Katharine Burr Blodgett Medal and Prize

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For inventions in the area of liquid crystal displays, and his role in the founding and commercial success of Displaydata – a leading supplier of graphic electronic labels for the retail sector.

Katharine Burr Blodgett Medal and Prize

In 2008 Council introduced a medal to recognise contributions to the organisation or application of physics in an industrial or commercial context.

Originally this medal was known as the Business and Innovation Medal; 2012 it was renamed the Swan Medal of the Institute of Physics in recognition of Sir Joseph Swan, and in 2016 it was renamed to the Katherine Burr Blodgett Medal and Prize to recognise her contributions to physics in industry.

Dr Blodgett was an American researcher and the first woman to be awarded a PhD in physics from the University of Cambridge, in 1926. After receiving her master’s degree, she was hired by General Electric, where she invented low-reflectance “invisible” glass, where the non-reflective coating is called a Langmuir-Blodgett film. Blodgett was issued eight US patents during her career and was the sole inventor on all but two of them.
Neutron Scattering
An Introduction
Properties of the neutron

Why use neutrons?

Neutron Production 1
Reactor Sources

Moderation
Detection
Scattering Processes
  Elastic and Inelastic
  Coherent and Incoherent

Much simplified – no or few equations
  Powder Diffraction
  Triple Axis Spectrometry
  Small-angle Scattering
  ..Reflectometry

Neutron Production 2
Spallation Sources
Neutron Properties

Theorized  
Ernest Rutherford (1920)

Discovered  
James Chadwick (1932)

Mass  
$1.675 \times 10^{-27}$ kg
$939.565$ MeV/$c^2$
$1.00866$ u

Mean lifetime  
$881.5$ s (free)

Electric charge  
$0$ e

Magnetic moment  
$-0.966 \times 10^{-26}$ J·T$^{-1}$

Spin  
$\frac{1}{2}$

Velocity and wavelength of neutron  
$h/\lambda = mv$

Proton mean lifetime  
$\sim 2 \times 10^{29}$ yrs

Electron mean lifetime  
$\sim 7 \times 10^{28}$ yrs
Why Use Neutrons to investigate Matter?

Absence of charge – highly penetrative

Energy / wavelength ~ atomic and molecular motion and atomic spacing

Scattering power varies in a random way across Periodic table, different isotopes may have very different scattering power
Production of Free Neutrons

Nuclear Reactor Sources
Single fuel element (97% $^{235}\text{U}$) sits in the centre of a tank of 2.5 m diameter of heavy water moderator.

Cooling and moderation is by heavy water circulation passing through heat exchangers.

The moderator partly reflects thermalized neutrons back towards the fuel element

Thermal power 58.3 MW
Max. perturbed thermal flux at the beam tubes
$1.2 \times 10^{15}$ neutrons cm$^{-2}$ s$^{-1}$
Coolant flow in fuel element 2400 m$^3$/h
Coolant temperature (outlet) 50 °C
Reactor cycle 50 days
Average consumption of $^{235}\text{U}$ 36 %
1eV = 1.6×10^{-19} \text{J};

E=(1/2)mv^2; \text{ wave particle duality neutron wavelength } \lambda=h/mv.

E=\frac{h^2}{2m\lambda^2} \quad \lambda=\sqrt{\frac{h^2}{2mE}}
Moderation

Peak flux of the neutron beams is shifted to longer or shorter wavelengths

Thermally equilibrating the neutrons with cold or hot moderator.

**Cold moderator** - liquid deuterium ~23K (-250°C); reduces the energy to around 5meV (λ~0.4nm);

hot source is carbon at 2400K.
Instrumentation must be surrounded by massive shielding - prevent contamination of the detected scattered neutrons by parasitic neutrons
**Neutron Detection**

Neutrons have no charge - cannot be detected directly.

Nuclei with large absorption cross section for neutrons - subsequent nuclear reactions emit charged particles; attracted to detector electrode - current is related the neutron absorption event.

