The Use of Neutron scattering in Bio-Physics

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Abstract

Method of neutron scattering has proven to be the most important a unique technique for elucidating the structure and dynamics of matter. In this paper, small angle neutron scattering experiment most often used in Bio- Physics research has been discussed.

A neutron is one of the fundamental spin $\frac{1}{2}$ neutral particle that make up matter. Neutron was identified in 1930s that resides in the nuclues of a typical atom along with proton. The magnetic moment of neutron is -1.913 nuclear magneton. The compositon of neutron is very high, that is more than the half of all visible matter present in the universe. The pioneering work of neutron scattering was performed by Wollan and Shull in 1946. Neutron Scattering is one of a unique and powerful tool to charatercize the structure of matter. In 1994, the Nobel prize for physics was awarded to Shull and Bert Brockhouse for "showing where are atoms and what atoms do". Neutron scattering provides new information those can't be obtained from other techniques such as x-ray diffraction, electron microscope and optical spectroscopies at an atomic level as well as the chemical and physical properties of matter. The most promising advances in materials science and other fields of science have been explained by research using neutron scattering technique such as high temprature superconductor, plastic polymers, new magnetic materials, amorphous semiconductor used in solar cells, medicine and biology. It will be particularly valuable for studies in nano technology and nano science.

Properties of Neutron

1. The de Brogile wavelength 'λ' of the neutron is given the relation, $\lambda = \frac{h}{p}$, $p = \hbar k = mv$
The de Brogile wavelength of thermal neutrons is comparble to atomic spacings. The energy of a neutron is purely kinetic energy because the neutron has a finite mass (m_n = 1.673 $\times 10^-27$ kg),
$E = \frac{mv^2}{2}$ = $k_B T$, E(mev) = $\frac{81.799}{\lambda^2}$ $\hbar = 6.626 \times 10^{-34} Js$, v = velocity of neutrons (measured by time of flight method), T = Temprature of moderator
2. It tracks down the positional parmeters as well molecular vibration, of atom during catalaytic reactions. The energy of thermal neutron matches to the energy of excitations of phonons.
3. The neutron has a small magnetic moment. This can interact with spin and orbital magnetic moments present in a sample containing atoms with unpaired electrons. It provides a unique probe for the study of magnetic structure, magnetic moment distributions and magnetic excitations.
4. The interaction of neutron with mattter is weak i.e. neutrons interact with atomic nucleus and not with orbiting electrons. The absorption by most material is correspondingly small. Because of their high penetration ability into most materials therefore bulk properties of mater can be studied.

Sources of Neutrons

There are two different sources avilable for neutron scattering.
1. Neutrons produced by the nuclear fission process in the reactor are very energetic and high-speed.These are quickly slow and cool as they pass through liquid hydrogen(-253^o C).These neutrons are used as sources in small angle neutron scattering process.
2. In Spallation technique, particle accelerators and synchotron are used to generate intense, high energy proton are directed to at a target heavy nuclei. Which will knock off or spalled some neutrons. These neutrons are slowed down in moderator and guided through beam lines to areas containings special instruments such as neutron detector.

Theory

The direction of propagation of the incident neutron beamt tavelling with velocity $\vec{v}_i$ is represented by the wave vector $\vec{k}_i$ and that of scattered neutron beam $\vec{v}_f$ and $\vec{k}_f$ respectively. The scattered beam makes an angle $\frac{\theta}{2}$ with the incident beam as shown in figure.

