Neutron Scattering for Condensed Matter Studies
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So far, I have discussed about the various components of a spectrometer starting from beam tailoring at the reactor to detectors. But neutron being a spin half magnetic nuclear particle, few more important topics are neutron polarization for some experiments and the capability to flip the neutron spin. Because often in magnetic neutron scattering, we need to polarize the beam of neutrons and then use it for scattering experiments and sometimes even analyze the polarization of the reflected beam. In this lecture I will introduce you to neutron polarization and very briefly about spin flippers

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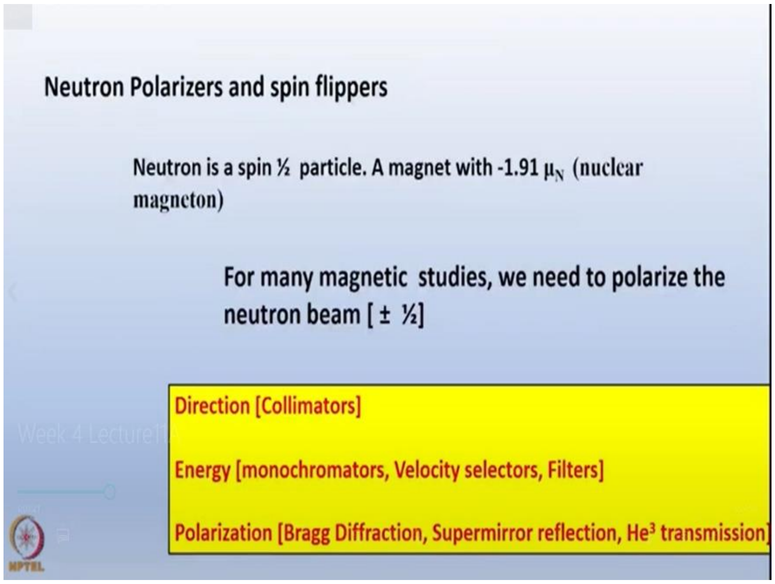

These designs can be intricate and elaborate and if you get in details then we might not be able to reach the target of neutron diffraction. Hence, I will be discussing spin flippers and neutron polarizers briefly. Now we know that neutron is a spin half particle, a magnet with -1.91 μ_N magnetic moment, which is much lesser than what we have for the electron, nearly two thousand times weaker. But it is a tiny magnet which can penetrate deep in material. Sometimes for magnetic studies we need to polarize the neutron beam, which means with respect to some direction the neutron beam will either have +1/2 spin or -1/2 spin. For such experiments, we often need to flip the polarization of the neutron beam.

We have already discussed about defining direction of beam using various kinds of collimators: in-pile collimators as well as soller collimators. We get the energy of the beam defined, using monochromators, if we want a broad beam then using velocity selectors or even sometimes using filtered neutron beams.

Polarization can be done by various means: using Bragg diffraction from a magnetized crystal, using super mirror reflection and also using He-3 transmission polarizer. I will give brief introduction to these techniques.

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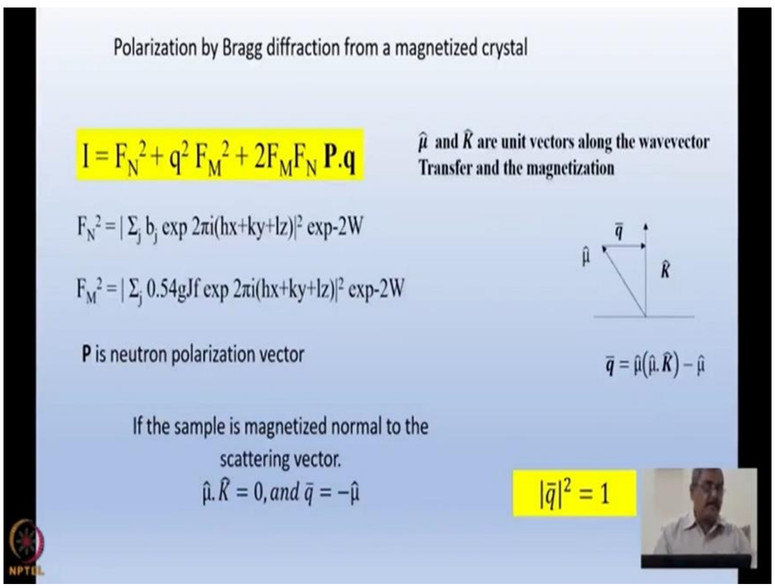

I will prefer to start with an expression for Bragg diffraction from a magnetic crystal. The derivation of this expression is long so I will skip that but I will give you the expression for intensity of the Bragg diffraction which has got nuclear part, magnetic part and various terms as I defined.

