Neutron Scattering for Condensed Matter Studies
Center for Distance Engineering Education Programme
Indian Institute of Technology, Bombay
Week 02
Lecture 03C
Scattering theory and introducing dynamics in the formalism

Keywords: Diffraction, form factor, Charge density, coherent scattering length, Fourier space

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In the previous part, I introduced the diffraction pattern as you expect from a neutron. The specific diffraction patterns are caused by a coherent scattering length. But, since neutron and x-ray diffractions: especially x-ray diffraction, are the most commonly used techniques, it is important that I provide a comparison of the two so that the subject becomes clearer. I am talking about neutron and x-ray diffraction on the same footing and I will show you that they are almost same except for a few differences like coherent and incoherent scattering length part.

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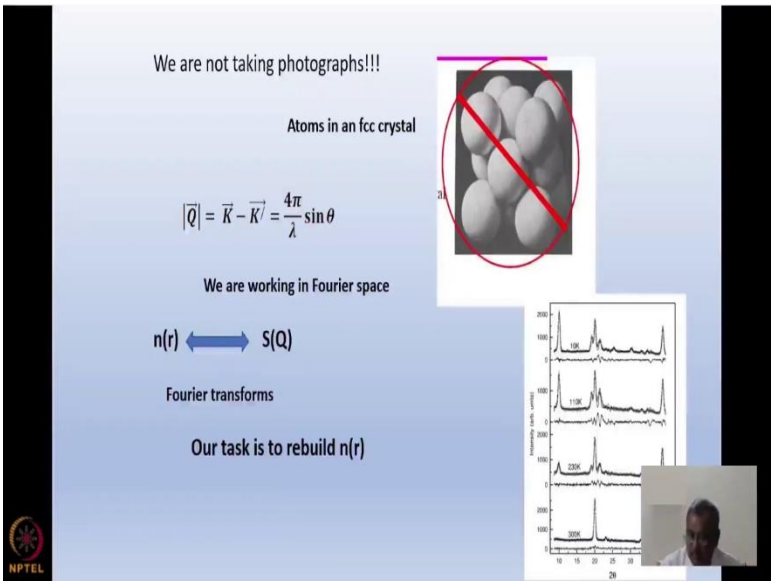

At the onset, I must mention clearly that in any diffraction experiment we are not taking photographs. I just showed you atoms in an fcc crystal that is how that arrange but to get this we do a diffraction experiment as a function of angle or we can write it as a function of the wave vector transfer Q which is K-K` given by $\frac{4\pi}{\lambda}\sin\theta$, when there is no energy transfer and we are working in Fourier space. On the right bottom, you can see a typical diffraction pattern of some samples at various temperatures.

You get this kind of patterns which are actually caused by the diffraction and the diffraction peaks signify various crystallographic arrangement like the one I have shown at the photograph. So, we are working in the Q space with what is known as scattering law, S(Q). I am working with S(Q) in Q space and the information I am getting is the real space distribution. They are Fourier transform of each other and in these experiments our task is to rebuild n(r). In a way, n(r) is the starting point.

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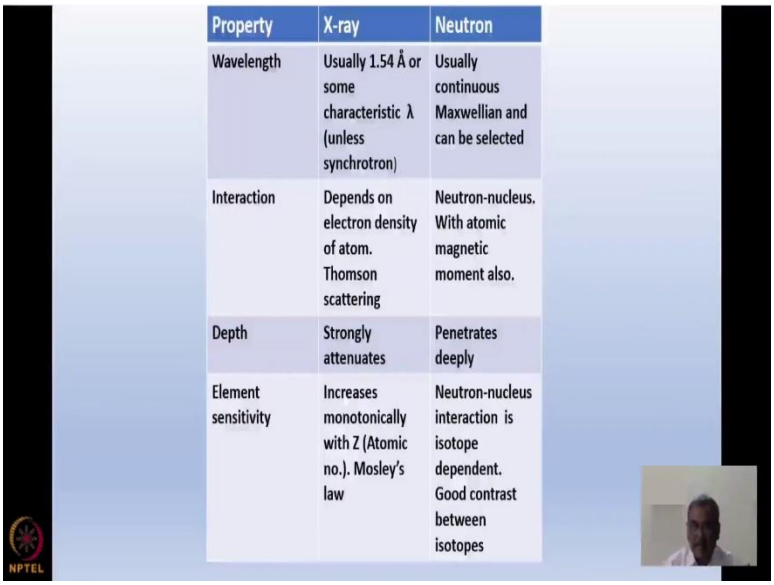

I will quickly give a comparison of the properties between x-ray and neutron which I repeatedly said. Their wavelengths are typically 1 Å (1.54 Å for Cu k_α), neutrons also have similar wavelengths. But in our table top x-ray experiment, 1.54 Å comes from a Cu target, characteristic wavelength of a specific target. For molybdenum it will be even lower: 0.6 or 0.7 Å. In case of neutron, there is a continuous Maxwellian distribution and we select the wavelength which are typically in this range.

Interaction of x-rays depends on the electron density distribution, not the free electrons, but the bound electron density distribution and caused by Thomson scattering. In case of neutron, it is neutron nuclear interaction and also interaction of neutron with the atomic magnetic moment. So far, I have not discussed it and it will be introduced a little later. Because x-ray is an electromagnetic wave it strongly attenuates in a medium and actually, we get information typically from few microns to tens of microns depth, while neutrons can penetrate very deeply. Even tens of centimeters it can go in because it is a charge less particle.

Another important difference is that in case of x-ray, the scattering length increases monotonically with Z. We know that it follows Mosley's law whereas in neutron nucleus interaction, it is fluctuating across the Z values in a periodic table and it provides good contrast between isotopes in many cases. In case of x-rays, the scattering intensity or scattering length varies $(Z-\mu)^q$.

