Neutron Optics and Instrumentation

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Oak Ridge National Laboratory

National School on Neutron and X-Ray Scattering
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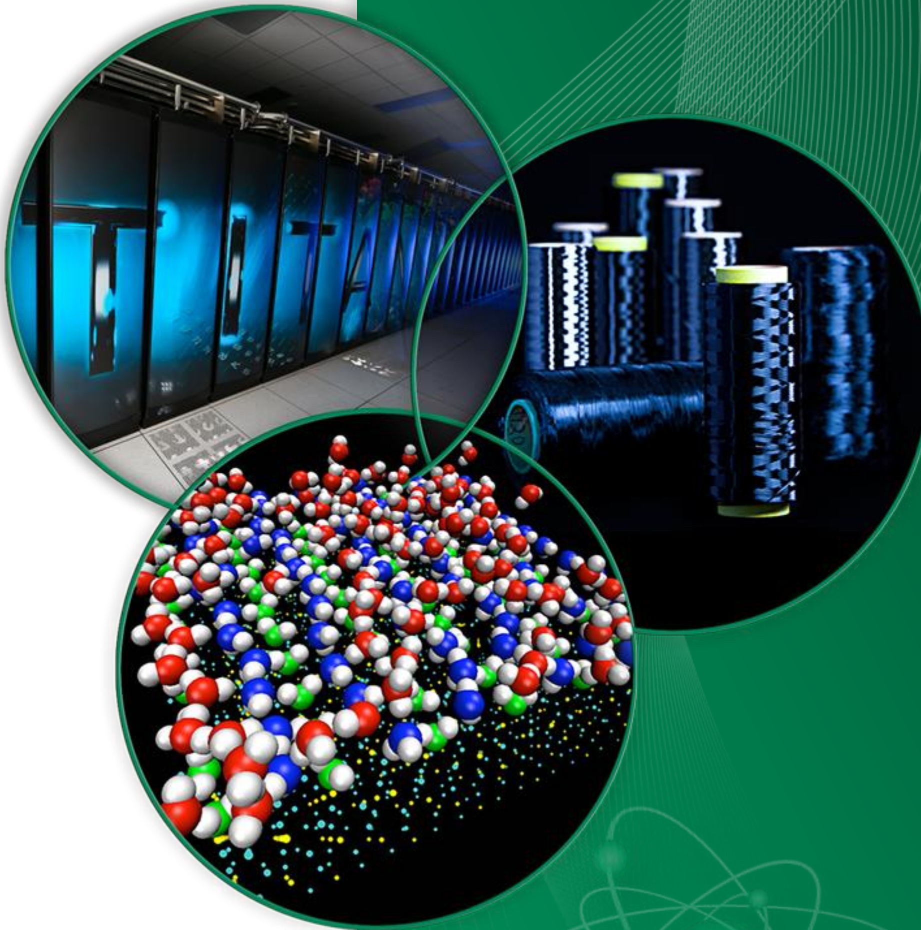
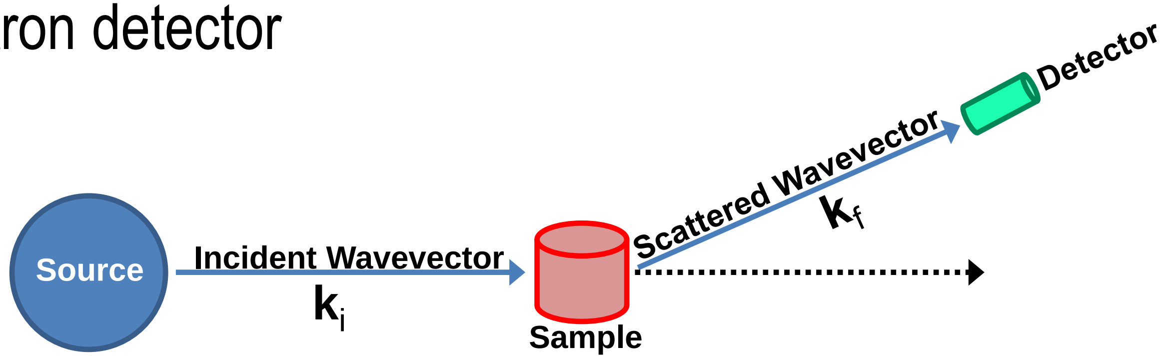
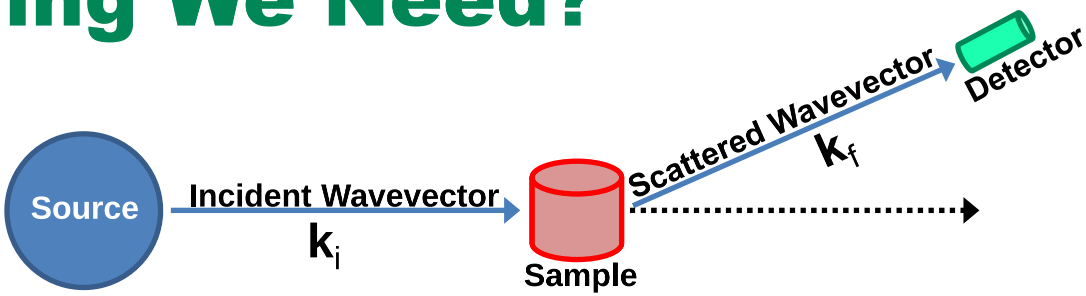


What is a Neutron Scattering Instrument?

- 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 ($\mathbf{k}_i$)
  3) A very interesting sample
  4) A method for determining the wavevector of the scattered neutrons ($\mathbf{k}_f$)
  5) A neutron detector



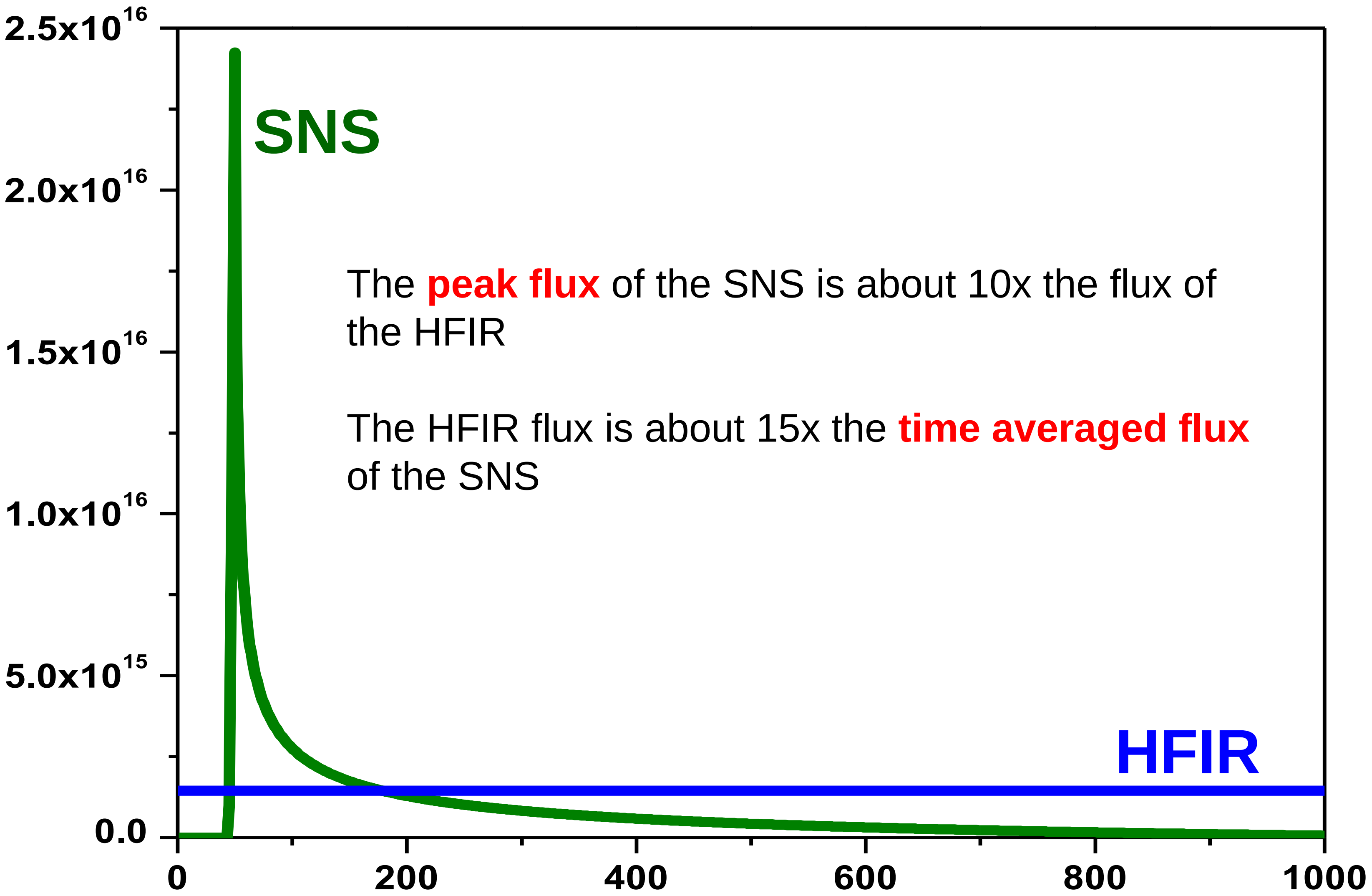
Why Not Just Build a Universal Neutron Scattering Instrument That Can Do Everything We Need?



- 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:

  $\lambda^2(Å^2) \sim 81.81/E(meV)$ and $v^2(m^2/s^2) \sim 191313 \times E(meV)$
- S(Q,E) the scattering properties of the sample depend only on Q and E, not on the neutron wavelength(λ)
- 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.

