Neutron Sources

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• Neutrons properties and their interactions

• How to generate intense neutron beams using high power proton linear accelerator: The example of the ESS

for further reading
• Applications using Neutrons
Electro-magnetic Spectrum

Penetrates Earth's Atmosphere?

Radiation Type

<table>
<thead>
<tr>
<th>Radiation Type</th>
<th>Wavelength (m)</th>
<th>Approximate Scale of Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radio</td>
<td>$10^3$</td>
<td>Buildings</td>
</tr>
<tr>
<td>Microwave</td>
<td>$10^{-2}$</td>
<td>Humans</td>
</tr>
<tr>
<td>Infrared</td>
<td>$10^{-5}$</td>
<td>Butterflies</td>
</tr>
<tr>
<td>Visible</td>
<td>$0.5 \times 10^{-6}$</td>
<td>Needle Point</td>
</tr>
<tr>
<td>Ultraviolet</td>
<td>$10^{-8}$</td>
<td>Protozoans</td>
</tr>
<tr>
<td>X-ray</td>
<td>$10^{-10}$</td>
<td>Molecules</td>
</tr>
<tr>
<td>Gamma ray</td>
<td>$10^{-12}$</td>
<td>Atoms</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Atomic Nuclei</td>
</tr>
</tbody>
</table>

Frequency (Hz)

- $10^4$
- $10^8$
- $10^{12}$
- $10^{15}$
- $10^{16}$
- $10^{18}$
- $10^{20}$

Temperature of objects at which this radiation is the most intense wavelength emitted

- Radio: $272^\circ C$ (1 K)
- Microwave: $173^\circ C$ (100 K)
- Infrared: $9,727^\circ C$ (10,000 K)
- Visible: ~$10,000,000^\circ C$ (10,000,000 K)
Neutron Microscope – Length scales

Length scale in nm
0.01 0.1 0.3 1.0 3.0 10 30 100

- atomic and magnetic structures
- organic molecules
- surfaces and multilayers inhomogeneities
- viruses
- cracks and voids
- internal strain
- magnetic defects
- pharmaceuticals
- supermolecules
- micelles
- proteins
- critical phenomena
- polymers

neutron wavelength in nm
0.1 0.3 1.0 2.0
Neutron Microscope – Time & energy scales

Time scale (seconds):
- $10^{-13}$
- $10^{-7}$

Excitation energy (eV):
- 1
- $10^{-1}$
- $10^{-2}$
- $10^{-3}$
- $10^{-6}$
- $10^{-9}$

Crystal fields:
- single particle excitations
- molecular excitations

Spin fluctuations:
- magnons and phonons
- tunneling diffusion

Spin relaxation:
- polymer reptation
- glassy dynamics libration
Ionizing Radiation

Ionizing radiation is radiation composed of particles that individually carry enough energy to liberate an electron from an atom or molecule without raising the bulk material to ionization temperature.

When ionizing radiation is emitted by or absorbed by an atom, it can liberate a particle. Such an event can alter chemical bonds and produce ions, usually in ion-pairs, that are especially chemically reactive.

Note: Neutrons, having zero electrical charge, do not interact electromagnetically with electrons, and so they cannot directly cause ionization by this mechanism.

→ High precision non-destructive probe … why?
Neutrons Properties

Note: X-rays are emitted by electrons outside the nucleus, while gamma rays are emitted by the nucleus.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>$1.675 \times 10^{-27}$ kg</td>
</tr>
<tr>
<td>Mean lifetime</td>
<td>15 min</td>
</tr>
<tr>
<td>Composition</td>
<td>udd</td>
</tr>
<tr>
<td>Electric charge</td>
<td>0</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>$-1.04 \mu_B$</td>
</tr>
<tr>
<td>Energy</td>
<td>939.57 MeV</td>
</tr>
<tr>
<td>Mass relation</td>
<td>$m_n \approx m_p + 2.5m_e$</td>
</tr>
<tr>
<td>Beta decay</td>
<td>$n \rightarrow p + e^- + \bar{\nu}_e$</td>
</tr>
</tbody>
</table>
Neutron Energy

\[ E = k_B T \]

\[ E = k_B T = \frac{1}{2} mv^2 = \frac{h}{2m}l^2 \]

Boltzmann distribution

De Broglie

\[ E \ [meV] = 0.0862 \ T \ [K] = 5.22 \ v^2 \ [km/s] = 81.81 \ \frac{1}{2} \ [\text{Å}] \]

<table>
<thead>
<tr>
<th>Source</th>
<th>Energy</th>
<th>Temperature</th>
<th>Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>cold</td>
<td>0.1-10</td>
<td>1-120</td>
<td>30-3</td>
</tr>
<tr>
<td>thermal</td>
<td>5-100</td>
<td>60-1000</td>
<td>4-1</td>
</tr>
<tr>
<td>hot</td>
<td>100-500</td>
<td>1000-6000</td>
<td>1-0.4</td>
</tr>
</tbody>
</table>
Why neutrons?

Neutron properties are used to understand the nature of the solid and liquid states of matter, as an analytical tool to aid the development of materials and as a tool to examine curiosity-driven research that spans from cosmology, superconductivity to the dynamics of the molecules of life.

1. Neutrons see the Nuclei
2. Neutrons see Elementary Magnets
3. Neutrons see light Atoms next to Heavy Ones
4. Neutrons measure the Velocity of Atoms
5. Neutrons penetrate deep into Matter
6. Neutrons are Elementary Particles
Why neutrons?

Electrically Neutral – neutrons are non-destructive and can penetrate deep into matter. This makes them an ideal probe for biological materials and samples under extreme conditions of pressure, temperature, magnetic field or within chemical reaction vessels.

Microscopically Magnetic – they possess a magnetic dipole moment which makes them sensitive to magnetic fields generated by unpaired electrons in materials. Precise information on the magnetic behavior of materials at atomic level can be collected. In addition, the scattering power of a neutron off an atomic nucleus depends on the orientation of the neutron and the spin of the atomic nuclei in a sample. This makes the neutron a powerful instrument for detecting the nuclear spin order.

