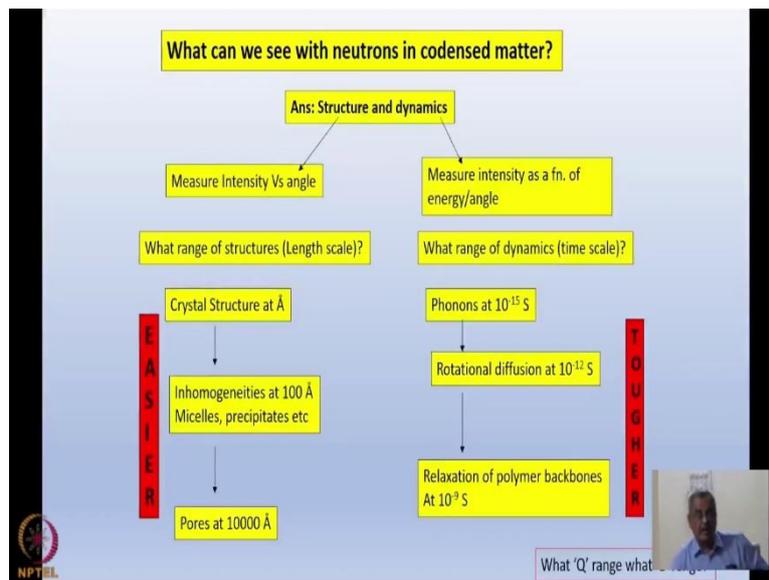


Neutron Scattering for Condensed Matter Studies
Professor Saibal Basu
Indian Institute of Technology Bombay
Week 3
Lecture 6B

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$$\int I(Q) e^{-iQ \cdot r} d^3q = g(r)$$

Structure at various length
 scales depending on Q'

$S(Q, \omega)$ 



Now we come to the fact that what can we see with neutrons in condensed matter, that is the question. Structure and dynamics are the broad answers. If we talk about X rays, you cannot see dynamics you can of course see structures. When I say structure that means measurements are intensity versus angle, we do not care about the outgoing energy, we just impinge neutrons on the system and we measure the intensity of the scattered neutrons as a function of angle and that gives me the Q vector and I get $I(Q)$. Fourier transform of $I(Q)$ over Q is related to $g(r)$. In

general diffraction is structure at various length scales depending on Q wave vector transfer because wave vector transfer and space are the Fourier transform of each other. This is the most general definition of diffraction, like in case of optical diffraction we know if you have rulings on a board then from the diffraction pattern, we can find out the spacing between lines. But this is a much larger length scale, maybe at micron level, because optical rays have wavelength in the range of 4000 to 7000 Å.

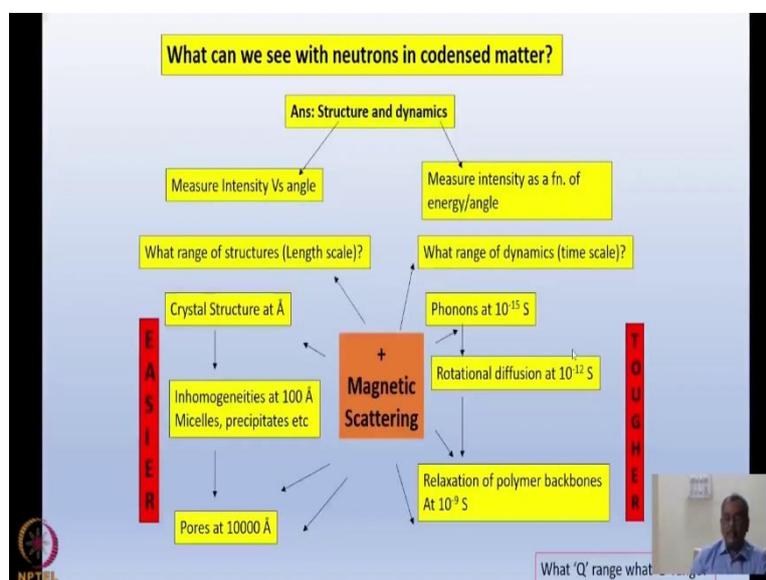
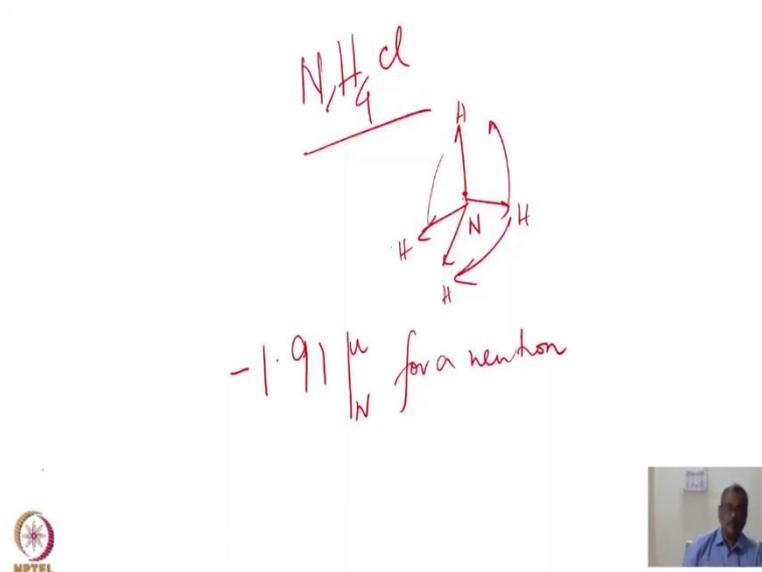
Basically, diffraction gives me structure at various length scales, and that is the purpose of our doing neutron diffraction. As I said, when I say measure intensity versus angle, what ranges of structures can we see? We can see crystal structure that is Å. We can see inhomogeneities at typically 100 Å means we can see things like Micelles, precipitates. Sometimes when you were mixing two materials depending on the miscibility one might start precipitating in the other, metallurgists often face this problem. There is something called a surfactant and surfactant has a head group, which might like or repel water and a tail group that is just the opposite. If I have a hydrophobic tail and the hydrophilic head, then the surfactants form conglomerations in a solution known as Micelles, and you can study them using neutron diffraction. If I go to very small Q values or smaller momentum transfers, we can see pores at 10,000 Å at micron size. Rocks are often made of pores and you can find out such pore distribution with diffraction.

