

**Indian Institute of Technology
Kanpur**

**NP-TEL
National Programme
on
Technology Enhance Learning**

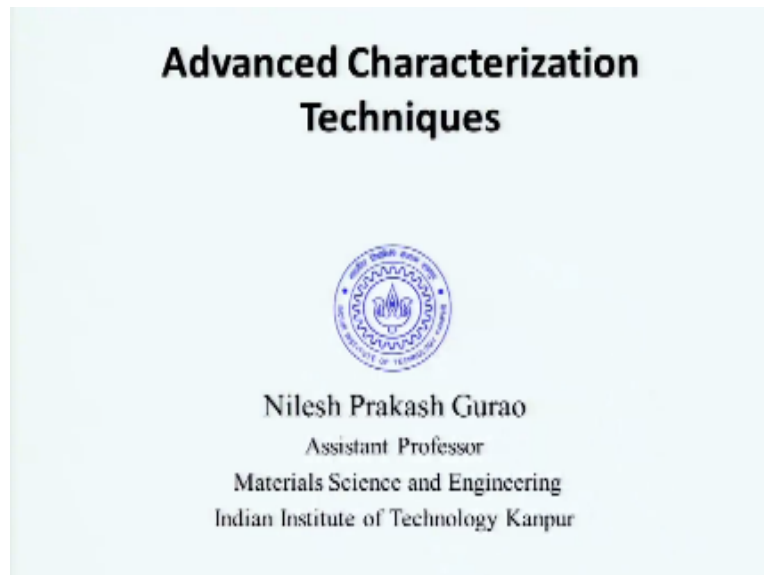
**Course Title
Advanced Characterization Techniques**

Lecture-32

**by...
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Hello everyone in today's class on advanced characterization techniques.

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We are going to be study of few things about.

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Module content

- a. Introduction to X-Rays and Review of basic diffraction theory
- b. Small Angle X-ray Scattering (**SAXS**)
- c. Grazing Incidence Small Angle X-ray Scattering (**GISAXS**)
- d. Low Energy Electron Diffraction (**LEED**)
- e. Reflection High Energy Electron Diffraction (**RHEED**)
- f. Extended X-ray Absorption Fine Structure (**EXAFS**)
- g. Surface Extended/Near Edge X-Ray Absorption Fine Structure (**SEXAFS/NEXAFS**)
- h. **Properties of neutron radiation and neutron sources**
- i. Small Angle Neutron Scattering (**SANS**)

Properties of neutron radiation and neutron sources. Up till now in this course or rather this module of the course dealing with x-ray diffraction and electron diffraction. But now we are going to look at a different class of radiation that is neutron diffraction.

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Introduction

- Neutrons are subatomic particles with no charge and mass of 1.675×10^{-27} kg
- Spin = $\frac{1}{2}$ and $\mu_n = 1.913 \mu_N$ (nuclear magneton $\sim 5.05 \times 10^{-27}$ J/T)
- With the exception of hydrogen-1, all atoms consist of neutrons and protons
- Neutrons bind the protons together in the nucleus
- Different number of neutrons \longrightarrow Isotopes
- Carbon-12 and Carbon-14

So all of us are aware what exactly neutrons are. So we know that neutron is essentially some subatomic particles which are there. So all of us are aware what exactly is neutron. So we know that neutrons are essentially subatomic particles which are there sitting in the nucleus along with the protons. These particles are characterized with no charge and have mass which is $= 1.675$ into 10^{-27} kg, we are also aware that this mass of neutron is slightly higher than that of protons.

Now in addition to the mass neutrons are also characterized with a spin of half and nuclear magnetic dipole moment of 1.93 times that of a nuclear magnet which is approximately equal to about 5.05×10^{-27} Joule/tesla. So having said that we know that neutron as such is a very different subatomic particles when compare to proton and an electron. Now with the exception of hydrogen one all atoms consist of neutrons and protons.

In fact the neutrons bind the protons together in the nucleus because the protons with all the positive charges have a tendency of repelling each other. The neutrons actually act as glue that holds all the protons together in the nucleus. Having said that we also aware that for the same atom we can have a situation where in the number of neutrons are different in the nucleus.

And such kind of atoms are actually know as isotopes, one of the classical example of an isotope is the carbon 12, and carbon 14 isotope, where in we know that the carbon 12 isotopes is actually characterized by 6 protons and 6 neutrons. While the carbon 14 isotopes that we are having has 6 protons, but in this case we will have 8 neutrons okay.

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- Bound neutrons in nucleus → Stable
- Unbound neutrons → Unstable
- Beta decay $n \rightarrow p + e^- + \bar{\nu}_e$
- β^- decay, where n is neutron, p is proton, e is electron and $\bar{\nu}_e$ is electron anti-neutrino
- Life time of 15 min
- Produced during nuclear fission and fusion

So moving ahead we also know that the bound neutrons in the nucleus are absolutely stable. However, the unbound neutrons which are just not associated with the nucleus are highly unstable. Well what exactly I mean when I say that they are unstable well. The neutrons center goes what is known as β decay. What happens in a β decay is that a neutron gets transformed into a proton, and a electron anti-neutrino.

Let us now getting to nuclear physics, but for the time being and assume and rather understand that it is not possible to have unbound neutrons as a source for carrying out neutron diffraction and neutron scattering experiments. Therefore, another important point that needs to be noted that all this association or decay mechanism that are told ensures that the life time of the neutrons is only about 15 minute.

And therefore, it is necessary to produce neutrons as and vend rick fire. Coming back how to produce neutrons well we can always produce them using nuclear fission as well as nuclear fusion, I am not going to talk much about fission and fusion.

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- Wave-particle duality
- de Broglie wavelength $\lambda = \frac{h}{mv}$
- Neutrons have wavelength of the order of X-rays (few Angstrom)
- Better penetration depth compared to X-rays
- Can be as high as few mm
- Neutrons see only the nucleus and not the electron cloud
- So they travel through a very open structure compared to X-rays or electron that see (interact) the electron cloud

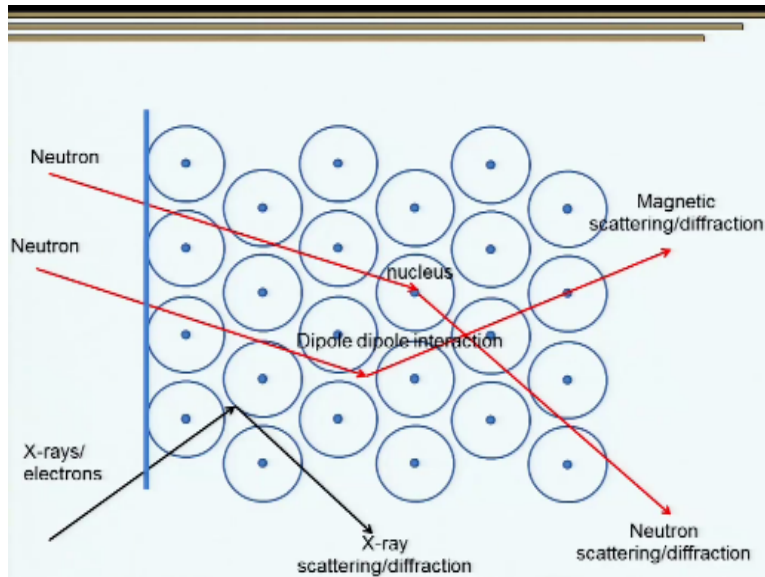
But let us talk about neutrons as a particle. We know that neutrons are subatomic particles and quantum mechanically they showed wave particle behavior. So for a neutron travelling at the particular velocity, we can always assign a particular wave length and treated as a wave with that particular wave length according to the wave length criteria.