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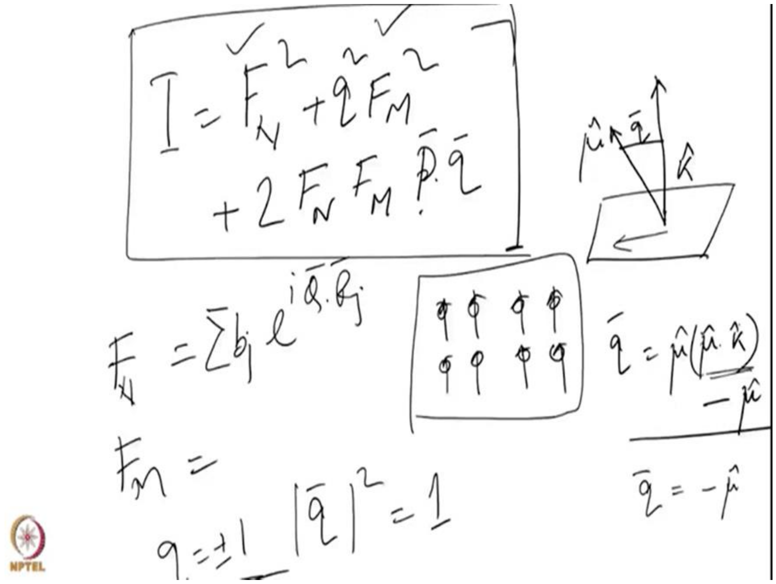

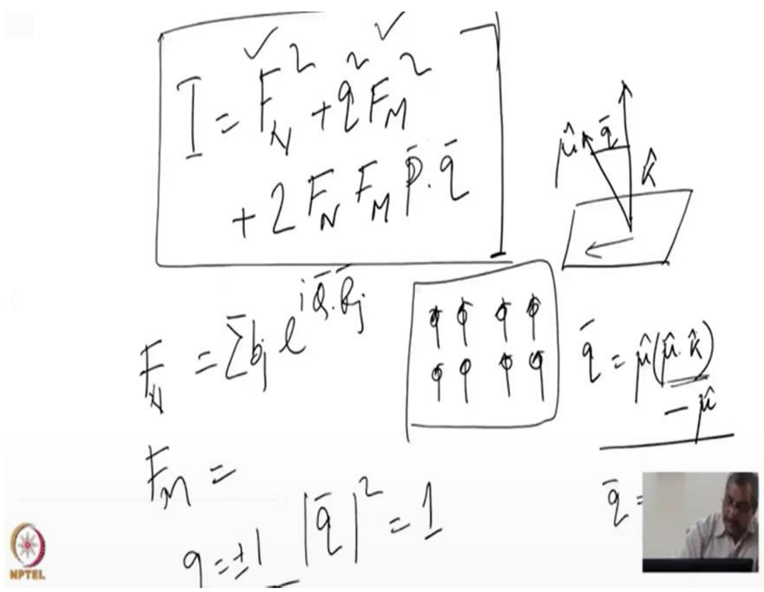

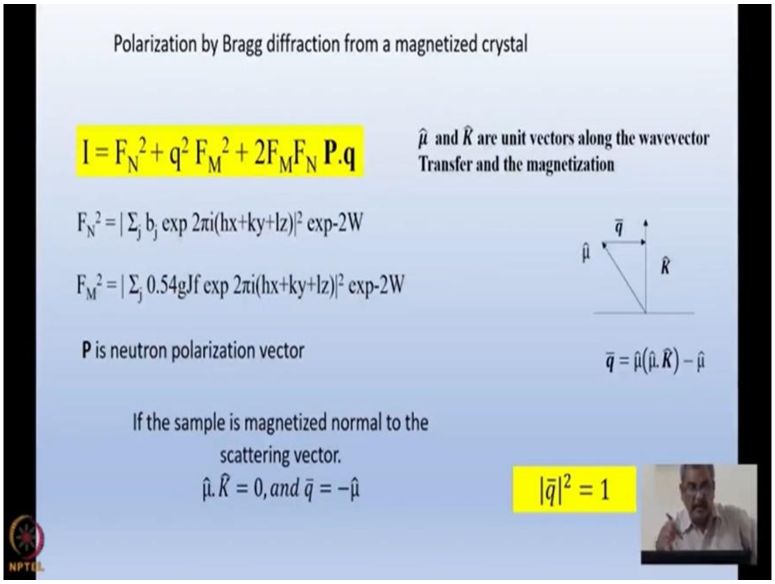

Consider a unit vector $\hat{k}$ along the momentum transfer and $\hat{\mu}$ the unit vector along the magnetic moment in general. Consider this (diffraction) happening from a (crystallographic) plane in the, sample then there is vector q which basically the component of $\hat{\mu}$ along the $\hat{k}$, $= \hat{\mu}\,(\hat{\mu}.\hat{k}) - \hat{\mu}$. Once I define the vector then the Bragg intensity is given as,

$$I = F_N^2 + q^2 F_M^2 + 2F_M F_N\, \bar{P}.\bar{q}$$

P is the polarization of the neutron.