Commonly used gases in detectors are $^3\text{He}$ and $^{10}\text{BF}_3$

$n(^3\text{He},p)^3\text{H}$

$n(^{10}\text{B,}\alpha)^7\text{Li}$

$^3\text{He}$ is a by product of the nuclear weapons industry - now in short supply.

$\text{BF}_3$ is very toxic (a Lewis acid used to initiate polymerisation).

Efforts are being made to replace both of these gases with e.g scintillation detectors.
Scattering Process

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$b_s$/fm</th>
<th>$\sigma_c$/B</th>
<th>$\sigma_{inc}$/B</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1$H</td>
<td>-3.74</td>
<td>1.76</td>
<td>80.27</td>
</tr>
<tr>
<td>$^2$H</td>
<td>6.67</td>
<td>5.59</td>
<td>2.05</td>
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</table>
Coherent Scattering
Neutron wave interacts with the whole sample - scattered waves from different nuclei interact with each other.
Elastic scattering - structure of matter.
Inelastic scattering - dynamics of atoms or groups in Matter.

Incoherent Scattering
Neutron wave interacts independently with each nucleus – no interference between scattered wave - no information on structure.
Inelastic, incoherent scattering - insight into certain types of motion in matter.
Rotation of functional groups; diffusive motions e.g. gases on catalyst surfaces; diffusion in polymer melts.
1. **Powder Diffraction**
2. **Triple Axis Spectrometry**

First areas of application of neutron scattering - Clifford Shull and Bert Brockhouse jointly awarded the Nobel Prize in Physics in 1994

3. **Small-Angle Scattering**
4. **Reflectometry**

Small-angle scattering - used in polymer, biological science, micellar structures.

Reflectometry - relatively recent addition – investigation of surfaces and interfaces in layered structures of a wide range of materials; liquid interfaces; magnetic multilayers; polymer interdiffusion; heterophase organisation.
theory for neutron diffraction – 1936 - proof demonstrated later that year
In neutron diffraction, neutrons of same wavelength incident on a sample atoms arranged in fixed positions on a lattice. Each nucleus is the centre of an elastically scattered spherical wave. Waves spread and overlap. In places reinforcement occurs, in others cancelation takes place.

Intensity of scattering measured as a function of scattering vector, $Q$, $Q=4\pi \sin \theta / \lambda$. 
Intensity variation with angle governed by structure factor $S(Q)$.

$Q$ values where intensity is non-zero are $Q = n(2\pi/d)$

d is the spacing of lattice planes. Replace for $Q$ $n\lambda = 2d \sin \theta$ Bragg's Law.

Neutron beams are not very bright - large cross section (~ cm$^2$) and single crystal measurement using neutrons are confined to large crystals

X-ray diffraction is much more suited for single crystal or fibre diffraction - X-ray sources are bright - micron sized beams can be employed. Spatial resolution is generally much better also.
In a powder - huge number of randomly oriented single crystal grains always some with correct orientation for diffraction.

<table>
<thead>
<tr>
<th>crystal</th>
<th>pyrolytic graphite (002)</th>
</tr>
</thead>
<tbody>
<tr>
<td>wavelength</td>
<td>2.52 Å</td>
</tr>
<tr>
<td>flux at sample/n cm(^{-2})s(^{-1})</td>
<td>6.5 x 10(^6)</td>
</tr>
<tr>
<td>crystal</td>
<td>Germanium (311)</td>
</tr>
<tr>
<td>wavelength</td>
<td>1.28 Å</td>
</tr>
<tr>
<td>flux at sample/n cm(^{-2})s(^{-1})</td>
<td>0.4 x 10(^6)</td>
</tr>
<tr>
<td>max beam size</td>
<td>5 x 2 cm(^2)</td>
</tr>
<tr>
<td>angular range 2(\theta)</td>
<td>-20° ... 130°</td>
</tr>
</tbody>
</table>
X-ray synchrotron sources data collection times are very short – milliseconds in some cases

**Neutrons - hours or days.**

For low AN atoms which are germane to structure and properties - neutrons may be the only method.