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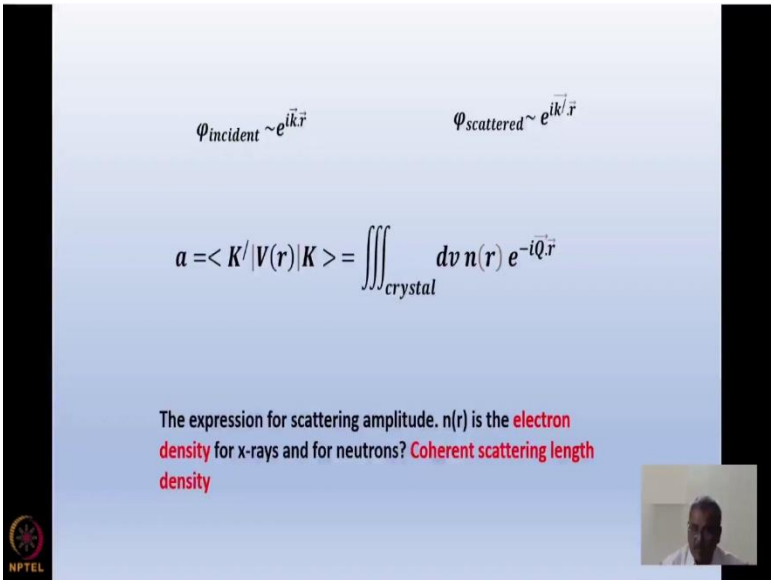

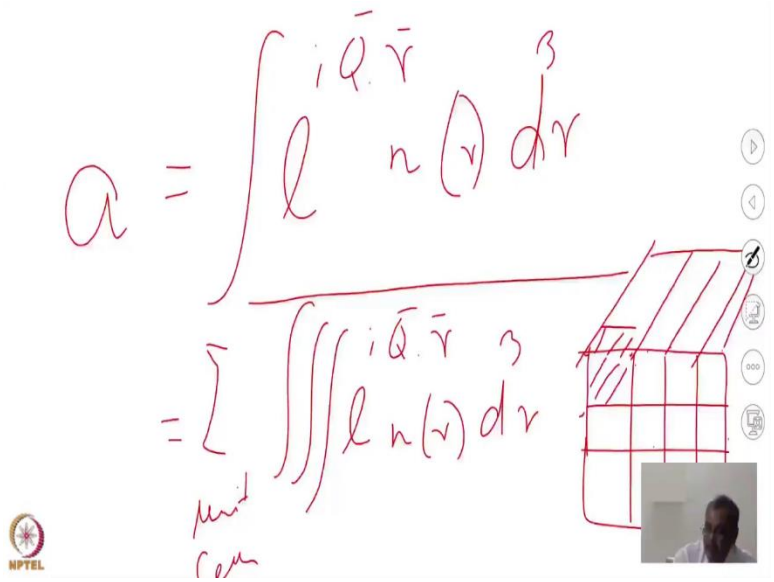

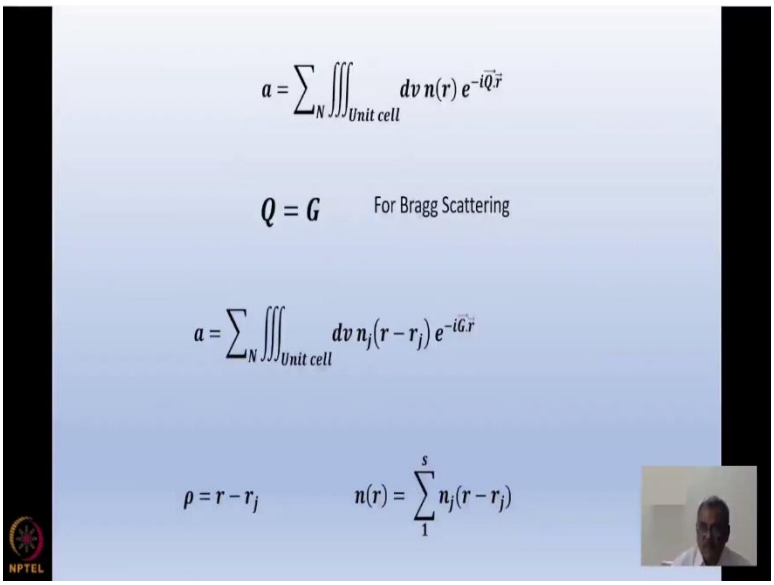

Primarily what I am trying to evaluate is this; I have got an incident wave function $e^{ik.r}$ and an outgoing wave function $e^{ik'.r}$. This 'k' to 'k'' change in direction is caused by the crystal scattering potential. Basically, the scattering amplitude a is given as a Fourier transform of the electron density in this case, over the entire crystal which I have written down as an integration over a Fourier transform of the density. I can write the volume as d^3r which means dv throughout, as I wrote there.

This is how scattering amplitude is expressed $a = \int e^{iQ.r}\, n(r) d^3r$. You can see that this is very similar to what I obtained from the Fermi Golden rule in case of neutrons. I will go ahead will show you the same. The expression for the scattering amplitude depends on the n(r) where n(r) is the electron density in case of any condensed matter for x-rays. By electron density I mean there are atoms at sites with electron clouds which causes Thomson scattering of the x-rays for diffraction and in case of neutrons it will be coherent scattering length density.

When I write that it is a Fourier transform over the entire crystal, the crystal consists of lattice. It is a combination of unit cells. This is one unit cell where I have just drawn a square lattice. I can easily extend it to three dimensions. Now this integration I can represent it as a sum over unit cells and the integration over a single unit cell. So, if I integrate over one unit cell and then sum over all the unit cells then I get the scattering amplitude because the crystal is built with the repetition of the unit cells.

The expression is,

$$a = \sum_{N} \iiint_{Unit\ cell} dv\, n(r) e^{-iQ.r}$$

dv = d^3r. For X ray scattering, we have been taught that all values of the wave vector transfers are not allowed, you have specific peaks in the Bragg scattering and actually when Q = G (reciprocal lattice vector) then the Bragg scattering occurs. That is what the Ewald's construction tells us.