Now the beauty about neutrons as a source for carrying out diffraction or scattering is essentially that the velocity at the which the neutrons travel when combine with their mass essentially ensures that the kind of wave length that we are going to get this order of angstrom which falls in the range of that of x-rays. And this is what ensures that we can use neutrons for carrying out diffraction experiments whereas the inter atomic another inter planner distances or of the order of few Angstrom.

But when compare to x-rays neutrons offer much better penetration depth and that is essentially because neutrons essentially interact with the nucleus of the atom. Now if we look at consider atom the nucleus occupies on much smaller region compare to the entire size of the atom, most of the region is occupied by the electronic cloud, having said that this ensures that the neutrons have a much better penetration depth compare to x-rays it can be as high as of few millimeter in materials with high density.

As I had already mentioned of this is essentially due to the fact that neutrons C or other field only the nucleus and not the electron cloud. So the travel essentially to a very open structure compare to x-rays or electron that see or interact with the electron cloud.

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The same philosophy or the same concept is shown over here in this figure. So if you look at of free surface over here and consider it comprises of all these atoms with the dark spot at the center being in the nucleus and the electron clouds surrounding it. You see that the neutrons actually interact with the nucleus. It can under go diffraction or scattering. While the x-rays interact with the outer electrons and it undergoes x-ray scattering or diffraction.

Therefore, we can assume that the probability of x-ray interacting with atom is much higher than that of a neutron, and therefore, the penetration depth of neutrons is much higher than that of x-rays. Having said that neutrons also have a tendency to interact with the dipole mind you, we can talk that neutrons have particular strength and a magnetic dipole moment associated with it. And therefore, the neutrons can interact with free electrons that also have a dipole moment.

And this dipole-dipole interaction can give us information about magnetic scattering or diffraction. I would like to bring to your notice that neutron diffraction is probably one of the most sophisticated techniques that can give us some information about the magnetic structure of the material.

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- Interference pattern similar to that of electrons is generated
- Diffraction theory for X-rays and electrons can be extended to neutrons
- Scattering and diffraction similar to X-rays
- Braggs law is valid
- Entire X-ray techniques can be performed with neutrons
- Magnetic information as neutrons have spin

Having said that let us try to understand how exactly diffraction takes place when neutrons are used as a source. Well the concept is exactly similar to that of x-rays. Only thing is instead of x-rays getting bounced off from the outer part of the atom we have neutrons which get bounced off or rather reflected from the nucleus of the atom. Therefore, we get a interference pattern very similar to that of x-rays or electrons.

The diffraction theory for x-rays and electrons can be easily extended to that of neutrons. And therefore the scattering and diffraction principles that will employ for x-rays and electrons can be borrowed one to one wave for neutrons also. This shows that Bragg's law is valid for neutron diffraction and that we can carry out all the x-ray diffraction and scattering techniques that we talk about using neutrons.

However, as I had already mentioned one of the best part rather the best kind of property of neutrons that is on offer which is not there for electrons and x-rays is that we can use the information about the magnetic structure. Now this information is not given either by x-rays or electrons, but neutrons can offer us information regarding the magnetic structure of the material under consideration in addition to the crystal structure.

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Generation of neutrons

- Neutrons have to be freed from the nucleus
- Fission reactor
 - Neutron source like radioisotope californium-252
 - Bombard n on ^{235}U nuclei
$${}_0^1n + {}_{92}^{235}\text{U} \rightarrow {}_{56}^{141}\text{Ba} + {}_{36}^{92}\text{Kr} + 3{}_0^1n$$
- Spallation source
 - use synchrotron to accelerate protons (GeV range)
 - focus the beam on depleted uranium target
 - neutrons produced by impact and hence spallation
 - Tantalum is most favoured target

So now when it comes to generation of neutron. So we had talked how we generate x-rays right in different ways of generating x-rays. Similarly, neutrons also can be generated in different ways. Essentially we have to draw off the neutrons from the nucleus of the atom. And this can be done using a fission reactor. In a fission reactor we use a neutron source like radio isotope californium 252.

Now this releases neutrons which are bombarded on a $\text{U}235$ nuclei, this leads to fission of the uranium nuclei and release of neutrons. Now with the use proper moderator we can control the number of neutrons that are released and this can act as a continuous source of neutrons right. Another important way of reducing neutrons is using what is known as a spallation source in which case we use synchrotron to accelerate protons to very high energy of the order of giga electron volt range.

And focus this beam on depleted uranium target or these face the most favored target is tantalum which ensures that neutrons actually fall off or rather spall off from this material that is from uranium target or tantalum target giving a pulsed source of neutrons. I would like to mention that a fission reactor can be used for producing nuclear fuel. And therefore, in most countries it is generally not used for atomic activities.

However, spallation source is more appropriate and is and most of the time is used tabular. However, one of the biggest problem is spallation source is that it produces a lot of radioactive waste, that comes from the target material. So once the accelerated photons hit the uranium and

tantalum target and use out neutrons the left over material is highly radioactive. This is one of the drawbacks of the spallation source.

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Type of neutrons	
➤ Neutrons produced in fission are at 1MeV	
➤ Slowed down by heavy water or carbon (moderator)	
➤ Hot neutrons	
▪ moderated at 2000° C	
▪ 0.1-0.5 eV, 0.3-1 Å, 10,000 m/s	
➤ Thermal neutrons	
▪ moderated at 40° C	
▪ 0.01-0.1 eV, 1-4 Å, 2000 m/s	
➤ Cold neutrons	
▪ moderated at 2000° C	
▪ < 0.01 eV, 0-40 Å, 200 m/s	

But having said that depending on the kind of energy that we have neutrons in two different neutrons can be classified into different regimes. So if you look at how neutrons, hot neutrons are moderated at 2000 degree centigrade of about 0.01 to 0.5 eV wavelength of about 0.3 to 1 angstrom and travel at the velocity of 1000m/sec. there are thermal neutrons which are moderated at about 40 degree centigrade, they have energy range of the order of 0.01 to 0.1 eV wavelength of the order of 1 to 4 angstrom and travel at a velocity of 2000m/sec.

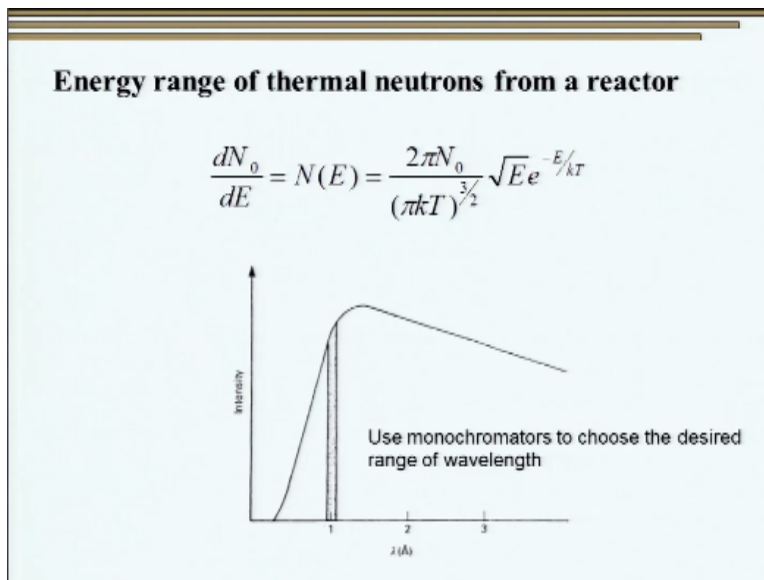
Mind you I hope you have noticed that the thermal neutrons probably are the most important neutrons because look at the wavelength, the wavelength is of the order of x-rays that we use in a

laboratory. Having said that, look at the energy level that we are having, the energy level is of the order of one 10^{th} to 1 100s of the electron volt that is in the range of a few linear electron volt.

