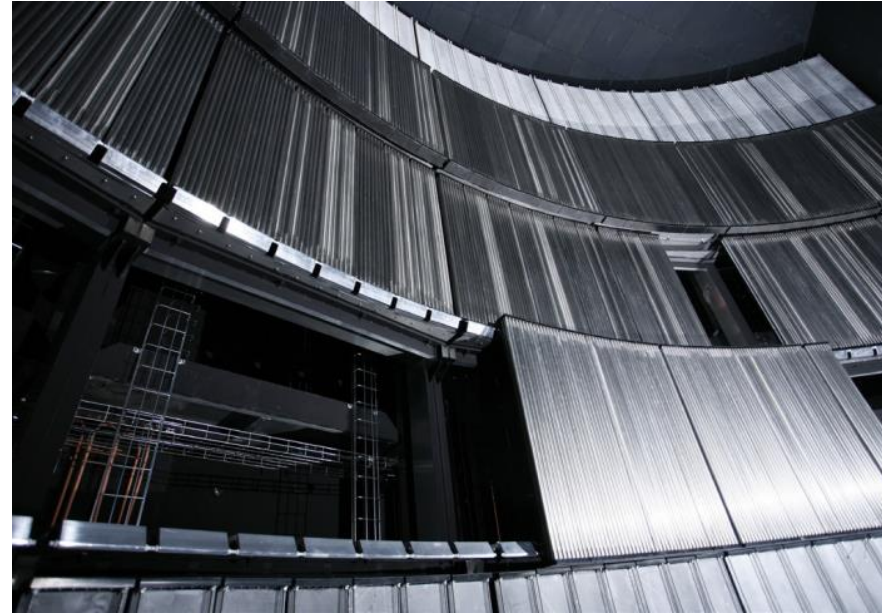
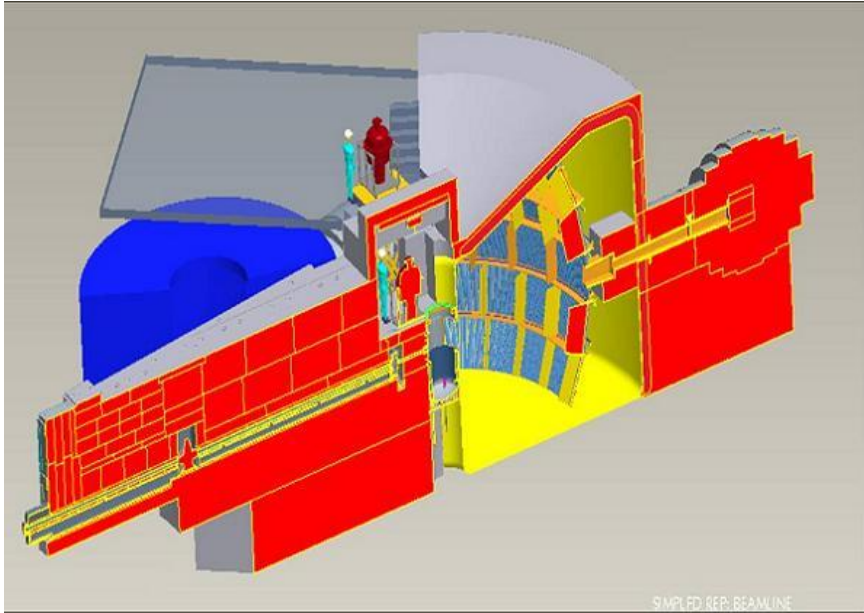


# Inelastic Neutron Scattering Instruments

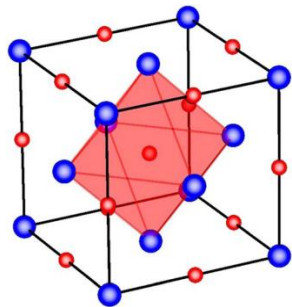
- Inelastic instruments include:
  - Direct Geometry TOF Spectrometers
  - Indirect Geometry TOF Spectrometers
  - Triple-Axis Spectrometers
  - Backscattering Spectrometers
  - Neutron Spin-Echo Spectrometers
- Used to study dynamics such as phonons, magnons, and diffusion (i.e. what the atoms are doing)