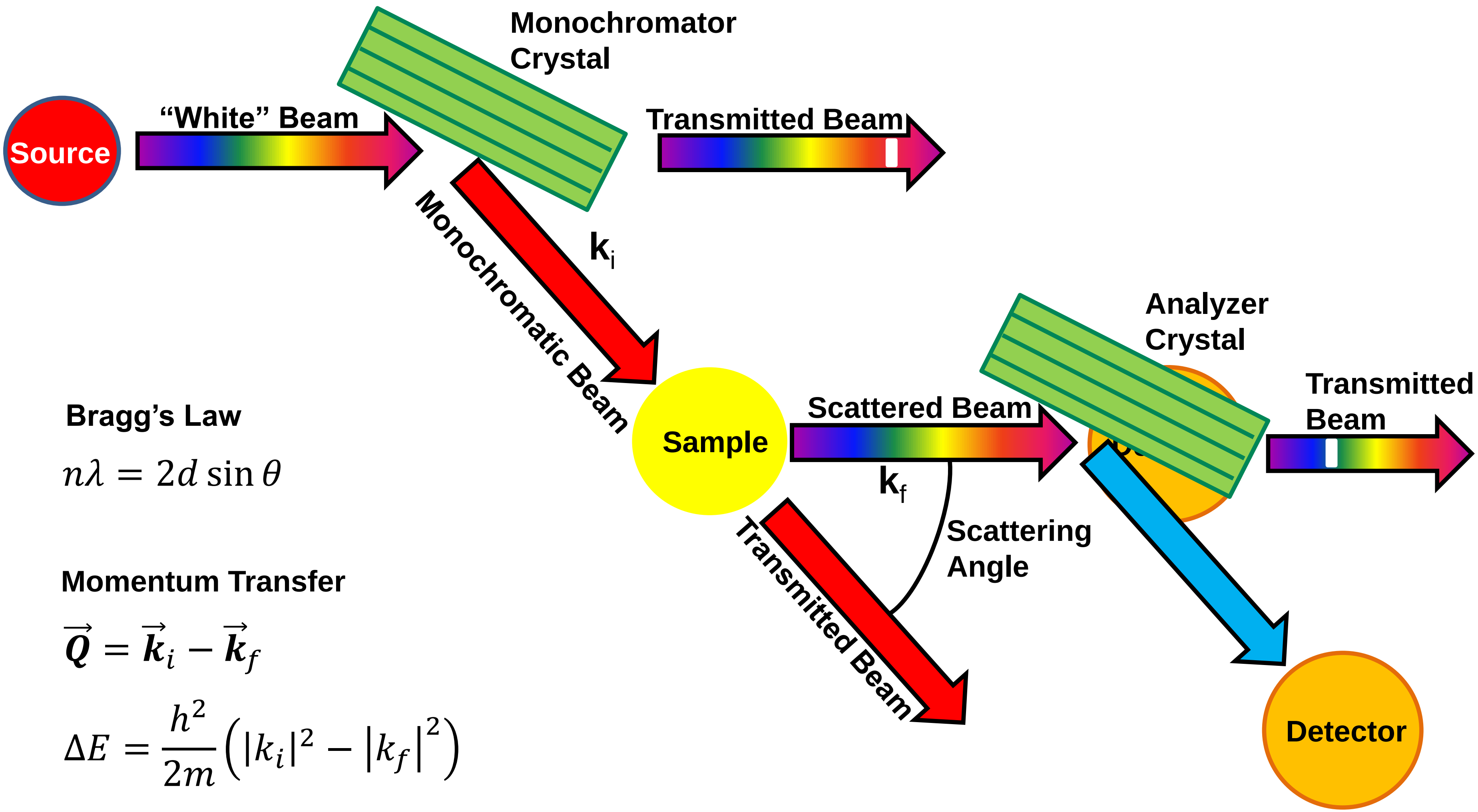
Pulsed vs Continuous



The **peak flux** of the SNS is about 10x the flux of the HFIR

The HFIR flux is about 15x the **time averaged flux** of the SNS

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



Bragg's Law

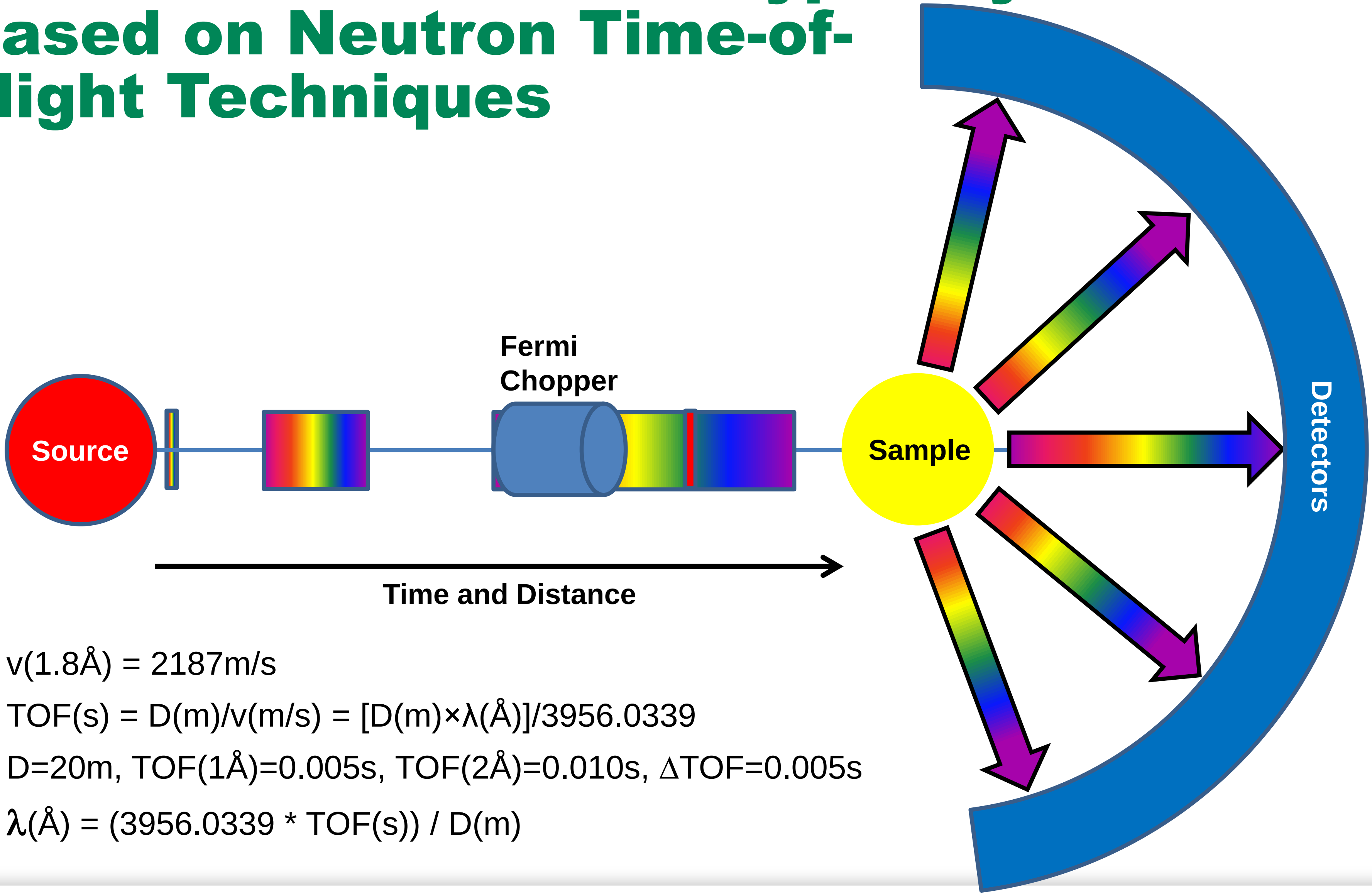
$$n\lambda = 2d \sin\theta$$

Momentum Transfer

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

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

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



v(1.8Å) = 2187m/s

TOF(s) = D(m)/v(m/s) = [D(m)×λ(Å)]/3956.0339

D=20m, TOF(1Å)=0.005s, TOF(2Å)=0.010s, ΔTOF=0.005s

λ(Å) = (3956.0339 * TOF(s)) / D(m)

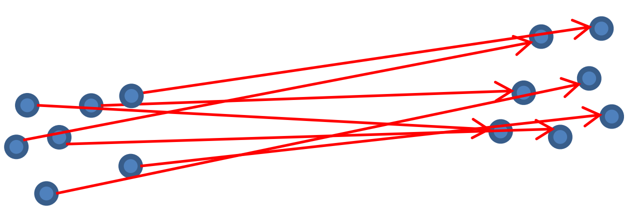
Neutron Optics

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

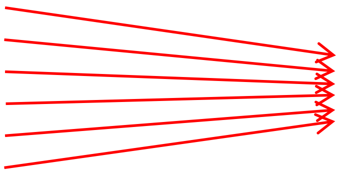
- **Monochromators / Analyzers:** Monochromate or analyze the energy of a neutron beam using Bragg's law
- **Choppers:** Define a short pulse of neutrons or select a small band of neutron energies
- **Guides / Mirrors:** Allow neutrons to travel large distances without suffering intensity loss
- **Polarizers / 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.

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

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

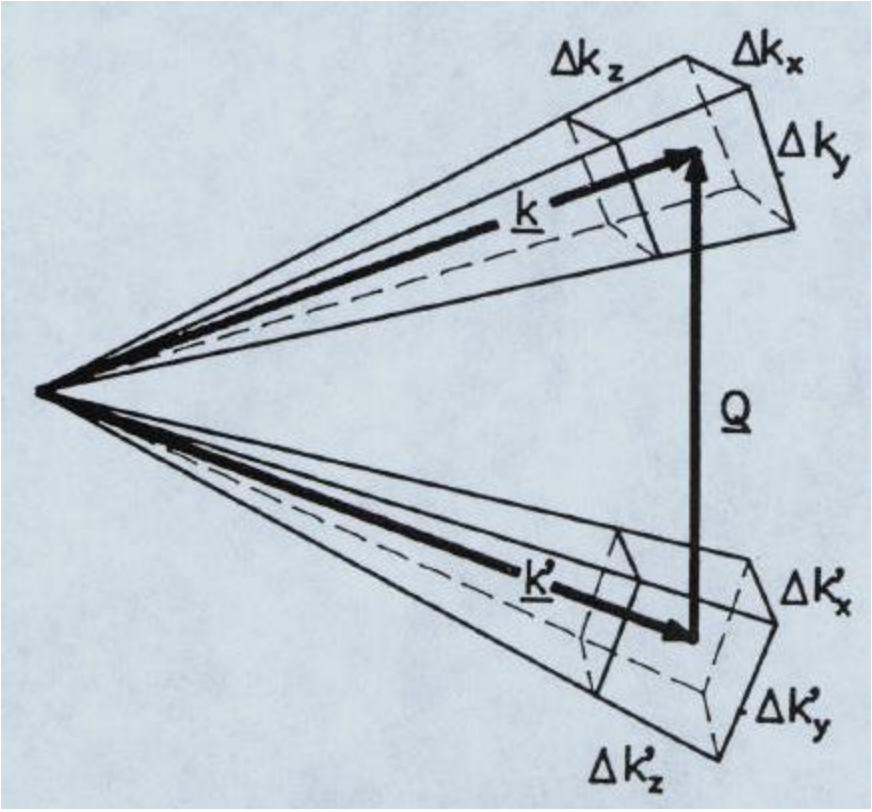
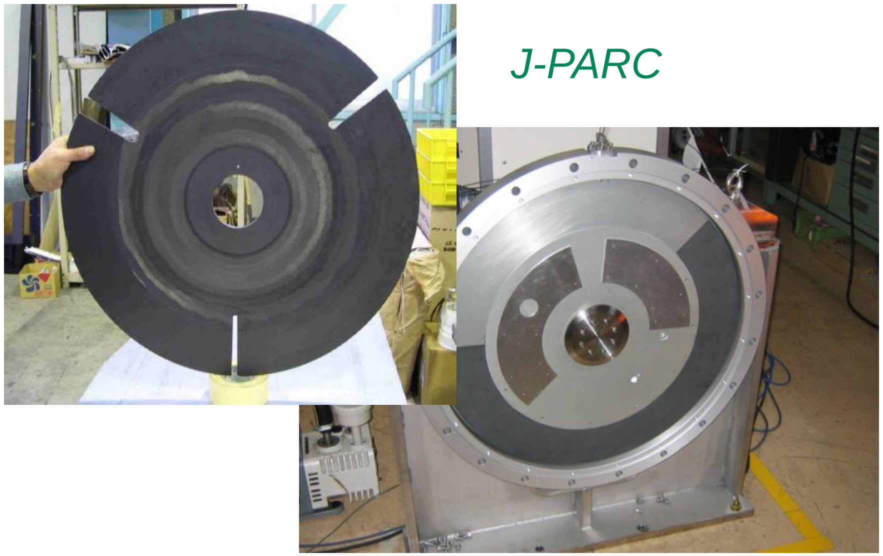