In order to produce the same wavelength if you remember you are using voltage of the order of kilo electron volt when it came to x-rays. So I hope this point it very well taken that we can get the same wave length of neutrons atom much lower energy level. Now there are what are known as cold neutrons. So this cold neutrons are actually moderated at 2000 degree centigrade and they have energy which is lower than 0.01 electron volt, and of wave length of the order of 0 to 40 and travel at speed 200 meter per second.

So most of the cases that we will talk mostly we will focus since we are keeping x-rays and electrons as our focus, I will talk mostly about thermal neutrons which form in the same range as that of our x-rays.

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So from all the sources what is the kind of spectrum like what is the kind of neutron that we did? Do we get neutrons of same frequency and energy or different energy? Well like x-rays also. We have continue spectrum and we have a characteristic it not here for neutron. In case of neutrons if you look at the intensity versus wave length. We see that the neutrons follow Maxwell distribution which is being effected over here.

Most of the time we do not need a wide range of energy distribution, and therefore, we use mono-chromaters to choose only a wavelength of our interest and use it for further use.

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Scattering Cross section

- Probability of a scattering event between neutron and nucleus
- For a plane wave e^{ikz} , scattered wave $f(\theta, \phi) (e^{ikr}/r)$
- Differential cross section $\frac{d\sigma}{d\Omega} = |f|^2$
- Integral cross section $\sigma = \int \frac{d\sigma}{d\Omega} d\Omega$
- A measure of effective surface area seen by impinging particles

Now what are the most important part like which we had talked about doing x-ray as well as electron diffraction is actually the scattering cross section. The scattering cross section essentially defines the probability of scattering event between neutrons and nucleus for a plane wave I, k, z are scattered wave which is $f(\theta, \phi)$ and is multiplied with e^{ikr}/r , now this gives us the scattering probability right.

If you remember this is exactly similar to what we add for x-rays and this term $f(\theta, \phi)$ is nothing but equivalent to the structure factor that we had used in case of x-rays. So the differential cross section if we are about to calculate is $d\sigma/d\omega$ which is nothing but proportional to square of the structure factor. Now this is nothing but we know the intensity that we did, you remember in x-rays we are also talked is in just a change in terminology, but in case of x-rays we have this intensity proportional to the I^2 .

Now if we go for integral cross section which is nothing but you know you integrate this differential cross section, so which is $\sigma = \int d\sigma/d\omega d\omega$ this $d\omega$ is the solid angle we will talk about it in the later slide. But this essentially gives us a measure of effective surface area seen by in fringing particles.

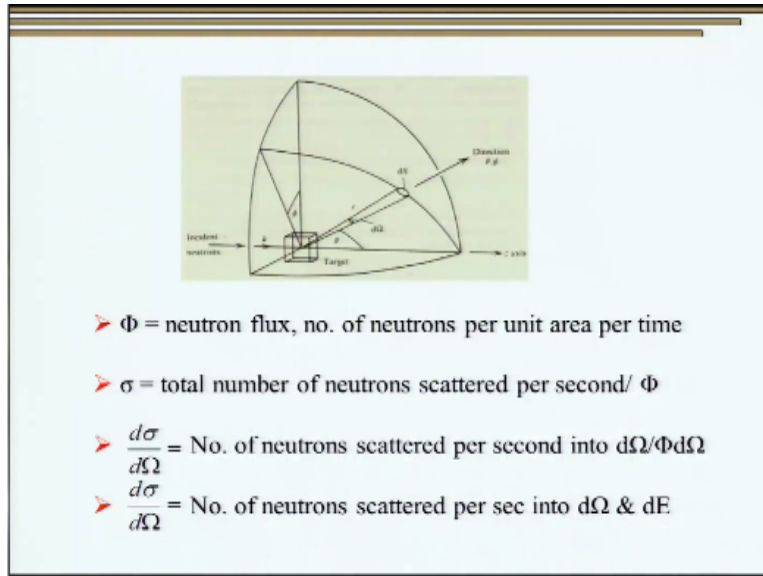
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- Effective area presented by a nucleus to an incident neutron
- Unit → Barn
- 1 Barn = 10^{-27} m^2
- Attenuation = $\exp(-N\sigma t)$ where N = no. of atoms per unit volume and t is thickness
- Cross section is proportional to square of structure factor
- Very important in determining the intensity of diffracted beams

So the effective area presented by nucleus to an incident neutron is actually represented in terms of a Barn which is nothing but a unit of area $1 \text{ barn} = 10^{-27} \text{ m}^2$. Having said that another important point that needs to be noted is that once the neutrons are travelling and the interactive matter they are going to get attenuated that means their velocity is going to change. And therefore, the attenuation is given as exponential – $N\sigma t$, where N is the number of atoms per unit volume and t is the thickness.

So the cross sectional is proportional to the square of structure factor. Now this is very important in determining the intensity of the diffracted beam. Coming back again the reason we are talking so much about neutron cross section is actually because of the wave nature and particle nature right. So here neutrons can also be considered as particle nature while in case of x-rays we just ensured that no intensity is proportional to the square of the structure factor.

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Having said that this will be more clear with this drawing over here wherein you see we have incident neutrons which are coming over here and this is the target. We see that how the neutrons get diffracted in a particular direction. So if at all we have a neutron flux or Φ which is nothing but the neutron, the number of neutron per unit area, per time and the σ is the total number of neutrons scattered per second for incident flux of Φ .

So our $d\sigma/d\omega$ where $d\omega$ is the solid angle that is covering is actually the number of neutrons scattered per second into $d\omega$ right. And this is for Φ $d\Phi$ is not it, and therefore, our $d\sigma/d\Phi$ is nothing but the number of neutrons scattered per second into $d\omega$ in a energy range of about dE right. So we see that we have incident and what is the probability of neutrons getting diffracted. So this is nothing but the fraction of neutrons that are getting diffracted in a particular direction ω .

So this is nothing but your neutron cross section, and this is absolutely proportional or rather directly proportional to the square of the structure factor.

