Lectures 9: Neutron Scattering Instrumentation
Neutron Scattering is Really Quite Simple.....
.....at least, in Principle

- Measure the number of scattered neutrons as a function of \( Q \) and \( \omega \)
- The result is the scattering function \( S(Q, \omega) \) that depends only on the properties of the sample
- All we need to do is to prepare a neutron beam with wavevector \( k_0 \) and measure the intensity of neutrons scattered with wavevector \( k \)

\[ \hbar Q = \hbar(k - k_0) \]
\[ \hbar \omega = E - E_0 \]

Momentum = \( \hbar k \); Energy = \( \hbar^2 k^2/2m_n \)
But, Neutron Sources are Comparatively Weak…

<table>
<thead>
<tr>
<th>Source</th>
<th>Brightness ($s^{-1} m^{-2} ster^{-1}$)</th>
<th>$\Delta E/E$ (%)</th>
<th>Divergence (mrad$^2$)</th>
<th>Flux ($s^{-1} m^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutrons</td>
<td>$10^{15}$</td>
<td>2</td>
<td>$10 \times 10$</td>
<td>$10^{11}$</td>
</tr>
<tr>
<td>Rotating Anode</td>
<td>$10^{16}$</td>
<td>3</td>
<td>$0.5 \times 10$</td>
<td>$5 \times 10^{10}$</td>
</tr>
<tr>
<td>Bending Magnet</td>
<td>$10^{24}$</td>
<td>0.01</td>
<td>$0.1 \times 5$</td>
<td>$5 \times 10^{17}$</td>
</tr>
<tr>
<td>Wiggler</td>
<td>$10^{26}$</td>
<td>0.01</td>
<td>$0.1 \times 1$</td>
<td>$10^{19}$</td>
</tr>
<tr>
<td>Undulator (APS)</td>
<td>$10^{33}$</td>
<td>0.01</td>
<td>$0.01 \times 0.1$</td>
<td>$10^{24}$</td>
</tr>
</tbody>
</table>

Neutron Scattering is a signal-limited technique
Instrumental Resolution

- Uncertainties in the neutron wavelength & direction of travel imply that Q and E can only be defined with a certain precision.

- When the box-like resolution volumes in the figure are convolved, the overall resolution width is the quadrature sum of the box sizes. Small “boxes” give good resolution.

- The total signal in a scattering experiment is proportional to the product of the “box” sizes.
  
  The better the resolution, the lower the count rate.
Neutron Scattering Instrumentation is Designed to Compromise between Intensity & Resolution

• Maxwellian distribution of neutron velocities
  \[ P(v) \sim \frac{1}{T^{3/2}} e^{-\frac{1}{2} \frac{mv^2}{kT}} \]

• Liouville’s theorem – the (6-dimensional) phase space density of non-interacting particles cannot be increased by conservative forces
  – Brighter sources => colder moderators or non-equilibrium neutron production

• We can only increase scattered intensity at a given \((\vec{Q}, E)\) by increasing the phase space volume

• Design instruments to have good resolution in the direction of \((\vec{Q}, E)\) space that is important for the science

• Neutron optics & instrumentation is designed to:
  – Maintain neutron brightness
  – Provide good resolution in a chosen direction in \((\vec{Q}, E)\) space
  – Simultaneously measure as many resolution elements [i.e. \((\vec{Q}, E)\) points] as is useful
Instrumental Resolution

\[
I(\vec{Q}_0, \omega_0) = \iiint \frac{d^2 \sigma(\vec{Q}, \omega)}{dE d\Omega} P(\vec{k}_i - \vec{k}_f) P(\vec{k}_f - \vec{k}_f) \delta(\hbar \omega - E_i + E_f) \\
\delta(\vec{Q} - \vec{k}_i + \vec{k}_f) d^3k_i d^3k_f d^3Q d\omega
\]

where \( \vec{Q}_0 = \vec{k}_i - \vec{k}_f \) and \( \hbar \omega_0 = E_i - E_f \) and \( P' \)'s are transmission probabilities

\[
I(\vec{Q}_0, \omega_0) = \iint \frac{d^2 \sigma(\vec{Q}, \omega)}{dE d\Omega} R(\vec{Q} - \vec{Q}_0, \omega - \omega_0) d^3Q d\omega
\]

- The resolution function, \( R \), is an ellipsoid in \( Q, \omega \) space, centered at \( Q_0, \omega_0 \), whose size is determined by:
  - Incident and final collimations
  - Incident and final energy band widths
- The resolution function can be written in diagonal form with respect to conjugate diameters of the resolution ellipsoid
- The integrated intensity is proportional to the product of the phase space volumes for the incident & scattered neutrons
  - Minimizing resolution broadening while maximizing the intensity -\( \to \) matching
Components of Neutron Scattering Instruments