Ångstrom wavelengths – neutron wavelengths range from 0.1 Å to 1000 Å, making them an ideal probe of atomic and molecular structures, be they single atomic species or complex biopolymers.
Why neutrons?

Energies of millielectronvolts – their energies are of the same magnitude as the diffusive motion in solids and liquids, the coherent waves in single crystals (phonons and magnons), and the vibrational modes in molecules. It is easy to detect any exchange of energy between a sample of between 1 microeV (even 1 neV with spin-echo) and 1 eV and an incoming neutron.

Randomly sensitive – with neutrons the variation in scattering power from one nucleus to another within a sample varies in a quasi-random manner. This means that lighter atoms are visible despite the presence of heavier atoms, and neighboring atoms may be distinguished from each other. In addition, contrast can be varied in certain samples using isotopic substitution (for example D for H, or one nickel isotope for another); specific structural features can thus be highlighted. The neutron is particularly sensitive to hydrogen atoms; it is therefore a powerful probe of hydrogen storage materials, organic molecular materials, and biomolecular samples or polymers.
Why neutrons?

In half a century we have developed neutron scattering science enormously with an effective gain in source performance of only a factor of 4!

- **Diffractometers - Measure structures**
  – Where atoms and molecules are 1 - 10 Ångström

  → To analyze the structure of a material from the scattering pattern produced when a beam of radiation or particles (such as X-rays or neutrons) interacts with it

- **Spectrometers - Measure dynamics**
  – What atoms and molecules do 1 - 80 meV

  → To measure properties of light over a specific portion of the electromagnetic spectrum
Why neutrons?

Cliff Shull – Neutron diffraction - showing where atoms are:

Bert Brockhouse – Spectroscopy - showing what atoms do:

Using nowadays technique..
Neutrons show us: where atoms are (left, Bragg scattering) and what they do (right, Spectroscopy). Energies of neutrons are on the same scale as excitations. 1 Neutron 6 orders of magnitude less than 1 A Synch.
Scientific challenges

Solid State Physics
*Dynamics of superlattices, wires and dots, molecular magnets, quantum phase transitions*

Liquids and Glasses
*Solvent structures, influence of molecular structures on protein folding*

Fundamental Physics
*Left and right handedness of the universe, neutron decay, ultracold neutrons*

Soft Condensed Matter
*Time resolution, molecular rheology, structures and dynamics*

Biology and Biotechnology
*Hydrogen and water, membranes, biosensors, functions*

Materials Science and Engineering
*Real time investigations with realistic dimensions under real conditions*

Chemical Structure, Kinetics and Dynamics
*Thin films, pharmaceuticals, supramolecules - structures and functionality*

Earth and Environmental Science, Cultural Heritage
*Extreme temperatures and pressures simulating the mantle*
Fields of interest

A wide range of length and timescales.

High sensitivity and selectivity.

Deep penetration.

A probe of fundamental properties.

A precise tool

An ideal probe for magnetism.
The visions

- Room Temperature Super Conductors
- Sterile neutrinos
- Hydrogen storage substrate
- Neutron electric dipole moment
- Efficient membrane for fuel cells
- Flexible and highly efficient solar cells
- Carbone nano-tubes for controlled drug release
- Self healing materials – smart materials
- Spin-state as a storage of data \((10^{23} \text{ gain in capacity})\)
- CO\(_2\) sequestration

Unobtainium

Avatar
Multi-science with neutrons

<table>
<thead>
<tr>
<th>Materials science</th>
<th>Bio-technology</th>
<th>Nano science</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy Technology</td>
<td>Hardware for IT</td>
<td>Engineering science</td>
</tr>
</tbody>
</table>

- Neutrons can provide unique and information on almost all materials.

- Information on both structure and dynamics simultaneously. "Where are the atoms and what are they doing?"

- 6000 primary users in Europe today and 6000 secondary users. Access based on peer review.

- Science with neutrons is limited by the intensity of today’s sources
Because of their unique properties, neutrons are a powerful tool for investigating Nature at all levels, from testing theories about the evolution of the Universe to elucidating the complex processes of life.
X-Ray and Neutron beam
Complementarity between X-rays and Neutrons

Consider ESS/MaxIV equal in terms of functionality
## Complementarity between X-rays & Neutrons

<table>
<thead>
<tr>
<th>Neutrons</th>
<th>Synchrotron radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Particle beam (neutral subatomic particle)</td>
<td>• Light beam (electromagnetic wave)</td>
</tr>
<tr>
<td>• Interactions with the nuclei and the magnetic moment of unpaired electrons (in the sample)</td>
<td>• Interactions with the electrons surrounding the nuclei (in the sample)</td>
</tr>
<tr>
<td>• Scattered by all elements, also the light ones like the hydrogen isotopes</td>
<td>• Mainly scattered by heavy elements</td>
</tr>
<tr>
<td>• Deep penetration depth (bulk studies of samples)</td>
<td>• Small penetration depth (surface studies of samples)</td>
</tr>
<tr>
<td>• Less intense beam measuring larger samples</td>
<td>• Very intense beam measuring small or ultra-dilute samples</td>
</tr>
</tbody>
</table>
## Complementarity between X-rays & Neutrons

<table>
<thead>
<tr>
<th>Neutrons Applications</th>
<th>SR Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Magnetic structures &amp; excitations</td>
<td>• Protein-crystal structures</td>
</tr>
<tr>
<td>• Organic structures using the H-D isotope effect</td>
<td>• Fast chemical reactions</td>
</tr>
<tr>
<td>• Bulk studies (strains, excitations)</td>
<td>• Surface studies (defects, corrosion)</td>
</tr>
<tr>
<td>• Low-energy spectroscopy e.g. molecular vibrations</td>
<td>• High-energy spectroscopy e.g. measurements of electron energy-levels</td>
</tr>
</tbody>
</table>
Complementarity between X-rays & Neutrons