Figure borrowed from Roger Pynn

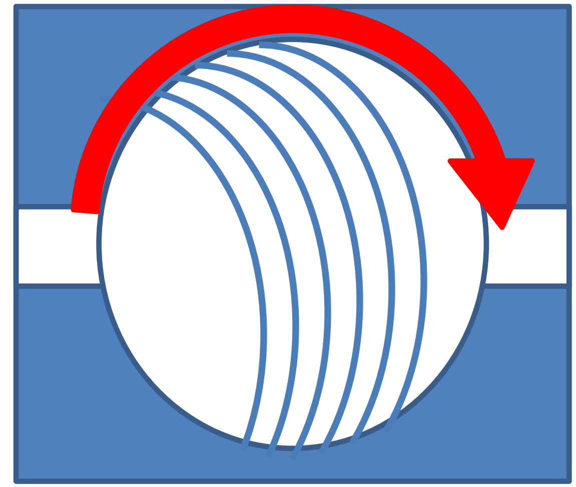
Choppers and Velocity Selectors

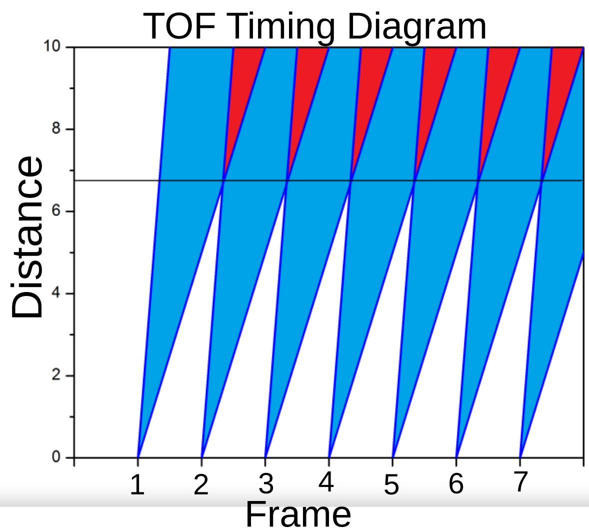
Disk Chopper



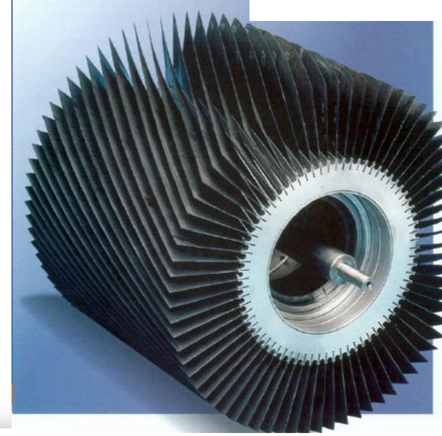
J-PARC

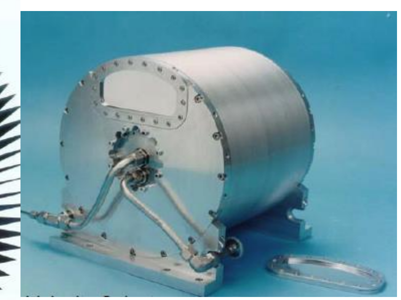
Fermi Chopper





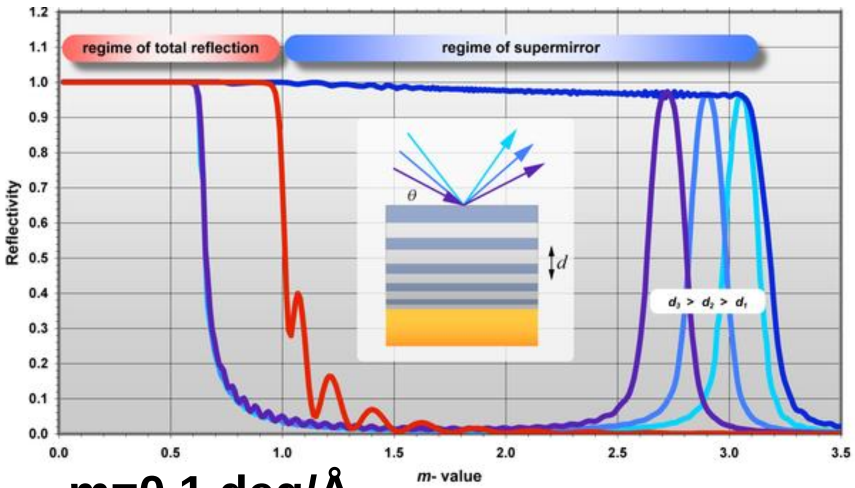
Velocity Selector



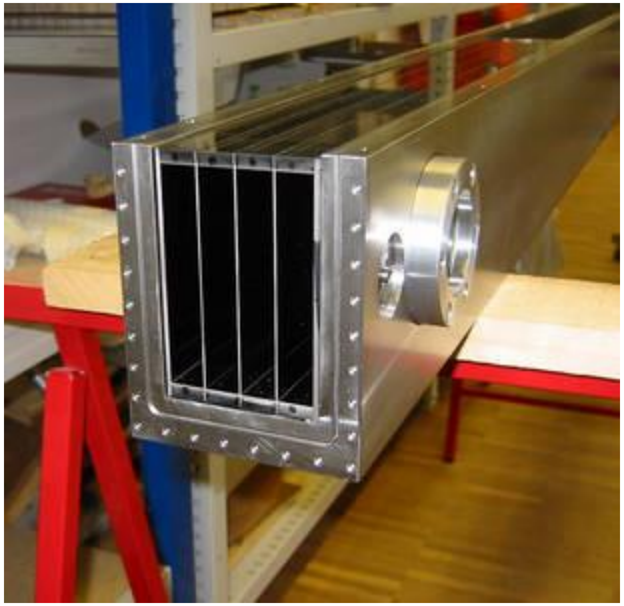


Astrium

Neutron Guides



m=0.1 deg/Å

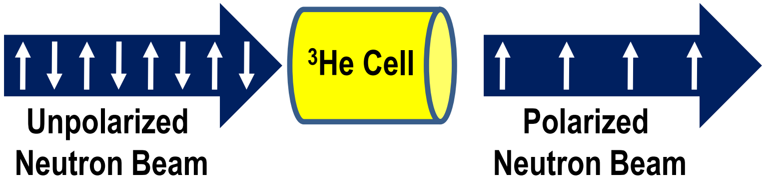


Multichannel Curved Guide
Fabricated by Swiss Neutronics

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

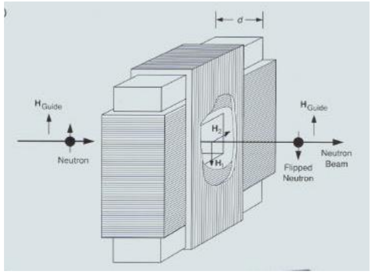
Guide Installation at ISIS

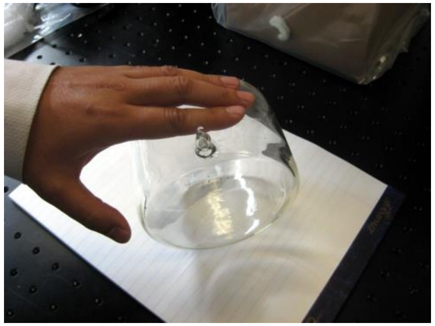
Polarizers and Spin Manipulators



Heussler Monochromator AlCuMn

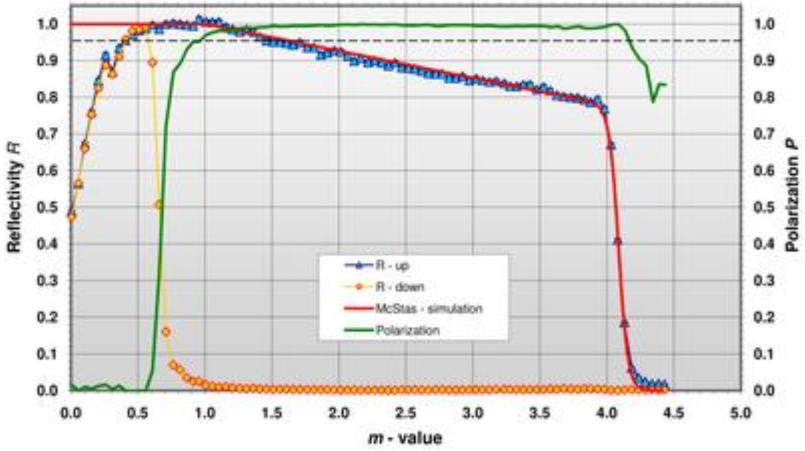
Larmor Precession Flipper





^{3}He Spin Filters

Polarizing Supermirrors

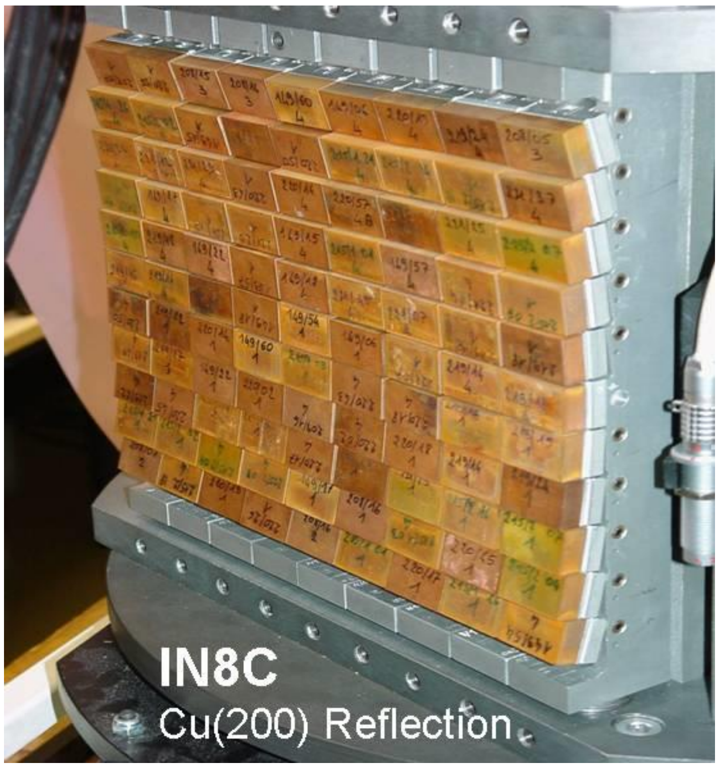


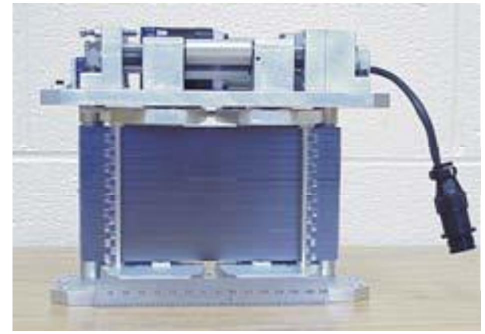
Spherical Neutron Polarimetry

POLI-HEiDi at FRMII

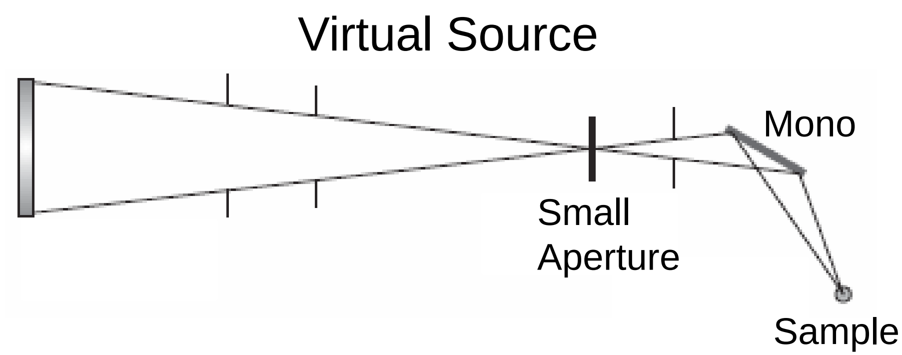
Neutron Optics: Focusing

Doubly focusing Cu monochromator at the ILL

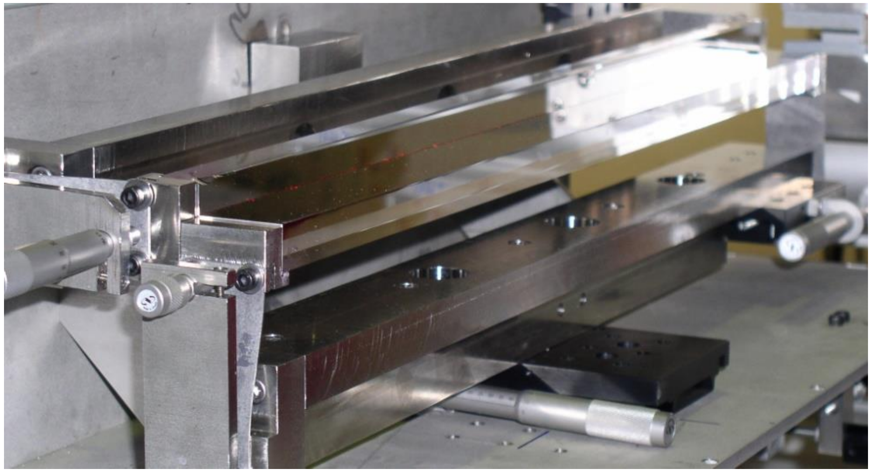


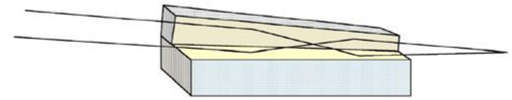


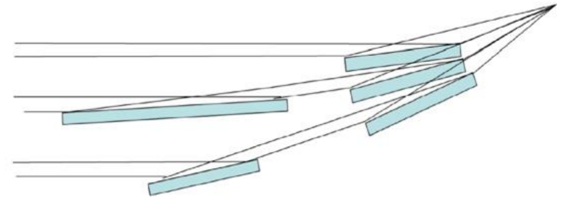
Double focusing "Popovici" monochromator. The vertical curvature is fixed while the horizontal curvature is variable by bending stacks of thin silicon wafers. The gain is achieved both by spatial focusing and 'wavelength focusing'.