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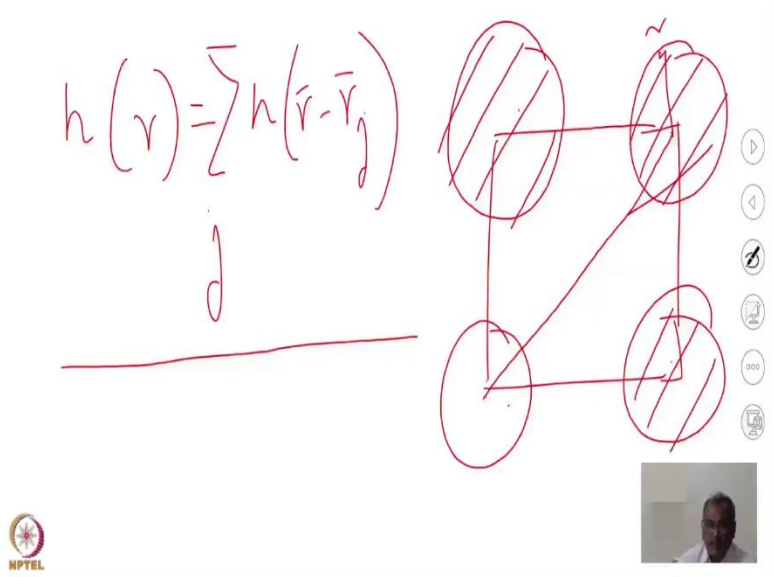

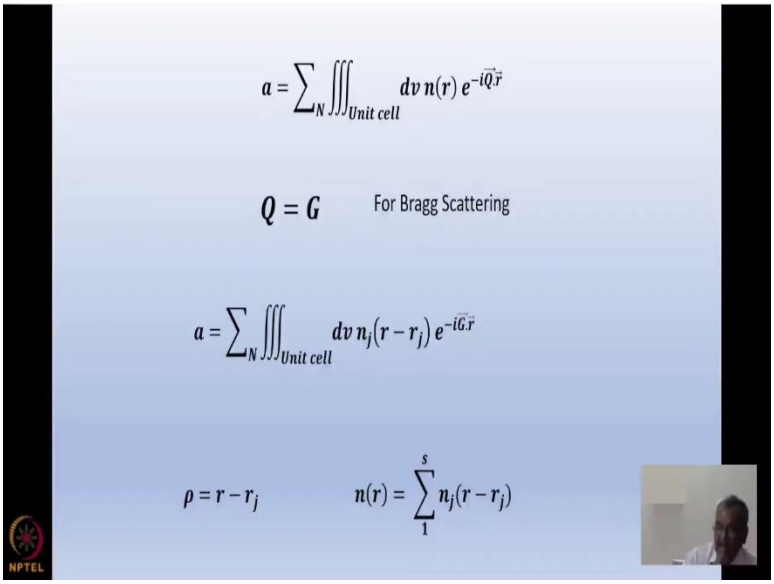

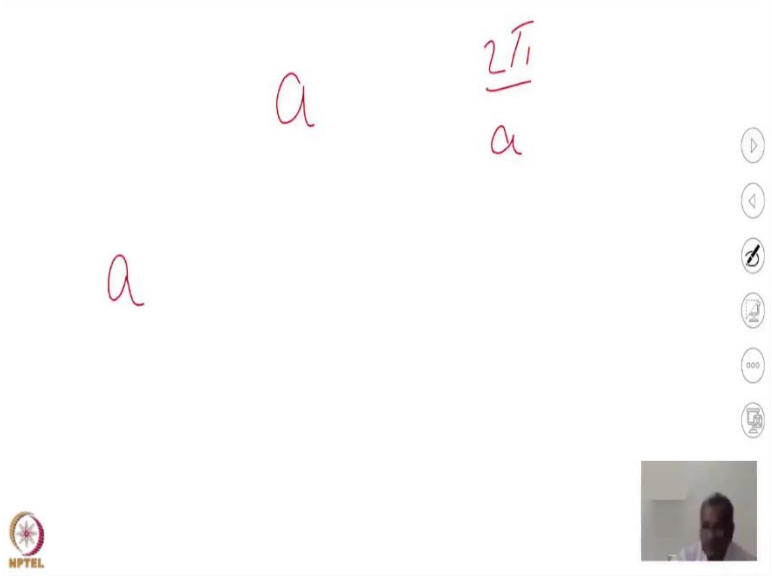

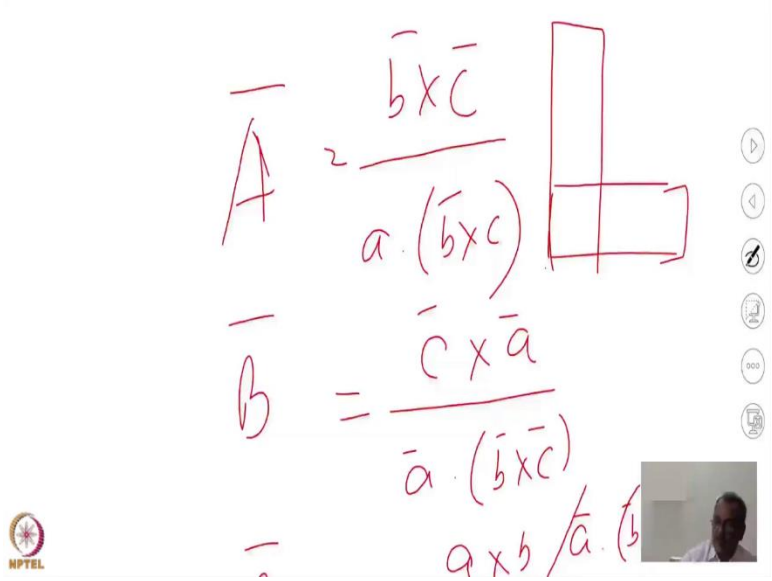

If I consider one of the lattice sites, then there is electron charge cloud around it. Consider j^{th} lattice site so the unit cell consists of these lattice sites where I have the electron charge cloud. In this case I can write $n(r) = \sum_j n(r - r_j)$ assuming an arbitrary origin. At any arbitrary point is r, the density of charge cloud is given by r - r_j and it is summed over all the points in the unit cell and that gives me one unit cell then I sum up over all the unit cells, so this is the expression for the density for the entire crystal.

I can write the scattering amplitude as integration over unit cell sum over all the unit cells then density which I wrote it as n(r-r_j) and then the factor $e^{-iG.r}$, giving

$$a = \sum_{N} \iiint_{Unit\ cell} dv\, n(r - r_j) e^{-iG.r}$$

because whenever the wave vector transfer Q is equal to a reciprocal lattice vector (G) then and then only Bragg scattering takes place. I understand that you are familiar of reciprocal lattice of a crystal lattice. In case of cubic lattice if a is the real lattice, then reciprocal lattice length will be $2\pi/a$. But, in general, the reciprocal lattice (A) is given by $\frac{b \times c}{a.(b \times c)}$. This is the definition of reciprocal lattice. Basically, because it depends inversely with the real lattice length, if in one direction it is 'a' in that direction it will contract to 1/a. So, if I have a real lattice like this in two dimensions then the reciprocal lattice will be like this

Let me get back to my point that whenever Q = G then I will have Bragg scattering. I have to add up over the all the charge clouds which are centered around j point. For the unit cell I have to sum over all the 'j' in unit cell and the general wave vector in a charge cloud is given by $n_j(r\text{-}r_j)$.