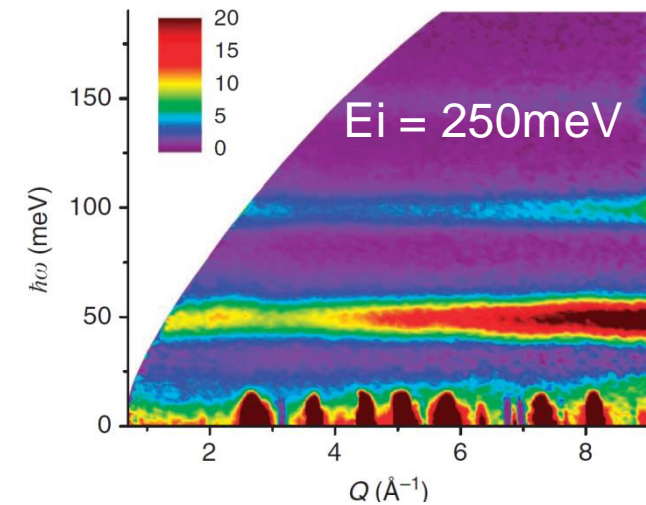
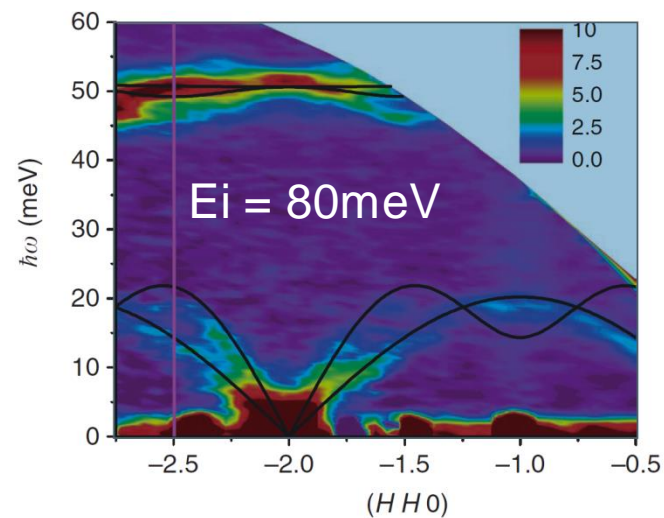
# SEQUOIA: A Direct Geometry TOF Spectrometer at the SNS



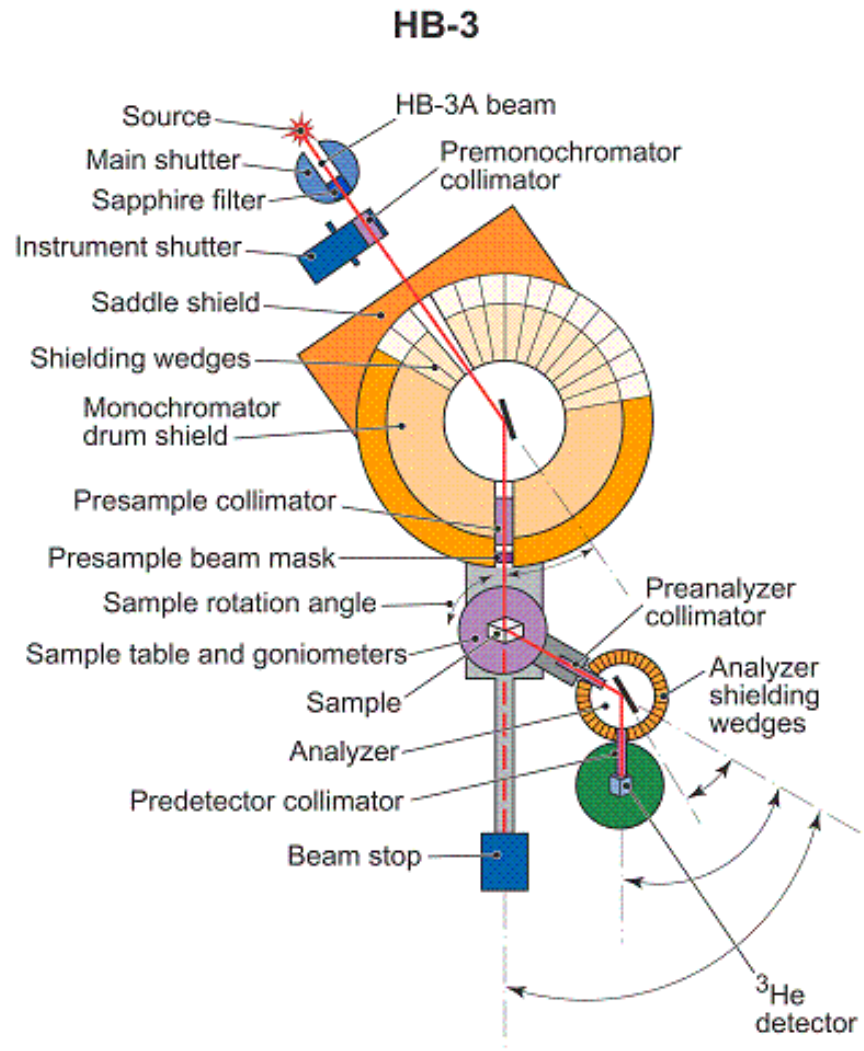
Quantum oscillations of nitrogen atoms in uranium nitride