X-ray interact with electrons → X-rays see high-Z atoms

Neutron interact with nuclei → Neutrons see low-Z atoms

Material for Li-battery seen by X rays (left) and Neutrons (right)

T. Kamiyama, et al.
Advantages of SANS over SAXS are its sensitivity to light elements, the possibility of isotope labeling, and the strong scattering by magnetic moments.
Complementarity between X-rays & Neutrons

Hen Egg-White Lysozyme

Water molecules Observed with neutrons

N. Niimura, et al.

X-rays

Neutrons

Protein

From structure to function

DNA

A protein molecule moving along the DNA chain
Complementarity between X-rays & Neutrons

- See magnetic atoms
- See inside materials
- See light atoms
- See atoms move
- See isotopes
Neutron beam and X-Ray for Medical Applications
Scattering and Diffraction
Scattering – coherence and incoherence

\[ \text{coh} = 4 \langle b \rangle^2 \]

\[ \text{incoh} = 4 \left( \langle b^2 \rangle - \langle b \rangle^2 \right) \]

Definition:
One depends on energy the other doesn't (where atoms are, what they do)

WHY NEUTRON SCATTERING IS USEFUL

When used as a probe for small samples of materials, neutron beams have the power to reveal what is invisible using other radiations. Neutrons can appear to behave either as particles or as waves or as microscopic magnetic dipoles, and it is these specific properties which enable them to uncover information which is often impossible to access using other techniques.

Isotopes and spin?
Inelastic Scattering of plane wave

Plane incident wave: \( \exp(ikr) \)

Scattered spherical wave: \(-b \exp(ikr)/b\)

Simple spherical object!!

\[ \sigma_{\text{tot}} = \text{number of neutrons scattered in all directions per sec/incident flux} \]

\[ d\Omega \]
Diffraction = Coherent Elastic Scattering of plane wave

\[ \sigma_{\text{tot}} = \text{number of neutrons scattered in all directions per sec/incident flux} \]

Plane incident wave: \( \exp(ikr) \)

Scattered spherical wave: \(-b \exp(ikr)/b\)

Simple spherical object!!

\[ \sigma_{\text{tot}} = 4b^2 \]
Scattering

- Cross section:

\[ d\sigma = \frac{\text{(# particles scattered into solid angle } \Delta\Omega/s)}{\text{( # particles incident/sec)(# scattering centers/area)}} \]

\[ \frac{d\sigma(Q)}{d\Omega} = N_p V_p \bar{\rho} P(Q) S(Q) \]

- Volume fraction
- Contrast
- Shape
- Interaction
The neutron diffraction pattern of sulfuric acid tetrahydrate at 4.2 K as seen by the 90 degree detectors on HRPD, and fitted with the existing X-ray derived structural model for the deuterated species.
**Neutron cross sections**

## Neutron scattering lengths and cross sections

<table>
<thead>
<tr>
<th>Isotope</th>
<th>conc</th>
<th>Coh b</th>
<th>Inc b</th>
<th>Coh xs</th>
<th>Inc xs</th>
<th>Scatt xs</th>
<th>Abs xs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>---</td>
<td>9.45</td>
<td>---</td>
<td>11.22</td>
<td>0.4</td>
<td>11.62</td>
<td>2.56</td>
</tr>
<tr>
<td>54Fe</td>
<td>5.8</td>
<td>4.2</td>
<td>0</td>
<td>2.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>56Fe</td>
<td>91.7</td>
<td>9.94</td>
<td>0</td>
<td>12.4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>57Fe</td>
<td>2.2</td>
<td>2.3</td>
<td></td>
<td>0.66</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>58Fe</td>
<td>0.3</td>
<td>15.7</td>
<td>0</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Select the element, and you will get a list. Feature section of neutron scattering lengths and cross sections.

*NOTE: The above are only thermal neutron dependent cross sections please go to the following site.*

Diffraction of X-rays or neutrons by polycrystalline samples is one of the most important, powerful and widely used analytical techniques available to materials scientists. For most crystalline substances of technological importance, the bulk properties of a powder or a polycrystalline solid, averaged throughout the sample, are required; in general a single-crystal data, even if they can be obtained, are usually of little interest except for determination of the crystal structure or for studying some other fundamental physical property. By Ian Langford and Daniel Louer.
Diffraction - Bragg

- Bragg / Laue scattering
- Coherent elastic scattering

Two beams with identical wavelength and phase approach a crystalline solid and are scattered off two different atoms within it. The lower beam traverses an extra length of $2d \sin \theta$. **Constructive interference** occurs when this length is equal to an integer multiple of the wavelength of the radiation.

\[ n\lambda = 2d \sin \theta \]

*Bragg’s Law*
Diffraction - Bragg

Using the grains as internal strain gauges

\[ \lambda = 2d \sin \theta \]
\[ \varepsilon = -\cot(\theta) (\theta - \theta_0) \]

Two ways to measure \( d \):
- keep \( \lambda \) fixed and measure \( \theta \) constant wavelength
- keep \( \theta \) fixed and measure \( \lambda \) time-of-flight

Bragg's law gives information about position of a diffraction peak from a type of lattice planes.
Rietveld approach calculated height, position and width of diffraction peaks from first principles, i.e.
Temperature, composition, vacancies, etc.
Diffraction: Texture

- ISIS: GEM instrument
- Near $4\pi$ coverage

Example:
- Cold rolled copper, simulating manufacturing process for archeometry
- 2mm thick disks
- 20x20mm$^2$ beam
- 2 min counting times

Neutron texture analysis on GEM at ISIS
W. Kockelmann, L.C. Chapon and P.G. Radaelli
Diffraction: Stress and Strain

Applications:
Residual stresses
Fatigue/Structural Integrity
Welds
Alloy development
Microstructure/Texture
Phase transformation
In-situ experiments
Example - Diffraction

D2B at the ILL, Grenoble, 50 years later
Fast, short-wavelength neutrons arrive earlier at detector!

