Neutrons.

Sources and theory basics.

A.V.Belushkin

Frank Laboratory of Neutron Physics, JINR, Dubna

View of J-PARC in May 2007

Site; Tokai, Ibaraki 150km to the north from Tokyo

The first neutrons from liquid mercury target 30 May 2008!

Linac (400MeV -> 200MeV)

Materials & Life Experimental Hall (MLF: JSNS+muon) (1MW, 25Hz ->0.6MW)

Hadron Experimental Hall

50 GeV

synchrotron (MR)

Neutrino to

Joint Institute for Nuclear Research

Super KAMIOKANDE (300km away)

600year old historic shrin

3 GeV-

(RCS)

synchrotron

The European Spallation Source

Brightness comparison of different radiation sources

ILL, Grenoble, France

Neutron as a particle

According to quark theory, neutron consists of two down (d) and one up (u) quarks.

Neutron

mass m_n= 1.175×10^{-27} kr el. charge = 0; спин = $\frac{1}{2}$ magnetic dipole moment μ_n = -1.913 μ_N , where nuclear magneton $\mu_N = e h/4\pi m_p = 5.051 \times 10^{-27}$ JT-1

Neutron as a particle

Neutron Beta Decay

Why it is important to know precisely the neutron life-time?

 $n \rightarrow p^+ + e^- + \overline{v}_e + 782 \text{ keV}$

$$
\tau_n = 885.7 \pm 1.0 \text{ sec}
$$

Neutron as a particle and a wave

Neutron possesses properties of both particle and a wave:

$$
E = m_n v^2 / 2 = k_B T = (hk/2\pi)^2 / 2m_n
$$
; $k = 2 \pi / \lambda = m_n v / (h/2\pi)$

Neutrons for condensed matter research

Neutrons for condensed matter

The diameters of the circles shown scale with the scattering amplitude $f_{\sf x}$ (sin θ =0) for X-rays, and $b_{\rm coh}$ 10 for neutrons. Hatching indicates negative scattering amplitudes

Penetration depth of thermal neutrons, low energy electrons and 8 keV X-rays into different elements

Disadvantages For neutrons: no regular wavelength dependence of scattering length (which is just a number, not the function of the scattering angle as in the case of X-rays!) and absorption coefficient from atomic number; enormous difference in scattering legths and absorption coefficients for H and D; huge absorption for Cd, B, Sm, Gd

Relatively low intensity of neutron sources \Rightarrow weak signal, large sample volumes required etc. Strong absorption of some elements, but isotope substitution can cure the problem. Kinematical restrictions limit the achievable energy-momentum range..

Neutrons for condensed matter

The Nobel Prize in Physics 1994

structure and dynamics

Neutrons hounce

against atomic nuclei

They also react to the

magnetism of the

atoms.

Research reactor

Neutrons reveal

techniques for studies of condensed matter.

Clifford G. Shull, MIT Cambridge, Massachusetts USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

Shull made use of elastic scattering i.e. of neutrons which change direction without losing energy when they collide with atoms.

Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. Even the placing of light elements such as hydrogen in metallic hydrides, or hydrogen, carbon and oxygen in organic substances can be determined. The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.

Lay a neutron diffraction map (showing the positions of the nuclei) over an X-ray diffraction
map (giving the distribution of the map (giving the distribution of
the dectrons). It is then clear
that the dectron density is

shifted in relation to the po-
tions of the atomic nuclei.
Since a chemical bond invo-
a shift in electron position.

direct picture of the chen
bond is obtained in this x

D.J. Hughes The Nudear Reator as a Research Internation, sciences Managean, vol., 189, AUGUST 1953, P. 23. .
Lengeler and J.L. Finney *The European Spallation Source,* EUROPHYSICS NEWS, VOL. 25, P.37, 1994.
miation about the Nobel Prize in Physics 1994 (presselence), THE ROYAL SWEDISH ACADEMY OF SCIEN

Neutrons see more than X-rays

Further reading

A version of the control of the control of the state of the state of the With X-rays it is easiest to see atoms that have many electric Hydrogen, for example, which has only one electron, is not control to exay to see. Wit

has changed and hence the

internal forces remaining
round the hole after it has
been punched.

The curves show local
expansion forces (positive)
and compression forces
(negative) in different
directions (red, green and
duo) in an aircraft part
(Saab39 Gripen).