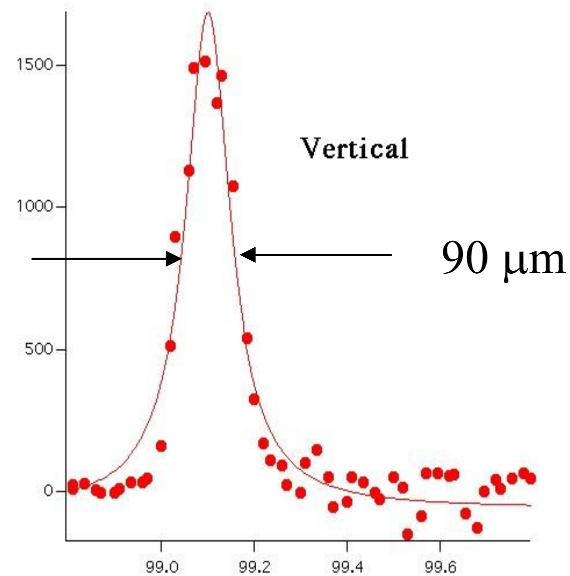
Neutron Optics: Focusing







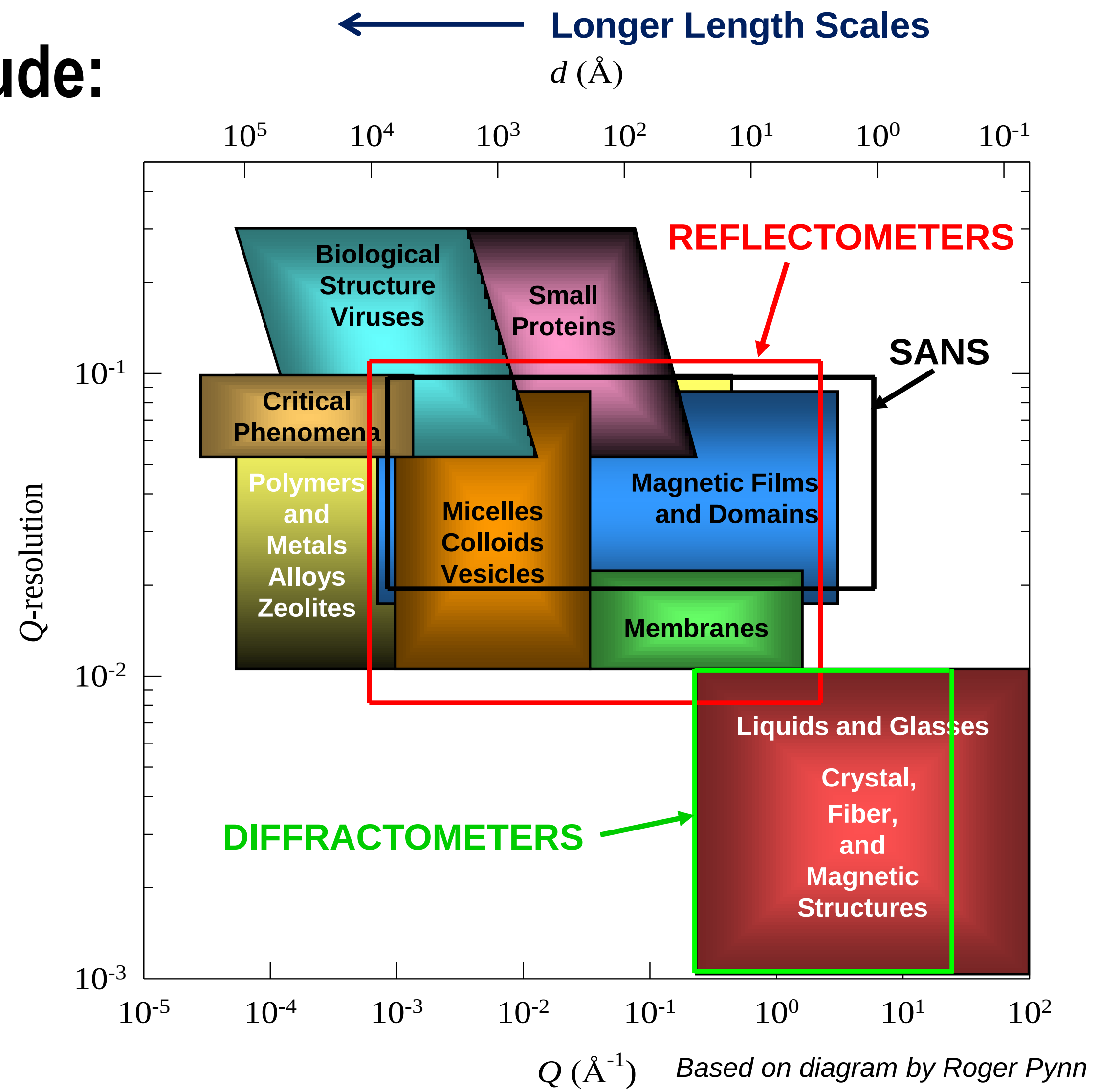
- Focusing Mirrors :
  - Develop a nested advanced KB mirror system to make a more compact assembly and to achieve the highest performance.
  - Identify applications where focusing optics can replace neutron guides and offer better performance.



Elastic Neutron Scattering Instruments

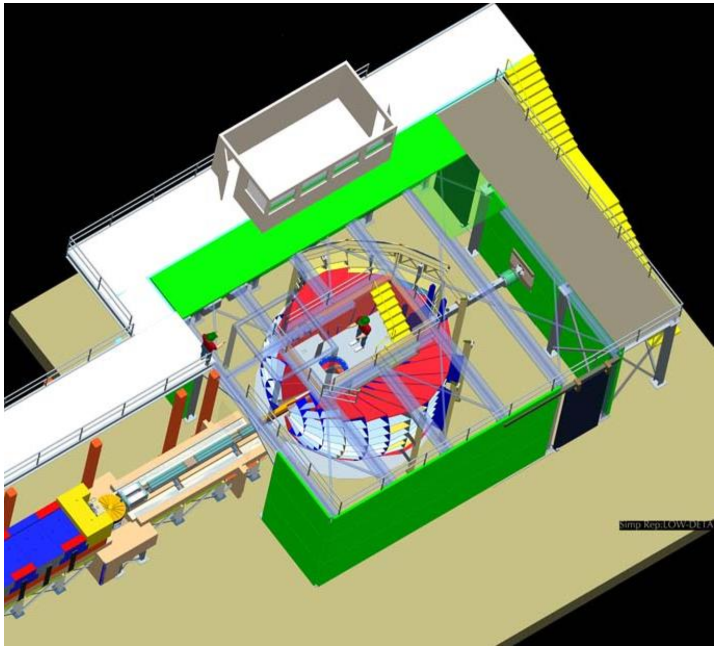
- Elastic instruments include:
  - Powder diffraction
  - Single Crystal diffraction
  - SANS (typical)
  - Reflectometry

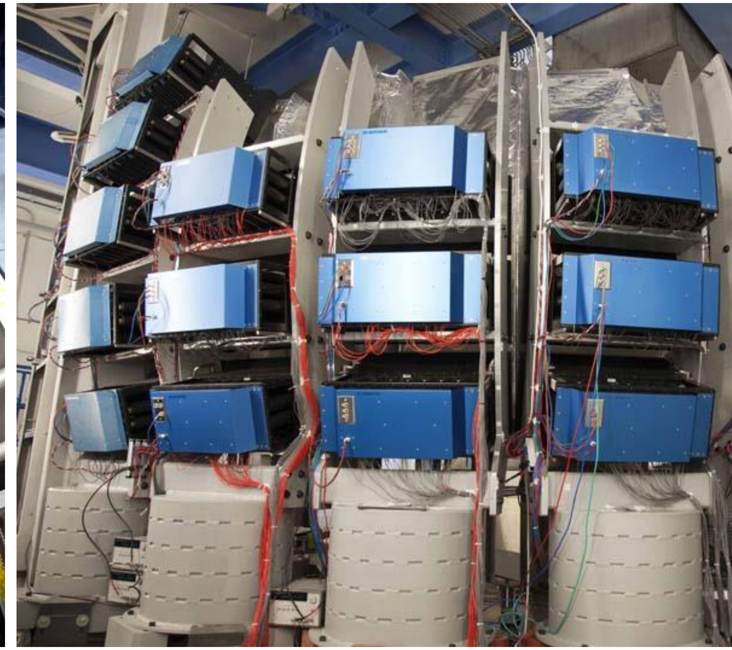
- Used to determine the average structure of materials (i.e. how the atoms are arranged)



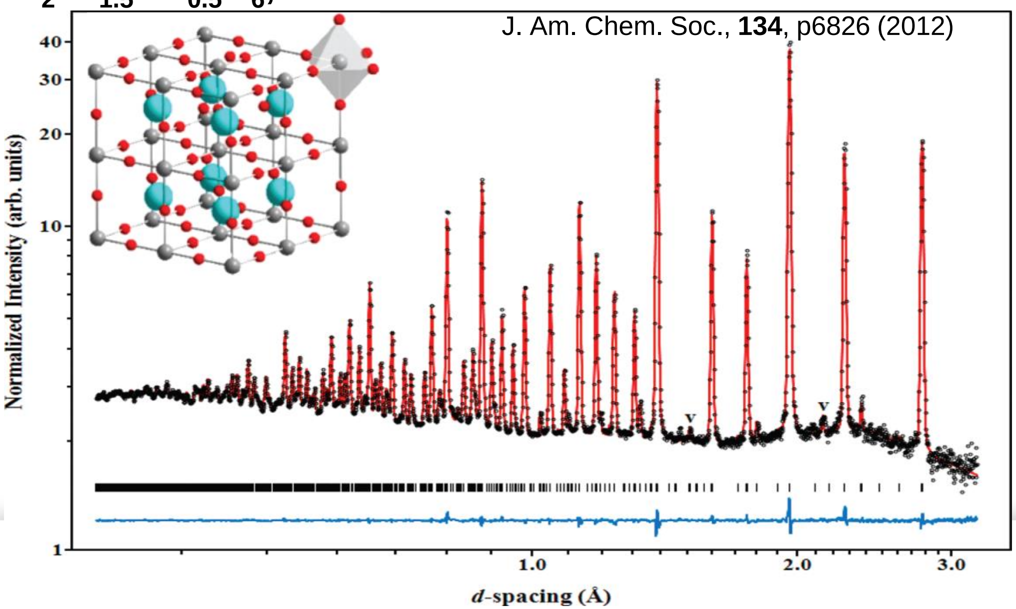
Based on diagram by Roger Pynn

TOF Powder Diffractometer: POWGEN (SNS)





$Sr_2Fe_{1.5}Mo_{0.5}O_6$, Electrode Material for Solid Oxide Fuel Cells



J. Am. Chem. Soc., **134**, p6826 (2012)

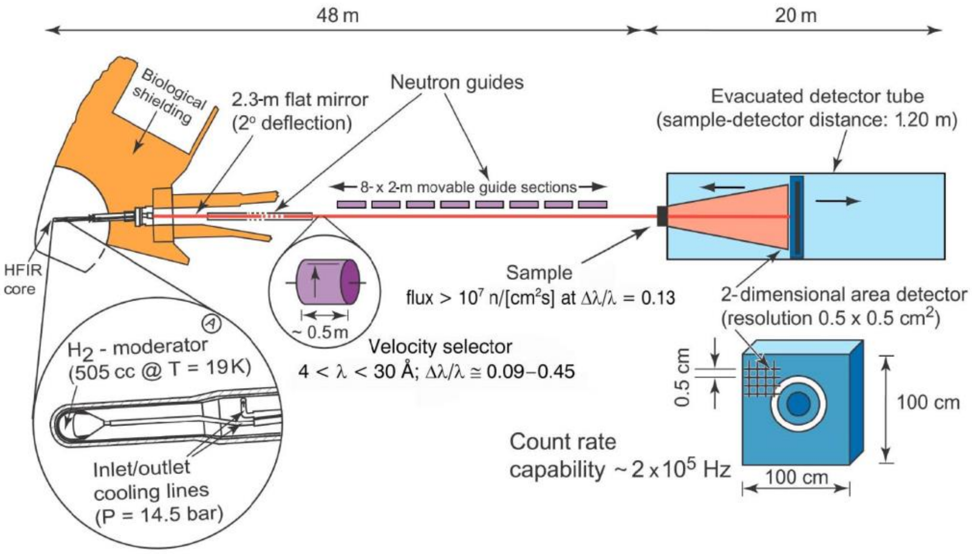
$$d = \frac{\lambda}{2\sin\theta} = \frac{2\pi}{Q}$$

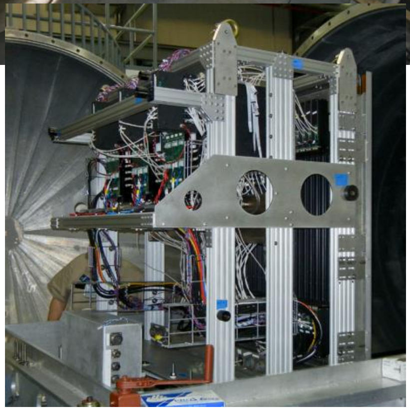
$$\lambda(\text{Å}) = (3956.0339 * TOF(s)/D(m)$$

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

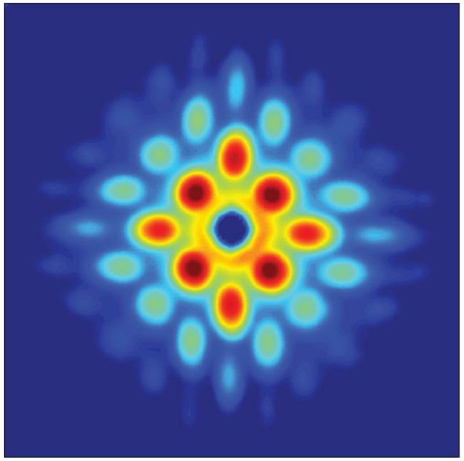
For POWGEN D = 64.5m

Small Angle Neutron Scattering (SANS)