**Example**

High $T_c$ superconductors discovered in the mid – 1980s; - ceramic type materials - stacked layers of metal oxides of different oxygen content - **only accessible via neutron diffraction.**
nickel-lanthanum hydride electrode materials in Ni-MH batteries

charge-discharge of the standard electrode cyclic transformation between two crystalline phases called α and β. Unit cell volumes differ by 20 % inducing large constraints - causes crystal structure to fragment.

Neutron diffraction during cycling shows a transitory intermediate γ phase with a cell volume between that of the α and β phases may appear - significantly reduces the constraints during the cycling process, leading to a better lifetime
Triple Axis Spectrometry

Molar Heat capacities of Elements – Dulong and Petit’s law
**Einstein solid**
- Each atom in the lattice is an independent non-interacting 3D quantum harmonic oscillator
- All atoms oscillate with the same frequency

**Debye model**

vibrations of the atomic lattice interact

quantization of the vibrational modes - **phonons** by Igor Tamm in 1936

**Phonons determine**; conductivity – thermal, electrical and sound; specific heat; reflectivity; inelastic scattering of light; X-ray scattering; **neutron scattering**.
Phonon frequency $\sim 10^{12}$ Hz; energy $\sim 4$ meV $\sim$ neutron energy

Interested is focussed on the **dispersion of phonons** - relation between phonon frequency and wave vector $k$ and $k=2\pi/\lambda$

In inelastic coherent neutron scattering - neutron can absorb energy from or pass energy to the phonon. Difference in energy before and after scattering = phonon energy.

Phonon frequency determination need the direction of propagation is also needed –obtained by measuring the neutron wavevector, $k$, before and after the scattering event.

Both energy and vector information are obtained using a **triple axis spectrometer**
The first experiments of this type were done by Bert Brockhouse at AEC Canada Chalk River in 1954

http://rsbm.royalsocietypublishing.org/content/roybiogmem/51/51.full.pdf
The Nobel Prize in Physics 1994
"for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

**Bertram N. Brockhouse**
"for the development of neutron spectroscopy"

**Clifford G. Shull**
"for the development of the neutron diffraction technique"
Small-Angle Scattering

Scattering techniques work in reciprocal space (Q \sim 2\pi/d).

As d becomes larger then the pertinent range of Q becomes smaller as does 2\theta.

For objects » \lambda - 2\theta must be very small.

Materials where small-angle neutron scattering is used

- Polymers and colloids
- Polymer blends, solutions; Micelles; Dendrimers; Liquid crystals; Gels; Reaction kinetics of mixed systems
- Materials science
- Phase separation in alloys and glasses; Morphologies of superalloys; Microporosity in ceramics; Interfaces and surfaces of catalysts
- Biological macromolecules
- Size and shape of proteins, nucleic acids; Biomembranes; Drug vectors
- Magnetism
- Flux line lattices in superconductors; Magnetic correlations
For SANS the wavelength » interatomic distance

Space pervaded by the molecule is a region of uniform scattering power.

In these cases the scattering is given by;

\[ I(Q) = (\rho_p - \rho_m)^2 N_p P(Q) \]

\( P(Q) \) is the particle form factor

Sphere  \( P(Q) = [(3/(QR)^3(\sin(QR) - QR\cos(QR)))^2 \]
Polymer molecule

\[ P(Q) = \frac{2}{(Q^2 R_g^2)} \left( \exp(-Q^2 R_g^2) - 1 + Q^2 R_g^2 \right) \]

This is the **Debye equation** first obtained in 1944 for light scattering from polymer solutions.
\((\rho_p - \rho_m)^2\) is the contrast factor

\(\rho_i\) is the scattering length density of the particle, (p) or medium (m).