I will explain this expression term by term. I am talking about a crystalline sample which also has got magnetic moments and these magnetic moments are aligned. And I am carrying out a Bragg diffraction from this sample. Now here the term F_N is the nuclear scattering amplitude which I had defined earlier to you and is given by $\sum b_j\, e^{iQ.R_j}$, b_j is the coherent scattering length. Replacing Q with reciprocal lattice vector and including the thermal term it can be written as,

$$F_N^2 = \left|\sum b_j\, e^{2\pi i(hx+ky+lz)}\right|^2 e^{-2W}$$

Thermal term, the Debye-Wallar factor e^{-2W}, is because of the atoms are oscillating around their mean position which reduces the Bragg intensity. Here, $W = \sigma^2 q^2$ where σ^2 is a root mean square displacement.

Similarly, there is magnetic scattering amplitude given by,

$$F_M^2 = \left|\sum 0.54gJf e^{2\pi i(hx+ky+lz)}\right|^2 e^{-2W}$$

You can see in the equation above that apart from the constant terms, for the time being just accept that 0.54g is the Lande splitting factor and J is the angular momentum of the nucleus, it is similar to that for F_N except that there is f in place of b_j which is the magnetic form factor.

So, we have very similar terms. Also, we have an interference term, $2F_M F_N\,\bar{P}.\bar{q}$. Here, $\bar{P}$ is the polarization of the neutron and $\bar{q} = \hat{\mu}\left(\hat{\mu}.\hat{k}\right) - \hat{\mu}$. Including all these terms, we have the expression of Bragg intensity coming from a certain plane of a crystal with magnetic moment at the sites.

If the magnetic moment is in plane then you can see that $\hat{\mu}.\hat{k} = 0$ and then $\bar{q} = -\hat{\mu}$, a unit vector. Hence, $\bar{q}^2 = 1$ and $q = \pm 1$ when the magnetization vector is in plane. In such a case $\bar{P}.\bar{q}$ can be +1 or -1. $\bar{P}$ will be -1 when it is opposite to the magnetization of the sample.

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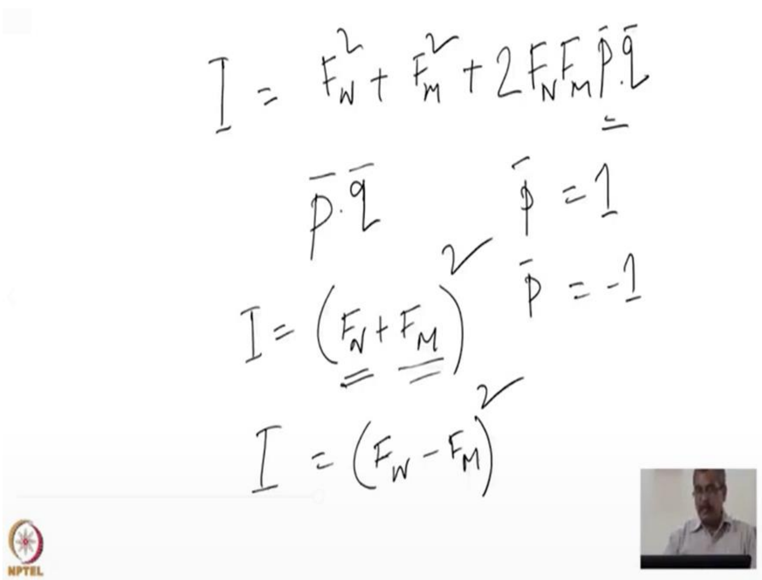

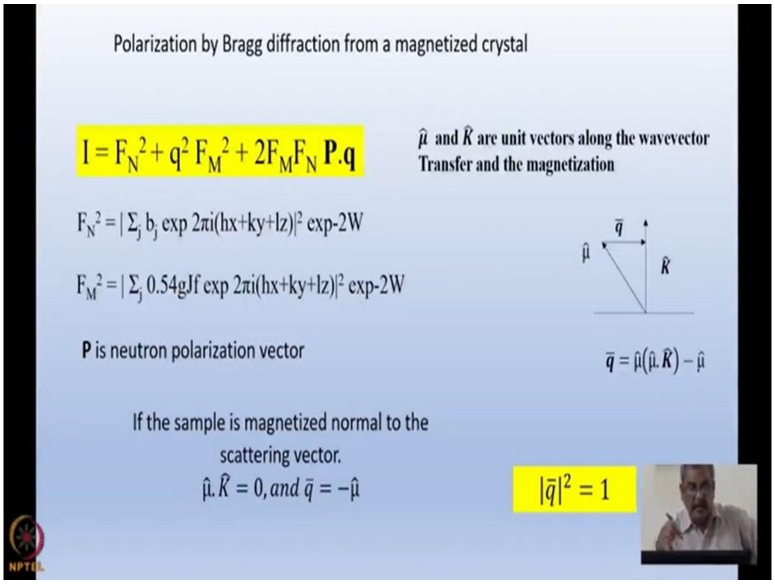

In case when $\bar{P} = +1$, then $I = (F_N + F_M)^2$ means the nuclear form factor or nuclear scattering amplitude interferes constructively with the magnetic scratching amplitude. When $\bar{P} = -1$ then $I = (F_N - F_M)^2$ then they are acting opposite to each other and they are destroying each other or interfering destructively.