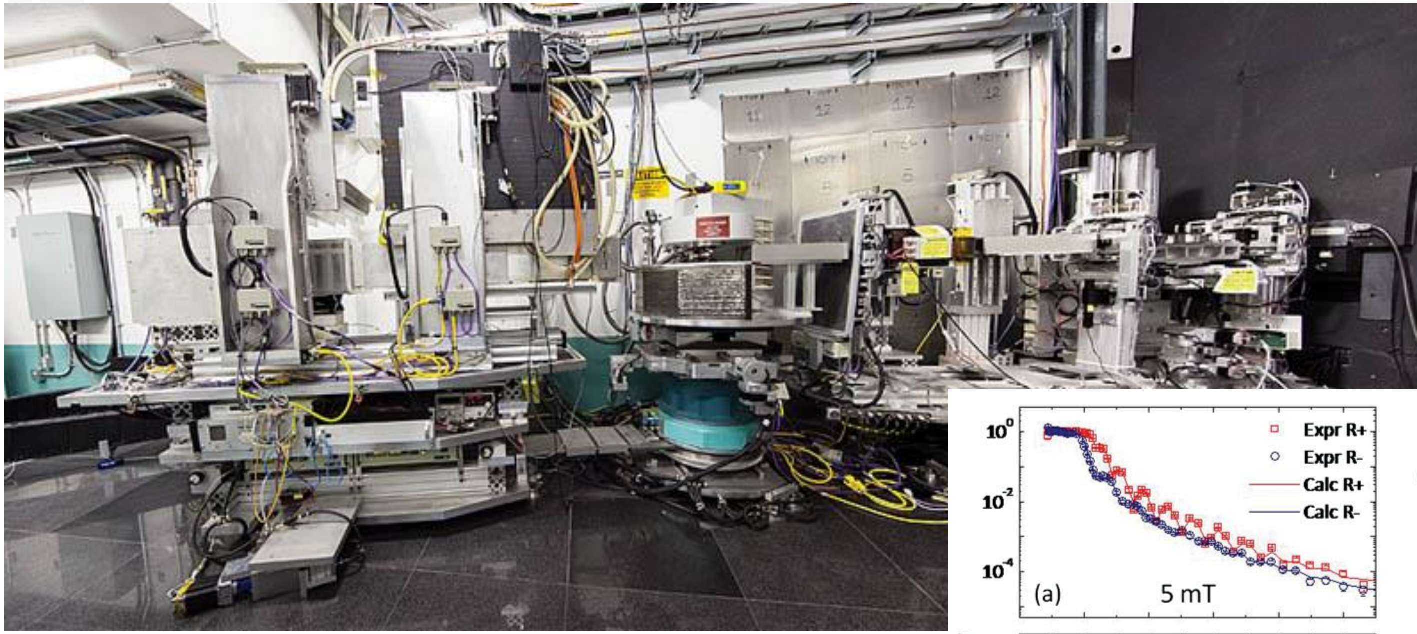


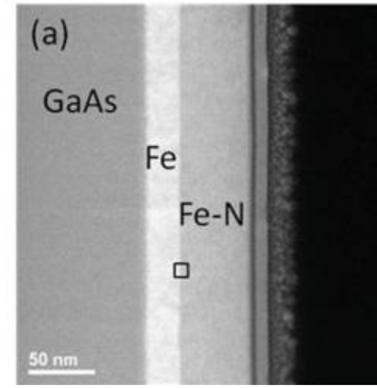
$TmNi_2B_2C$ Vortex Lattice

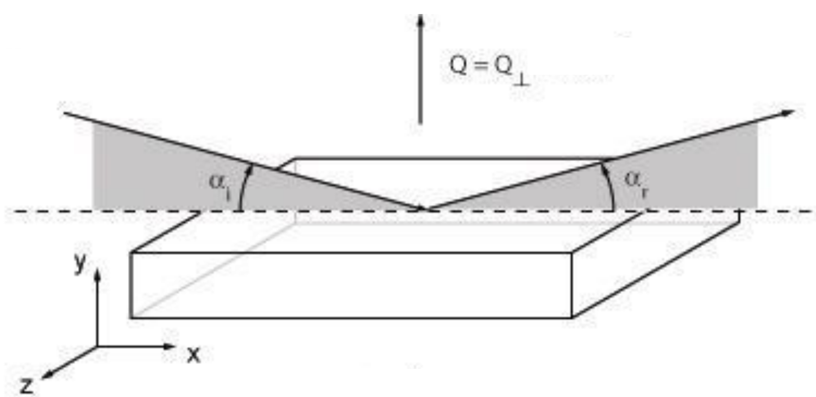


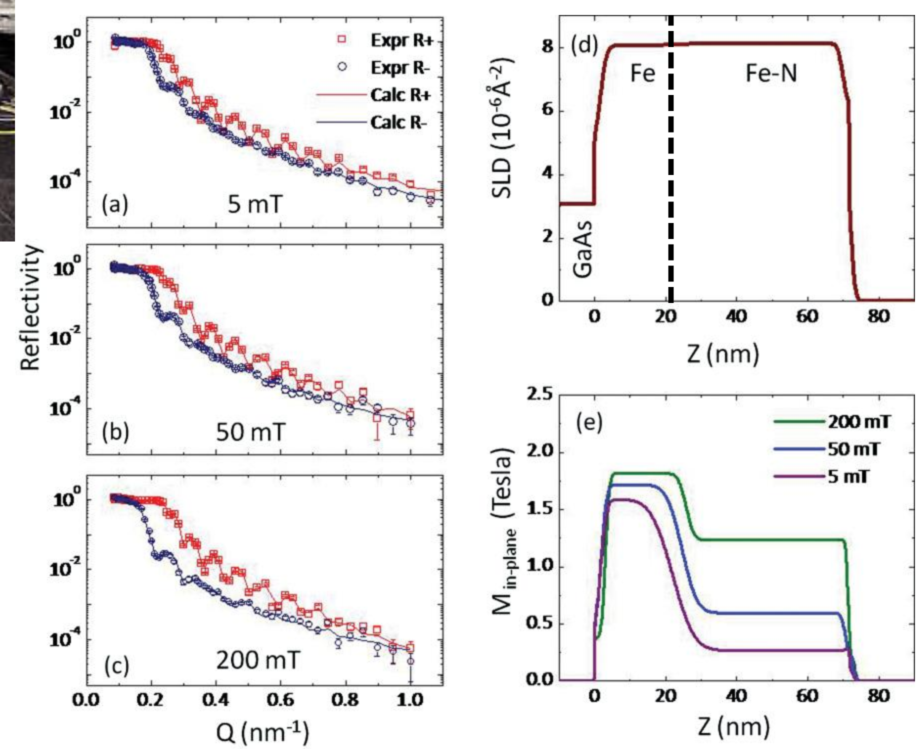
PHYS REV B **86**, 144501 (2012)

Magnetism Reflectometer (SNS)



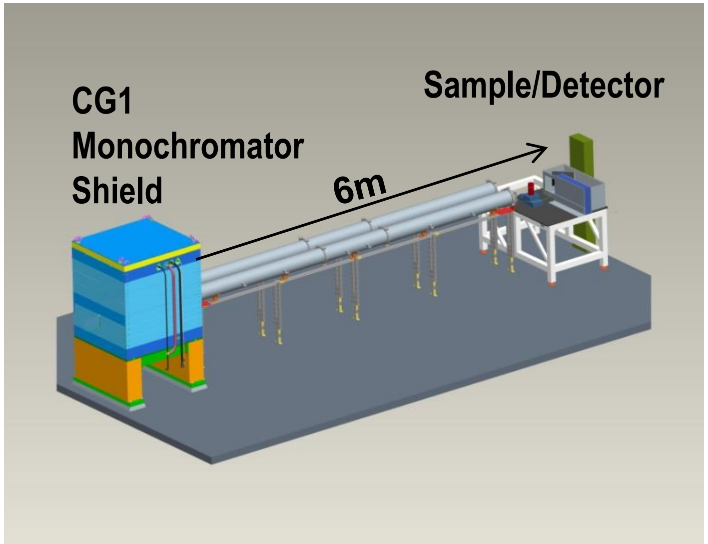




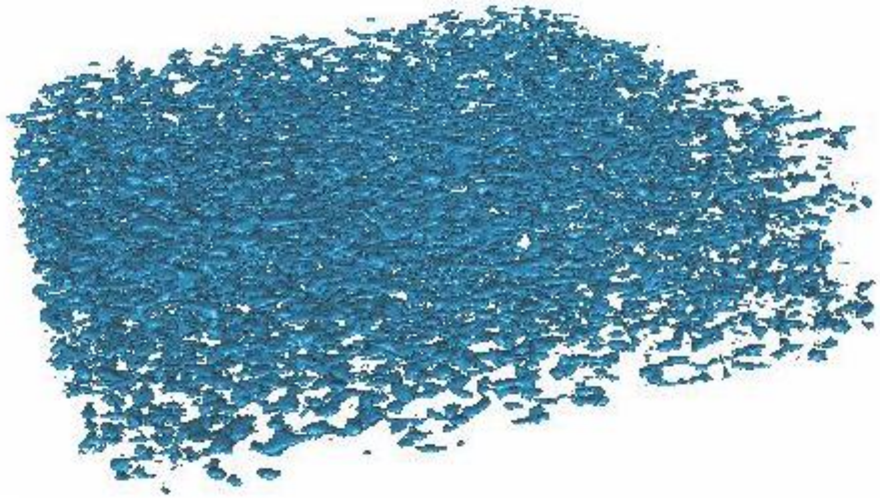


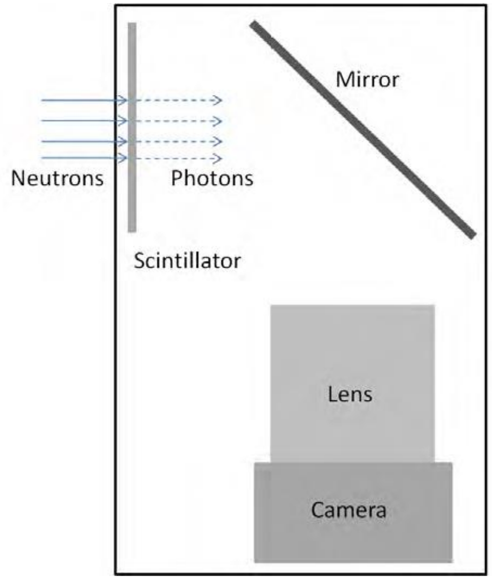
PHY REV B **84**, 245310 (2011)