Nature Communications v3, p1124 (2012)

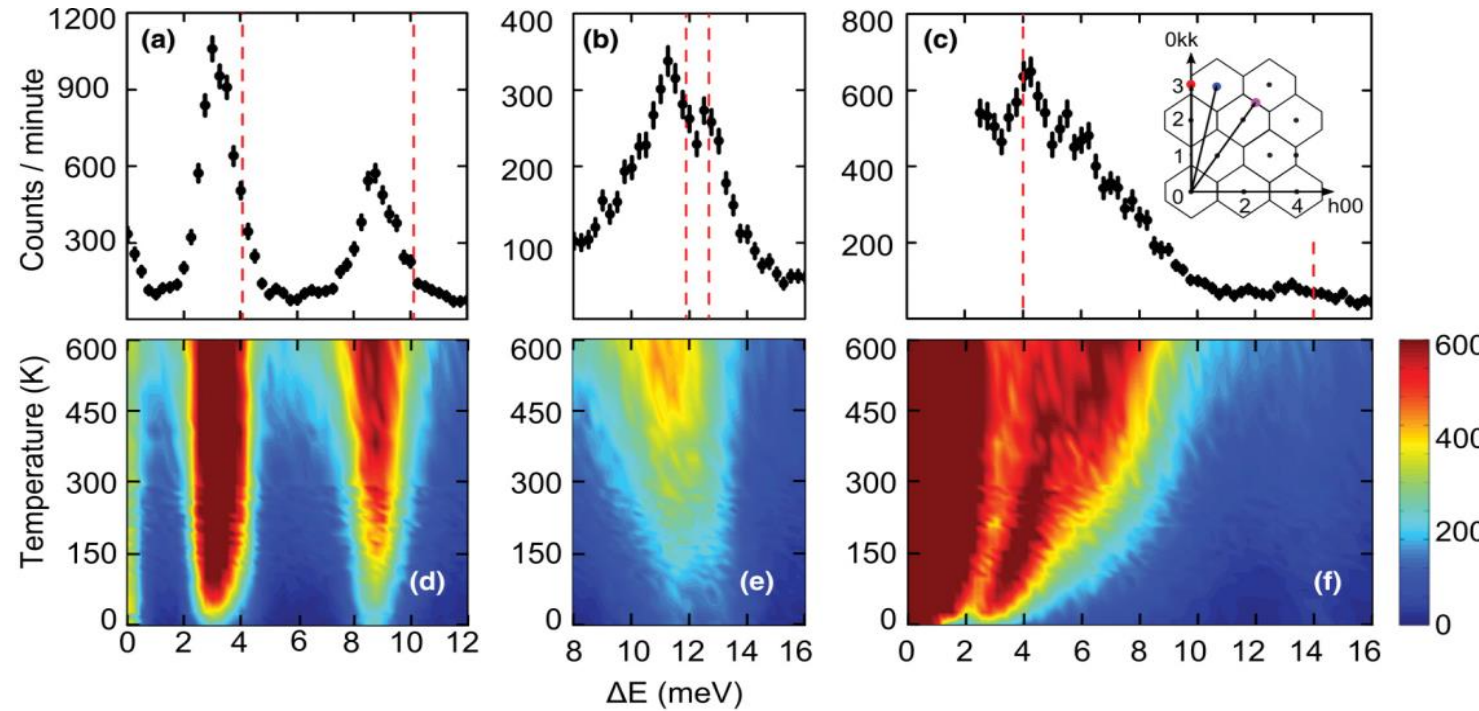


# Triple-Axis Spectrometer



Lattice Dynamics of PbTe

PHYS REV B 86, 085313 (2012)



# HFIR Instrument Suite

## Fixed-Incident-Energy Triple-Axis Spectrometer • HB-1A

Low-energy excitations, magnetism, structural transitions  
neutrons.ornl.gov/fietax

## Polarized Triple Axis Spectrometer • HB-1

Polarized neutron studies of magnetic materials, low-energy excitations, structural transitions  
neutrons.ornl.gov/ptax

## Neutron Powder Diffractometer • HB-2A

Structural studies, magnetic structures, texture and phase analysis  
neutrons.ornl.gov/powder

## WAND<sup>2</sup> • HB-2C

Diffuse-scattering studies of single crystals and time-resolved phase transitions  
neutrons.ornl.gov/wand

## Polarized Neutron Development Station • HB-2D

Development of new components and techniques for utilizing polarized neutrons  
neutrons.ornl.gov/ntd

## Neutron Residual Stress Mapping Facility • HB-2B

Strain, texture, and phase mapping in engineering materials  
neutrons.ornl.gov/nrsf2

## Triple-Axis Spectrometer • HB-3

Medium- and high-resolution inelastic scattering at thermal energies  
neutrons.ornl.gov/tax

## Four-Circle Diffractometer • HB-3A

Small unit-cell nuclear & magnetic structural studies  
neutrons.ornl.gov/hb3a

## Polarized Neutron Development Station • CG-4A/4B

Development of larmor precession techniques  
neutrons.ornl.gov/ntd

## Cold Neutron Triple-Axis Spectrometer • CG-4C

High-resolution inelastic scattering at cold neutron energies  
neutrons.ornl.gov/ctax

## Image-Plate Single-Crystal Diffractometer (IMAGINE) • CG-4D

Atomic resolution structures in biology, chemistry and complex materials  
neutrons.ornl.gov/imagine

## Reactor Pressure Vessel

## Cold Neutron Source

## Development Beam Line • CG-1A

Detector development and testing  
neutrons.ornl.gov/ntd

## Optics Development Beam Line • CG-1B

Sample alignment and optics  
neutrons.ornl.gov/ntd

## Cold Neutron Imaging Beam Line • CG-1D

Transmission imaging of natural and engineered materials  
neutrons.ornl.gov/imaging