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Scattering by single nucleus

- Range of nuclear force (R) is of the order of fm
- $\lambda_n \gg R$
- $E_n \ll E_N$ no energy transfer between neutron and nucleus
- Scattering is always elastic \longrightarrow no change in v_N
- Scattering is far from nuclear resonance
- Negligible neutron absorption

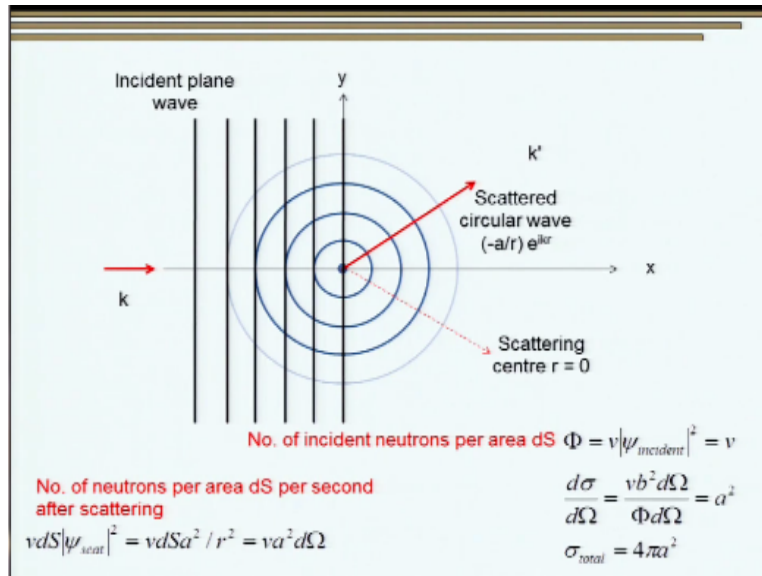
So let us talk as I have already mentioned that you know the neutrons actually interact with the nucleus of the atom and not with the electron cloud. So if you look at the nucleus you know, that there is a nuclear force associated with the nucleus. Now the range of the nuclear force is very small and of the order of few femtometers. We are also aware that the kind of wavelength that we are using for neutrons is of the order of few angstroms.

Therefore, we have a situation where the wavelength of the neutrons is much, much larger than the range of the nuclear force. Therefore, the energy of the neutron is much, much lower than the energy of the nucleus. And this ensures that there is no energy transfer between neutron and nucleus. This actually ensures that once you have a neutron interacting with a nucleus it does not lose its energy.

And therefore, all the scattering and the diffraction phenomena that are occurring are essentially elastic. The wavelength as I had already mentioned is actually decided by the velocity because $\lambda = h$ divided by the momentum term which is nothing but a V , so the velocity of the neutrons does not change. However, their angle the θ part right in the last slide we are talking about may change.

So the scattering is far from nuclear resonance and there is no absorption of neutrons during the interaction of a neutron with the nucleus of an atom.

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A semantic diagram of the same is shown over here, where we have this incident beam of the planar neutron beam right. And here we see that the number of neutron per area ds per second after scattering is $v ds$ 5 scattering square, this is again your wave equation which is square that gives the intensity ds is the area, and V is velocity. So at the end of the day we end up getting equal to $va^2 d\omega$ where $d\omega$ is the angle it is not been shown over but it is a solid angle right.

And you know that the scatter circular way as the equation of $-a/r e^{ikr}$ right. So now the number of incident neutrons per area ds which is your Φ is nothing but $v\Psi$ incident square which is nothing but equal to V . And the cross section $d\sigma/d\omega = d^2$ right. So depending on the scattered circular wave amplitude we are going to get the $d\sigma/d\omega$. And as you can see the total scattered neutron is nothing but in a solid angle right once you integrate you get $4\pi a^2$ right.

This is the where this term is very similar to that of the surface area of the sphere. So we are considering all spherical waves. So the point is, I would like to repeat again that the neutron cross section is actually proportional to the square of amplitude right, this is the what we got even for x-rays only things is we are trying to derive it in a slides different way, because here we are going instead of having of a way of approximation we are trying to explain the same thing using a particles of approximation.

Having said that at the end of the day we will end of getting the same solution. So x-rays or for that matter electrons right, like electrons we talked about coherence scattering and in coherence scattering.

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Coherent and Incoherent Scattering Cross section

- Scattering length $a_i = \langle a \rangle + \delta a_i$
- The random component of scattering vector contributes to incoherent scattering
- Information about collective motion and relative position of nuclei \longrightarrow Coherent Scattering
- Motion of individual nucleus \longrightarrow Incoherent Scattering
- H has low coherent scattering cross section than D while for incoherent scattering cross section the situation is reversed

So the actual scattering length for neutrons with the nuclear is actually given say a_i which is nothing but $a + \Delta a_i$. Now this Δa_i essentially indicates or random component, so the random component of scattering vector contributes to incoherent scattering. So the contribution of A this summation of a or other bracket of a actually corresponding to elastic while this Δa_i corresponds to inelastic scattering.

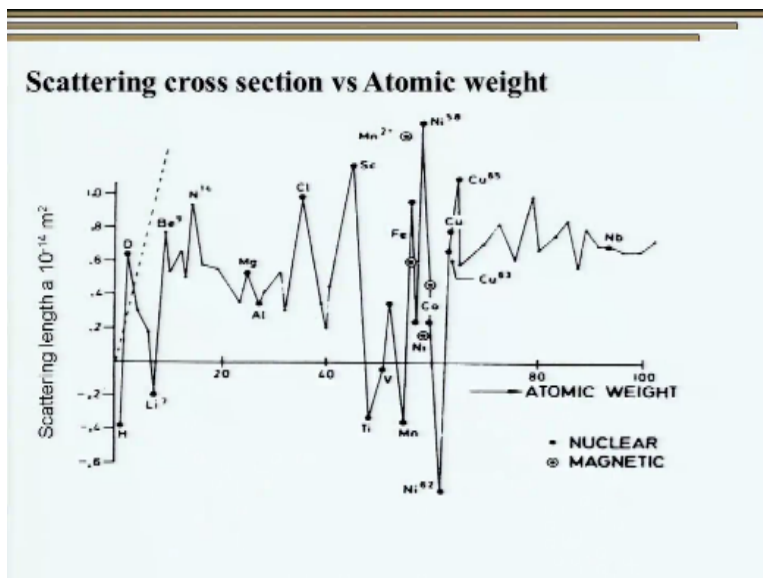
Now the information about collective motion and relative position of nuclei is given by coherent scattering. So this is very similar to what we are having right where you atoms are sitting that means where you nuclei are sitting. And where your neutrons are getting interacting with this with the nucleus and getting scattered, so this is because of coherent scattering. However, we also know we have seen this d/l like term that you know only at 0 Kelvin all the atoms are sitting at there are own places in the unit cell.

In fact at any temperature other than zero there actually vibrating right. So we actually get a motion of individual nucleus and that actually leads to incoherent scattering. Now this contributes actually to this Δa_i term. Now this term is slightly different then the D while term because that is taken care of. But any small perturbation in the nucleus actually captured using incoherent scattering.

To just give an example I will mention that you have cross sections associated with both coherent as well as incoherent scattering. Having said that a classical example is that of hydrogen which has a very low coherent scattering cross section, and therefore it cannot be detected using normal neutron, you know coherent scattering neutron experiments. However, it has a very nice or other very high incoherent scattering cross-section.

Therefore, if you want to study in fraction experiments mostly hydrogen is replaced with deuterium which has a very good either of very high elastic or other coherent scattering cross section but as very poor incoherent scattering cross-section. So this way you can see that we think use different kind of scattering events namely coherent and incoherent to detect the presence of a particular element or rather to be more precise a particular isotope in neutron scattering or diffraction.