Sum of the coherent scattering lengths of the atoms that make up the constituent units of the scattering body

<table>
<thead>
<tr>
<th>Material</th>
<th>Formula</th>
<th>(\rho \ (10^{-6}\text{Å}^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H polystyrene</td>
<td>C(_8)H(_8)</td>
<td>1.4</td>
</tr>
<tr>
<td>D polystyrene</td>
<td>C(_8)D(_8)</td>
<td>6.92</td>
</tr>
<tr>
<td>H polyethylene oxide</td>
<td>C(_2)H(_4)O</td>
<td>0.56</td>
</tr>
<tr>
<td>D polyethylene oxide</td>
<td>C(_2)D(_4)O</td>
<td>6.33</td>
</tr>
<tr>
<td>Water</td>
<td>H(_2)O</td>
<td>-0.28</td>
</tr>
<tr>
<td>Heavy water</td>
<td>D(_2)O</td>
<td>6.68</td>
</tr>
</tbody>
</table>
1949 P J Flory (NP 1974) - solid state amorphous polymer molecule should adopt its random walk configuration

First experiments in 1973 (Dennis Ballard, George Wignall – ICI; Jim Schelten IFF Julich)
Small % of PSD with PSH of same MW - scattering as predicted by Flory.

Considerable research on polymer systems of all types followed - contributed to the NP in Physics awarded to P G de Gennes in 1991
Contrast Variation

Polymer Contrast

Film Contrast

Bulk Contrast
Neutron Reflectometry

If the angle of incidence of the neutron beam is sufficiently small then, just like light, the neutron beam will be reflected to an extent.

Intensity and variation with incident angle of reflected beam $\alpha$ reflecting power of material normal to the surface.

from its beginnings in the UK in circa 1986 on a single ‘black’ instrument - now 15 – 20 instruments world wide
Adsorption at the liquid surface
Adsorption / tethering at solid liquid interface
liquid / liquid interfaces
L-B films
polymer films and interfaces
in situ electrochemistry
metal multilayers
Magnetic surface phenomena

Film Factor = \( Q^4 R(Q) / 16\pi^2 \)
What’s Missing?
Incoherent inelastic scattering – rotational motions

Quasi-elastic scattering – QM Tunneling

Spin echo scattering – diffusion

Magnetic scattering.
Spallation Sources

ISIS is a high power accelerator that fires high energy protons into two targets to release neutrons for experiments.

The ISIS synchrotron accelerates protons to 84% of the speed of light then fires them into two tungsten targets.

**Target Station 1**
Neutrons are released from both targets via spallation. Using neutrons, scientists can study the atomic structure of materials and can even measure the forces between atoms.

**Target Station 2**
The second target station is optimised for low energy neutrons providing greater capacity at ISIS and opening up new areas of research.
Detection at a Spallation Source

neutrons at spallation sources are produced in pulses – 50 times a second.
Each pulse has a distribution of neutron wavelengths (velocities)
Measure the time of flight of each neutron as it arrives at the detector.
start time of the neutron is fixed, due to the pulse structure
Measure the arrival time at its destination, i.e. in the detector.
Instrument geometry is fixed - distance travelled is known –
from arrival time at the detector the velocity is calculated –
wavelength obtained and value of Q evaluated.

All the techniques used at reactor sources can be done at spallation sources – savings in space and cooling requirements
Sources

www.ill.eu
www.isis.stfc.ac.uk/Pages/home.aspx
www.ill.eu/about/what-is-the-ill/history/jacrots-book-neutrons-for-science/
www.youtube.com/watch?v=1zOsSx_Yd7w  Didcot Atom Village (1947)
www.youtube.com/watch?v=o_Z6ax6J-Go  Decommissioning of DIDO and PLUTO reactors
http://www.harwellcampus.com/
www.ornl.gov

*Theory of Neutron Scattering from Condensed Matter* S W Lovesy  
*Polymers at Surfaces and Interfaces* R A L Jones and R W Richards  
*Polymers and Neutron Scattering* J S Higgins and H Benoit

Original publications