Diffraction in ToF mode at pulsed source. Flight time is propre to wavelength
Ice

Figure 1. Neutron diffraction patterns measured in the course of heating of the recovered D₂O high-pressure phase ice VIII from 94 to 273 K.

Figure 2. Neutron diffraction patterns of D₂O ices before and after phase transitions: (a) from ice VII (dashed line) to a mixture of hda + lda ices (solid line) at 125 K; (b) from the mixture of hda + lda ices (solid line) to ice 'e' (dashed line) at 160 K; (c) from ice 'e' (solid line) to the hexagonal phase, "smectic B" type structure (dashed line), at 190 K; (d) from "smectic B" type ice (dashed line) to ice Ih (solid line) at 230 K. The diffraction patterns also contain peaks from the aluminium sample can and cryostat.
The application of diffraction in battery research: patterns as function of temperature. Peak position and intensity give structure. Peak broadening give anisotropic atomic oscillations and hence likely migration path (the ellipses), then diffraction in other fields of research, from chemistry to engineering measuring stresses...

Figure 2 Neutron diffraction patterns measured at room temperature (RT) and 620 K for the FePO₄−LiFePO₄ binary phase diagram. a, Rietveld refined powder neutron diffraction profile measured for RT (a) and the angle-dispersive neutron diffraction profile measured for 620 K (b). Two different neutron diffractometers were used for each measurement as explained in the main text. All error points are plotted using the common scale $Q = 4\pi \sin(\theta)/\lambda$. The $Q$ range for VEGA and HERMES for comparison. Specific details of composition and temperature are given in the inset phases of Delacourt et al. and Dodd et al. Observed intensity $I_{obs}$ are represented by red plus signs and the green squares are the calculated intensity $I_{calc}$. The blue curve at the bottom represents the residual difference between $I_{obs}$ and $I_{calc}$. Parameters are summarized in Supplementary Information, Table S1. The structure can be described as a distorted two-dimensional square lattice perpendicular to the basal plane, with LiO$_4$ octahedra aligned in parallel chains along the [001] direction. The FeO$_6$ octahedra are arranged in trigonal close-packed oxygen subarray, in which Li, Fe, P atoms, respectively. The lithium migration paths: c, along the [010] direction; and d, along the [001] direction. One-dimensional diffusion along the [010] direction using the computational method.

Figure 3 Anisotropic harmonic lithium vibration in LiFePO₄ shown as green thermal ellipsoids and the expected diffusion path. The ellipsoids were refined with 95% probability by Rietveld analysis for room-temperature neutron diffraction data. Expected curved one-dimensional continuous chains of lithium motion are drawn as dashed lines to show how the motions of Li atoms evolve from vibrations to diffusion.
Fuel Cells

Application in fuel cells, neutrons used for optimization of microstructural crystal structure, composition of membrane material (proton transport) and engineering (water transport) on macro scale.

Table 1
Summary of results obtained from Rietveld analysis of neutron powder diffraction data for BaZr_{1-x}In_{x}O_{3-δ}, collected at 10 K on the NPD diffractometer.

<table>
<thead>
<tr>
<th></th>
<th>x=0.0</th>
<th>x=0.0</th>
<th>x=0.25</th>
<th>x=0.25</th>
<th>x=0.50</th>
<th>x=0.50</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(as-prepared)</td>
<td>(deuterated)</td>
<td>(as-prepared)</td>
<td>(deuterated)</td>
<td>(as-prepared)</td>
<td>(deuterated)</td>
</tr>
<tr>
<td>Space group</td>
<td>Pm-3m</td>
<td>Pm-3m</td>
<td>Pm-3m</td>
<td>Pm-3m</td>
<td>Pm-3m</td>
<td>Pm-3m</td>
</tr>
<tr>
<td>a (Å)</td>
<td>4.1879(1)</td>
<td>4.1880(1)</td>
<td>4.1916(1)</td>
<td>4.1983(1)</td>
<td>4.1942(2)</td>
<td>4.2260(4)</td>
</tr>
<tr>
<td>Thermal parameters, $B_{eq}$ (Å²)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ba on 1(b) 1/2,1/2,1/2</td>
<td>0.08(3)</td>
<td>0.08(2)</td>
<td>0.10(3)</td>
<td>0.21(4)</td>
<td>0.48(6)</td>
<td>0.97(10)</td>
</tr>
<tr>
<td>Zr on 1(a) 0,0,0</td>
<td>0.14(2)</td>
<td>0.11(2)</td>
<td>0.19(3)</td>
<td>0.23(3)</td>
<td>0.43(5)</td>
<td>0.37(9)</td>
</tr>
<tr>
<td>In on 1(a) 0,0,0</td>
<td></td>
<td></td>
<td>0.19(3)</td>
<td>0.23(3)</td>
<td>0.43(5)</td>
<td>0.37(9)</td>
</tr>
<tr>
<td>O on 3(d) 1/2,0,0</td>
<td>0.24(2)</td>
<td>0.26(2)</td>
<td>0.63(2)</td>
<td>0.56(2)</td>
<td>1.16(4)</td>
<td>1.17(5)</td>
</tr>
<tr>
<td>Oxygen site occupancy</td>
<td>2.98(1)</td>
<td>2.99(1)</td>
<td>2.82(1)</td>
<td>2.90(2)</td>
<td>2.68(2)</td>
<td>2.98(3)</td>
</tr>
<tr>
<td>$\chi^2$</td>
<td>1.96</td>
<td>1.99</td>
<td>1.85</td>
<td>1.64</td>
<td>1.72</td>
<td>3.16</td>
</tr>
<tr>
<td>Weighted $R_{wp}$</td>
<td>4.17%</td>
<td>5.16%</td>
<td>4.7%</td>
<td>4.74%</td>
<td>5.28%</td>
<td>6.62%</td>
</tr>
<tr>
<td>Bragg $R_B$</td>
<td>3.97%</td>
<td>3.86%</td>
<td>4.63%</td>
<td>4.40%</td>
<td>8.16%</td>
<td>6.62%</td>
</tr>
<tr>
<td>Fitted parameters</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
</tr>
</tbody>
</table>