Atoms in a

crystalline sample

 \bullet

Neutrons show

When the neutrons
collide with atoms in the
sample material, they

Neutrons reveal inner stresses

Dr

change direction (are

scattered) - elastic
scattering.

where atoms are

forwards neutrons of
a certain wavelength (energy) - mono chromatized neutrons

Neutrons show what atoms remember **VEGIT HITTELY STEESSES**

hed in an important metal aircraft part.

Does the part match up?

Neutron diffraction can

show how much the dis-

time between the atoms

A volume of their extreme solver when they move randomly in relation to
not their rather positions when they move randomly in relation to
calch ofter in liquids and media. Even here there is in fact some local
often the ad \bullet $(1 ps = one$ s snow now
lionth of a m onth of a se pring, Corresponding "memory fi
ets e.g. near the Curie temperat

Crystal that sorts and
forwards neutrons of
a certain wavelength
(energy) – mono-

(energy) - mono-
chromatized neutrons

1940s and 1950s. It was then that the resources of the reactors became available for peacetime research.

advanced neutron scattering installations have been built and
more are planned in Europe, the USA and Asia. At these super-installations the researchers are studying the structure of

new ceramic superconductors, molecular movements on surfaces of interest for catalytic exhaust cleaning, virus
structures and the connection between the structure and the

... now it continues
Thousands of researchers are now working at the many

How it started

.. how it continues

elastic properties of polymers

Brockhouse made use

Bertram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize

in Physics for the development of neutron spectroscopy.

of inelastic scattering i.e. of neutrons, which change both direction and energy when they collide with atoms. They then start or cancel atomic oscillations in crystals and record movements in liquids and melts. Neutrons can also interact with spin waves in magnets.

With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structures in liquids change with time.

and the neutrons then counted in a
detector.

Neutrons for condensed matter **Interdisciplinary character of research with neutrons**

Fission reactions Slow neutron **Production of neutrons**

Each fission act produces in average ~2.5 neutrons with energy release about 200 MeV. In the case of chain (self sustained) reaction 1 neutron is necessary to ensure the next fission, 0.5 is lost because of absorption inside the neutron source and 1 neutron can be extracted for use in the experiment

Production of neutrons

Steady state nuclear reactor

Production of neutrons

Spallation reaction gives up to 30 neutrons per 1 proton. There exists *empirical* expression for the estimation of neutron yield from the target when proton energy exceeds 120 MeV

$$
N_n(E,A) = \begin{cases} 0.1 \times E_{GeV} \times (A+20) - \text{for non-fissile target} \\ 50 \times E_{GeV} - \text{for uranium} - 238 \end{cases}
$$

Production of neutrons

Principal scheme of spallation neutron source

Components of neutron scattering instruments

What do we need to perform good neutron experiment?

- **❖ Intense neutron source with efficient moderator**
- neutron shaping, guiding and velocity selection system
- \div interesting sample for the study
- ❖ system to analyse parameters of scattered neutron beam
- advanced neutron detector

Typical scheme of neutron scattering experiment

Examples of registered patterns on a detector

From the analysis of the signal on a detector, using advanced mathematical models one can extract information about characteristics of a sample under investigation

Cross-sections definitions

Let the sample is irradiated by flux Φ_{in} of neutrons per unit area per unit time. We define I*^s* and I*^a* as ^a number of neutrons scattered and absorbed by the sample per unit time, respectively. Then the total cross sections of scattering and absorption of neutrons by the sample are defined as:

 $I_s = \Phi_{in} \sigma_s$

 $I_a = \Phi_{in} \sigma_a$

Dimensionality of the total cross sections is [barn]:

1barn = 10^{-24} cm².

By definition the flux Φ_{in} = $1/S$ *·t* = v_o /V, where S – is the area irradiated by neutrons, $t -$ time of irradiation, $v_0 -$ velocity of neutrons, *V* – volume of the irradiated sample.

The interaction of neutron with nuclei is described by Fermi pseudopotential:

$$
H = \frac{2\pi\hbar^2}{m_n}b\delta(\vec{r}-\vec{R})
$$

Where m_n – neutron mass, b – scattering length, R – vector defining the position of a nucleus in space.