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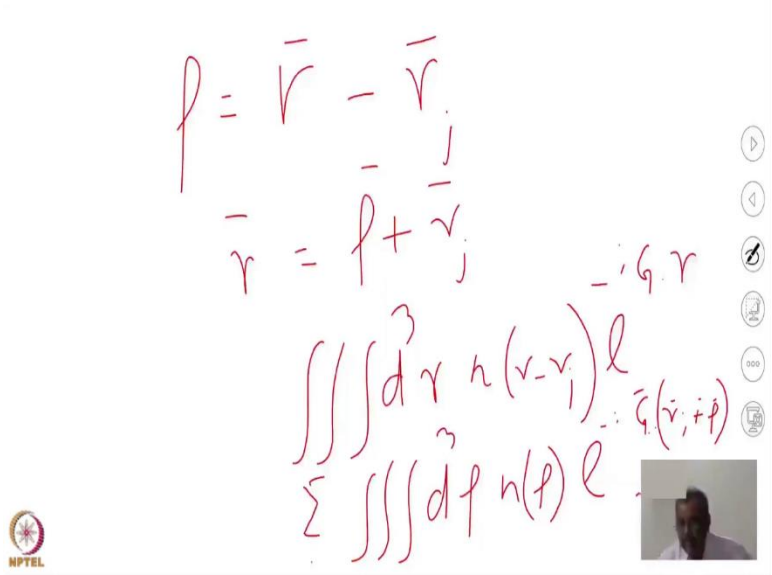


$$a = \sum_j e^{-G.r_j} \int dv\, n_j(\rho)\, e^{-iG.\rho}$$

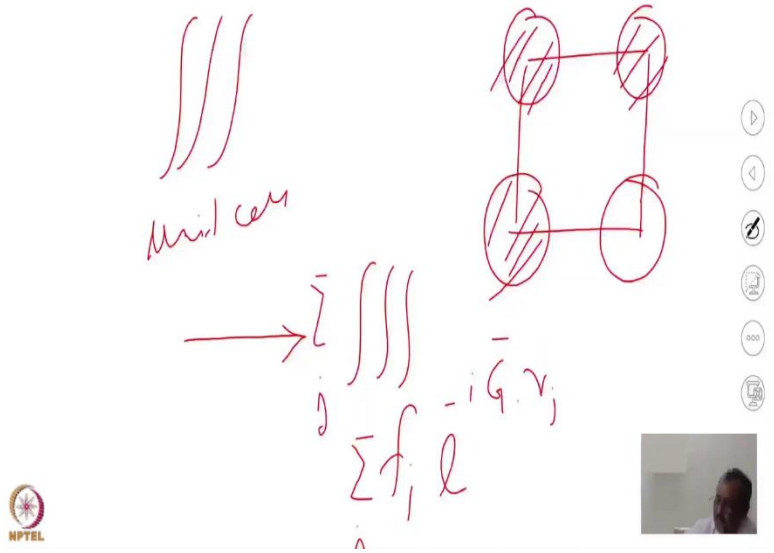
$$= \sum_j f_j e^{-iG.r_j}$$

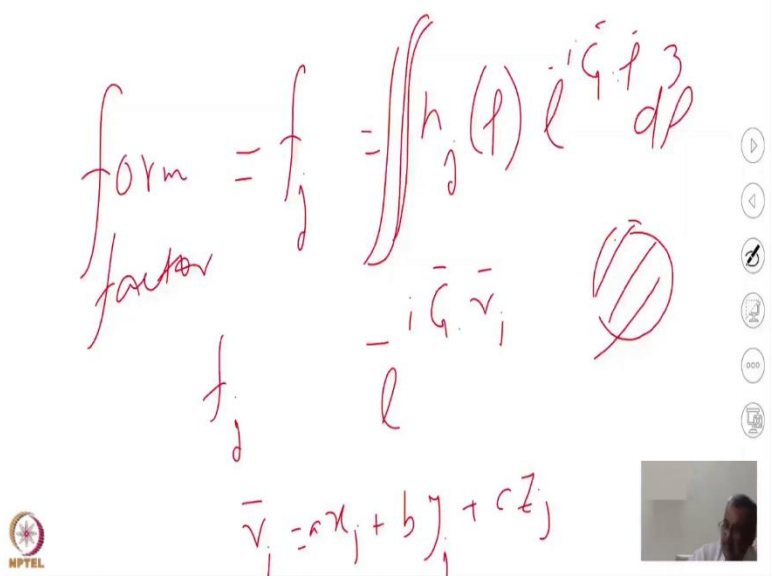
where $f_j = \int dv n_j(\rho) e^{-iG.\rho}$

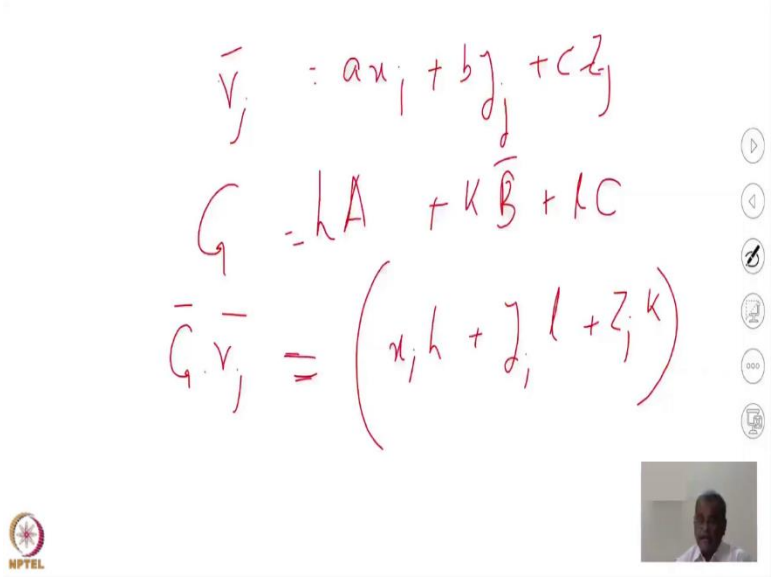
$r_j = ax_j + by_j + cz_j$ Crystal lattice

