Neutron Generation and Detection
Neutron Optics and Instrumentation

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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:
  \[ \lambda^2(\text{Å}^2) \sim 81.81/E(\text{meV}) \]  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

The peak neutron production of the SNS is about 10x that of the HFIR.

The HFIR neutron production is about 15x the time averaged production 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

\[ \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f \]

\[
\Delta E = \frac{h^2}{2m} \left( |k_i|^2 - |k_f|^2 \right)
\]
Neutron Scattering Instruments at Pulsed Sources Are Typically Based on Neutron Time-of-Flight Techniques

\[ v(1.8\text{ Å}) = 2187 \text{ m/s} \]

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

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

\[ \lambda(\text{Å}) = \frac{(3956.0339 \times \text{TOF(s)})}{D(\text{m})} \]
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!
Choppers and Velocity Selectors

Disk Chopper

Fermi Chopper

Velocity Selector

TOF Timing Diagram
Neutron Mirrors and Supermirrors / Neutron Guides

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

Multichannel Curved Guide
*Fabricated by Swiss Neutronics*

Guide Installation at ISIS
Polarizers and Spin Manipulators

Heussler Monochromator
AlCuMn

Larmor Precession Flipper

Spherical Neutron Polarimetry

POLI-HEiDi at FRMII

3He Cell

Unpolarized Neutron Beam

POLARIZING

Supermirrors

Polarized Neutron Beam

3He Spin Filters
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)

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

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

$$\lambda (\text{Å}) = (3956.0339 \times \text{TOF(s)}/D(\text{m}))$$  
For POWGEN D = 64.5m

Sr$_2$Fe$_{1.5}$Mo$_{0.5}$O$_6$, Electrode Material for Solid Oxide Fuel Cells

Small Angle Neutron Scattering (SANS)

PHYS REV B 86, 144501 (2012)
Magnetism Reflectometer (SNS)
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)
Quantum oscillations of nitrogen atoms in uranium nitride

Nature Communications v3, p1124 (2012)

Ei = 80meV

Ei = 250meV
Triple-Axis Spectrometer

HB-3

Source
Main shutter
Sapphire filter
Instrument shutter
Saddle shield
Shielding wedges
Monochromator crum shield
Presample collimator
Presample beam mask
Sample rotation angle
Sample table and goniometers
Sample
Analyzer
Precollimator
Beam stop

\(^{3}\text{He}\) detector

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/fttax

- 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 • 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/nld

- 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/nld

- Cold Neutron Triple-Axis Spectrometer • CG-4C
  - High-resolution inelastic scattering at cold neutron energies
  - neutrons.ornl.gov/tcx

- Cold Neutron Imaging Beam Line • CG-1D
  - Transmission imaging of natural and engineered materials
  - neutrons.ornl.gov/imaging

- Optics Development Beam Line • CG-1B
  - Sample alignment and optics
  - neutrons.ornl.gov/nld

- General-Purpose SANS • CG-2
  - Materials structure and processing, metallurgy, polymers, geophysics, high-Tc superconductors, complex fluids, magnetism and spin textures
  - neutrons.ornl.gov/gpssans

- Image-Plate Single-Crystal Diffractometer (IMAGINE) • CG-4D
  - Atomic resolution structures in biology, chemistry and complex materials
  - neutrons.ornl.gov/imagine

- Cold Neutron Source
Advanced Neutron Optics: IMAGINE

- Entrance Slit 1
- Flight Tube
- Entrance Slit 2

CG-4 Guide
CTAX
Mono

Beamstop/Slit
Multimirrors
Flat Mirror

INSTRUMENT ENCLOSURE

- Beamstop/Slit
- Drop-In Apertures
- Elliptical Mirror 1
- Elliptical Mirror 2
- Monitor
- Diffractometer

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

beam focus at sample position

4 mm
2 mm
Future Instruments: Larmor Pression

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