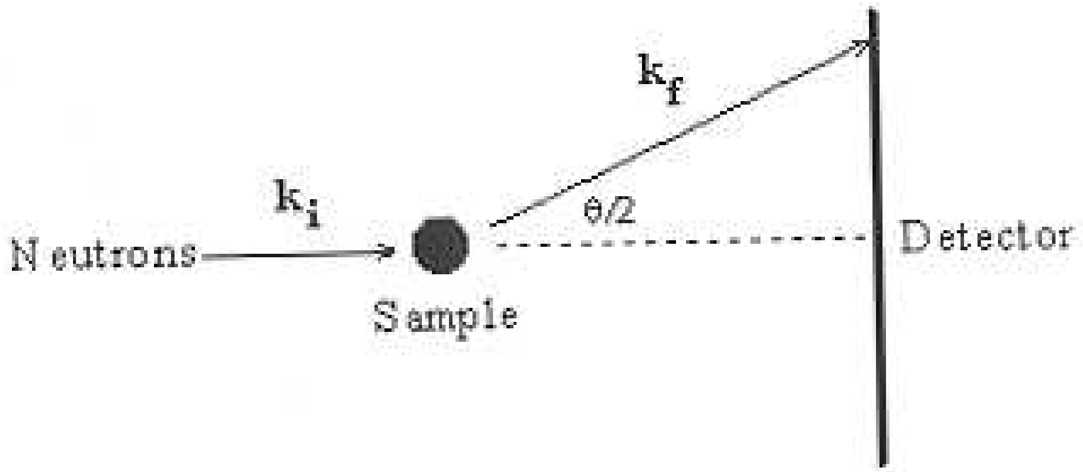

Figure 1: *Geometry of Neutron scattering event [1].*

The scattering vector,
$\vec{Q} = \vec{k}_f - \vec{k}_i$,
$\hbar\vec{Q} = m\vec{v}_f - m\vec{v}_i$
$Q^2 = k_f^2 + k_i^2 - 2k_f k_i cos\frac{\theta}{2}$
The energy change on Scattering in the form,
$\Delta E = E_f - E_i$
$\hbar\omega = \frac{mv_f^2 - mv_i^2}{2}$
$\Delta E = \hbar^2(k_f^2 - k_i^2), \leftrightarrow \hbar\omega = \hbar^2(k_f^2 - k_i^2)$
Because of the conservation of energy and momentum, the momentum $\hbar\vec{Q}$ and $\hbar\omega$ are transfered to the sample.
In elastic scattering,
$\Delta E = 0$
$E_f = E_i \leftrightarrow \mathrm{k}_f = k_i$
$\mid k_f \mid = \mid k_i \mid$
$Q = 2k sin\frac{\theta}{2}$
$Q = \frac{4\pi \sin\frac{\theta}{2}}{\lambda}$
$k = \frac{2\pi}{\lambda}$
we have, Bragg's law of diffraction,
$\lambda = 2d\sin\frac{\theta}{2}$
which yields,
$d = 2\frac{\pi}{Q}$,
Elastic scattering provides information about the position of the atom or the size and distribution of imhomgeneities in a sample. However, inelastic scattering provides the time and

the frequency dependent properties of the sample.

Small Angle Neutron Scattering

Neutron spectrometers are classified into two groups.

1. The simplest diffractometer measure the scattered intensity in a specific direction without determing energy and wave vector. Assuming that$E_i = Ef$ for elasctic scattering.

2. In other class of spectrometer k_f and E_f are measured by the detector (velocities are measured by time of flight method).