This whole lot of experiments on the left of this slide tells me about diffraction experiments at various length scales. Diffraction experiments are easier because we are not measuring energy.

For dynamics, I need to measure intensity of neutrons as a function of energy and angle. When you measure energy difference then of course, we are trying to probe dynamics in the systems and depending on how much energy transfer we have seen in an experiment. It will sort of look at one specific kind of dynamics in the system and at various Q values. In a dynamics experiment what I actually get is $S(Q,\omega)$ from where we try to get the dynamics at various time ranges.

I have just listed a few such experiments. We can measure phonons with the timescales of typically 10^{-15} seconds or we can study rotational diffusion with the timescales of typically 10^{-12} seconds. Let me give you an example of rotational diffusion.

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Suppose, I have got an NH_4Cl crystal. This crystal lattice has got this tetrahedra of NH_4 where all NH bond lengths are the same, but interestingly with time NH_4 does not remain static. Suddenly it might just undergo a rotational jump. It is continuously undergoing a kind of rotational diffusion. Energies and the timescales of the diffusion are measured using neutron inelastic scattering.

Also, we can look at dynamics using very small energy transfer and when you talk about very small energy transfer, we are talking about longer or slower processes. Such an example is relaxation of polymer backbones at nanosecond that is 10^{-9} second timescale. So, timescale is increasing here, and the demand on doing experiments at lower and lower energies is increasing.

When you want to do experiments at lower energies, then you also need neutrons who themselves have very low energies, because we are supposed to measure the energy difference in an experiment. If the neutron has very high energy it will be difficult to measure a small energy transfer as a percentage change. That is why, we will also need neutrons with lower energy or what are known as cold neutrons in the parlance of neutron scatterers.

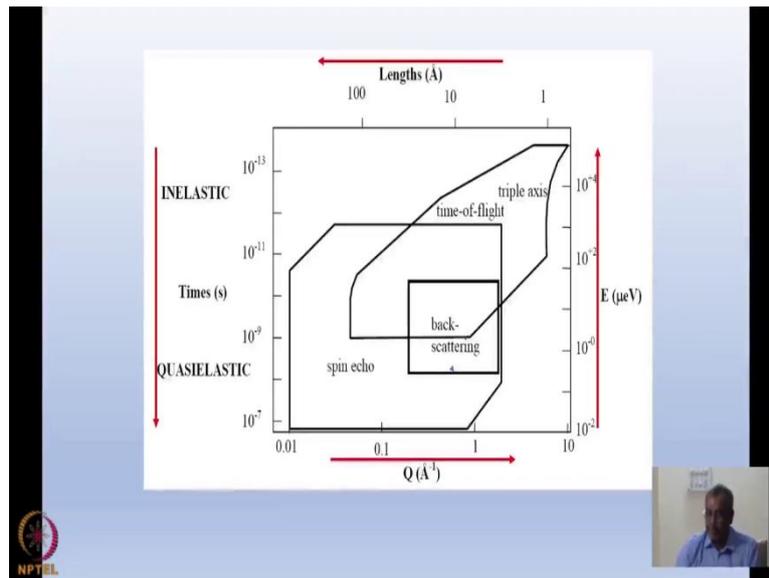
On top of everything, the structure at various length scales and the dynamics at various time scales, we have the magnetic moment of -1.91 nuclear magneton for a neutron. It is a tiny magnet for us. So, I can do magnetic measurement at all these length scales and at all these time scales using polarized neutrons or using a sample, polarized and the neutron unpolarized. Both of these kinds of experiments give us magnetic information.