I must mention here one thing clearly. When I discussed about nuclear scattering, I mentioned that the nuclear scattering potential is a delta function and does not have any drop as a function of Q because Fourier transform of the delta function is 1 all over Q-space.

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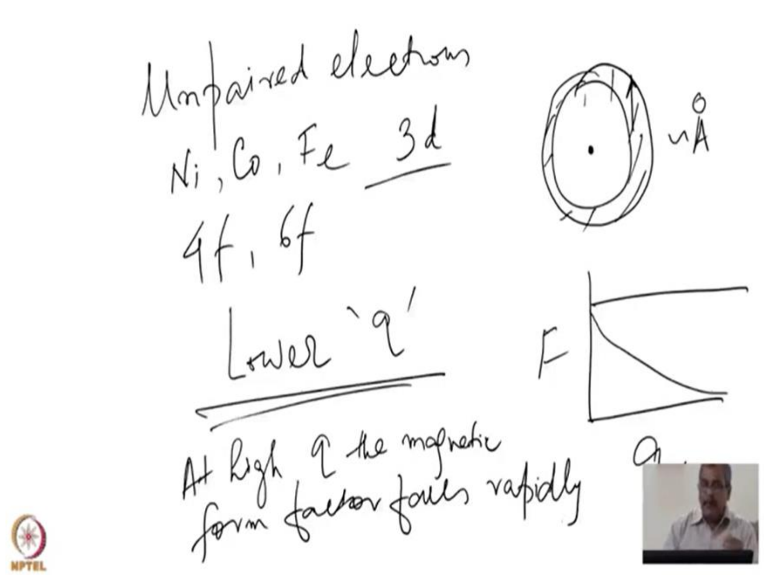

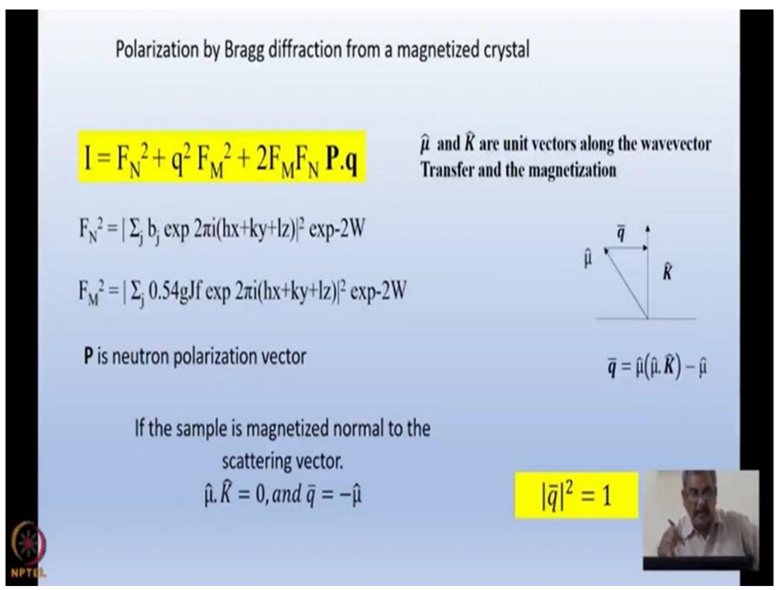

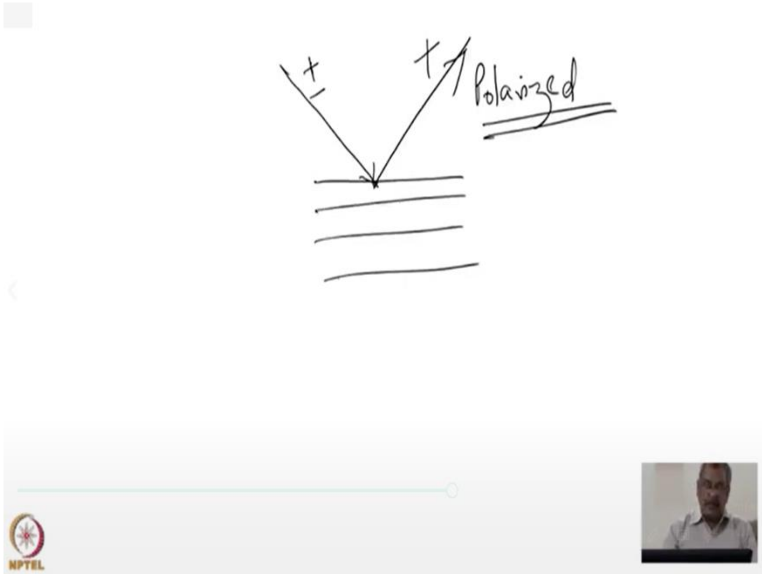

I cannot say the same thing for the magnetism. One must understand the fact that nucleus is tiny of ~ femtometer size. But the magnetism comes from unpaired electrons, for example, *d*-shells for transition metals while *f*-shells for rare earth metals which are partially filled. That is why I can consider it as a shell classically in which we have a magnetic moment. The shells have got a finite dimension, that is of the order of angstrom. Magnetic form factor falls even faster than the (x-ray) form factor with 'q', which I calculated for x-rays for an atom because there you consider the whole sphere while here it is only the shell. Hence, the magnetic peaks or magnetic contribution appear at lower Q's because at high Q the magnetic form factor falls rapidly.