Mind you if you want to study diffraction where we need to carry out which corresponds to coherence scattering, we have to use material or like we will get better signal for deuterium. Therefore, people who work on ice most all which is H₂O solid actually replaced hydrogen with deuterium to carry out neutron diffraction studies to determine the crystallographic texture, while if you are more interested in studying the spectroscopic aspect of it we can always use hydrogen. (Refer Slide Time: 26:11)



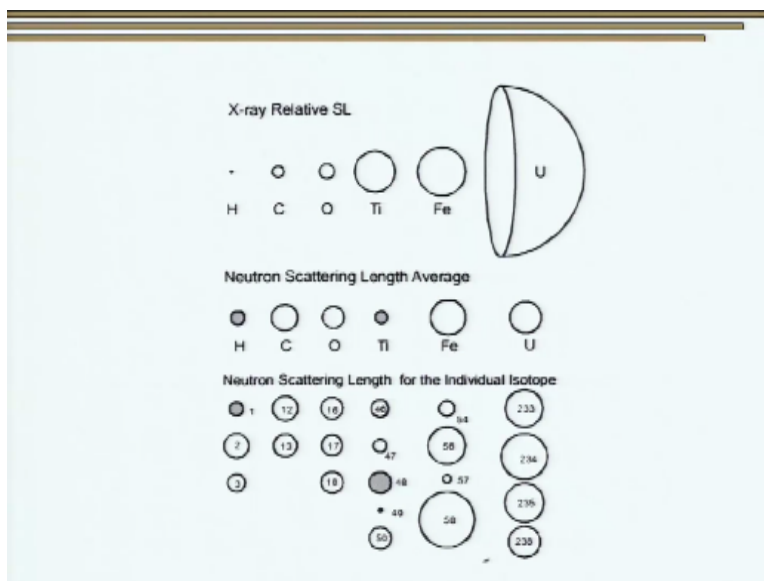
Having set that another important aspect with neutron diffraction if you remember for x-ray diffraction does not have to offer is the scattering cross section. So if you remember we had the

scattering cross-section or rather the intensity of proportional to f^2 in case x-rays, and f is nothing but it was a atomic number. So it was not possible to differentiate between two element which are very close to each other in the periodic table.

However, look what happens when you look at neutron cross- section which is given over here in terms of scattering length, we see that two atoms or like two elements which are very close to each other have very different right you see aluminum and caloric with they have quieted different scattering cross-section. This is essentially ensures that we can easily separate out these two elements which are very close in periodic table using neutron diffraction.

At the same time we will also see that we get information about the magnetic cross section also, see here we have nickel 62 here, and we have another nickel, so this scattering cross-section for nickel and the magnetic cross section, there are two different. So we can actually find out where our nickel atom is sitting, and where the magnetic moment sitting right lead to for cobalt. And you see here for different isotopes of nickel you see the huge amount of nickel in the scattering cross section. Now this information is offered only and only by neutron diffractions.

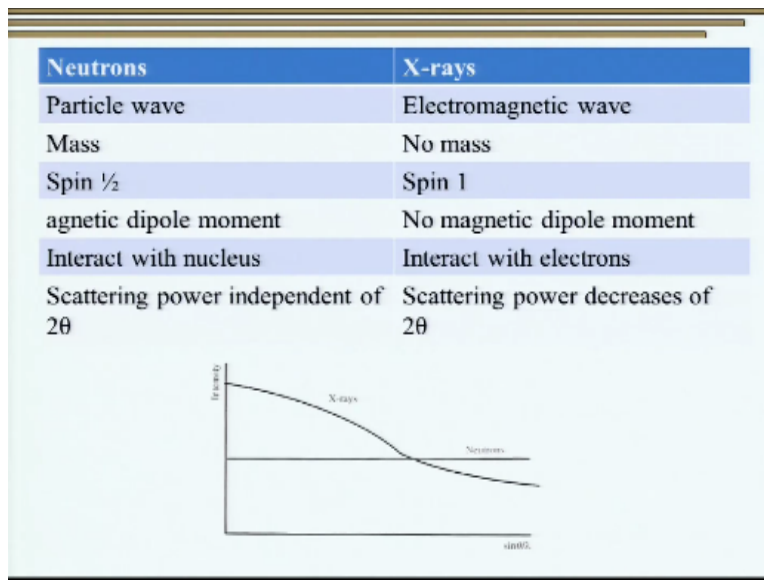
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The similar information is presented in a very nice work here, so you can see here the x-rays relative scattering length, we see hydrogen is small, carbon bigger as it most as function of g . However, when we look at neutron we see there is no one to one corresponds between side that is

atomic number and then the scattering length. And see we can easily separate out between at joining elements.

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Taking forward our comparison between neutrons and x-rays. We have seen that neutrons actually behave like particle and wave and x-rays are actually electromagnetic wave. Now neutrons have a mass associated with it, while x-rays have no mass associated with them. Neutrons have a spin of half while x-rays have spin of one or they have a magnetic dipole moment while x-rays have no magnetic dipole moment.

The neutron actually interacts with the nucleus while the x-rays interact with the electrons. Now the neutrons are scattering power independent of 2θ which as be shown over here so see what happens the intensity vs $\sin\theta$ well it is almost a straight line, it is always a straight line because as not dependent of the angle. While when we talk about x-rays we know that this value decreases.

Remember we had seen this f versus $\sin\theta$ value how it was decreasing which started from z , and it was to do things continuously as a function of θ not sure for neutrons.

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Neutrons	X-rays
Lower absorption	Higher absorption
Large amount of sample	Small amount of sample
Neighbours and isotopes can be discriminated	Neighbours and isotopes cannot be discriminated
Light element detection	Light elements not detected
Magnetic structure determination	No Magnetic structure determination
Weak	Intense (Lab source is 1000 times brighter than neutron source)
Low availability	Very high availability

Now neutrons with their kind of energy they have and since they interact only with the neutrons have very low absorption while x-rays absorb a lot. But there is a problem since neutron interaction is weak we need large amount of sample, while with the x-rays we can leave with the small amount of sample. Now neutrons the neighbors as well as isotopes can be easily discriminated, while for x-rays the neighbor isotopes there is no way we can isotopes neighbors discrimination is very, very difficult.

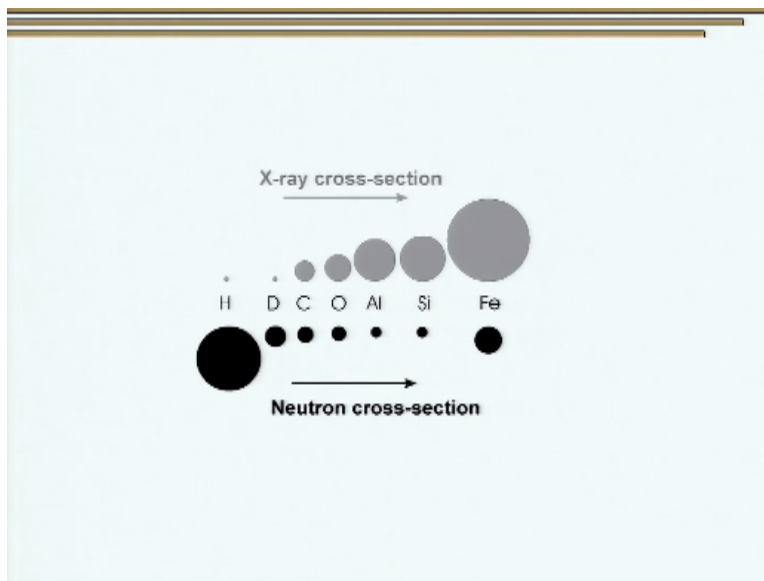
The detection of light element is very difficult in x-rays while it can be done on a routine basis in neutrons. One of the biggest USBs of neutrons is that it can be used to determine the magnetic structure, while no magnetic structure information is obtained from x-rays diffraction. As we had already seen that the neutron is very weak source or rather of very weak probe, but this is not a disadvantage.

Because a weaker probe ensures that the kind of interaction that we had seen is not because of an artifact or any change in the state of matter that we are studying. I would likely mention that the x-rays of the internal sources where as in terms I am not really talking about synchrotron. But even

on normal x-rays laboratory source is most 1000 times brighter than neutron source. Having said that we should always remember that neutron source or not available every at every place.