Neutrons are possibly the only tool which can tell you about magnetic structure. Crystallographic structures have always been done using X rays. Many of us are familiar with the powder diffraction data table where we try to identify a sample, we have prepared fresh, from their Bragg peaks and say that phase has formed or not.

But here in addition, we can also find out the magnetic structure. The magnetic structure means, you have for example, for $3d$ transition elements like cobalt, iron, nickel, where you have unfilled shells in d orbit and they have their own magnetic moment. So, the atom has a magnetic moment and the neutron has a magnetic moment, it is an interaction between these two magnetic moments. Similarly, inhomogeneities, there can be magnetic inhomogeneities and I can use polarized neutron to study them.

Similarly, when I come to dynamics, I have talked to you about phonons, but, we can also talk about magnons which is the counterpart of phonon where the magnetic moments precess around their mean position. Elementary particles of these spin waves are known as magnon and magnons are also measured using magnetic neutron scattering. This is possibly a unique tool, which can give you an idea about crystal structure, a magnetic crystal structure and also magnetic dynamics among all other probes.

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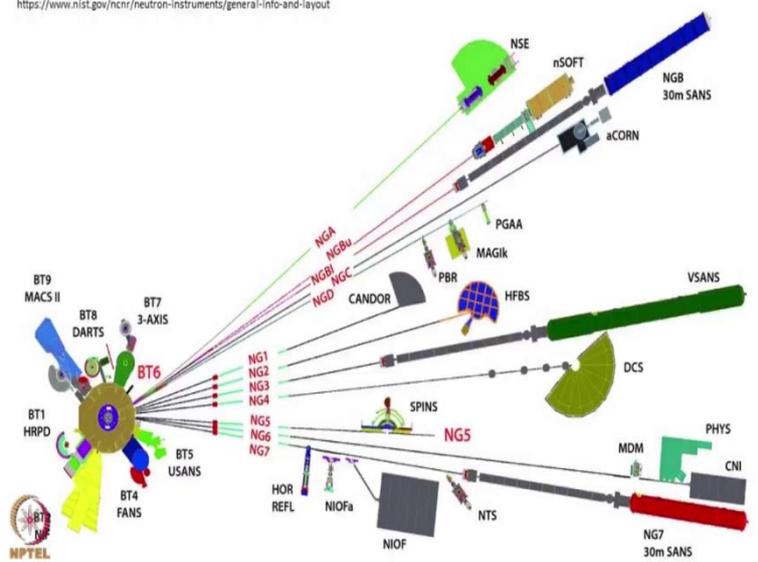
Now, we will talk about a Q - ω space, ω is basically energy, so, energy and momentum space. In Q - ω space these are representations shown, you can see that the Q space is covered by various kinds of spectrometers like spin echo, backscattering, time of flight, etc. And the energy space is also covered by many of them.

These are typical slices of this Q - ω space, that means the Q - ω values in the Q - ω space that you can measure using various instruments like triple axis, backscattering, spin echo etc. These are dynamics and one instrument with which you can measure dynamics is triple axis an instrument, which can measure phonons. I will discuss them and time of flight machines that can measure structure and dynamics. The only thing I want to point out to you is that, neutrons cover a very large range of Q - ω space, which gives us a good handle to use them to understand dynamics and structure for various kinds of materials and length scales.

Also, I would like you to notice, Q and length scales are inverse of each other, as Q goes up your length scale goes down. For lower Q experiments, length scales are about 100 \AA . Similarly, when the time goes up, that means things become slower, we talk about energy transfers which are smaller and when the time because faster or smaller, we talk about energy transfers which and larger, they are inverses of each other. This is just a schematic representation of how we cover the Q omega space in various spectrometers.

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<https://www.nist.gov/ncnr/neutron-instruments/general-info-and-layout>



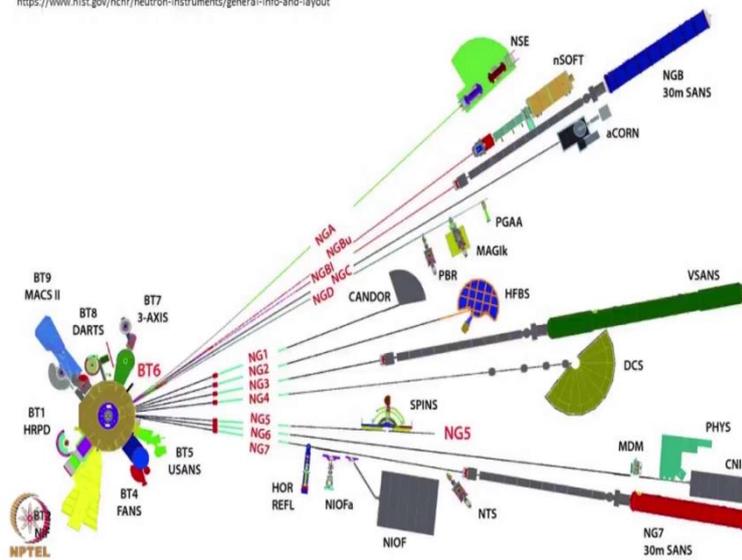
To cover this, we need various kinds of arrangements.