Let us first consider the scattering of a neutron on isolated nucleus under the following assumptions:

neutron wavelength is much larger than the scattering length which is the radius of action of nuclear force (this is the limitation of applicability of Fermi pseudopotential)

 \triangleright the scattering is purely elastic, e.g. the energy of neutron is conserved before and after the scattering

 \triangleright the absorption of neutrons by the nucleus can be neglected

$$
\Phi_{out} = v_0 \Psi_{out}^* \Psi_{out} = \left| b \right|^2 \frac{1}{r^2} \frac{v_0}{V}
$$

The number of neutrons passing through the element of spherical surface $S = r^2 d\Omega$ is equal

$$
dI_{out} = \Phi_{out}(\vec{r})r^2d\Omega = |b|^2 \frac{v_0}{V}d\Omega
$$

And differential scattering cross section (i.e. the probability that neutron is scattered in a direction defined by a vector *r* into an element of solid angle $d\Omega$) is equal

$$
\frac{d\sigma}{d\Omega} = \frac{dI_{\text{out}}}{\Phi_{\text{in}} d\Omega} = |b|^2
$$

And the total scattering cross section will be

 $\sigma = \int (d\sigma/d\Omega) d\Omega = 4\pi |b|^2$ **ISOTROPIC!!!**

Let us now consider the scattering by a nucleus which position is defined by a vector R_i . The wave function of incident neutrons will again be a plane wave:

$$
\Psi_{in}=\frac{1}{\sqrt{V}}e^{i\vec{k}_0\vec{r}}
$$

And for the scattered neutrons

 \overrightarrow{a}

$$
\Psi_{out} = \frac{1}{\sqrt{V}} e^{i\vec{k}_0\vec{R}_i} \left[\frac{-b_i}{|\vec{r} - \vec{R}_i|} e^{ik_0|\vec{r} - \vec{R}_i|} \right]
$$

$$
\vec{r} - \vec{R}_i \Big| = r - \frac{\vec{r}}{r} \vec{R}_i + O\left(\frac{1}{r}\right)
$$

For $r \rightarrow \infty$ we have:

$$
e^{ik_0|\vec{r}-\vec{R}_i|}=e^{ik_0r}e^{-ik_0\frac{\vec{r}}{r}\vec{R}_i}=e^{ik_0r}e^{-i\vec{k}_1\vec{R}_i}
$$

$$
\Psi_{out}=\frac{1}{\sqrt{V}}e^{-i\vec{k}_1\vec{R}_i}\left(\frac{-b_i}{r}e^{ik_0r}\right)
$$

r

The resulting neutron flux after scattering on the nuclei R_i and R_j will be equal \vec{r}

$$
\Phi^{i,j}_{out} = \frac{v_0}{V} \Psi^{i}_{out}{}^* \Psi^{j}_{out} = \frac{v_0}{V} b_j b_j e^{i \vec{k}_1 \vec{R}_i} e^{-i \vec{k}_1 \vec{R}_j}
$$

Therefore, differential cross section for N nuclei:

$$
\frac{d\sigma}{d\Omega}=\sum_{i,j}^{N}b_{i}b_{j}e^{i\vec{Q}(\vec{R}_{i}-\vec{R}_{j})},\text{ where }\vec{Q}=\vec{k}_{1}-\vec{k}_{0}
$$

Now, consider more common case, when the velocity of neutron is changing during the scattering process due the fact that atoms perform thermal vibrations and their coordinates in space become time dependent. This means that $v_1 \neq v_0$ and *Ri=Rⁱ (t)*. Then the above formula can be written in a more common form giving the double differential cross section. This cross section defines the probability of neutron being scattered in a direction *r* into an element of solid angle $d\Omega$ with the neutron energy change *E=E¹ -E⁰* in an interval *dE*.

$$
\frac{d^2\sigma}{d\Omega d\omega}=\frac{k_1}{k_0}\sum_i\sum_j\int\limits_{-\infty}^{+\infty}\!\!\left\langle b_ib_je^{i\vec{Q}\vec{R}_i(t)}e^{-i\vec{Q}\vec{R}_j(0)}\right\rangle\!e^{-i\omega t}dt
$$

Angular brackets mean averaging over all values of nuclei coordinates in a space *Rⁱ (t)* , isotope content and all possible spin states of nuclei. It is known, that the scattering length depends on a relative orientation of nucleus and neutron spins. For parallel spins denote the scattering length as b^+ , and for anti parallel as b^- . Scattering length is also different for different isotopes of the chosen chemical element. Then one obtains:

$$
\left\langle b_{i}b_{j}\right\rangle =\begin{cases}\left\langle b_{i}\right\rangle \!\!\left\langle b_{j}\right\rangle &\text{for}\;\; i\neq j\\\left\langle \left|b_{i}\right|^{2}\right\rangle &\text{for}\;\; i=j\end{cases}
$$