$G = hA + kB + lC$ Reciprocal lattice

$$G.r_j = (ax_j + by_j + cz_j).(hA + kB + lC)$$
$$= 2\pi(x_j h + y_j k + z_j l)$$







In a simple way, I write $r - r_j = \rho$, then $r = \rho + r_j$ and putting this in that integration, a becomes

$$a = \sum_{N} \iiint_{Unit\ cell} dv\, n(r - r_j) e^{-iG.r} = \sum_{N} \iiint_{Unit\ cell} d^3\rho\, n(\rho) e^{-iG.(\rho + r_j)}$$

here, $dv = d^3r$. You can see that here my integration breaks up into a summation over all the lattice points in the unit cell and integration over a single charge cloud.

What I am left with actually is an integration over a single charge cloud which gives me, if it is the j^{th} charge cloud then it is $f_j = n(\rho) e^{-iG.\rho}$ and there is a summation over all these charge

clouds in a single unit cell. What I mean is that, let me take one unit cell so I have these charge clouds around each point so that integration over one unit cell goes to integration over a single charge cloud and summation over all the charge clouds.

I will write this so that in the previous expression summation over all the charge clouds, and an integration, $f_j = \iiint n_j(\rho) e^{-iG.\rho} d^3\rho$. This integral is basically known as form factor. Many of you are familiar with this term, 'form factor' and now what we have for the scattering amplitude is this form factor multiplied by $e^{iG.rj}$; $\sum_j f_j e^{-iG.r_j}$.

In real space, any point $r_j = ax_j + by_j + cz_j$ in terms of a, b, c and in the reciprocal space with the Bragg coefficients h k l, it is given G = hA+kB+lC. One part is the Fourier transform over the charge cloud around one point which is f_j and the other is $G.r_j = (ax_j + by_j + cz_j).(hA+kB+lC)$ which gives $2\pi(x_jh + y_jk + z_jl)$.

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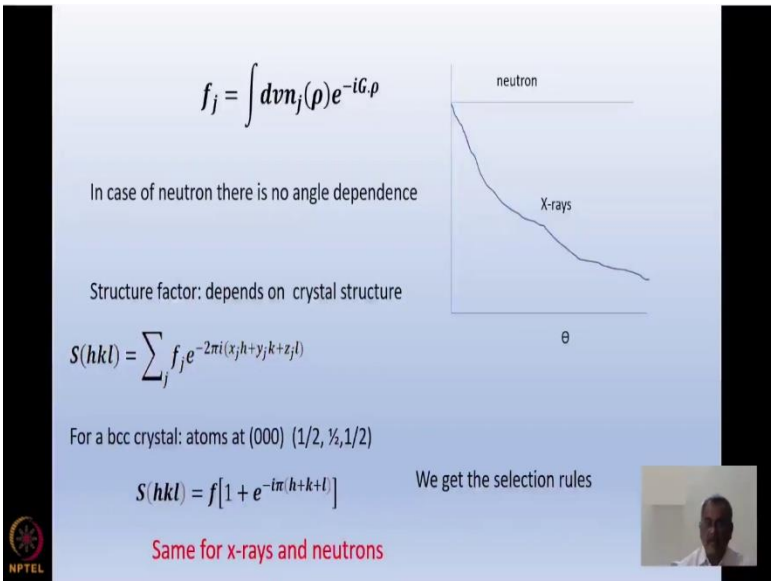

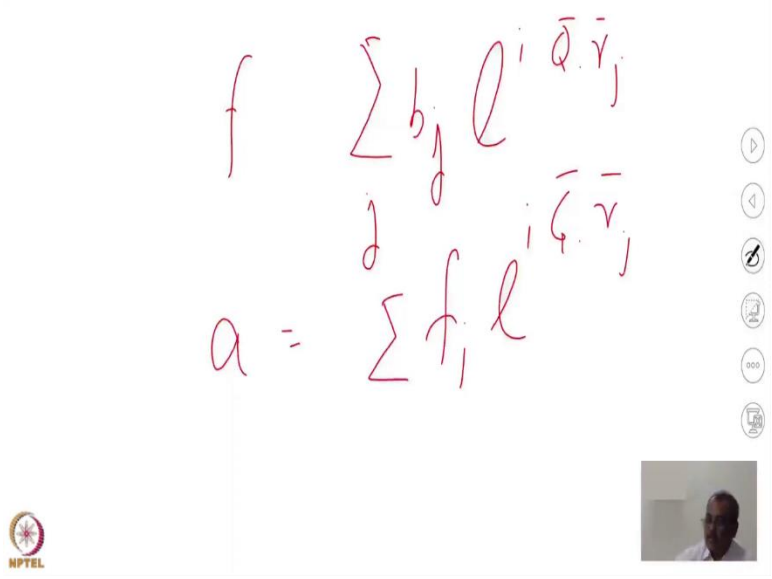

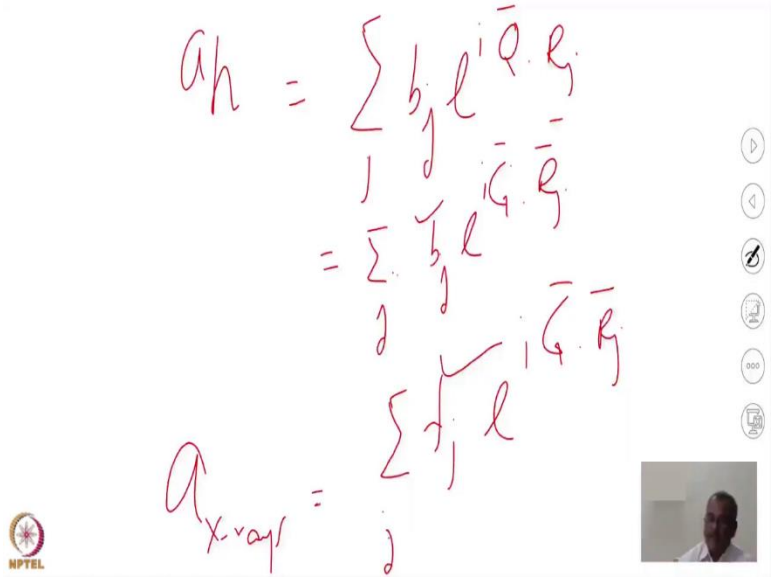

Interestingly, this gives me the selection rules. But before that let me discuss what is f_j. The expression for scattering amplitude in case of neutron was $\sum_j b_j e^{iQ.r_j}$, Q becomes G for a crystal lattice otherwise it remains same. In case of x-rays, scattering amplitude is $\sum_j f_j e^{iQ.r_j}$.