And in fact there are very they hardly of few places in the world while x-rays source the x-ray diffractometers are available at every university. And therefore, then we used on a day today basis.

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What having said that it is not like x-rays are gone then neutrons are back. In fact these two techniques are completely complement to each other, and this particular slide kind of encompasses the basic complimentary nature of both the techniques. So look at different elements we have shown different elements over here and see how with the neutron cross section, and the x-ray cross section various.

So you see that materials with high x-ray cross section have low neutron cross section. Therefore, you can see that if there is a situation where we have material with high x-ray cross section and high neutron cross section at the same time, we can always use x-ray and neutron diffraction or scattering technique to compliment and get complete information from the sample under investigation.

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Advantages of neutrons over X-rays

- Comparable wavelength to that of X-rays (in Angstrom) at lower energy
- For $\lambda \sim 1\text{\AA}$
 - neutrons have energy of tens of meV
 - X-rays have energy of tens of keV
- Ping-pong vs. Cannon ball
- ND can exactly predict where atoms (nuclei) are and what they do
- Atomic structure and dynamics can be estimated directly

Now just to compile what are the advantages of neutrons over x-rays. Well both of them have comparable wave length in the angstrom level. However, the energy of neutrons is much lower. The neutron lower energy as I had already mentioned ensures that there is no harm to the sample. There is no damage to the sample. The interaction of neutrons with the sample is more of that of a what happens pink pong ball right and will get trashed on one place to the other.

While in case of x-rays the x-ray photon is like a canon ball which is going through the structure. Neutron diffraction therefore can predict where atoms that is the nuclei and what they do, this is something that x-rays cannot tell, x-rays just tell us where the atoms are right, but they do not tell where the nuclei are. And therefore, atomic structure and dynamics can be estimated directly mind you only using neutrons.

The dynamics part come because neutron diffraction not only tells us where the atoms or rather the nuclear but also what they are doing. So this is one of the biggest advantage of neutron diffraction.

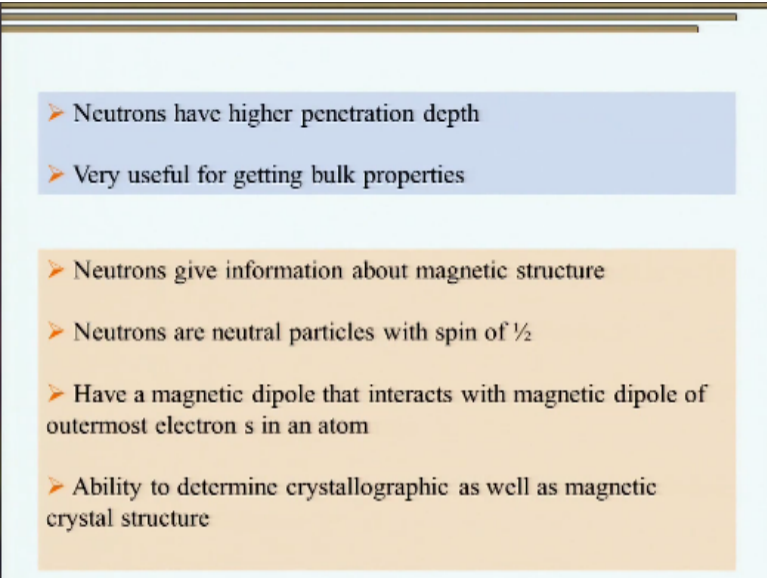
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- Neutron scattering cross section varies randomly unlike for X-rays
- Easy to differentiate close elements in periodic table
- Neutrons are sensitive to isotopes not X-rays
- Neutrons offer a weak probe
- Better signal
- However weaker signal

We know that neutron scattering cross section varies randomly right, we had seen those curve that you know it is not dependent on Z . Now this ensures that we can easily differentiate close elements in the periodic table. At the same we also have this ability to differentiate between isotopes different isotopes of the same element using neutrons. X-rays have no capability to differentiate between the isotopes.

As we had seen neutrons offer a very weak probe and therefore it gives us a very better signal. Though the signal is very weak and it takes some time to collect and amplify the signal the weak probe actually ensures that no damage is caused to the material under investigation. More importantly no damage is caused to this structure of the material under consideration.

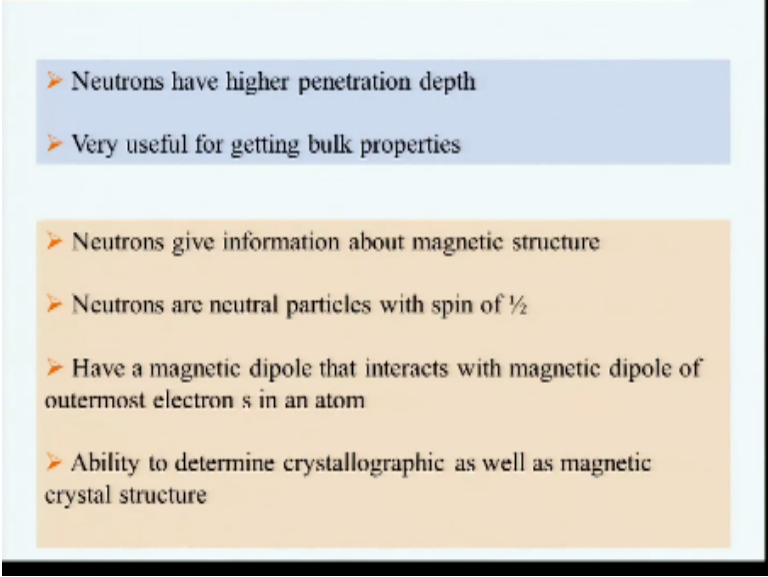
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- 
- Neutrons have higher penetration depth
 - Very useful for getting bulk properties
-
- Neutrons give information about magnetic structure
 - Neutrons are neutral particles with spin of $\frac{1}{2}$
 - Have a magnetic dipole that interacts with magnetic dipole of outermost electrons in an atom
 - Ability to determine crystallographic as well as magnetic crystal structure

We have seen that neutrons have higher penetration depth. And they're very, very useful for getting bulk properties. Many of times, the size is very large, if the grain size is very large x-rays cannot penetrate and they cannot give us complete information about the kind of pieces and say for that matter preferred orientation that is present in a material. This is where neutron diffraction becomes very, very important.

And this is something that can be done only with neutron diffraction. So whenever it comes to getting statistically relevant data for a normal diffraction data, we can always use neutron diffraction. The biggest advantage and which I am reiterating again and again for neutrons.

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- 
- Neutrons have higher penetration depth
 - Very useful for getting bulk properties
-
- Neutrons give information about magnetic structure
 - Neutrons are neutral particles with spin of $\frac{1}{2}$
 - Have a magnetic dipole that interacts with magnetic dipole of outermost electrons in an atom
 - Ability to determine crystallographic as well as magnetic crystal structure

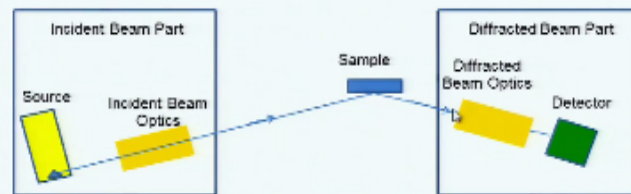
Is that they give information about the magnetic structure. Neutrons are essentially neutral particles which spin of half and have a magnetic dipole that interacts with the magnetic dipole of outermost electrons in an atom. This ensures that we can determine not only the crystallographic as well as but also the magnetic crystal structure of the material under investigation. Now this is one of the best advantages of neutron compared to that of X-rays.