Consequently, neutron cross sections will consist of two terms – coherent and incoherent:

$$
\sigma = \sigma_{coh} + \sigma_{inc}; \qquad \sigma_{coh} = 4\pi b_{coh}^2; \qquad \sigma_{inc} = 4\pi b_{inc}^2
$$
\n
$$
\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{coh} + \left(\frac{d\sigma}{d\Omega}\right)_{inc} = \underbrace{\left|\sum_{i}^{N} \langle b_i \rangle e^{i\vec{Q}\vec{R}_i}\right|^{2}}_{coh} + \underbrace{\left(\left\langle \left| b_i \right|^{2} \right\rangle - \left| \langle b_i \rangle \right|^{2}}_{inc}\right)}_{coh}
$$

$$
\frac{d^2\sigma}{d\Omega d\omega} = \left(\frac{d^2\sigma}{d\Omega d\omega}\right)_{\text{coh}} + \left(\frac{d^2\sigma}{d\Omega d\omega}\right)_{\text{inc}}
$$
\n
$$
\left(\frac{d^2\sigma}{d\Omega d\omega}\right)_{\text{coh}} = \frac{k_1}{k_0} \sum_{i} \sum_{j} b_i^{\text{coh}} b_j^{\text{coh}} S(\vec{Q}, \omega), \text{ r,}
$$
\n
$$
S(\vec{Q}, \omega) = \frac{1}{2\pi} \iint d\vec{r} dt \ e^{i(\vec{Q}\vec{r} - \omega t)} G_n(\vec{r}, t)
$$
\n
$$
G_n(\vec{r}, t) = \sum_{i} \sum_{j} \int \left\langle \delta[\vec{r} - \vec{r}' + \vec{R}_j(0)] \cdot \delta[\vec{r}' - \vec{R}_i(t)] \right\rangle d\vec{r}'
$$
\n
$$
S(\vec{Q}, \omega) \qquad \text{Is called the SCATTERING LAW}
$$
\n
$$
G_n(\vec{r}, t) \qquad \text{Is called PAIR CORRELATION FUNCTION,}
$$

Which is the probability, that if the arbitrarily chosen nucleus j at a time **t=0** had a coordinate $\mathbf{R}_{\mathbf{i}}$ (0), then at a moment t≠0 another atom i will have a coordinate **Rⁱ** (t).

$$
\left(\frac{d^2\sigma}{d\Omega d\omega}\right)_{inc} = \frac{k_1}{k_0} \sum_{i} \left(b_i^{inc}\right)^2 S^{inc}(\vec{Q}, \omega)
$$

\n
$$
S^{inc}(\vec{Q}, \omega) = \frac{1}{2\pi} \iint d\vec{r} dt e^{i(\vec{Q}\vec{r}-\omega t)} G_a(\vec{r}, t)
$$

\n
$$
G_a(\vec{r}, t) = \sum_{i} \int \left\langle \delta[\vec{r} - \vec{r}' + \vec{R}_i(0)] \delta[\vec{r}' - \vec{R}_i(t)] \right\rangle
$$

 $G_{a}(\vec{r},t)$ - Is called an AUTOCORRELATION FUNCTION,

Which is the probability, that if at a time t=0 the arbitrary chosen atom i had a coordinate $\underline{\mathbf{R}}_{\underline{\textbf{\textit{i}}}}(0)$, then at a time t≠0 its coordinate will be **Rⁱ** (t).

Possible types of neutron scattering experiments and corresponding scientific applications

© А.В.Белушкин, 2006

Magnetic neutron scattering

The detailed evaluation of the expressions for cross sections of elastic and inelastic neutron scattering on different magnetic structures is rather complicated. Therefore, let's see only the final result for several most common cases.