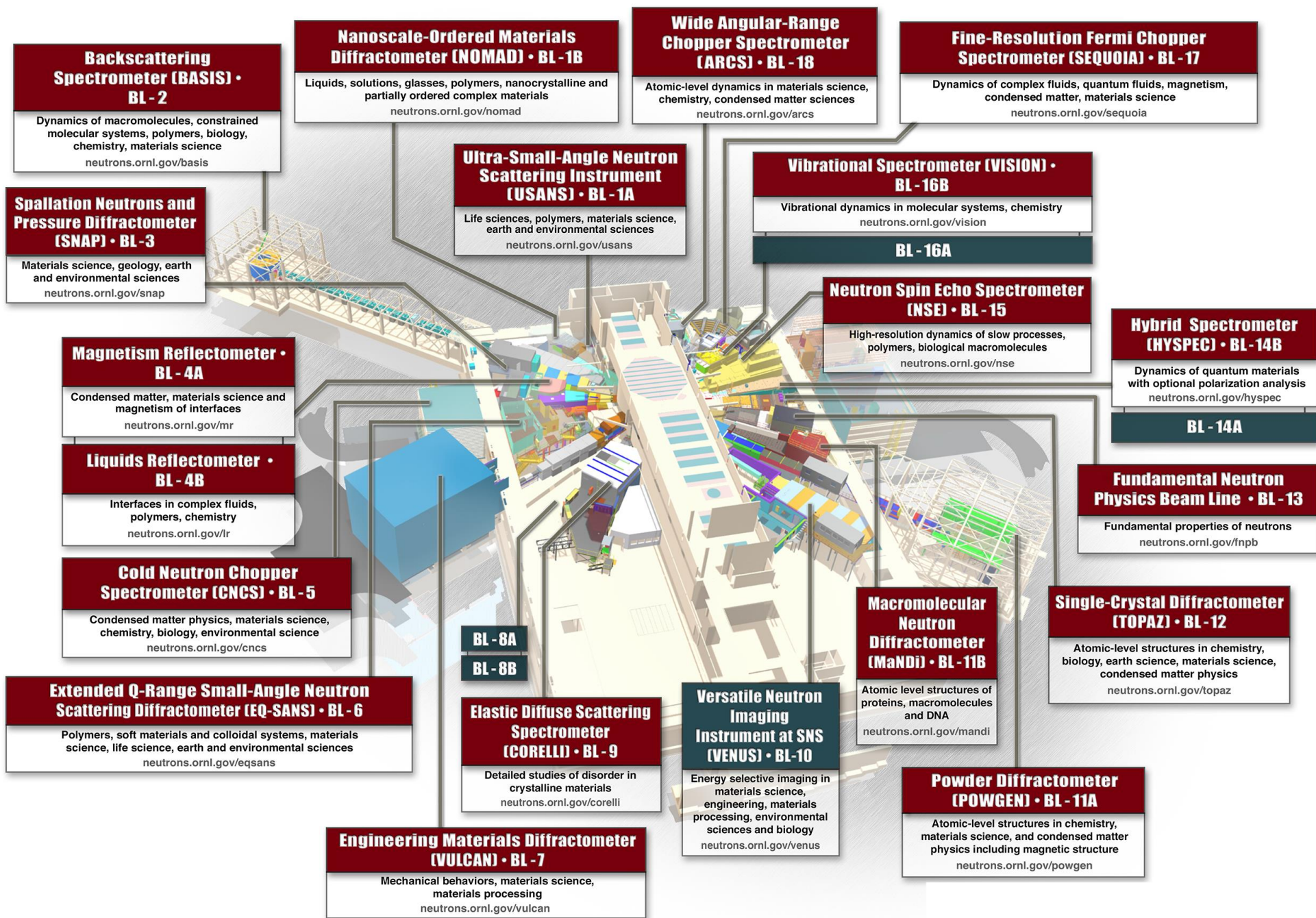
## General-Purpose SANS • CG-2

Materials structure and processing, metallurgy, polymers, geophysics, high-Tc superconductors, complex fluids, magnetism and spin textures  
neutrons.ornl.gov/gpsans