Hence, scattering amplitude for a crystalline material,

for neutrons, $a_n = \sum_j b_j e^{iG.R_j}$

for x-rays, $a_{x-rays} = \sum_j f_j e^{iG.R_j}$

Expressions are identical for both the cases. Except for the terms b_j and f_j they are identical. b_j is the coherent scattering length we wrote it as b average.

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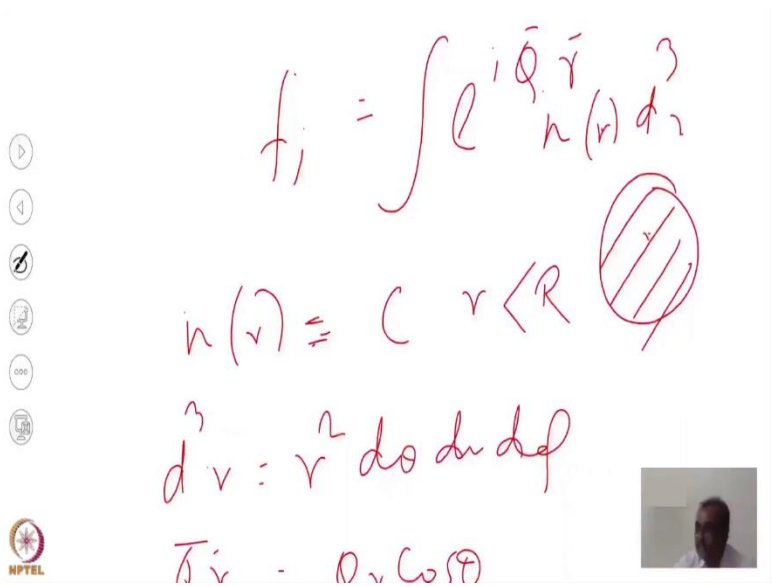

f_j is the Fourier transform of a charge cloud at the site j. This is an important difference between x-rays and neutrons. This Fourier transform for a spherical charge cloud can be written as, $f_j = \int e^{iQ.r}\, n(r)\, d^3r$. You can write n(r) equal to some constant when r is less than radius 'R'. I can assume a constant density charge cloud and then you use the relation $d^3r = r^2 d\theta dr d\varphi$ and Q.r = Qr cosθ. You can try this integral as my aim is not to evaluate this integral over here. But, the fact is, it is an extended charge cloud so the Fourier transform will look somewhat like this.

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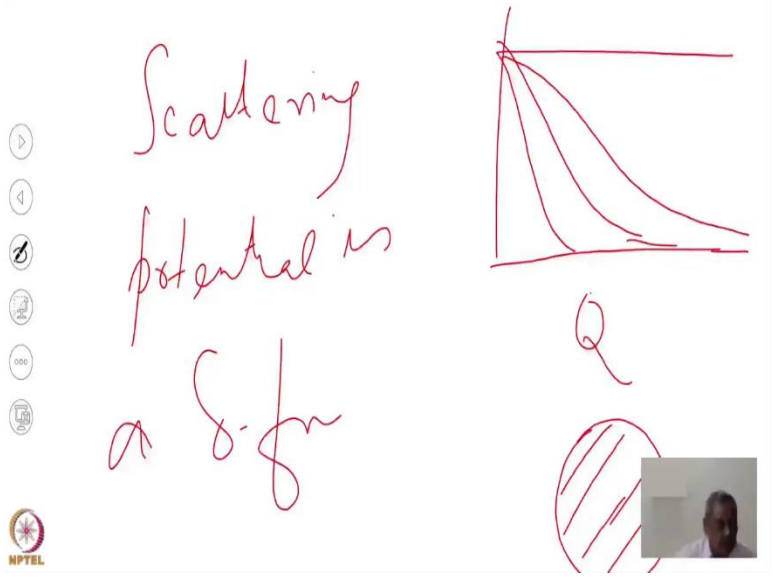

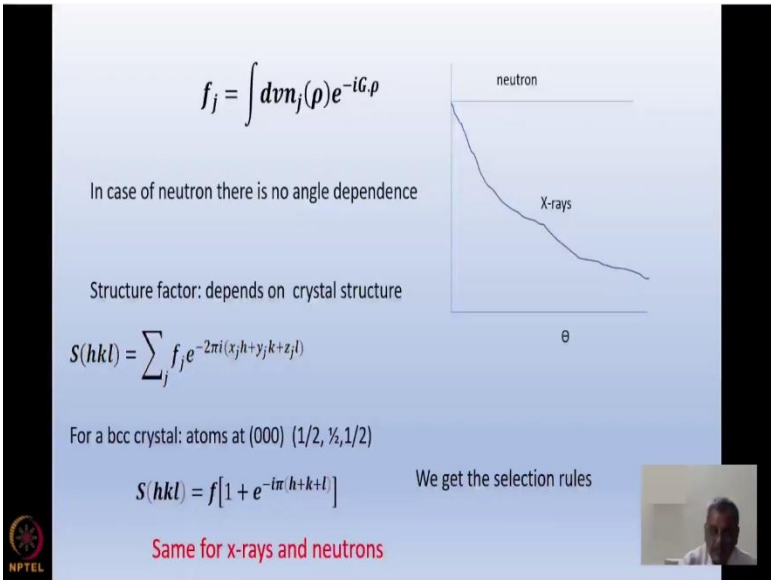

So if I draw it, the Fourier transform will fall in space (Q). But if you think in terms of the average scattering length for neutron, it does not have any angle dependence and it is constant with respect to 'Q'. It is because your scattering potential for neutrons is a delta function and the Fourier transform of a delta function is constant with Q. Delta function in real space will give a constant value in all over Q whereas in case of x-rays because it is an extended charge cloud, By extended I mean the extension is of the order of the wavelength of x-rays, you have this form factor falling in Q and larger your atom, the faster it will fall. That means, the form factor for uranium will fall much faster than the charge cloud for an aluminum.