Fig. 2. Low temperature (10K) neutron powder diffraction patterns of as-prepared and respective deuterated (marked with D) BaZr_{1-x}In_{x}O_{3-δ} (x=0.00, 0.25 and 0.50) samples.
Small Angle Scattering

• Scattering Vector

\[ Q = k_i - k_j \]

\[ k_i \]

\[ k_j \]

\[ \sin \theta = \frac{Q\lambda}{4\pi} = \frac{\lambda}{2d} \]

\[ \rightarrow d = \frac{2\pi}{Q} \]

Small angle \( \rightarrow \) small \( Q \) \( \rightarrow \) large distances

\( \lambda \) (cold neutrons) = 6 Å, \( d = 200 \) Å, \( 2\theta = 1.7^\circ \)

\( \rightarrow \) The larger the object, the smaller the angle
SANS: Experimental Setup

Beam:
Neutron (SANS) or X-ray (SAXS)

\[ |Q| = \frac{4\pi \sin \theta}{\lambda} \]

\[ Q_{\text{min}} \approx 0.03^\circ, \quad Q_{\text{max}} \approx 3^\circ \]

In a standard crystallography experiment, theta_max is typically 45 degrees
Scattering

- Cross section:

\[ d\sigma = \frac{\text{(# particles scattered into solid angle } \Delta\Omega/\text{s})}{\text{(# particles incident/sec)(# scattering centers/area)}} \]

\[ \frac{d\sigma(Q)}{d\Omega} = N_p V_p \bar{\rho} P(Q) S(Q) \]

- Volume fraction
- Contrast
- Shape
- Interaction
SANS: Scattering of plane wave

\[ \sigma_{\text{tot}} = \text{number of neutrons scattered in all directions per sec/incident flux} \]

Plane incident wave: \( \exp(ikr) \)

Scattered spherical wave: \( -b \exp(ikr)/b \)

Simple spherical object!!

\[ \frac{d\sigma(Q)}{d\Omega} = N_p V_p \bar{\rho} P(Q) S(Q) \]

Volume fraction

Contrast

\[ \text{tot} = 4 \ b^2 \]
SANS: Particles: contrast!

Contrast! \[ \frac{p}{s} = \frac{v}{s} \]

Solvent: \( S \)
Volume: \( V \)

Density: \( \rho_s \)

6.4 Water

RNA
Phospholipids
Protein

-0.56 %D\textsubscript{2}O
Protein based drugs:
• Typically proteins in solution to be injected
• Long shelf life (up to 2 years)
• Control of release profile is desirable

Fast action: Monomeric and dimeric insulin

Medium action: Hexameric insulin

Slow action: Large complexes of hexameric insulin

Knowledge and control of solution properties of the proteins are crucial

Source: L Arleth, Uni Copenhagen
SANS versus SAXS

SAXS contrast

SANS contrast 1

SANS contrast 2

SANS contrast 3

SANS gives the possibility of not seeing everything at the same time….
SANS: Different Shapes

- Spheres: 
  \( R = 60 \, \text{Å} \)

- Rods: 
  \( R = 60 \, \text{Å} \)
  \( L = 1200 \, \text{Å} \)

- Worms: 
  \( R = 18 \, \text{Å} \)
  \( L = 5000 \, \text{Å} \), 
  Kuhn Length = 300 Å
SANS: Selective Deuteration

sensitivity and selectivity
isotopic substitution/contrast variation
Neutron Reflectivity

• Basic principle

\[ n = 1 - \lambda^2 \frac{\sum_i b_i V}{2\pi} \]
Neutron reflectometry to investigate the delivery of lipids and DNA to interfaces (Review)

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(Received 6 May 2008; accepted 1 August 2008; published 19 December 2008)

The application of scattering methods in the study of biological and biomedical problems is a field of research that is currently experiencing fast growth. In particular, neutron reflectometry (NR) is a technique that is becoming progressively more widespread, as indicated by the current commissioning of several new reflectometers worldwide. NR is valuable for the characterization of biomolecules at interfaces due to its capability to provide quantitative structural and compositional information on relevant molecular length scales. Recent years have seen an increasing number of applications of NR to problems related to drug and gene delivery. We start our review by summarizing the experimental methodology of the technique with reference to the description of biological liquid interfaces. Various methods for the interpretation of data are then discussed, including a new approach based on the lattice mean-field theory to help characterize stimulus-responsive surfaces relevant to drug delivery function. Recent progress in the subject area is reviewed in terms of NR studies relevant to the delivery of lipids and DNA to surfaces. Lastly, we discuss two case studies to exemplify practical features of NR that are exploited in combination with complementary techniques. The first case concerns the interactions of lipid-based cubic phase nanoparticles with model membranes (a drug delivery application), and the second case concerns DNA compaction at surfaces and in the bulk solution (a gene delivery application). © 2008 American Vacuum Society. [DOI: 10.1116/1.2976448]
Fission and Spallation
Spallation is a non-elastic nuclear interaction induced by a high-energy particle producing numerous secondary particles.
Fission and Spallation

[D. Filges and F. Goldenbaum, Handbook of Spallation Research]
Energy efficiency is key for high intensity neutron beam production

Fast neutrons produced / joule heat deposited in target station

Fission reactors: $\sim 10^9$ (in $\sim 50$ liter volume)
Spallation: $\sim 10^{10}$ (in $\sim 2$ liter volume)
Fusion: $\sim 1.5 \times 10^{10}$ (in $\sim 2$ liter volume)
   (but neutron slowing down efficiency reduced by $\sim 20$ times)
Photo neutrons: $\sim 10^9$ (in $\sim 0.01$ liter volume)
Nuclear reaction (p, Be): $\sim 10^8$ (in $\sim 0.001$ liter volume)
Laser induced fusion: $\sim 10^4$ (in $\sim 10^{-9}$ liter volume)

Spallation: most favourable for the foreseeable future
Spallation Process

**Spallation Neutron Yield** (i.e. multiplicity of emitted neutrons)

determines the requirement in terms of the accelerator power (current and energy of incident proton beam).