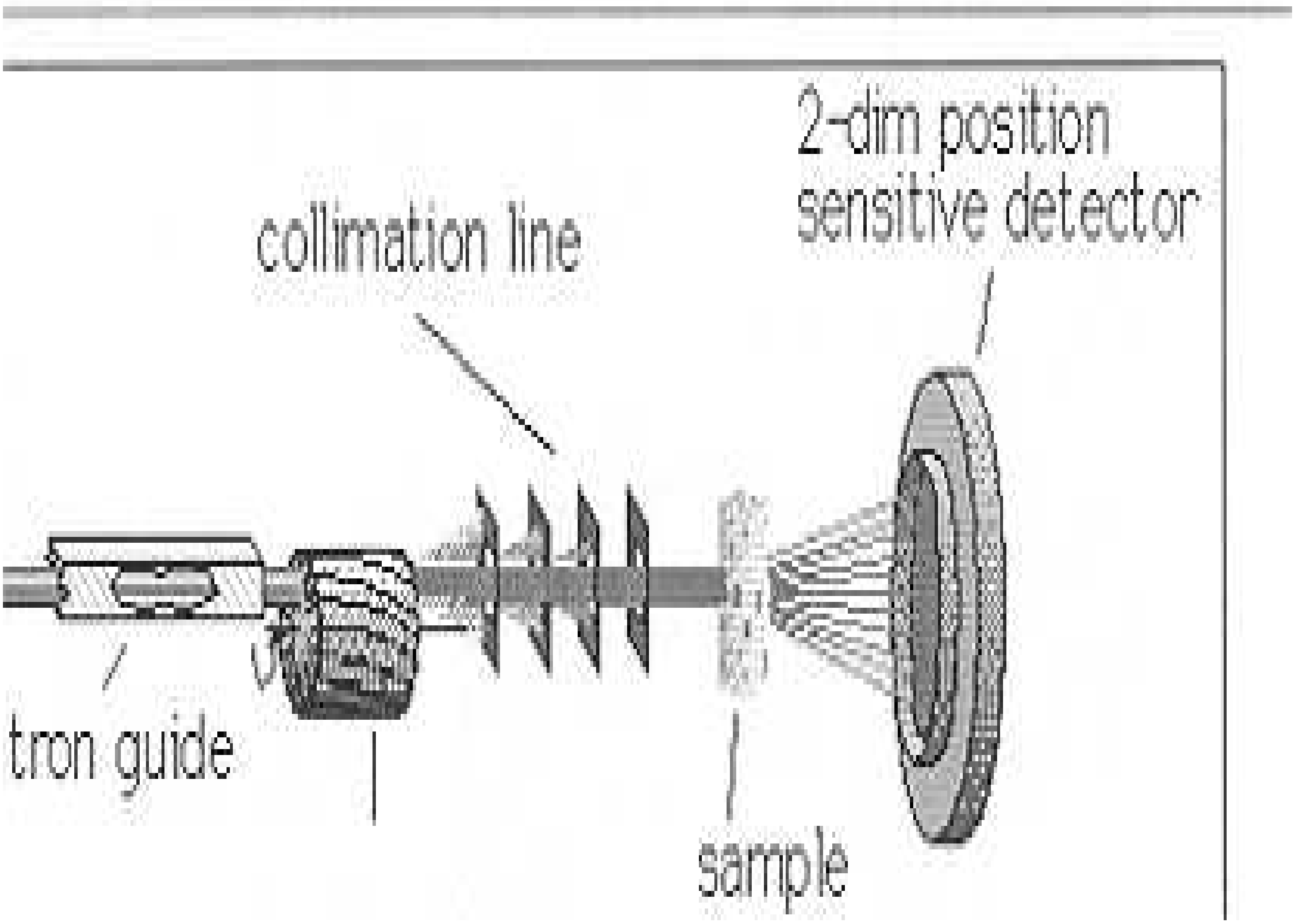

Figure 2: *Schematic view of a small angle scattering instrument [1].*

Small angle neutron scattering (SANS) is a low resolution technique applicable for studying the structure of solutions and non crystalline materials.With SANS one obtains informationon the shape, size and structure of materials in the mesoscopic size about 1- 400 nm. scattering occurs in a radically symmetric fashion and is measured on a 2D detector shown above.

In this method, a collimated incident beam, though not necessairly monochromatic, radiation is directed at a sample illuminating a small volume V. Some of the incident radiation is transmitted by the sample, some is absorbed, and rest part is scattered. A detector of dimension dx $\times$ dy positioned at some distance, L_{sd}(30 m) and scattering angle θ from the sample, then records the flux of radiation scattered into a solid angle element, $\Delta\Omega = \frac{dx \times dy}{L_{sd}^2}$.
This flux may be expressed in a general terms in the following way.
$I(\lambda, \theta) = I_0 \Delta\Omega \eta(\lambda) TV \frac{\partial\sigma}{\partial\omega}(Q)$
where , I_0 = Incident flux
η = detector efficiency
T = sample transmission, V = volume
$\frac{d\sigma}{d\omega}$ = differential cross-section
$\frac{\partial\sigma}{\partial\omega}(Q) = N_p V_P^2 \Delta(\delta)^2 P(Q) S(Q) + B_{inc}$
N_p= no fo concentration of scattering bodies, v_p= volume of one scattering body
$P(Q)$ = forrm factor , $S(Q)$ = structure factor
B_{inc} = the isotropic incoherent background signal
$(\Delta\delta)^2$ = square of the distance in neutron scattering length density
If the detector measures also the energy of the scattered particles then $\frac{d^2\sigma}{d\Omega dE_f}$is measured. It provides the no. of particles that are scattered into $d\Omega$ having an energy between $E_f$and E_f+dE$_f$, the total cross-section is,
$\sigma = \int \frac{d\sigma}{d\Omega} \times d\Omega$

Application of Neutron scattering in Bio-Physics

Molecular biology describes living organism interms of physical and chemical laws. Understanding the function of bio- molecule is very complex in its spatial organization. Biomolecules such as cellulose and starch are polymers of glucose. The most important classes of biomolecules are (1). Proteins and (2). Nucleic acids

Proteins

Understanding how proteins work is a key to unlocking the secrets of life. Proteins are made up of string of amino acids. Proteins, among their many functions are (1). bio-chemical catalysis (as enzymes) (2). structural (the main components of connective tissue and muscle) and (3). direct the activities of its organ(hemoglobin which carries oxygen i.e. the electron carriers in the energy conversions reactions)

Nucleic Acids

Nucleic Acid converse the genetic message and play essential roles in its replication and translation.Thus the life of a cell is regulated by proteins which it synthesizes. These are, in turn determined by the genetic information contained in the DNA molecules.The molecular mechanism by which the proteins and nucleic acids involved in DNA replication, transcription, translation and genetic recombination achieve their biological function.
DNA is the basic hereditary material in a cells and contains all the information necessary to make proteins. It is a linear polymer that is made of necletide unit (deoxyribose, sugar and a phosphate). RNA is a polymer that contains ribose rather than deoxyribose sugar.