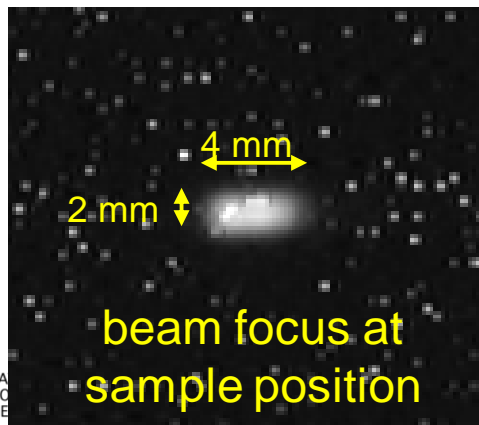
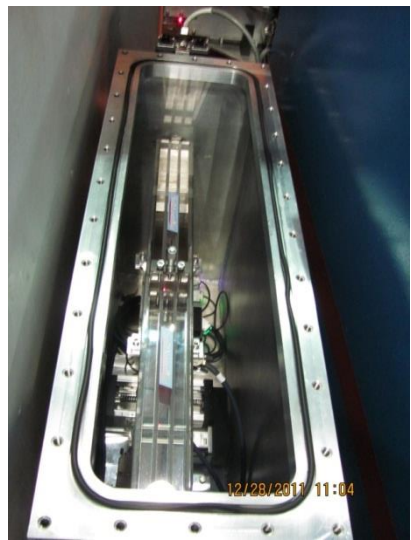
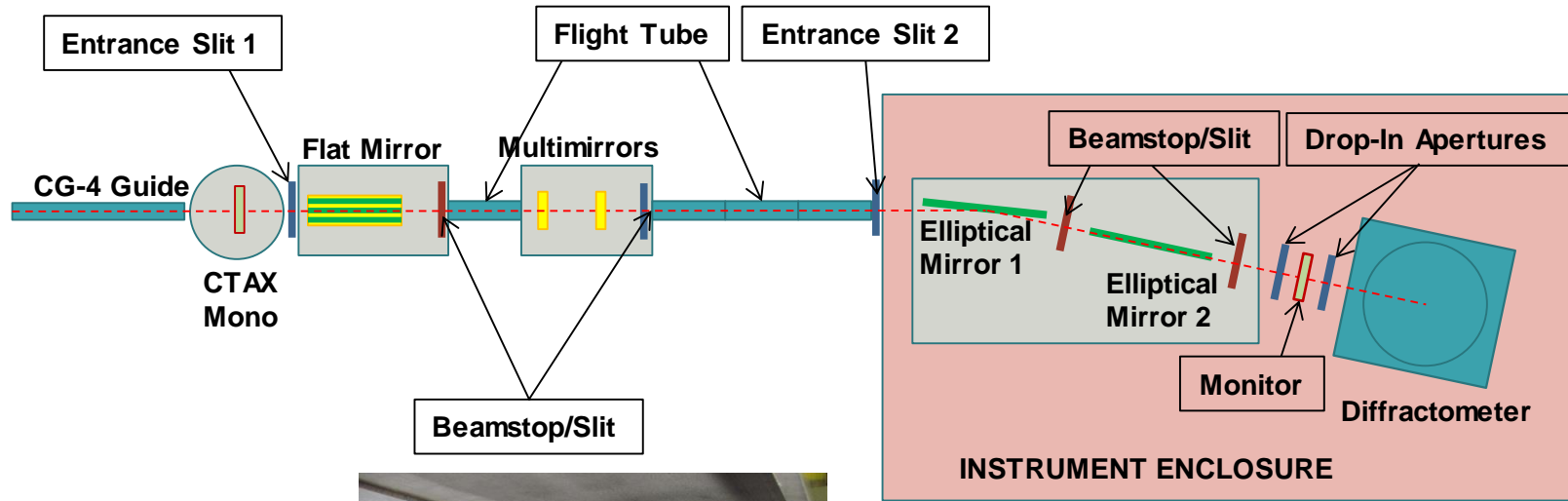
## Bio-SANS • CG-3

Proteins and complexes, pharmaceuticals, biomaterials  
neutrons.ornl.gov/biosans