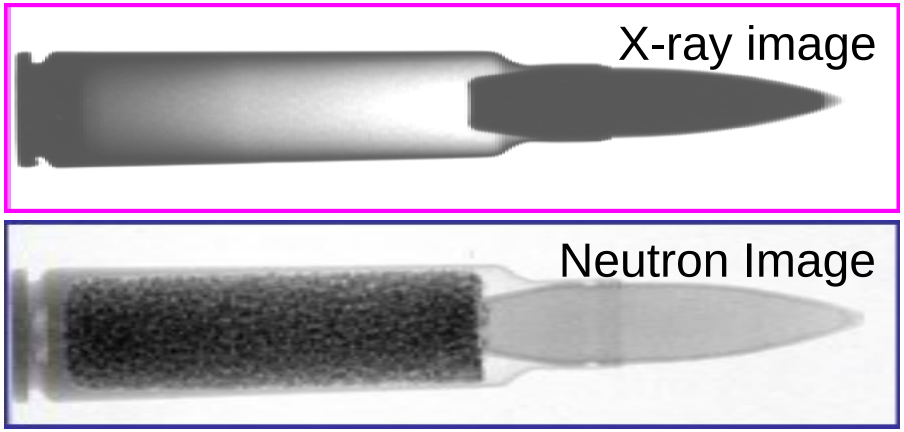
Neutron Imaging



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

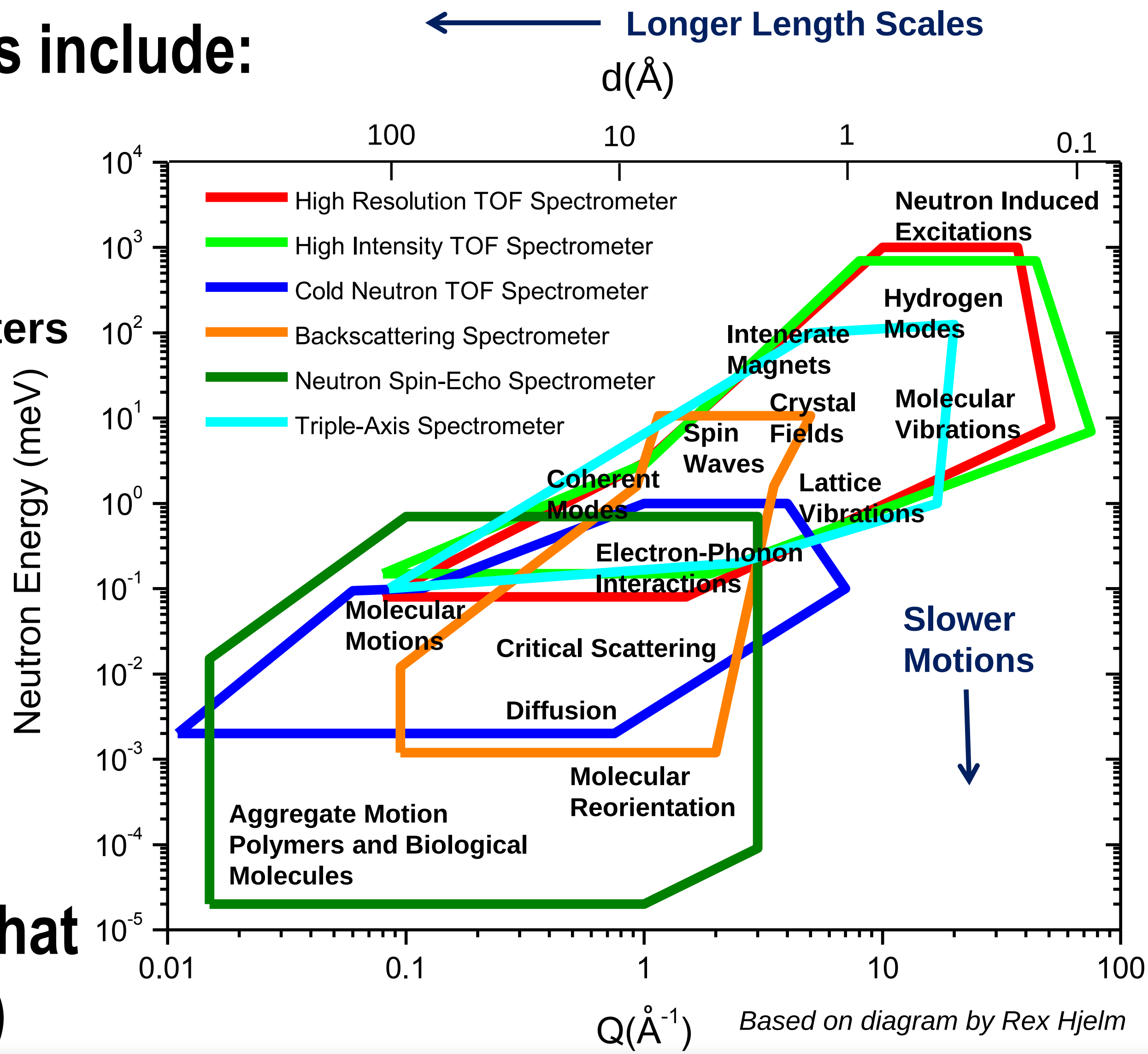






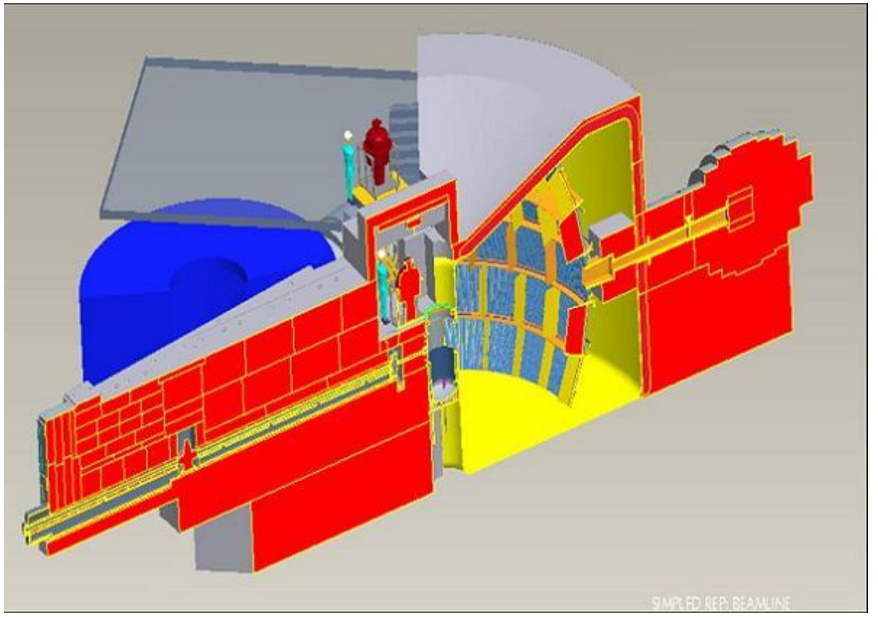
Inelastic Neutron Scattering Instruments

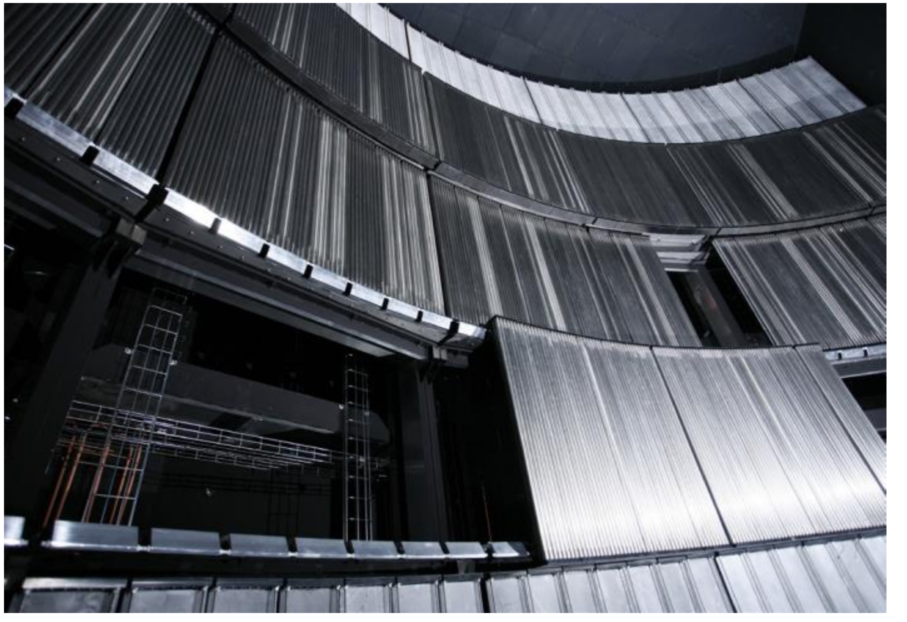
- **Inelastic instruments include:**
  - Direct Geometry TOF Spectrometers
  - Indirect Geometry TOF Spectrometers
  - Triple-Axis Spectrometers
  - Backscattering Spectrometers
  - Neutron Spin-Echo Spectrometers
- **Used to study dynamics such as phonons, magnons, and diffusion (i.e. what the atoms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



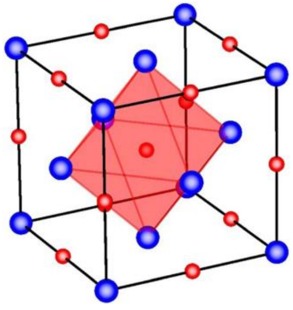
Based on diagram by Rex Hjelm

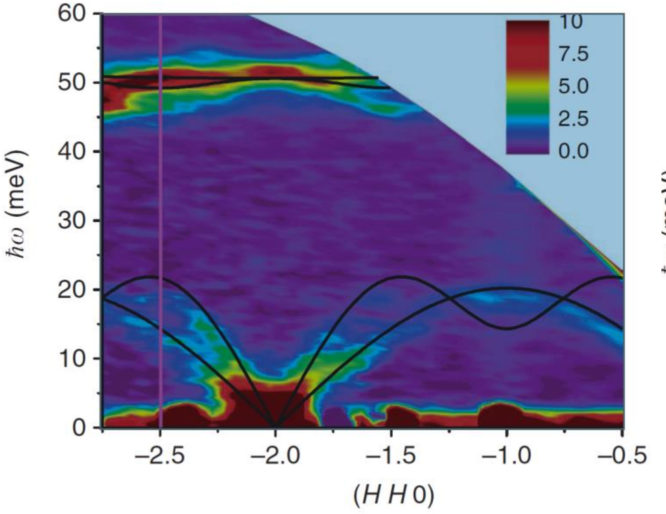
SEQUOIA: A Direct Geometry TOF Spectrometer at the SNS

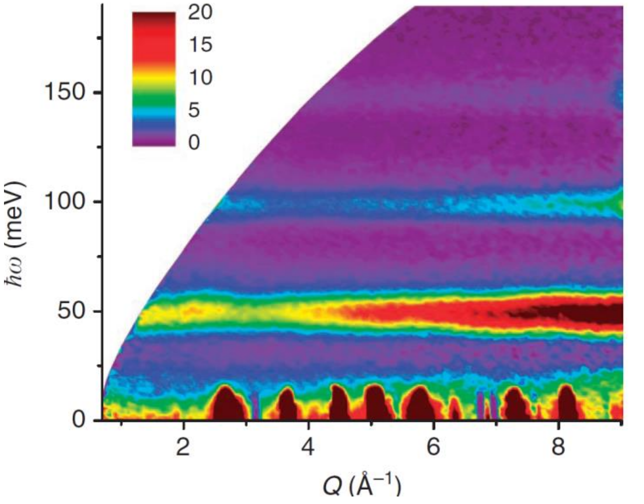




Quantum oscillations of nitrogen atoms in uranium nitride



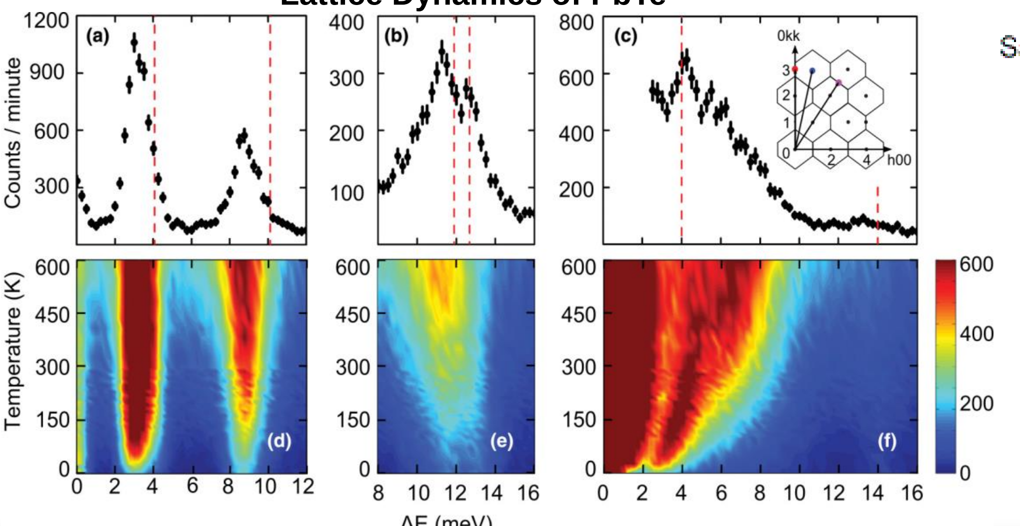




Nature Communications v**3**, p1124 (2012)