The ability of neutron scattering technique to distinguish (1). (H_2) and deuterim (D_2) because a protein has active structure only in an aqueous medium and a few water molecules

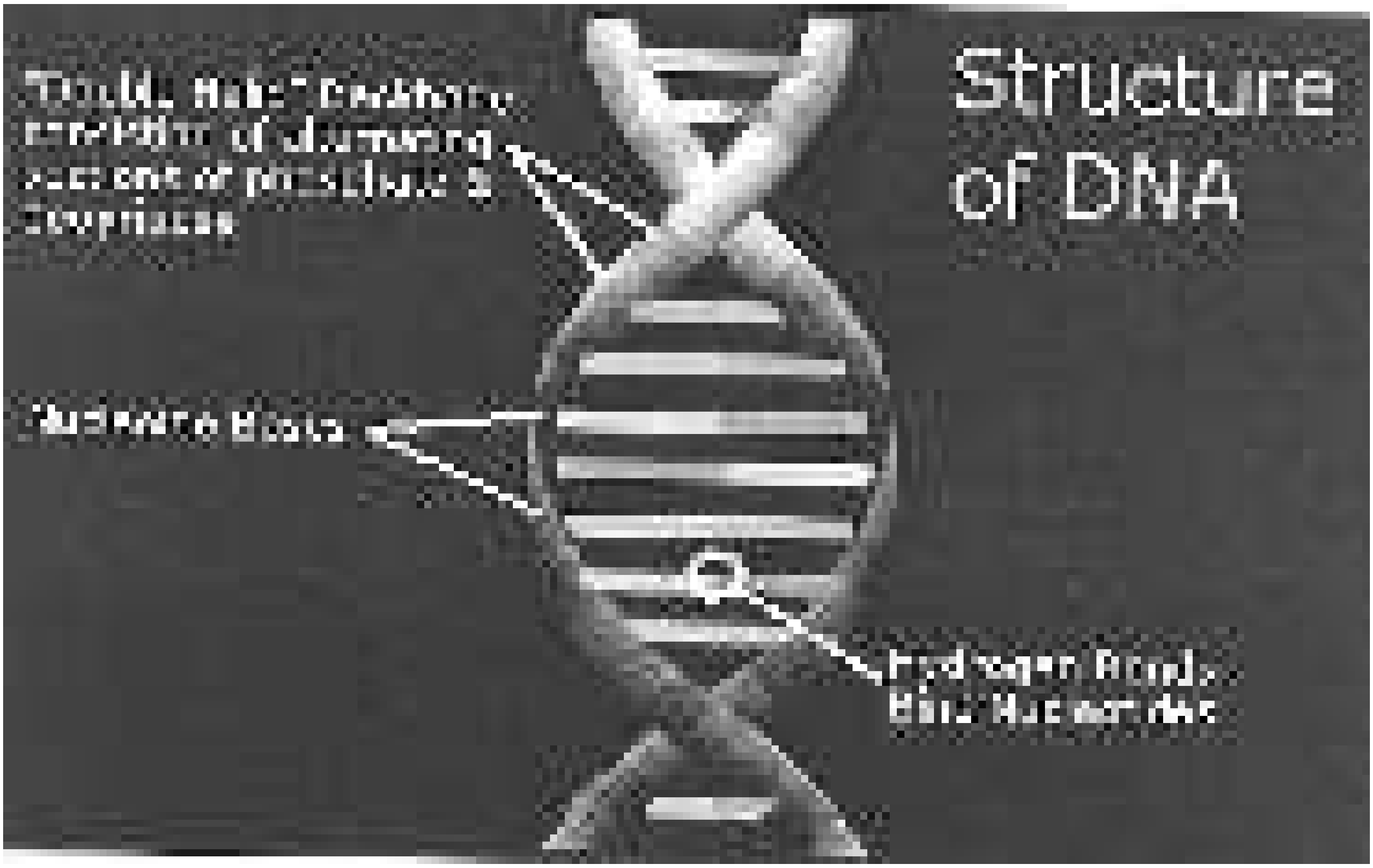

Figure 3: *structure of DNA [2].*

are inherent in its structure (2). cross section are same for all nuclei so that heavier elements donot dominate their scattering. (3). The radiation is nondestructive to the cells.

As we know , proteins defend against infection but in their mutant from they contribute to the development of disease scuch as Cancer and AIDS. Thus it is essential to know the real strucutre of protein and DNA. Aging and Cancer are caused partially by the abnormal functioning of DNA and protein. Knowing the individual structures of these macro-molecules will aid understanding of the chemical nature of disease at the atomic level.

References

[1] Stephen M. King, *Small Angle Neutron scattering* , www.isis.rl.ac.uk, 2000.

[2] G. Zaccai, *Neutron Scattering IN Biology in 1998 and beyond* , Journal of Physics and Chemistry of Solids, 1999