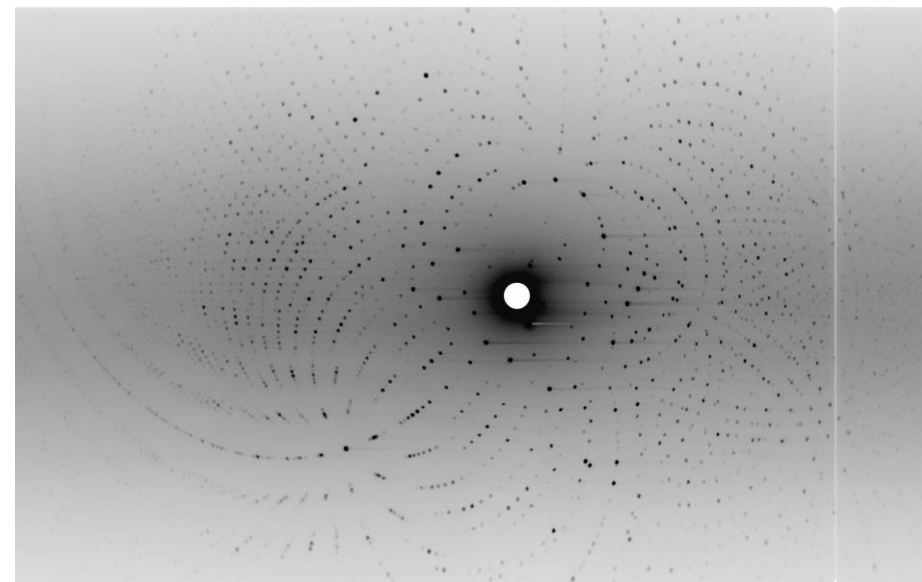
# SNS Instrument Suite



# Advanced Neutron Optics: IMAGINE



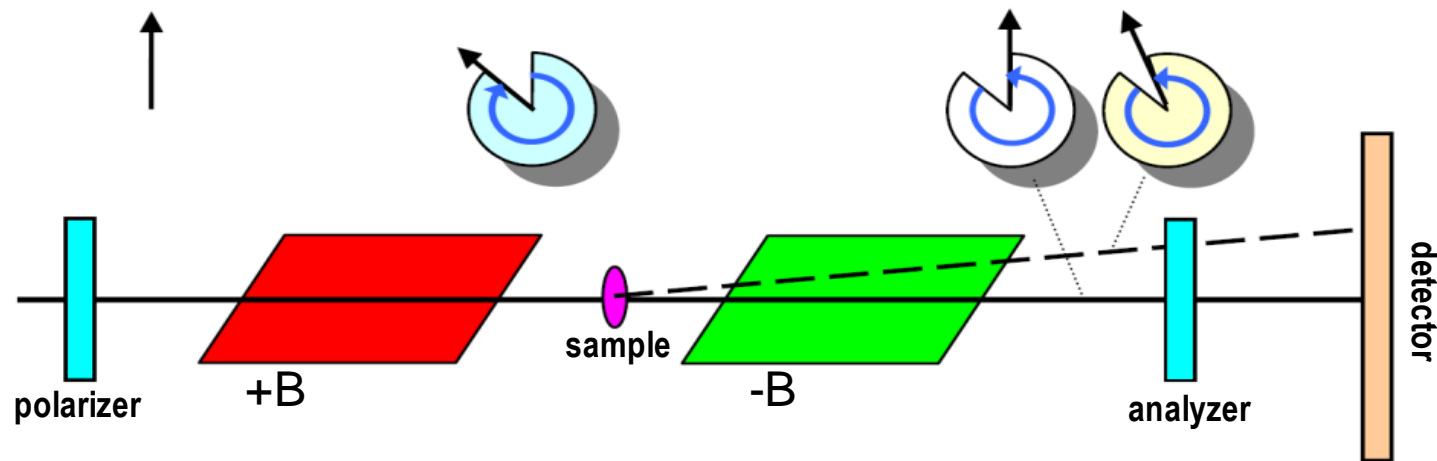
Short wavelength filter @ 2.0, 2.78, and 3.33 Å  
 Long wavelength filter @ 3.0, 4.0, and 4.5 Å  
 Elliptical mirrors for focusing the beam



# Future Instruments: Larmor Precession

## Spin-Echo Scattering Angle Measurement:

The neutron spin precesses through two magnetic regions with opposite field directions. For scattered neutrons the path-length through the two regions is different resulting in a net change in the spin procession.



- Real space correlation lengths up to 20 microns (and beyond?)
- Does not require tight collimation for high resolution
- Can be used to probe the in-plane correlations of thin films and interfaces.



# Concluding Remarks

- Instrument design is driven by the needs of the scientific community coupled with the source capabilities along with advances in neutron optics and detectors.
- In the near term instrument development will be primarily focused on:
  - Focusing optics
  - Neutron transport
  - Polarization
  - Detectors
  - Instrument development infrastructure (computer simulations)
  - New techniques and applications