Hence, this form factor falls with the size of charge cloud whereas in case of neutron the form factor's equivalent is b which is the coherent scattering length and it does not have any angular dependence. This is a very interesting difference. Hence, in case of x-rays you may not see large angle peaks

This is one part of the form factor, the other part depends on the structure of the crystal $2\pi(x_jh+ y_jk + z_jl)$. Hence, the structure factor is given by the form factor multiplied by part which depends on the structure.

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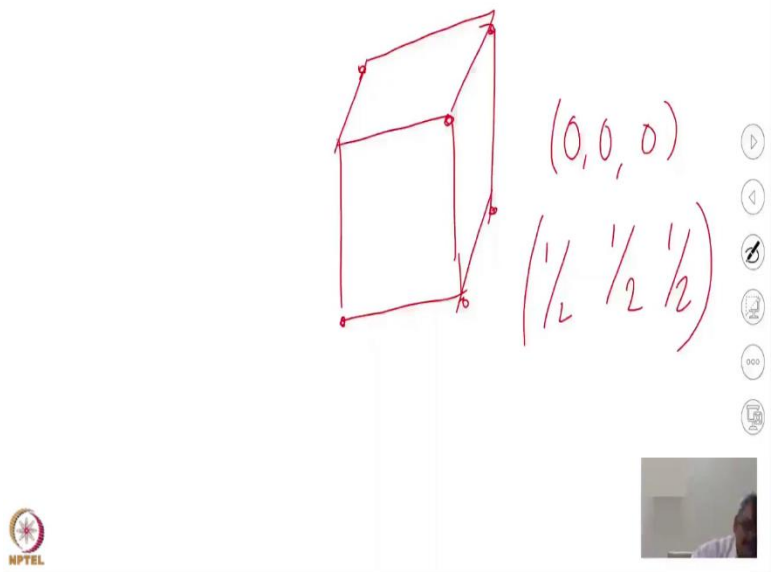

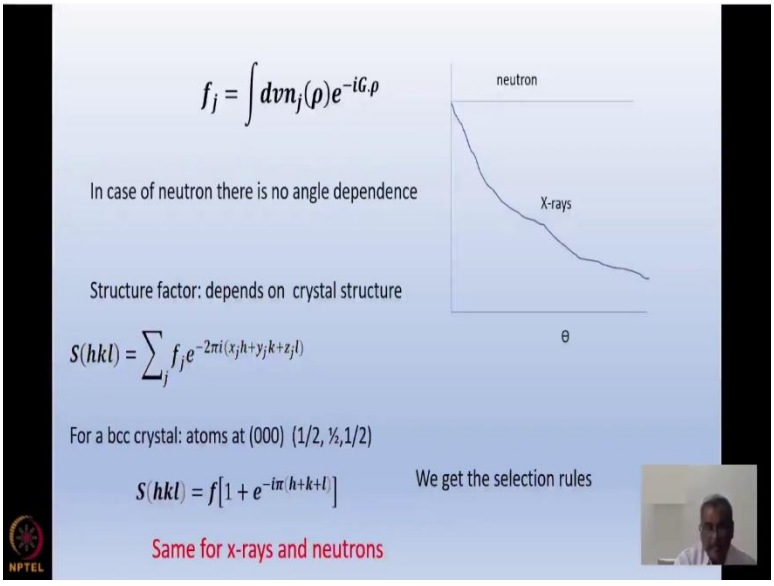

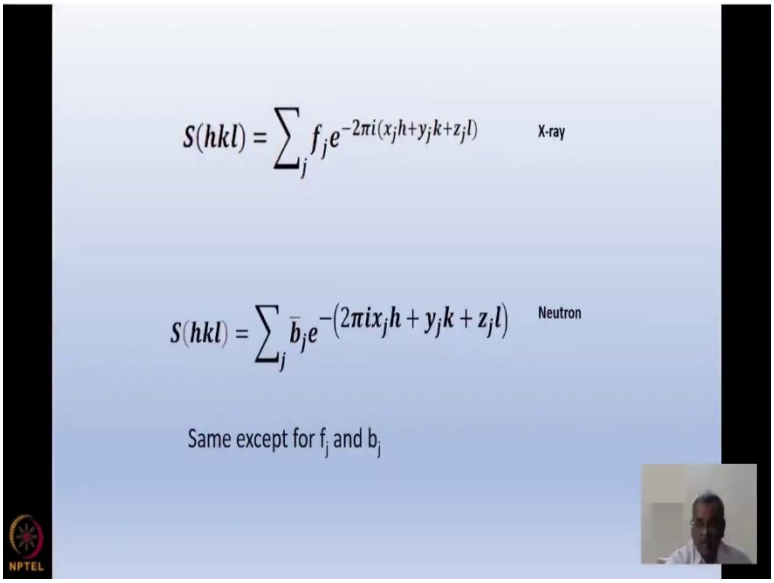

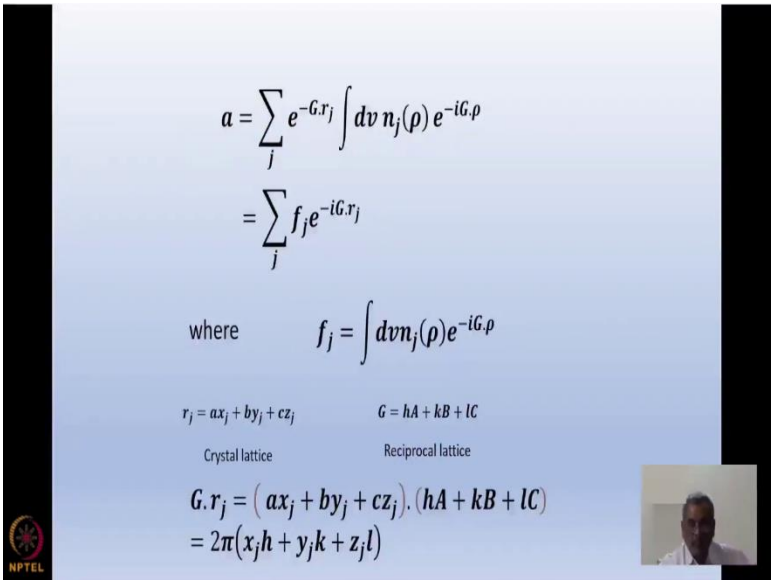

For example, if you have a bcc crystal which is a cubic crystal and you have an atom at the body center and another at (1/2,1/2,1/2). That means, if I consider the atomic coordinates for bcc unit cell there is one at 0, 0, 0 one is at (1/2,1/2,1/2). Here, if I consider only one type of atom then f_j = f (f is same for similar atoms). Hence for a bcc lattice, the structure factor reduces to,