General expression for double differential cross section (unpolarised neutrons)

Magnetic neutron scattering

Magnetic form factor F(**Q**) is the Fourier transform of the magnetisation density in a crystal. It is important to note, that neutron magnetic form factor is defined by distribution of electrons with uncompensated spins only.

 r_0 = e²/m_ec² – electromagnetic radius of the electron

 $y = -1.913$ – neutron magnetic moment in Bohr magnetons

Kroneker symbol 1, if $i = j$ 0,if i \neq j $\mathbf{y} = \left\{ \begin{matrix} 0, & \cdots & 1 \\ 1, & \cdots & 1 \end{matrix} \right\} \overline{\mathcal{L}}$ $\left\{ \right.$ \int $=$ \neq $\delta_{\rm ii} =$

) Q $\mathsf{Q}_{\alpha} \mathsf{Q}$ $\left(\delta_{\alpha\beta} - \frac{\alpha}{\Omega^2}\right)$ Polarisation factor $\left(\delta_{\alpha\beta} - \frac{\mathcal{Q}_{\alpha} \mathcal{Q}_{\beta}}{\Omega^{2}}\right)$ indicates that neutrons interact only with the components of atomic spin which are perpendicular to the scattering vector **Q**. This fact allows uniquely measure in an experiment the directions of atomic spins and polarisation of spin waves. r_0 value indicates that the magnetic neutron scattering cross section is of the order 10⁻²⁴ cm², therefore comparable with nuclear scattering cross section.

Uses of neutron scattering in magnetism

Static properties (elastic scattering)

Spin arrangements in ordered magnetic structures Static spin correlations in disordered or frustrated magnets Magnetisation density (magnetic form factor) Flux distributions in superconductors Magnetism of surfaces (reflectometry)

 etc

Dynamic properties (inelastic scattering)

Crystal field excitations

Inter-multiplet atomic excitations

Spin waves in ordered magnetic structures

Spin fluctuations in strongly correlated or frustrated magnets

Magneto-phonon coupling

etc

Magnetic scattering
\n
$$
S^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar} \int dt \ e^{-i\omega t} \frac{1}{N} \sum_{\mathbf{R}\mathbf{R}'} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R}')} < S^{\alpha}_{\mathbf{R}}(0) S^{\beta}_{\mathbf{R}'}(t) >
$$

Modern challenges - novel fields of neutron scattering application **"There are no such things as applied sciences, only applications of science." "A bottle of wine contains more philosophy than all the books in the world."**

What neutron autoradiography tells us about Old Masters: The genesis of Jan Steen's "Wie die Alten sungen, so zwitschern die Jungen"

By Dr. K.Kleinert (HZB, Berlin) and M.Reimelt (Gemaldegalerie, Berlin)

Jan Steen, "Wie die Аltеп suпgеп, so zwitschern dte Jungеп", 1665/66, сапvаs, 84.8х 100.4 cm, Gemaldegalerie Berlin

The X-ray image already shows that large areas of the painting, like the drapery on the upper part of the archway on the right have been changed during the painting process.

Neutrons allow the visualisation of structures and layers beneath the surface and, in addition, enable the detailed identification of the elements contained in the pigments. Neutrons immediately clearly reveal the drapery and the landscape in the archway.

Today's version of the painting

Contour drawing of the reconstructed original version

(IBR-2, FSD, October 2011)

Travel and Transport Travel and Transport

Date 8 January 1989 **Summary** Engine fan blade fracture (design flaw), **Pilot error Site** Kegworth, Leicestershire, England 52°49′55″N 1°17′57.5″WCoordinates: 52°49′55″N 1°17′57.5″W **Passengers** 118 **Crew** 8 **Injuries (non-fatal)** 79 **Fatalities** 47 **Survivors** 79 **Aircraft type** Boeing 737–4Y0 **Operator British Midland Flight origin** London Heathrow Airport **Destination** Belfast International Airport

Neutron Reflectivity Reveals Suspected Air Layer under Water Drops on Lily Pads

• **Hydrophobic forces govern protein folding, lipid aggregation, and hence life itself**

• Dew drops roll off lily pads because their surfaces are hydrophobic ("water fearing")

An air layer has been long-suspected under such a drop

Removal of dissolved gases reduced the layer thickness; aeration increased it

Dhaval A. Doshi, Erik B. Watkins, Jaroslaw Majewski, Jacob Israelachvilli, PNAS

Hydrophobic Polymer $Q(A^{-1})$ **Quartz**

Water

Air (10 Å)

Clean transport based on hydrogen technology requires synthesis of advanced proton conducting materials

Neutrons are unique to study light atoms positions in structurally disordered phases

CsDSO₄

Tomography of padlock