Now talking about instrumentation, now this is some slide that we had already seen. We saw that this was for X-rays. So we had a source or incident beam optics or sample or diffracted beam optics and a detector.

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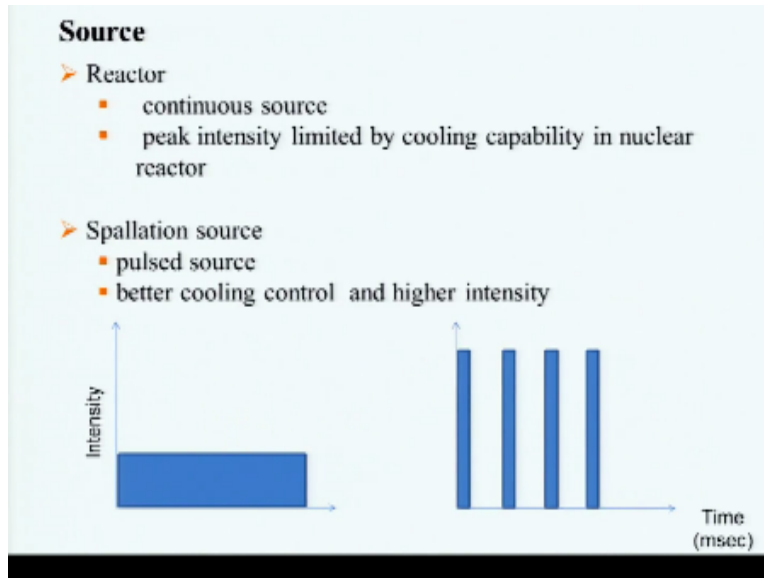
Instrumentation

- Source
- Optics
- Detector



We have something similar, not exactly the same but something very similar for neutrons. We will try to see how actually we have instruments for carrying out neutron diffraction. So let us start with the source.

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So as we had seen earlier like we have a reactor as a source for neutron diffraction, for producing neutrons. The reactor is a continuous source and which is shown over here. So we intensity, there is a constant intensity. Peak intensity is limited by cooling capability in nuclear reactors. Usually intensity is quite low.

However if we have a splicing source which we had talked about earlier, it is a pulse source. We see here instead of having a continuous energy level, we do get pulses. This is as a function of time and here the intensity of the pulses is much higher because of vector cooling control. But having said that we know that we do not get a continuous spectrum.

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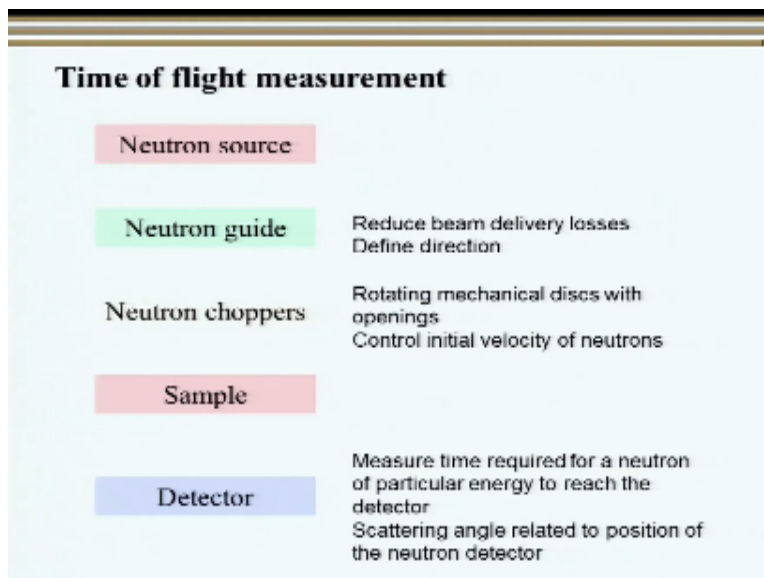
- Diffractometer for continuous source for normal I-2 θ scan
- Time of flight (TOF) measurement for spallation source for complete I-2 θ scan
- TOF is fast and gives high neutron flux
- Diffractometer data acquisition and analysis is simple and is good for magnetic studies
- Better resolution at low angles for diffractometer

But the intensity is nevertheless higher. Now for the continuous spectrum this is very similar to what we have for X-rays and once you put a mono-chromator you can use a normal diffractometer for continuous source and do the same kind of study that we did for X-ray diffraction. However if you are using a pulse source, mind you, you have to use a time of flight measurement wherein we measure the time taken by the neutrons to travel the same distance. Mind you, once the neutrons get scattered at different angles after interacting with the material they are going to take different time.

To reach the detector and this can be used to measure the scattering angle and intensity using time of flight measurement. In time of flight we know that the velocity or rather the mass of the neutrons is the same. Their velocity is also the same but depending on the angle of scattering there we are going to take different times to reach the detector. So this technique is actually known as time of flight technique.

This technique is very fast and however we need very high flux for it. Now this diffracted data acquisition and analysis is very simple and very well suited for magnetic studies and gives us a very good resolution at low angles. However at high angles we don't have any other choice but to go for time of flight measurements.

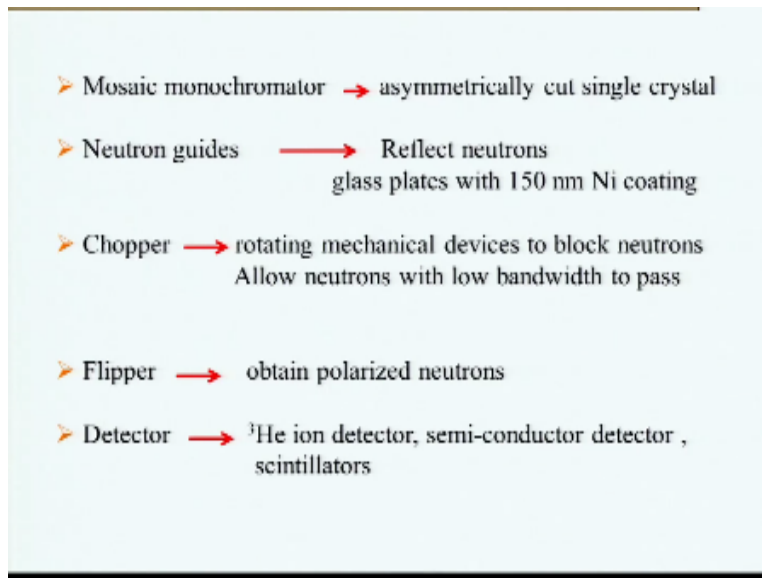
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So just to talk about, we talked about the optics. So let us talk about the optics, we have seen the source. Now we have what are known as neutron guides. Now what the neutron guides do? Essentially they deduce the beam delivery losses and ensure that the neutrons are travelling in a particular direction. Then we also have what are known as neutron choppers. Now these neutron choppers actually are rotating mechanical discs with openings that actually control the initial velocity of the neutrons.

Remember that we have to this initial velocity of the neutrons when, I say actually ensures that you are getting neutrons in a particular energy range, that is what we are aiming at. So this is what we want. Then all this neutrons that is incident that interacts with the sample and then we have a detector which requires the time required for a neutron of a particular energy to reach the detector. The scattering angle is related to position of the neutron detector.