$$S(hkl) = f[1 + e^{-i\pi(h+k+l)}]$$

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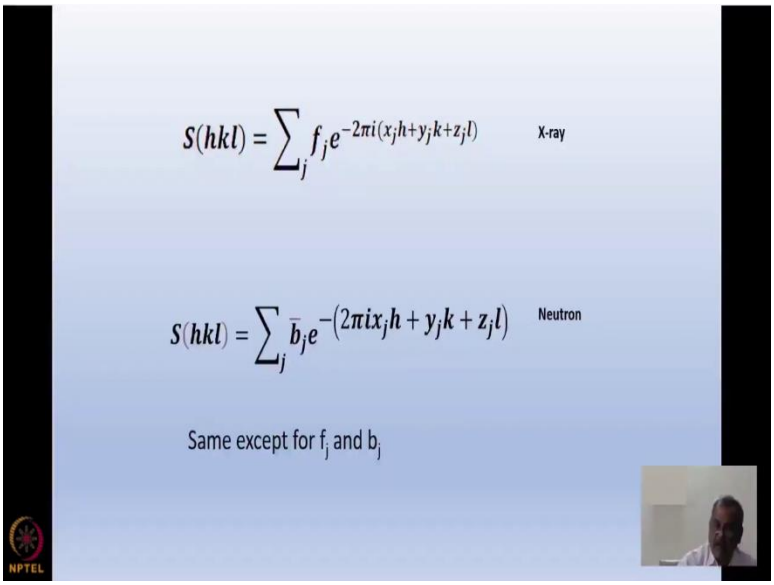

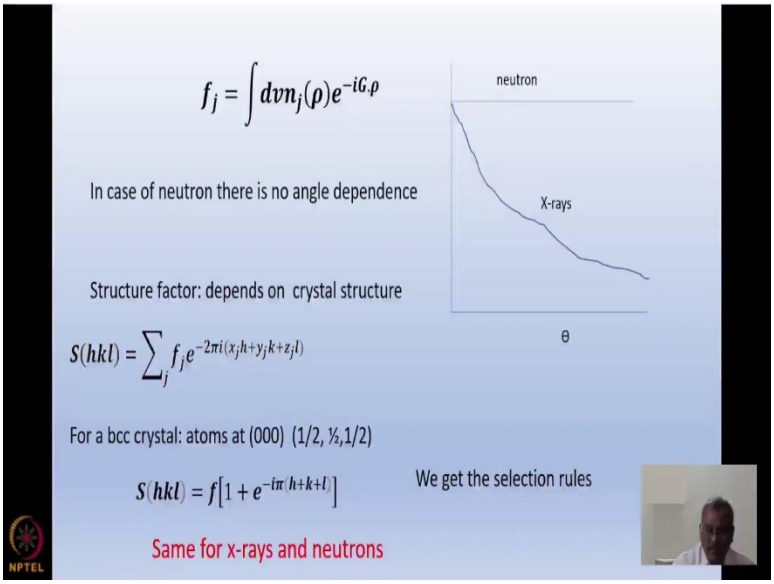

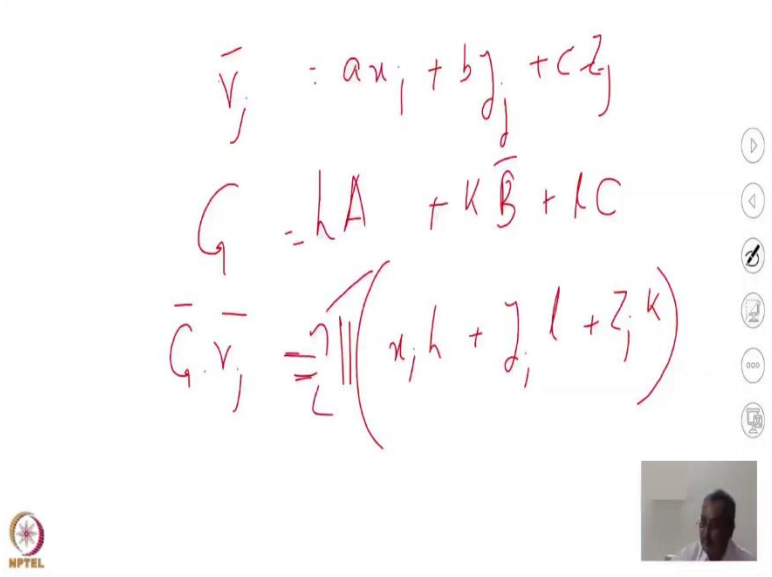

Hence, the structure factor of hkl reflection

for x-rays, $S(hkl) = \sum_j f_j e^{-2\pi i(x_j h + y_j k + z_j l)}$

for neutron, $S(hkl) = \sum_j \bar{b}_j e^{-2\pi i(x_j h + y_j k + z_j l)}$

Again, a reminder, that for x-rays there is a form factor and for neutrons there is a coherent scattering length. This relation of structure factor describes certain selection rules based on the values of h, k, l. For bcc lattice, if h + k + l is even then S = 2f. These rules are the same, irrespective of whether we use neutron or x-rays, but the form factors are different. That is why your high angle peaks for x-rays may be less intense because this f is multiplying structure factor. Your structure factor has a pre-factor f which is falling in Q space or falling in theta but b does not fall in theta. Hence, apart from this, the expression remains same and depending on the hkl values certain peaks will be allowed, certain peaks will be forbidden.

You get the selection rules which are same for x-rays and neutron, form factors are different. This way, I have established an equivalence between neutron diffraction and the way many of you have learned x-ray diffraction, they are identical, I started from slightly different points and reached at the same place.

Next, I need to discuss the thermal effect before I go forward, because so far, I have considered a lattice which is at 0 K, there are no fluctuations or no thermal effects in this lattice, I will introduce the thermal effect and then I will go ahead, thank you.