• Monochromators (crystals, velocity selectors, choppers)
  – Select the energy of a neutron beam by various means
• Choppers
  – Define a short pulse or pick out a small band of neutron energies
• Collimators
  – Define the direction of travel of the neutron
• Guides
  – Allow neutrons to travel large distances without suffering intensity loss
• Filters (Be, benders, S-bend guides)
  – Reject unwanted neutron wavelengths
• Detectors
  – Most commonly, neutrons are absorbed by $^3$He and the gas ionization caused by recoiling particles is detected
• Shielding
  – Minimize background and radiation exposure to users
Wavelength Selection

- Crystal monochromators are often used at CW neutron sources for diffractometers & three-axis machines
  - Bragg scattering from mosaic crystals defines the neutron wavelength
  - Crystal mosaic in the horizontal scattering plane controls intensity and $\delta\lambda/\lambda$
  - Crystal mosaic in vertical plane determines image beam size at the sample when focusing is used
  - Neutrons are often focused vertically – does not affect $\delta\lambda/\lambda$ but does worsen vertical Q resolution (often unimportant)
  - Neutrons are sometimes focused horizontally – degrades $\delta\lambda/\lambda$ and Q resolution in the scattering plane, but gains intensity

\[ \lambda = 2d \sin \theta_B \]
Neutron Monochromators

A simple, vertically focusing monochromator produced by Riso National Lab in Denmark comprised of 15 single crystals

A vertical and horizontally focusing monochromator fabricated by a Johns Hopkins team for the NCNR. See:
www.pha.jhu.edu/~broholm/homepage/talks/MACSmonochromatoracns.pdf
The Workhorse of Inelastic Scattering Instrumentation at Reactors Is the Three-axis Spectrometer

“scattering triangle”
Helical Velocity Selectors often used for SANS

30m SANS velocity selector at NCNR
Time of Flight

- At pulsed neutron sources (or with a chopped beam at a reactor), the neutron’s TOF is used to determine it’s speed (and, hence, wavelength).

- For elastic scattering (diffraction, SANS, reflectometry) no neutron monochromatization is needed.

\[
\Delta \lambda_{res}(nm) \approx 0.4 \Delta \lambda(ms) / L(m)
\]

\[
\Delta \lambda_{BW}(nm) \approx 0.4 T(ms) / L(m)
\]
Simultaneously Using Neutrons With Many Different Wavelengths Enhances the Efficiency of Many Neutron Scattering Experiments

Potential Performance Gain relative to use of a Single Wavelength is the Number of Different Wavelength Slices used i.e. $T/\Delta T$ or $\Phi_{\text{peak}}/\Phi_{\text{average}}$
Caveats

Different scattered neutron wavelengths correspond to different values of wavevector transfer. There may be no information of interest at some values of Q. Example – SANS at a pulsed source

The wavelength resolution and spectral intensity of the incident beam may vary with wavelength. Example – reflectometry at a pulsed source
For Inelastic Scattering at a Pulsed Source, Choppers are used as Monochromators

- Fermi chopper – rapidly rotating collimator

ARCS Fermi chopper housing and slit package (courtesy B. Fultz)
Band-Width-Limiting and T-zero Choppers are used to Clean Up the Beam

- T-zero choppers made of Fe-Co are used at spallation sources to absorb the prompt high-energy pulse of neutrons.
- Cd is used in frame overlap choppers to absorb slower neutrons.

Fast neutrons from one pulse can catch-up with slower neutrons from a succeeding pulse and spoil the measurement if they are not removed. This is called “frame-overlap”
Neutron Choppers at SNS

Viewgraph courtesy of Kent Crawford
Collimators Define the Direction of Travel of the Neutrons

- A Soller collimator is a set of parallel neutron-absorbing plates that define the direction of the neutron beam.
- More sophisticated arrangements are possible.

Honeycomb collimator for the Brillouin scattering instrument BRISP at ILL

Mylar collimator by Jens Linderholm, Denmark

Radial collimator for the ARCS spectrometer to be installed at SNS
Neutron Guides Transport Neutrons over Long Distances with Little Loss

- Critical external reflection of neutrons for $\theta_c = \lambda \sqrt{\rho / \pi}$
  - Critical angle for Ni in degrees $\sim 0.1 \times$ neutron wavelength in Å
  - Guides can be coated with supermirror (e.g. NiTi) to extend the critical angle by a factor of up to $\sim 7$ (8000 layers) but reflectivity drops

Neutron guide being installed on SMARTS at the Lujan Center

TEM of unpolished & ion-polished NiTi layered supermirrors produced at JAEA in Japan – polishing allows high critical angle to be achieved
Guides at Spallation Sources need Heavy Shielding Close to the Neutron Source

Backscattering spectrometer at SNS. Viewgraph courtesy of Kent Crawford
Be Filters, Benders and Optical Filters

A Be filter removes wavelengths below ~ 4 Å. A guide S-bend (bottom right) can be more efficient (below).