I just wanted to show you some schematics. Basically, this is one very famous reactor at NIST USA known as NCNR [NIST center for neutron research]. I may tell you that you can see that the core is here on the left bottom [schematic] and there are various instruments in the hall. You can see long lines going out. These are actually neutron guides; I will discuss them also in my course., There are various instruments accommodated on them.

And actually, in reality it looks like this [photograph]. What I showed you here as long lines, the guides, they actually look like this., You can see the brick shielding around the guides. In any experiment with a reactor or spallation neutron source using neutrons, we have to take care of the radiation that accompanies the neutron often, when it comes out from the source. So,



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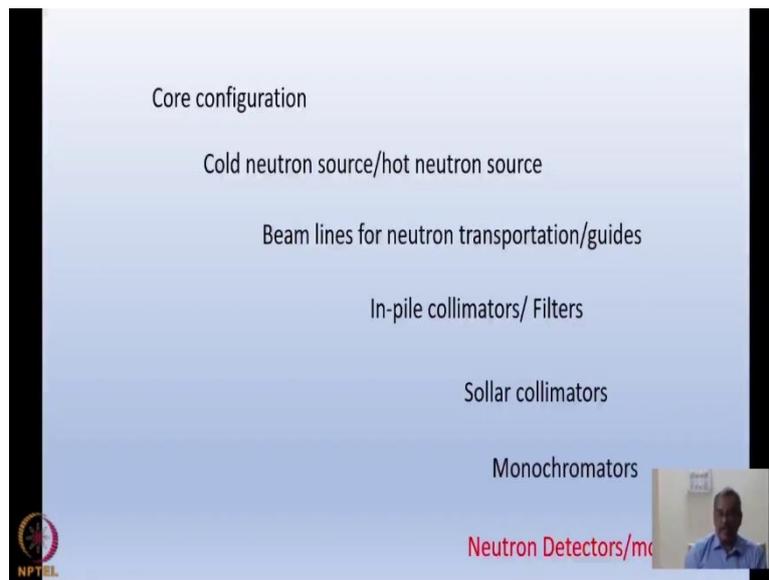


Similarly, I may talk about the best reactor in the world, Institute Laue Langevin (ILL) in Grenoble. This is a typical look for the reactor, the reactor hall and the guides. There are 64 instruments in this place. And this is how they are accommodated on the guides.

Then we come to our own neutron scattering facility at Dhruva. Dhruva is a 100-megawatt thermal reactor, because the moderator is close to room temperature. The thermal flux of 1.8×10^{14} neutrons/cm²/sec. I must tell you that neutrons are very expensive, because the flux, when you compare it to even to a tabletop x-ray source, is much smaller.

And so, our design of instruments has to be judicious and proper, so that we do not waste neutrons. And this is how a schematic looks like., This is the reactor, the small circle at the center is the reactor core. And then you can see the beam lines, some of them are radial, some of them are tangential, I will discuss, why! And then at the end of the beam lines or at the end of the beam hole we say, we put our instruments and they are used for various experimental purposes. We also have two guides, like you found the guides in ILL and in NIST, which are running into a guide hall next to the laboratory. And this is how the photograph looks like. Again, it is a large hall. These large cylindrical drums that are at the at the beam hole mouth, they are called monochromator drums. I have used this word earlier, but their utility I will be discussing briefly later.

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For neutron diffraction, I gave you the theoretical formalism and the reasons for doing several experiments at several angles from the point of view of Q range and structures we are trying to see. There are several points which I will bring to you such as the core configuration and the optimal use of neutrons.

For very slow dynamics, we need slow neutrons. For this, we have something called cold neutron source. Similarly, we also have hot neutrons. I will describe them to you. Then we have beamlines that transport neutrons. Beamlines transfer the neutrons to the outside of the reactor. And then the guide takes them far away from the reactor. To define the energy and direction of the neutrons, we have in-pile collimators, filters, solar collimators. I will describe all of them.

Neutron detectors and monitors are very important part of neutron experiments and I will try to discuss them in reasonable details during my talk. I will also tell you how neutron guides work and how they are designed. With this, I will stop here and come back with the next lecture.