**Spallation Neutron Spectrum** (i.e. energy distribution of emitted neutrons)

determines the damage and activation of the structural materials (design of the beam window and spallation target)

**Spallation Product Distributions**

determines the radiotoxicity of the residues (radioprotection requirements).

**Energy Deposition**

determines the thermal-hydraulic requirements (cooling capabilities and nature of the spallation target).

⇒ **Sub-critical Reaction**
Spallation: choice of target materials

\[ Y(E,A) = 0.1 \times [A+20] \times [E \text{ (GeV)} - 0.12] \text{ n/p} \]
High time average and peak flux

Evolution of the performance of neutron sources

Effective thermal neutron flux $n/cm^2-s$

• Neutrons properties and their interactions

• How to generate intense neutron beams using high power proton linear accelerator: The example of the ESS

for further reading
• Applications using Neutrons
ESS: Materials, Life Science and Society

EU Horizon 2020 – strategy

The structure which the EC proposed consists of three basic priorities:

1. Excellent Science
2. Industrial Leadership
3. Societal Challenges

Europe 2020 Priorities

- Creating Industrial Leadership and Competitive Frameworks
- Leadership in Enabling & Industrial Technologies
- Information & Communication Technologies (ICT)
- Nanotechnology, Materials, Manufacturing and Processing
- Biotechnology
- Space
- Access to Risk Finance
- Innovation in SMEs

Tackling Societal Challenges
- Health, Demographic Change & Well-being
- Food Security & the Bio-Based Economy
- Secure, Clean & Efficient Energy
- Smart, Green and Integrated Transport
- Climate Action, Resource Efficiency, incl. Raw Materials
- Inclusive, Innovative and Secure Societies

EIT and JRC will contribute to addressing these challenges

Simplified Access

Common Rules, Toolkit of Funding Schemes

Coherent with Other EU and MS Actions
Spallation Sources

Philosophie de “Pré-vert”: Greenfield

- Will bring new insights to the grand challenges of science and innovation
- Collaborative project: more than 17 countries
- 2014: Start of construction phase of the world's most powerful linear proton accelerator
- 2019: Provide the world's most advanced tools for studying materials with neutrons (~450 employees; >2500 users/year)
Helicopter view of ESS

Proton Accelerator
Energy: 2 GeV
Frequency: 14 Hz
Current: 62.5 mA

Target Station
Solid Rotating W
He or Water Cooled
5MW average power
>22 beam ports

Instrument
22 Instruments in construction budget

5 times more powerful than SNS
30 times brighter than ILL

Total Cost of Project
1843 (2013) Mil €
Collaborative projects

• ESS is an emerging research laboratory with (still) very limited capacity in-house

• Two possibilities:
  • Limit the scope of the project so that it can be done with in-house resources
  • Work in a collaboration where the scope of the project can be set by the total capacity (distributed) of the partners

• The accelerator part of the project well suited for this as this community has a strong tradition of open collaboration (e.g. E-XFEL, FAIR, LHC, European Commission Framework Programs and design studies)

• To keep cost down and to optimize schedule this requires that investments in required infrastructure is done at the partner with best capacity to deliver
Linac redesign to meet ESS cost objective

**Beam power (MW)** | 5
---|---
**Beam current (mA)** | 62.5
**Linac energy (GeV)** | 2
**Beam pulse length (ms)** | 2.86
**Repetition rate (Hz)** | 14

<table>
<thead>
<tr>
<th>Style</th>
<th>Spoke</th>
<th>Medium-β</th>
<th>High-β</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freq. (MHz)</td>
<td>352.21</td>
<td>704.42</td>
<td>704.42</td>
</tr>
<tr>
<td>Cavity #</td>
<td>26</td>
<td>36</td>
<td>84</td>
</tr>
<tr>
<td>Velocity range</td>
<td>0.42 to 0.58</td>
<td>0.58 to 0.78</td>
<td>0.78 to 0.95</td>
</tr>
<tr>
<td>Nom. Acc. Voltage (MV)</td>
<td>5.74</td>
<td>14.3</td>
<td>18.2</td>
</tr>
<tr>
<td>Loaded quality factor</td>
<td>$2.85 \times 10^5$</td>
<td>$8 \times 10^4$</td>
<td>$7.6 \times 10^5$</td>
</tr>
</tbody>
</table>

Accelerator collaborations for ESS “start-up”
Cavity Cryomodule Technology Demonstrators

One full scale 704 MHz medium and high-beta cavity cryomodules
A staged approach towards the series industrialization and the ESS Linac tunnel installation

- Validate designs and construction capability of SRF components
- Prepare the industrialization process by validating component life-cycles (incl. assembling process, QA)
- Validate component performances (incl. RF, mechanical, thermal)
- Develop ESS 704 MHz SRF linac operating procedures
- Validate control command strategy (Control box, PLC, EPICS, LLRF)
- Validate ESS integration and interfaces with RF, cryogenics, vacuum and control systems
- Train people in ESS SRF Technology and build an ESS collaboration