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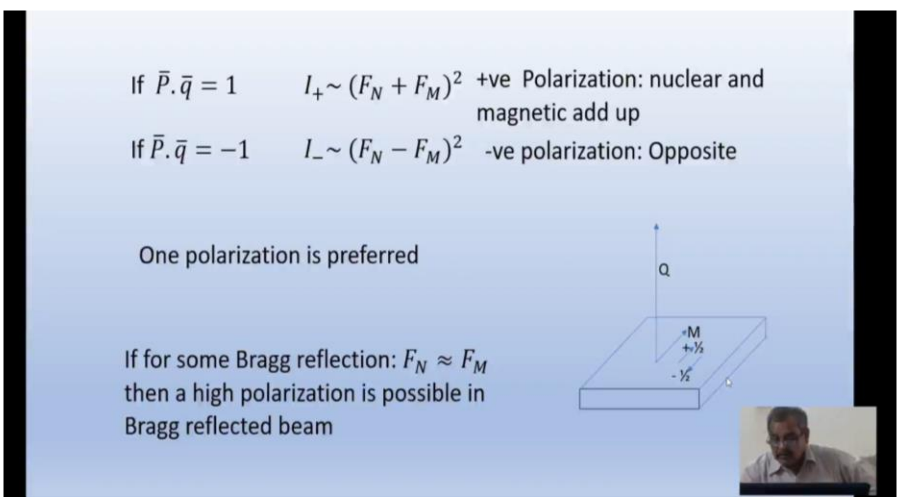

In summary, with the scenario where the sample is magnetized in plane, if the polarization is parallel to $\bar{q}$ and with $\bar{P}.\bar{q} = 1$ then $I_{+} \sim (F_N + F_M)^2$. When the neutron has opposite polarization in then they do not add up but the magnetic part gets subtracted from the nuclear part that is, $I_{-} \sim (F_N - F_M)^2$. This is shown in the figure above.

Now I have to look for a reflection in crystallographic parlance.

There is also a possibility that for some Bragg reflection $F_N \sim F_M$ then $F_N - F_M \sim 0$ and $F_N + F_M \sim 2F_N$ so we have only one polarization. So, in that case, the Bragg diffracted neutrons are polarized and the crystal acts as polarizer. High polarization is possible in Bragg reflected beam.

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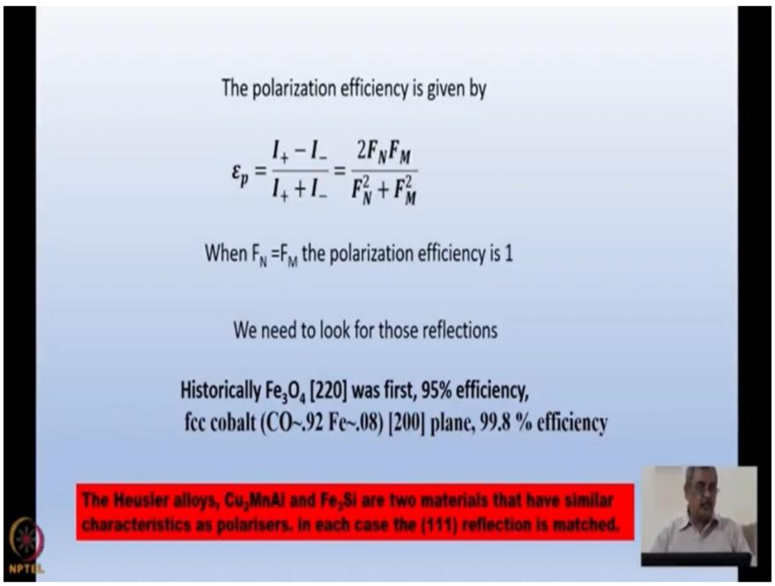