Triple-Axis Spectrometer

Lattice Dynamics of PbTe



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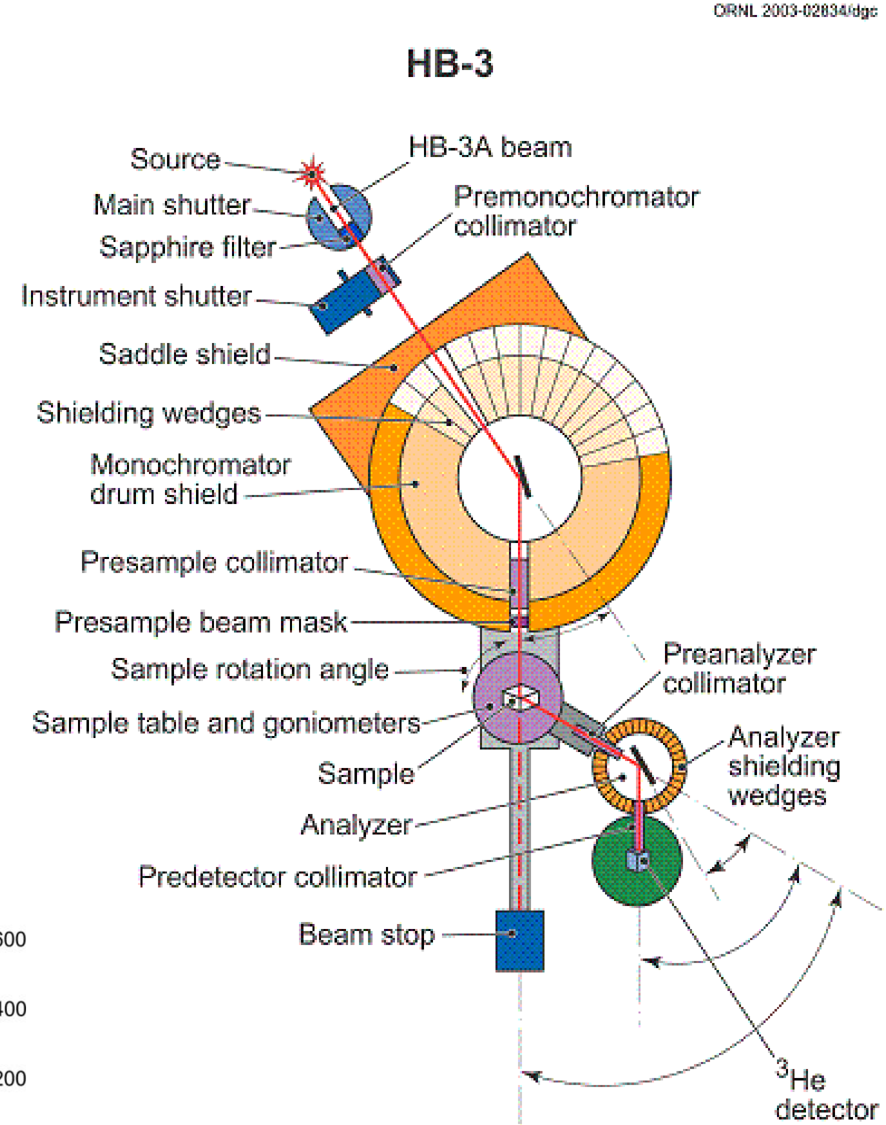
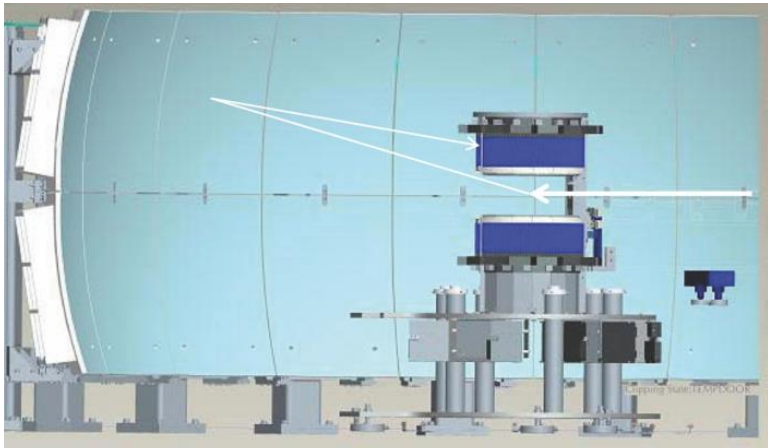
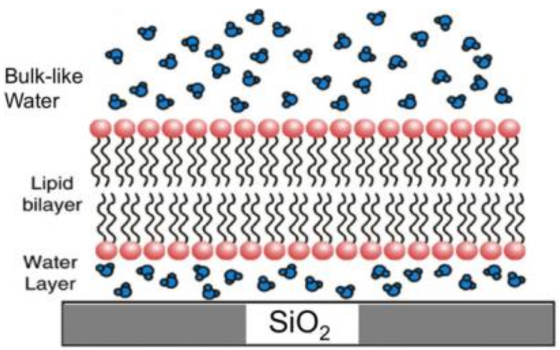
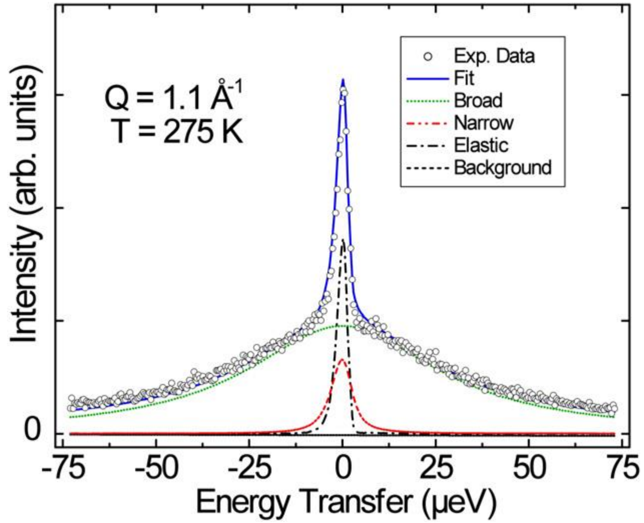


BASIS: An Inverted Geometry Backscattering Spectrometer

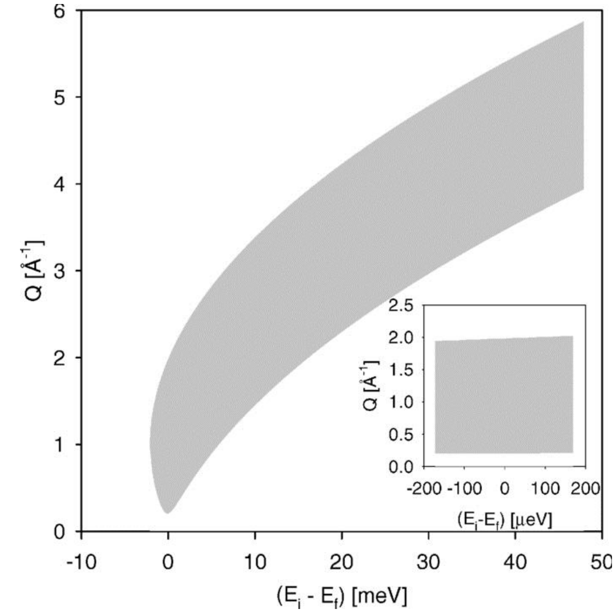


Study of water diffusion on single-supported bilayer lipid membranes by QENS





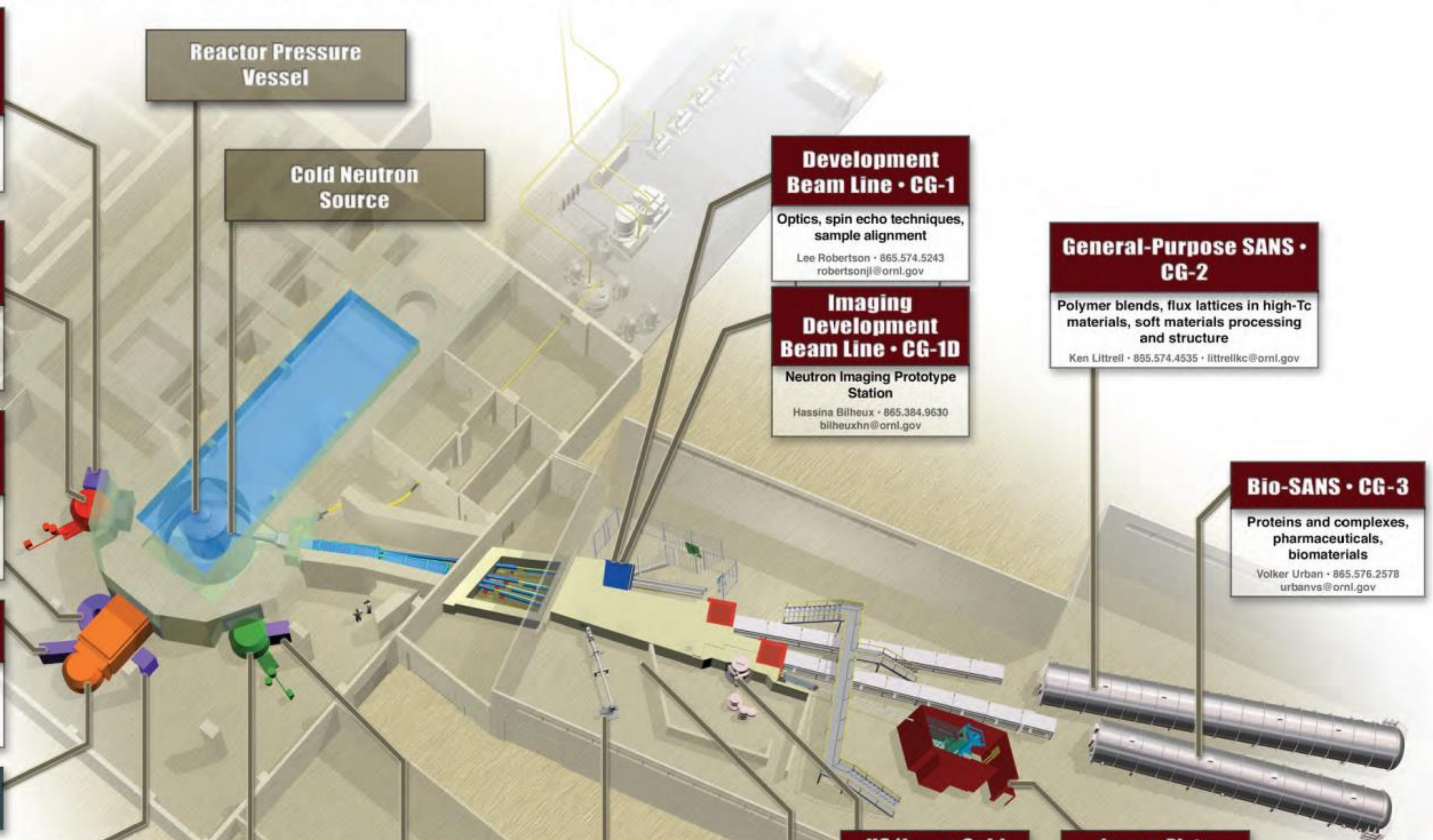
Bai M., *EPL* **98**, 48006 (2012)



High Flux Isotope Reactor at Oak Ridge National Laboratory

The United States' highest flux reactor-based neutron source

HFIR



Reactor Pressure Vessel

Cold Neutron Source

Fixed-Incident-Energy Triple-Axis Spectrometer • HB-1A
Low-energy excitations, magnetism, structural transitions
Wei Tian • 865.574.6427 tianwn@ornl.gov

Polarized Triple Axis Spectrometer • HB-1
Polarized neutron studies of magnetic materials, low-energy excitations, structural transitions
Masaaki Matsuda • 865.574.6580 matsudam@ornl.gov

Neutron Powder Diffractometer • HB-2A
Structural studies, magnetic structures, texture and phase analysis
Ovidiu Garlea • 865.574.5041 garleao@ornl.gov

US/Japan WAND • HB-2C
Diffuse-scattering studies of single crystals and time-resolved phase transitions
Jaime Fernandez-Baca • 865.576.8659 fernandezbja@ornl.gov

Future Development • HB-2D

Neutron Residual Stress Mapping Facility • HB-2B
Strain and phase mapping in engineering materials
Andrew Payzant • 865.235.4981 • payzanta@ornl.gov

Triple-Axis Spectrometer • HB-3
Medium- and high-resolution inelastic scattering at thermal energies
Andy Christianson • 865.574.1181 christiansad@ornl.gov

Four-Circle Diffractometer • HB-3A
Small unit-cell crystal structural studies, particularly H-bonding
Huibo Cao • 865.241.9428 caoh@ornl.gov

Future Development • CG-4A

Future Development • CG-4B

US/Japan Cold Neutron Triple-Axis Spectrometer • CG-4C
High-resolution inelastic scattering at cold neutron energies
Tao Hong • 865.574.8659 hongt@ornl.gov

Image-Plate Single-Crystal Diffractometer (IMAGINE) • CG-4D
Chemical, organic, metallo-organic, protein single crystals
Flora Meilleur • 865.241.2897 meilleurf@ornl.gov

Development Beam Line • CG-1
Optics, spin echo techniques, sample alignment
Lee Robertson • 865.574.5243 robertsonjl@ornl.gov

Imaging Development Beam Line • CG-1D
Neutron Imaging Prototype Station
Hassina Bilheux • 865.384.9630 bilheuxhn@ornl.gov

General-Purpose SANS • CG-2
Polymer blends, flux lattices in high-Tc materials, soft materials processing and structure
Ken Littrell • 865.574.4535 • littrellkc@ornl.gov

Bio-SANS • CG-3
Proteins and complexes, pharmaceuticals, biomaterials
Volker Urban • 865.576.2578 urbanvs@ornl.gov

* Scheduled commissioning date.