→ Similar process for the spoke cryomodules
ESS SRF Cavity Cryomodules

2 Spoke Cavities per Cryomodule

- Ti. Helium tank
- Cold tuning System
- Power coupler

Segmented SRF linac with RT focusing elements

4 Elliptical Cavities per Cryomodule
SRF Cavities Development

**Spoke cavity**
- Stiffeners on the Spoke bars (vacuum pressure)
- Ti He vessel
- Power coupler port

**Elliptical cavities**
- No HOM power couplers
- Hydroformed Ti bellows (+/- 3mm range)

- NbTi flange (w/bore holes for alignment & assembly tool) +Al hex. gaskets

**Stiffeners**

**Medium beta:**
- 6 cells – beta=0.67
- Length 1259,40mm

**High beta:**
- 5 cells – beta=0.86
- Length 1316,91mm
<table>
<thead>
<tr>
<th>Spoke cavities</th>
<th>Elliptical cavities</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Frequency (MHz)</strong></td>
<td>Medium</td>
</tr>
<tr>
<td><strong>Optimum beta</strong></td>
<td>0.50</td>
</tr>
<tr>
<td><strong>Operating temperature (K)</strong></td>
<td>2</td>
</tr>
<tr>
<td><strong>Nominal Accelerating gradient (MV/m)</strong></td>
<td>9</td>
</tr>
<tr>
<td>Lacc (βopt.x nb gaps x λ/2) (m)</td>
<td>0.639</td>
</tr>
<tr>
<td>Bpk (mT)</td>
<td>79 (max)</td>
</tr>
<tr>
<td>Epk (MV/m)</td>
<td>39 (max)</td>
</tr>
<tr>
<td>Bpk/Eacc (mT/MV/m)</td>
<td>&lt;8,75</td>
</tr>
<tr>
<td>Epk/Eacc</td>
<td>&lt;4,38</td>
</tr>
<tr>
<td>Beam tube diameter (mm)</td>
<td>50</td>
</tr>
<tr>
<td>RF peak power (kW)</td>
<td>335</td>
</tr>
<tr>
<td>G (Ω)</td>
<td>130</td>
</tr>
<tr>
<td>Max R/Q (W)</td>
<td>427</td>
</tr>
<tr>
<td>Qext</td>
<td>2.85 10^5</td>
</tr>
<tr>
<td>Q0 at nominal gradient</td>
<td>1.5 10^9</td>
</tr>
<tr>
<td><strong>Geometrical beta</strong></td>
<td>0.67</td>
</tr>
<tr>
<td><strong>Frequency (MHz)</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Number of cells</strong></td>
<td>6</td>
</tr>
<tr>
<td><strong>Operating temperature (K)</strong></td>
<td>2</td>
</tr>
<tr>
<td><strong>Epk max (MV/m)</strong></td>
<td>45</td>
</tr>
<tr>
<td><strong>Nominal Accelerating gradient (MV/m)</strong></td>
<td>16.7</td>
</tr>
<tr>
<td>Q_0 at nominal gradient</td>
<td>&gt; 5e9</td>
</tr>
<tr>
<td>Q_{ext}</td>
<td></td>
</tr>
<tr>
<td>Iris diameter (mm)</td>
<td>94</td>
</tr>
<tr>
<td>Cell to cell coupling k (%)</td>
<td>1.22</td>
</tr>
<tr>
<td>p,5p/6 (or 4p/5) mode sep. (MHz)</td>
<td>0.54</td>
</tr>
<tr>
<td>Epk/Eacc</td>
<td>2.36</td>
</tr>
<tr>
<td>Bpk/Eacc (mT/(MV/m))</td>
<td>4.79</td>
</tr>
<tr>
<td>Maximum. r/Q (W)</td>
<td>394</td>
</tr>
<tr>
<td>Optimum β</td>
<td>0.705</td>
</tr>
<tr>
<td>G (Ω)</td>
<td>196.63</td>
</tr>
<tr>
<td>RF peak power (kW)</td>
<td></td>
</tr>
</tbody>
</table>
Medium-β Elliptical Cavities

KL reduction using compensation rings for medium and high-beta

<table>
<thead>
<tr>
<th>Nominal wall thickness [mm]</th>
<th>3.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cavity stiffness Kcav [kN/mm]</td>
<td>2.59</td>
</tr>
<tr>
<td>Tuning sensitivity Df/Dz [kHz/mm]</td>
<td>197</td>
</tr>
<tr>
<td>KL with fixed ends [Hz/(MV/m)²]</td>
<td>-0.36</td>
</tr>
<tr>
<td>KL with free ends [Hz/(MV/m)²]</td>
<td>-8.9</td>
</tr>
<tr>
<td>Pressure sensitivity Kp [Hz/mbar] (fixed ends)</td>
<td>4.85</td>
</tr>
</tbody>
</table>

RF/mechanical design

Lorentz detuning

\[ K_L = \frac{\Delta f}{E_{acc}^2} \]

\[ K_L = K_{L\infty} + \frac{\Delta f F_\infty \cdot \bar{u}_z / E_{acc}^2}{\Delta z K_{ext} + K_{cav}} \]

\[ K_{ext} \text{ (tank + tuner)} \approx 30 \text{ kN/mm} \]
\[ \rightarrow K_L \approx -1 \text{ Hz/(MV/m)}^2 \]
\[ \rightarrow \Delta f \approx 325 \text{ Hz @ 18 MV/m} \]
(1/3 of cavity bandwidth)
Cryomodule Interfaces

- Most AD internal Work Packages (beam optics, RF, cryo, vacuum, test stands, electrical, cooling, installation)
- External WPs cryomodule, cavity and designers and potential In-Kind collaborators
- Control command (Control Box, PLC, LLRF, MPS, EPICS)
- Data-logging ICS teams
- ESS ES&H
- Conventional Facility
- ESS system engineer, QA
- Survey experts
- Transport

Previous Linac version for comparison ➔
Cold Tuning System

**Slow tuner**
Main purpose: Compensation of large frequency shifts with a low speed
Actuator used: Stepper motor

**Fast tuner**
Main purpose: Compensation of small frequency shifts with a high speed
Actuator used: Piezoelectric actuators

Stepper motor and planetary gearbox (1/100e) at cold and in vacuum

Elliptical CTS
Type V; 5-cell prototype +/- 3 mm range on cavity

Spoke CTS
2 piezo stacks

Stainless steel ball screws with MoS2 dry lubricant
Cold stepper motor and planetary gearbox
2 rolling rods
2 piezo actuators

Elliptical CTS

&
Fundamental Power Coupler

- Antenna
- Vacuum
- Outer conductor (LHe-cooled)
- Inner conductor (water-cooled)
- Al₂O₃ ceramic disc
- WR2300
- Doorknob
- Short circuit
- RF input

Spoke: 335 kW
Elliptical: 1.1 MW
Magnetic shield, e.g. Elliptical cavity

Achievable with 1.5 mm, \( \mu_r = 20000 \) shielding material

- Limit contribution of the trapped flux to the surface resistance to 4 \( \text{n}\Omega \)
- Limit the external static field to \( B_{\text{ext}} = 14 \text{ mG} \).
  \[ \rightarrow \text{Required shielding efficiency equal to 35.} \]
Heat load due to the beam losses deposit a maximum of 0.5 W/m to the Spoke, medium and high-beta cavities sections 2 K temperature levels.