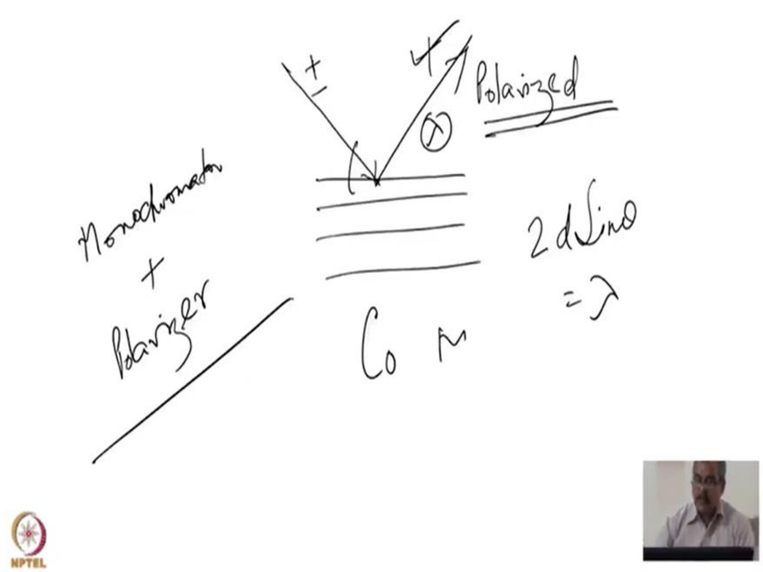

The polarization efficiency is defined as,

$$\varepsilon_P = \frac{I_+ - I_-}{I_+ + I_-} = \frac{2F_N F_M}{{F_N}^2 + {F_M}^2}$$

when $F_N = F_M$ then the polarization efficiency will be 1.

Historically, Fe_3O_4 [220] was the first reflection used for polarization with the polarization of 95%. FCC cobalt gives very good polarization. [200] plane of the alloy with 92% Co and 8% Fe gives very high efficiency but the issue is that cobalt is a strong newton absorber so we lose intensity in the absorption.

At present, Heusler alloy which is Cu_2MnAl and Fe_3Si are materials with very similar characteristics as polarizers. In both of them the 111 reflections are matched, means F_N is nearly equal to F_M and these are used as neutron polarizing monochromators. Here we not only choose the polarization depending on the Bragg angle we also choose the wavelength λ. These act as monochromators as well as polarizers. Heusler alloy is used in one of the magnetic neutron diffractometers at Dhruva.

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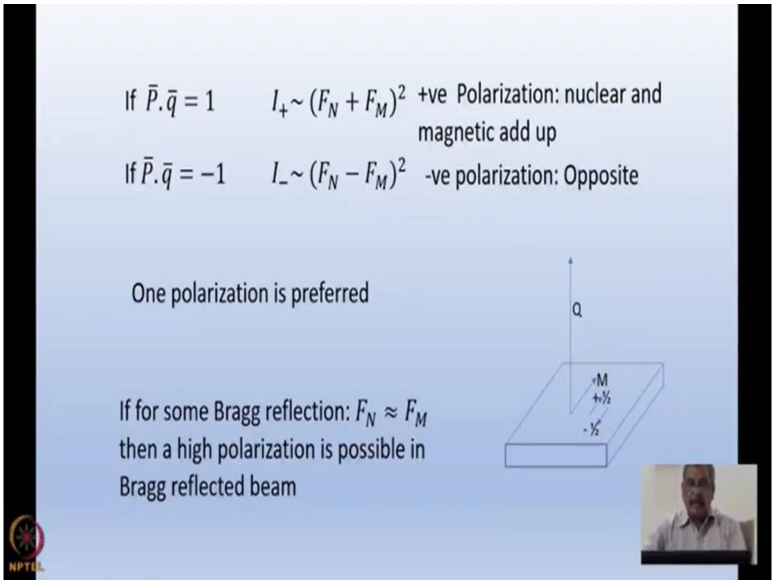

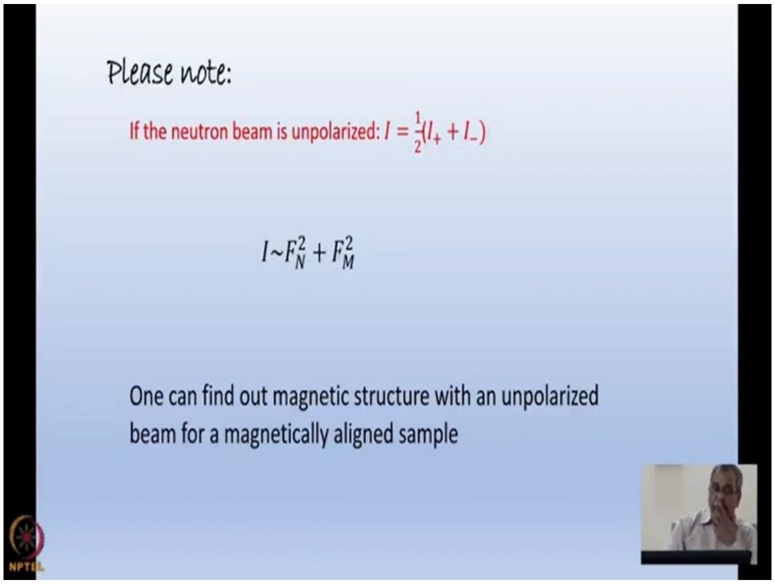

Next, I will discuss with you about mirror-based polarizers. Before that, I want to bring to your notice one thing. Suppose that we are doing diffraction from a magnetized sample. It means apart from crystallographic long-range order there is magnetic long-range order also. Then using these expressions, for unpolarized neutrons,

$$I = \frac{1}{2}(I_+ + I_-) \sim F_N^2 + F_M^2$$

because the beam is unpolarized so half of the neutrons are coming with up spin with respect to the sample magnetization and half of them are coming with minus of orientation with respect to the sample.