LEGEND
Installed, commissioning, or operating
In design or construction
Under consideration

07-G00244L/gim

U.S. DEPARTMENT OF ENERGY Office of Science

OAK RIDGE National Laboratory

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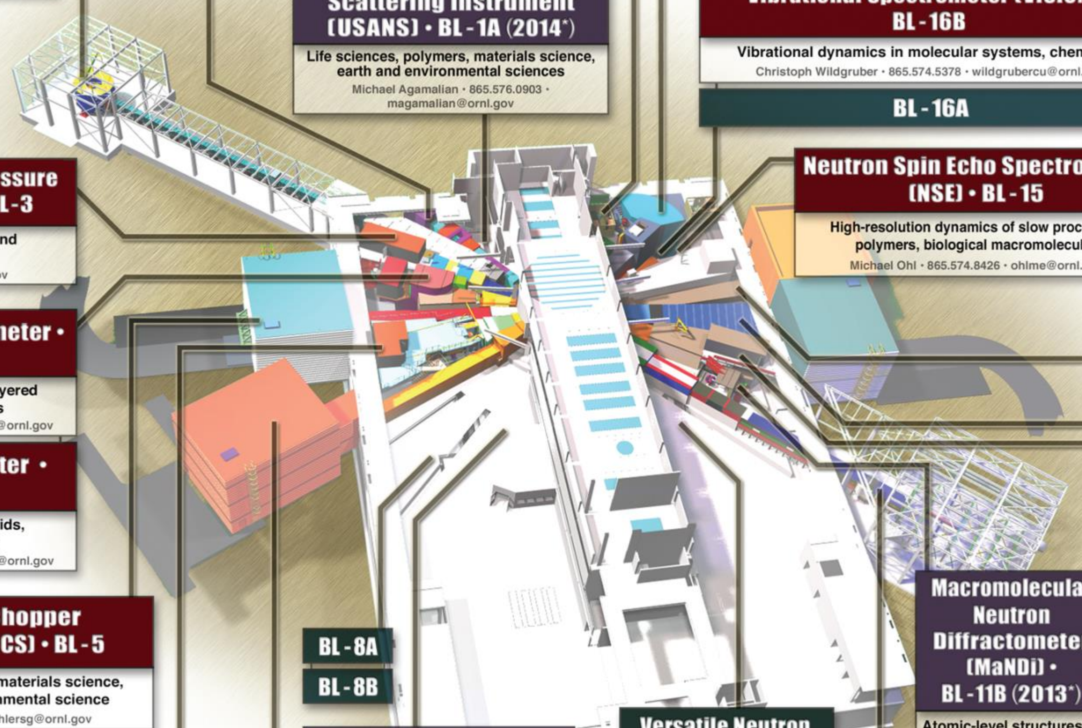
Spallation Neutron Source at Oak Ridge National Laboratory

The world's most intense pulsed, accelerator-based neutron source

SNS SPALLATION NEUTRON SOURCE



Backscattering Spectrometer (BASIS) • BL-2
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Eugene Mamontov • 865.574-5109 • mamontove@ornl.gov

Nanoscale-Ordered Materials Diffractometer (NOMAD) • BL-1B
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuefeind • 865.241.1635 • neuefeindjc@ornl.gov

Wide Angular-Range Chopper Spectrometer (ARCS) • BL-18
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Doug Abernathy • 865.576.5105 • abernathydl@ornl.gov

Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) • BL-17
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Garrett Granroth • 865.576.0900 • granrothge@ornl.gov

Ultra-Small-Angle Neutron Scattering Instrument (USANS) • BL-1A (2014*)
Life sciences, polymers, materials science, earth and environmental sciences
Michael Agamalian • 865.576.0903 • magamalian@ornl.gov

Vibrational Spectrometer (VISION) • BL-16B
Vibrational dynamics in molecular systems, chemistry
Christoph Wildgruber • 865.574.5378 • wildgrubercu@ornl.gov

BL-16A

Spallation Neutrons and Pressure Diffractometer (SNAP) • BL-3
Materials science, geology, earth and environmental sciences
Chris Tulk • 865.576.7028 • tulkca@ornl.gov

Neutron Spin Echo Spectrometer (NSE) • BL-15
High-resolution dynamics of slow processes, polymers, biological macromolecules
Michael Ohl • 865.574.8426 • ohlme@ornl.gov

Hybrid Polarized Beam Spectrometer (HYSPEC) • BL-14B
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Barry Winn • 865.809.6819 • winnbl@ornl.gov

BL-14A

Magnetism Reflectometer • BL-4A
Chemistry, magnetism of layered systems and interfaces
Valeria Lauter • 865.576.5389 • lauterv@ornl.gov

Liquids Reflectometer • BL-4B
Interfaces in complex fluids, polymers, chemistry
John Ankner • 865.576.5122 • anknerjf@ornl.gov

Fundamental Neutron Physics Beam Line • BL-13
Fundamental properties of neutrons
Geoffrey Greene • 865.574.8435 • greenegl@ornl.gov

Cold Neutron Chopper Spectrometer (CNCS) • BL-5
Condensed matter physics, materials science, chemistry, biology, environmental science
Georg Ehlers • 865.576.3511 • ehlersg@ornl.gov

BL-8A

BL-8B

Macromolecular Neutron Diffractometer (MaNDi) • BL-11B (2013*)
Atomic-level structures of membrane proteins, drug complexes, DNA
Leighton Coates • 865.963.6180 • coatesl@ornl.gov

Single-Crystal Diffractometer (TOPAZ) • BL-12
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
Christina Hoffmann • 865.576.5127 • hoffmanncm@ornl.gov

Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) • BL-6
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
William Heller • 865.241.0093 • hellerwt@ornl.gov

Elastic Diffuse Scattering Spectrometer (CORELLI) • BL-9 (2014*)
Detailed studies of disorder in crystalline materials
Feng Ye • 865.576.0931 • yef1@ornl.gov

Versatile Neutron Imaging Instrument at SNS (VENUS) • BL-10
Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology
Hassina Bilheux • 865.384.9630 • bilheuxhn@ornl.gov

Powder Diffractometer (POWGEN) • BL-11A
Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures
Ashfia Huq • 630.986.7321 • huqa@ornl.gov

Engineering Materials Diffractometer (VULCAN) • BL-7
Mechanical behaviors, materials science, materials processing
Ke An • 865.919.5226 • kean@ornl.gov

* Scheduled commissioning date

LEGEND
Installed, commissioning, or operating
In design or construction
Under consideration

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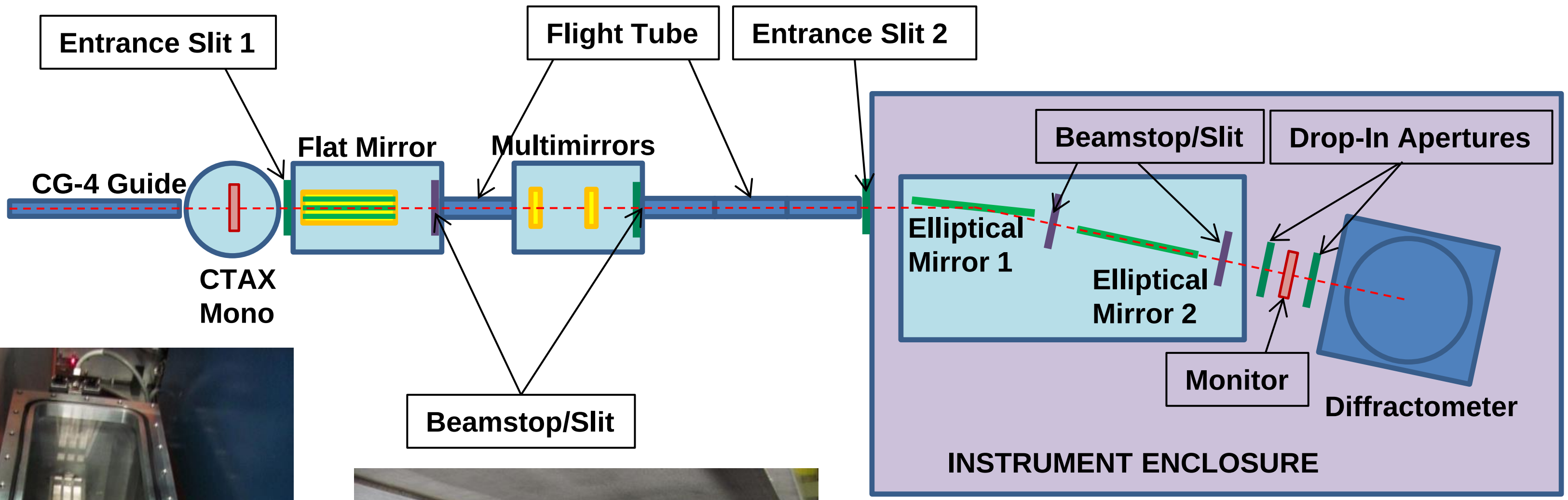
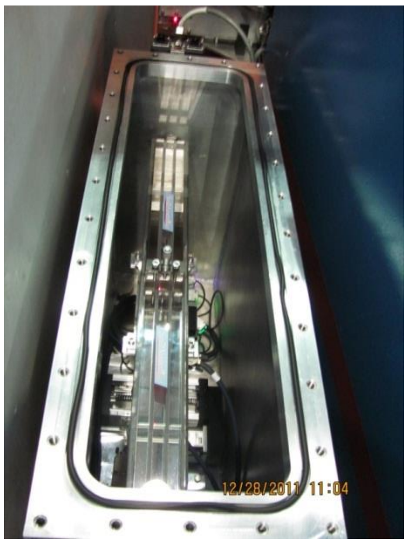
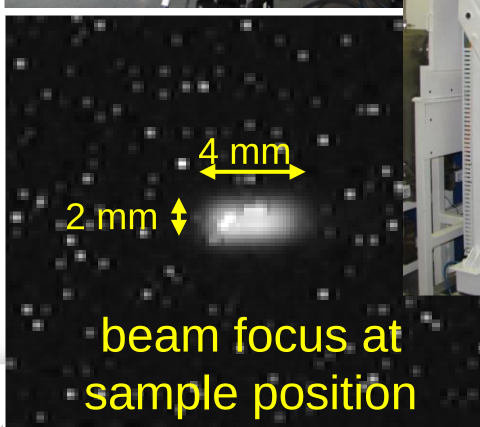
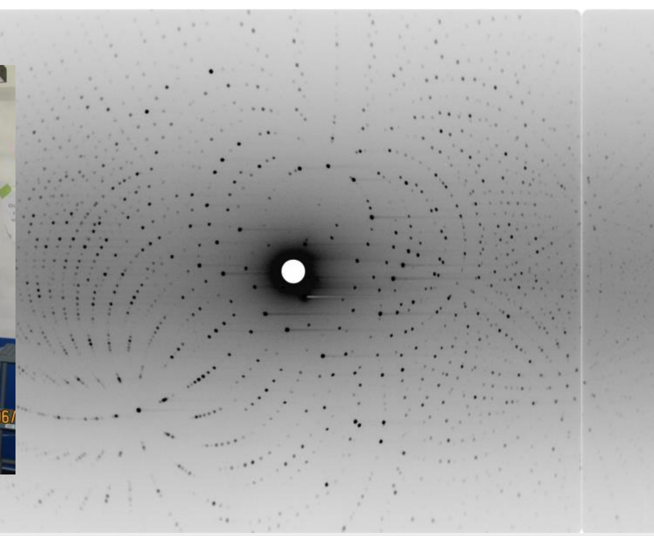
New Instrument: IMAGINE



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



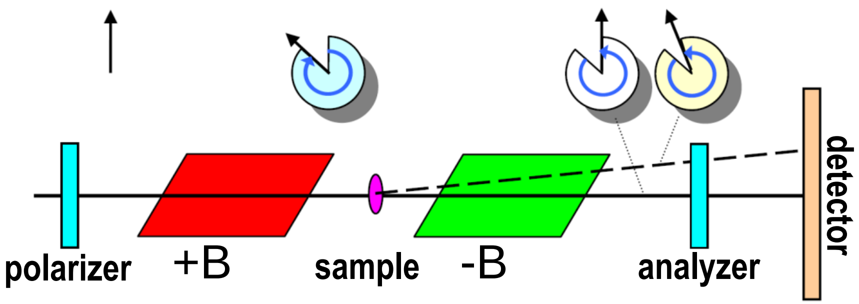




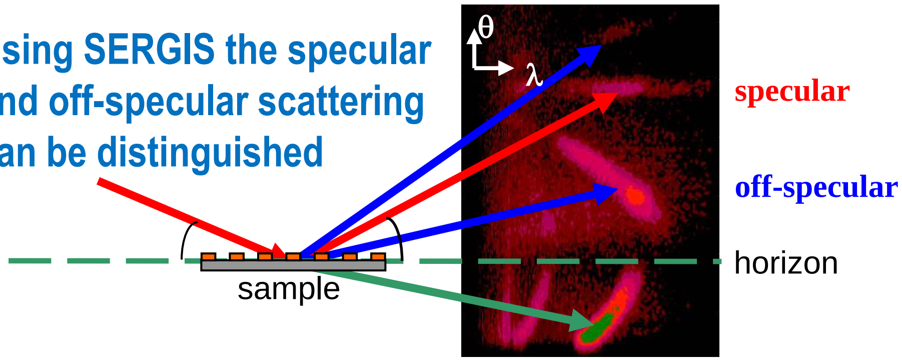
Future Instrument: SESANS/SERGIS

Spin-Echo Scattering Angle Measurement:

The neutron spin precesses through two parallelogram-shaped magnetic fields in opposite directions. For scattered neutrons the path-length through the two parallelograms is different resulting in a net change in the spin angle.



Using SERGIS the specular and off-specular scattering can be distinguished



- 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
  - Polarization
  - Detectors
  - Instrument development infrastructure (computer simulations)
  - New techniques and applications