### Cryomodule Heat Load Distribution

**Per cryomodule**

<table>
<thead>
<tr>
<th></th>
<th>Watts to 2 K</th>
<th>4.5 K Liquefaction (g/s)</th>
<th>Watts to ~50 K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Static</td>
<td>Dynamic</td>
<td>Total</td>
</tr>
<tr>
<td></td>
<td>Others</td>
<td>Valves</td>
<td>Coupler</td>
</tr>
<tr>
<td>1 Spoke</td>
<td>3.3</td>
<td>0.2</td>
<td>3.5</td>
</tr>
<tr>
<td>1 MB</td>
<td>6.3</td>
<td>0.2</td>
<td>6.8</td>
</tr>
<tr>
<td>1 HB</td>
<td>6.3</td>
<td>0.2</td>
<td>6.8</td>
</tr>
</tbody>
</table>

**Sum for the Linac cryoplant** (incl. 14 extra HB for contingency space)

<table>
<thead>
<tr>
<th></th>
<th>Watts to 2K</th>
<th>4.5K Liquefaction (g/s)</th>
<th>Watts to ~50K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Static</td>
<td>Dynamic</td>
<td>Total</td>
</tr>
<tr>
<td>Number of CMs</td>
<td>Static</td>
<td>Dynamic</td>
<td>Total</td>
</tr>
<tr>
<td>Spoke</td>
<td>13</td>
<td>91</td>
<td>84.5</td>
</tr>
<tr>
<td>Medium beta</td>
<td>9</td>
<td>119.7</td>
<td>209.7</td>
</tr>
<tr>
<td>High beta</td>
<td>35</td>
<td>472.5</td>
<td>627.9</td>
</tr>
<tr>
<td>Total</td>
<td>57</td>
<td>683.2</td>
<td>922.1</td>
</tr>
</tbody>
</table>
Cryomodule life-cycle

- High pressure rinsing
  In clean room (ISO5 or ISO4)
- Validation test of the cavity in vertical cryostat
- Qualified cavity storage
- Processed couplers storage
- Coupler RF processing
- Assembling in clean room
- Power coupler fabrication
- Cavity fabrication
- Chemical treatment
- Cryomodule components fabrication
- Cavity string assembling in clean room
- Cryomodule assembling
- Tools fabrication
- Transport
- Cryomodule reception and storage
- Validation test of the cryomodule
- Cryomodule storage
- Cryomodule on beam line

*Courtesy of Pierre Bosland CEA/IRFU*
Elliptical Cavity Preparation

High beta cavity fabrication (Zanon and RI)

Vertical Electropolishing system@ CEA

Study of the tooling in progress @ CEA

Example of the tooling for the assembling of the coupler on the cavity in clean room
Elliptical Assembly Procedure

Cavity string assembly in clean room

Cold mass assembly (outside the clean room)

Design concept of the tooling: Most of parts will be used for both types of elliptical cryomodules

Build on existing knowledge (SNS, XFEL)
- Develop Training and “Fabrication file”
- Pre-industrialization
- Industrialization

Thermal shield

Spaceframe

Vacuum vessel
Infrastructure in Saclay

Clean room for the M-ECCTD (and H-ECCTD)

Possible IKC for the assembly by industry at Saclay (XFEL cryomodules assembly)
- Uses the current infrastructure at Saclay
- Benefits from the experience of the XFEL cryomodule assembly (ALSYOM)

The clean room inauguration ➔ May 13th 2014
Assembly of elliptical cryomodules

Detailed procedures will be defined for every phases

- Components and tools
- Operations
- Controls and tests
Assembly: outside clean room

Cavity string assembled in the clean room → Assemble partially the magnetic shield → Install the tuning system → Connect the half rings on the helium tank → MLI on cavities → Complete the assembly of the magnetic shield

Assemble the Thermal shield → MLI on the thermal shield

Leak test of the cryogenic circuit → Insertion of the thermal shield in the spaceframe

Place the spaceframe on the cold mass insertion tool

Final leak test of the cryogenic circuits → Connect the remaining elements of the cryogenic circuits → Control of the alignment

Adjust of the spaceframe position in the vacuum tank

Insertion of the assembly inside the vacuum tank → Connect the blocks between the thermal shield and the tie rods

Completion of the thermal shield → Closing the cryomodule

Cryomodule OK

Check the electrical connections → Leak test of the insulation vacuum

Installation of the tie rods → Removing the trolley supporting the cold mass

MLI on the helium circuit → Connect other pieces of the helium circuit

Weld the helium return gas

Cold mass

Courtesy of N. Bazin / CEA
Spoke assembling in clean room/IPNO

Courtesy of D. Reynet / IPNO
Road to realizing the world’s leading facility for research using neutrons

- **2009**: Decision: ESS will be built in Lund
- **2003**: First European design effort of ESS completed
- **2012**: ESS Design Update phase complete
- **2014**: Construction work starts on the site
- **2019**: First neutrons on instruments
- **2023**: ESS starts user program
- **2025**: ESS construction complete
EXTRA SLIDES
Secondary particle produced at J-PARC

Target Nucleus

- Proton (p)
- Neutron (n)

Proton (p)
3 GeV, 50 GeV

Need to have high-power proton beams
→ MW-class proton accelerator (current frontier is about 0.1 MW)

Materials & Life Science from RCS
Nuclear & Particle Physics from MR
R&D toward Transmutation from LINAC