Even for an unpolarized beam, we can find out F_M^2 through fitting processes and we can find out the magnetic structure with an unpolarized beam for a magnetically aligned sample. This technique is used for many magnetic diffraction studies.

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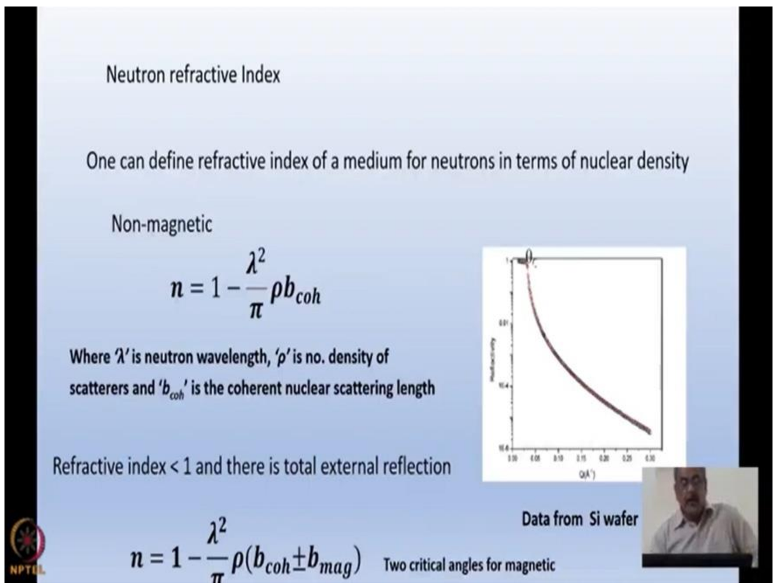

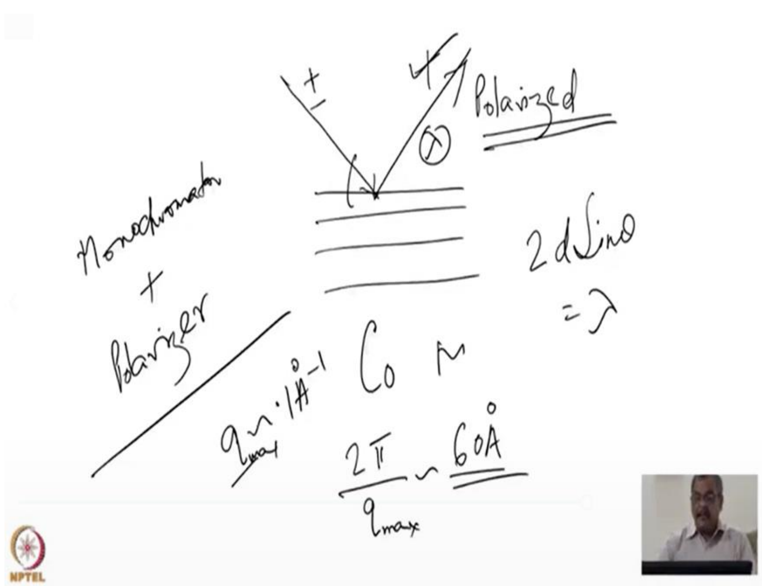

Now I will talk about mirror-based neutron polarizers. One can define refractive index of a medium for neutrons. So far, we have been talking about the atomic structure of the medium when we talked about neutron diffraction. But at a much lower Q, let us say of the order of 0.1 Å^{-1} then $\frac{2\pi}{Q_{max}}$ is about 60 Å, in a scattering experiment the medium does not come as a medium comprising atoms and molecules but as a uniform medium, the way we see the medium in case of light. Hence, in terms of non-magnetic sample and unpolarized beam, in this case we can define the refractive index of a medium as,

$$n = 1 - \frac{\lambda^2}{\pi}\varrho b_{coh}$$

here λ is a wavelength of the neutron ρ is the number density of the scatterer and b_{coh} is the coherent scattering length density. In this case you can see for, in general, n is less than 1.

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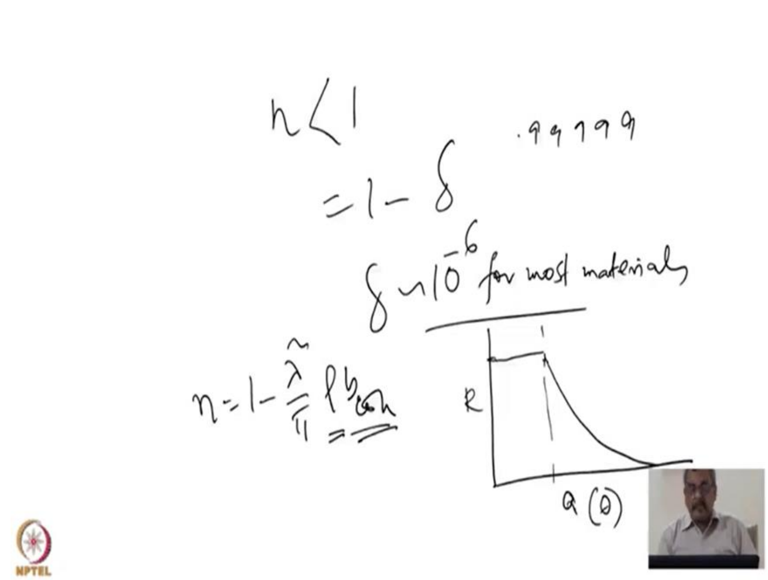