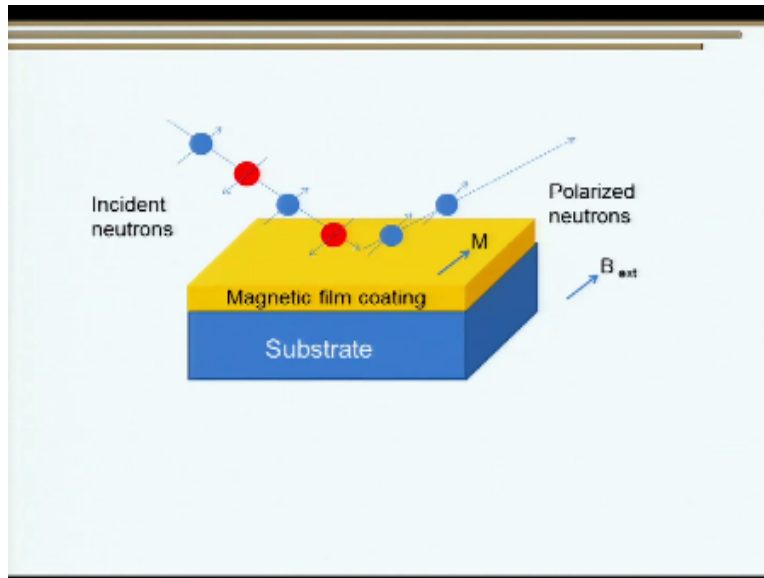
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Now talking in details we know that in X-ray optics also to get a radiation of a particular wavelength we use what are known as mono-chromators. For neutrons also we use mosaic mono-chromators which are nothing but asymmetrically cut single crystals. These ensure that neutrons with only a particular wavelength are able to pass through. Similarly the neutron guides actually reflect the neutrons and thereby kind of reduces the path that is available for the neutrons to travel.

These comprises of the last plates with about 150 nanometer of Nickel coating. So the neutrons which are incident get reflected and are guided to a particular region. The chopper as I had mentioned comprises of rotating mechanical devices that block neutrons of various energy and allow only neutrons with very low bandwidth to pass. So we had seen that there is a Maxwell distribution. Maxwell distribution will allow only a small part to pass using chopper. There are certain investigations wherein we need polarize neutrons for doing magnetic study. So in that case we use a flipper. Now how does a flipper work? I will show you in the next slide but keep in mind which is shown over here.

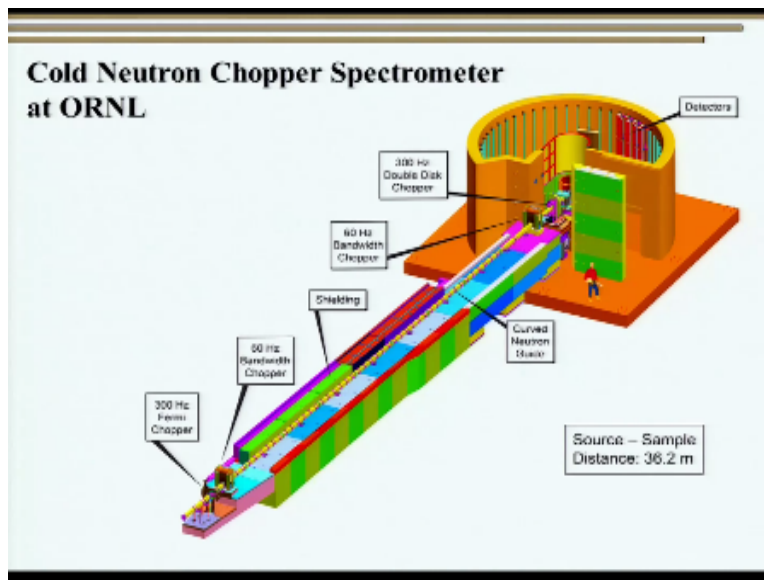
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So you see here we have neutrons which are having both kinds of spin, $+1/2$ and $-1/2$. Now we have a substrate which is essentially silicon and a magnetic film coating on it. So you can have Iron or Niobium and we see that all the neutrons which are incident on it get polarized so only one direction. So you will have neutrons coming in two opposite directions, all of them going in one particular direction. Now this single layer can be replaced with multi layer, and we can get multi layer mirrors or super mirrors to get highly polarized neutron source.

These are actually very important for carrying out magnetic structure determination. Having said that another most important part of neutron diffraction is actually the detector. Most often the most common detector is the Helium-Iron detector which comprises of a gas filled detector. We also use semi conductor detectors as well as centiliter detectors for analyzing neutrons.

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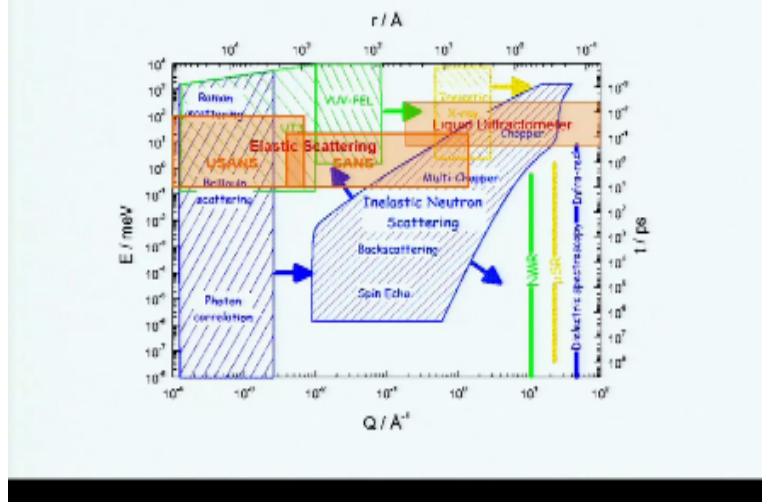


I have shown a few schematic of the gold neutron chopper spectrometer at Oakridge National Laboratory, we just give you a feel for things and here you can see that we have a Fermi chopper. Let us not talk about it but it is like more of a chopper that controls the kind of wavelengths which is going in. We have a bandwidth offer, then we have shielding, this is your nuclear guide and here you see, here is where our sample is and these are all your detectors. So these are pretty big and you see this entire source to sample.

If this your source over here to sample, this distance is used so write 36.2 m and everything, all of this is shielded and all this you can see that why very high angles we can get information using the spoliation source.

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Why Neutrons?



I did not talk so much about neutrons. Let us now sum up with why at all neutrons are important and for this you have to go to the energy momentum space diagram and here you see that this is our energy and momentum diagram or reciprocal space and angular velocity diagram and here we see that for different amount of Q and our energy, this is I mean you can also plot it as your R versus T . R is spatial distance and T is the time we see that neutron scattering.

We see there are various other techniques, we see Raman scattering over here. It is giving us some information about the time related stuff and the distance related stuff about what is happening at an atomic level. So you see Raman scattering gives us very small information which is even better than what we are getting using an MR or certain other techniques like dielectric spectroscopy or infrared spectroscopy that is shown over here.

But look at neutrons. You see neutrons gives us a lot of information see in inelastic neutron scattering because of back scattering gives us a lot of information. Similarly here we have small angle neutron scattering and ultra small angle neutron scattering. So we see when we compare at the Q vs E plot for structure of different materials we see that neutrons offer the ability to probe and cover the maximum region in the Q vs E space and therefore neutrons are very important source for carrying out material characterization. I hope you appreciate the importance of neutrons in materials characterization. In the next class which is also the last class of this module, we will talk about small angle neutron scattering and wind it up. Thank you.

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