A supermirror “bender” (above) or a guide S-bend (below) deviates useful neutrons, not hot neutrons.

Magnetism
Reflectometer, SNS

NG3 optical filter, NCNR
Most Neutron Detectors Use $^3$He

- $^3$He + n -> $^3$H + p + 0.764 MeV
- Ionization caused by triton and proton is collected on an electrode
- 70% of neutrons are absorbed when the product of gas pressure x thickness x neutron wavelength is 16 atm. cm. Å
- Modern detectors are often “position sensitive” – charge division is used to determine where the ionization cloud reached the cathode.

A selection of neutron detectors – thin-walled stainless steel tubes filled with high-pressure $^3$He.
Modern Instruments use Large Detector Arrays

Detector tank for the ARCS spectrometer at SNS. 26 m² covering 2.9 Str

D2b detector

PCS at Lujan
Much of the Improvement in Powder Diffraction has come from Larger Detectors
Modern Detectors and Electronics can Operate in Vacuum

Detector module for the ARCS spectrometer at SNS.

Viewgraph courtesy of Kent Crawford
To Obtain High Count Rate and Large Pixilated Areas, Arrays of Linear PSDs are Often Used

3 metre-long PSD (ILL)

5 metre-long PSD (ILL)
Examples of Specialization of Spectrometers: Optimizing the Signal for the Science

• **Small angle scattering** \[Q = 4\pi \sin\theta/\lambda; \quad (\delta Q/Q)^2 = (\delta \lambda/\lambda)^2 + (\cot\theta \delta \theta)^2\]
  - Small diffraction angles to observe large objects => long (20 m) instrument
  - Poor monochromatization (\(\delta \lambda/\lambda \sim 10\%\)) sufficient to match obtainable angular resolution (1 cm\(^2\) pixels on 1 m\(^2\) detector at 10 m => \(\delta \theta \sim 10^{-3}\) at \(\theta \sim 10^{-2}\))

• **Back scattering** \[\theta = \pi/2; \quad \lambda = 2 d \sin \theta; \quad \delta \lambda/\lambda = \cot \theta +\ldots\]
  - Very good energy resolution (\(~\text{neV}\)) => perfect crystal analyzer at \(\theta \sim \pi/2\)
  - Poor Q resolution => analyzer crystal is very large (several m\(^2\))
Accurate Assembly is Required

Perfect silicon crystals being assembled for the analyzer of the backscattering spectrometer at the SNS.
On-Going Research Aims to Improve Neutron Instrumentation

Examples of Japanese R&D provided by Prof. H. Shimizu
Lenses Can be Used to Reduce $Q_{\text{min}}$ for SANS

- Because $n < 1$ for neutrons, concave lenses are converging
- Ideal materials have low absorption and incoherent scattering and high scattering length density — e.g. MgF$_2$
- Since $n - 1$ is very small, compound lenses are needed

Compound MgF$_2$ lenses, 1” in diameter on the 30 m SANS at NCNR. More lenses are needed at short wavelength because $f \sim 1/\lambda^2$
Magnetic Focusing SANS lowered $Q_{\min}$ by 1/10 or less compared with conventional pin-hole SANS, in two dimensional imaging.

→ 2-dimensional USANS
New Idea for SANS with 50 μm Samples from Roland Gaehler at ILL

multi hole mask
\(\varnothing_{\text{hole}} \approx 0.1-1 \text{ mm} \)
15×15 cm²; 900 holes

\(a_e = 5 \text{ mm}\)

2D detector resolution \(\leq 0.1 \text{ mm}\)

\(\varnothing_{\text{image}} \approx 0.12 \text{ mm}\)

Single hole mask
\(\varnothing 50 \mu\text{m}\)

900 micro guides feeding the 900 holes

Kumakhov lens

\[ I = 900 I_0 \left(\frac{50}{10000}\right)^2 = 0.02 I_0; \]

\(I_0\) for standard SANS

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Conclusions

- Neutron scattering is a signal-limited technique
- Neutron instrumentation is designed to compromise between intensity and resolution
  - Many different types of instrument are needed to achieve the best compromise for different types of measurement
- The greatest gains (by far) in performance have come from improvements in instrumentation, not from better sources
  - The enormous gains in parallel data collection enabled by PSDs have been made possible by increases in computing power and storage
- The biggest single limitation currently is probably the speed and position resolution of detectors
- There are still many improvements that are understood on paper that have not yet been tried in practice