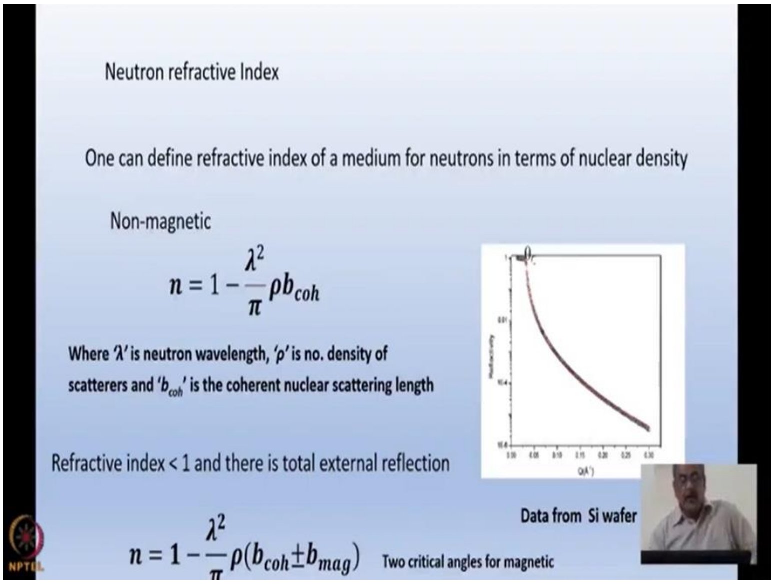

We can also write, n = 1-δ where δ is of the order of 10^{-6} for most materials in case of neutrons. Comparing it with our experience with light rays traveling from a denser medium to a rarer medium here any medium behaves like a lighter medium with respect to air or vacuum because its refractive index is less than 1. Hence, for most materials, in case of neutron, total external reflection will take place as compared to the total internal reflection in optics.

Since δ value will increase for larger b_{coh} or larger ρ this means our total external reflection will takes place to a up to a larger angle for larger ρb_{coh}. In general, if I take a reflectivity profile as a function of Q or θ then the reflected intensity up to certain point in 'Q' will be 1 because total external reflection takes place and then beyond that critical angle the intensity starts falling. This is a typical reflectivity curve of a medium.

I have shown you the experimental data from a silicon wafer and here you can see that up to the critical angle the reflectivity is 1 and then it falls. Actually, when I go to large Q value that falls as $\frac{1}{Q^4}$ known as Fresnel reflectivity.

If there is a magnetized medium, similar to what I did in case of Bragg scattering, then apart from b_{coh} for a magnetic medium we also have a magnetic scattering length which is b_{mag}. Depending on the magnetization direction with respect to the neutron spin we can either have b_{coh} + b_{ma} or b_{coh} - b_{ma}. So refractive indices are different for two different spins of neutron.

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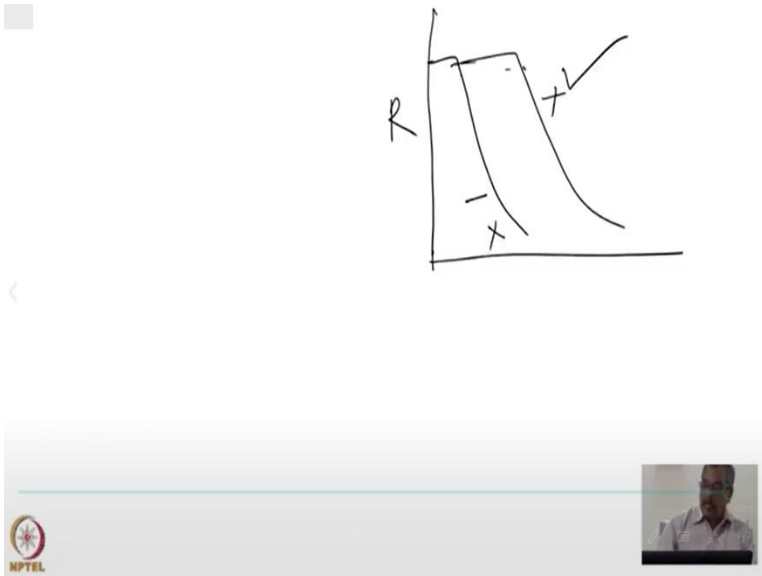

This means, now, we can have two different critical angles. This is very interesting and you can see, in the figure, that if I go beyond this angle one spin component gets reflected but the other spin component does not get reflected.

I will stop now and then I will continue with the same topic and will talk to you about neutron super mirror polarizers.