# Electron Diffraction and Imaging
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## Lecture - 12
## Diffraction – Structure and Shape Factor

Welcome you all to this course on diffraction and imaging. In the last class, we discussed how a words sphere can be used to find out what all reflections which will appear in the diffraction pattern; and also how evolves the construction of they evolves sphere has been used. To consider different types of a defractometers, then we also started talking about how to find out the intensity of the spot in the diffraction. What all factors will decide the intensity of the spots first?

Student: (Refer Time: 00:54).

Orientation other than that; what is the most important thing scattering angle other than that? Majority of oriented planes the problem is that the planes we do not talk about the atoms.

Student: Atoms.

It is.

Student: (Refer Time: 01:10).

Essentially like this how many atoms are going to diffract correct; that is essentially we have if the beam falls on n number of atoms.

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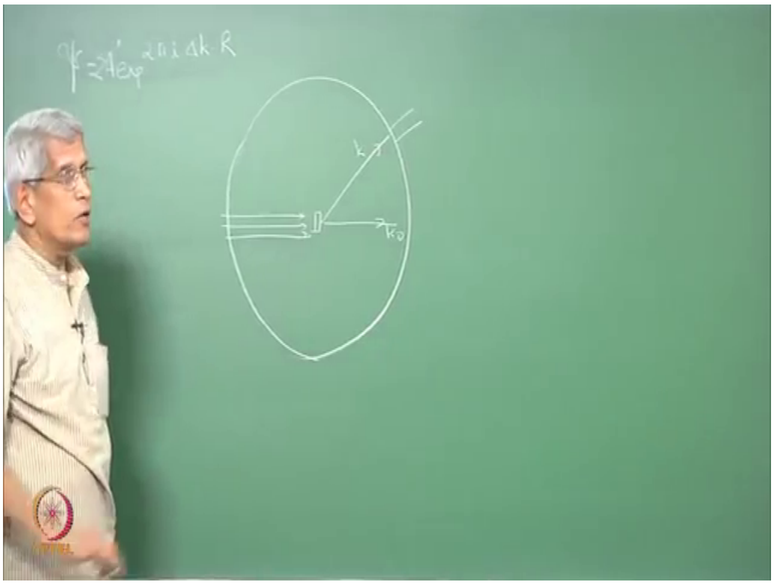

All of them contribute to intensity in each k direction, am I right? is it not that is if we have a sample if we keep it, and then electromagnetic radiation is falling onto the sample, this is the incident beam direction k 0 if you take you take in this direction k, this we define a separate different vectors because those are magnitude remains that same angle is different, so then they are distinct vectors. So, if you put a detector here and try to find out; what is going to be the intensity? The first thing which the intensity depends on is that each of them are contributing to it. So, the intensity is nothing, but amplitude squared right. So, amplitude from each of the wave which is coming, the vectorial sum is taken that sum could all add up or that sum could some cases be different that will decide the net amplitude of the density. If all add up then we say that a constructive interference has taken place correct and maximum intensity is observed. In between regions intensity will be different, is it right.

So, essentially the intensity of the diffracted spot are the amplitude of the diffracted spot first depends upon the number of atoms which are diffracting, then what is the phase relationship with which this diffraction takes place that is one also which will come into the picture to decide what is going to be the overall intensity. So, what is the way we can write the scattered wave? Then amplitude A dash was there this is sigma A dash is because if each atom the scattering amplitude could be different that is why we are taking that sort of a term, correct. What does this R depend on now? This R is essential to the position of each of the atom which we are considering it.

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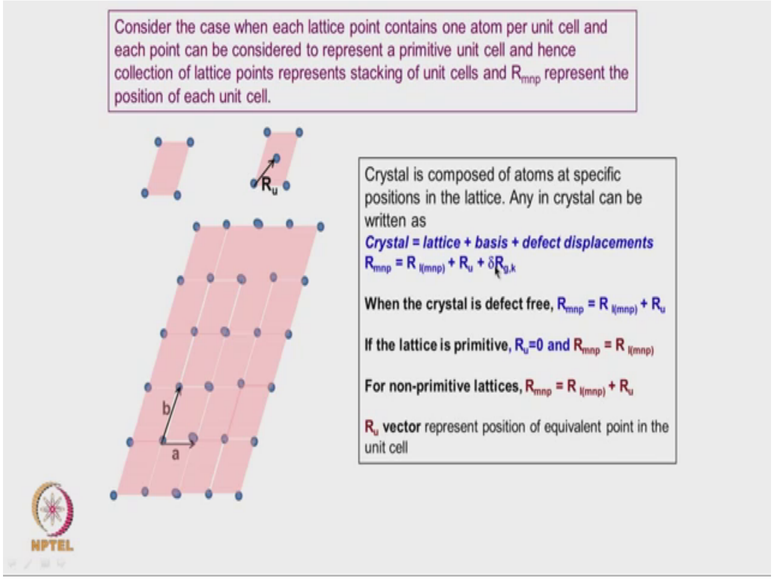

Consider the case when each lattice point contains one atom per unit cell and each point can be considered to represent a primitive unit cell and hence collection of lattice points represents stacking of unit cells and $R_{mnp}$ represent the position of each unit cell.

Crystal is composed of atoms at specific positions in the lattice. Any in crystal can be written as

*Crystal = lattice + basis + defect displacements*

$R_{mnp} = R_{l(mnp)} + R_u + \delta R_{g,k}$

When the crystal is defect free, $R_{mnp} = R_{l(mnp)} + R_u$

If the lattice is primitive, $R_u = 0$ and $R_{mnp} = R_{l(mnp)}$

For non-primitive lattices, $R_{mnp} = R_{l(mnp)} + R_u$

$R_u$ **vector** represent position of equivalent point in the unit cell

Suppose we assume that the lattice is something like a primitive lattice, then each point represents position of that what is going to be the scattering from the unit cell we can take it to be that value scattering from this point correct.

Then suppose the unit cell itself is non primitive then we can consider it in 2 ways, we can assume that the though the point represents a primitive lattice each corresponding to each of this a point other than that, there has to be some more position which should be there in the unit cell in the case of a non primitive lattice correct. This can be dealt with in a different way also, what we can tell is that it is a primitive lattice, in that the basis per lattice point could be one for primitive, could be more for others correct? That way if we consider a b c c itself, we can consider it as a simple cubic lattice with 2 basis that is 2 atoms per lattice point, but only the position where they are coming will be fixed in space that is what essentially it is that way also we can consider that.

So, essentially what will happen is that this vector R which we decide will be 1 is the lattice vector, plus the vector which corresponds to a basis which are occupying different positions in the lattice, plus this is suppose there is going to be a deviation from the exact position because there is a some defect is present. So, atom is not at the correct position then that deviation will be represented by this vector. Let us assume the case where it is a perfect crystal then this factor will turn out to be 0, correct. So, only these 2 terms have to be taken.

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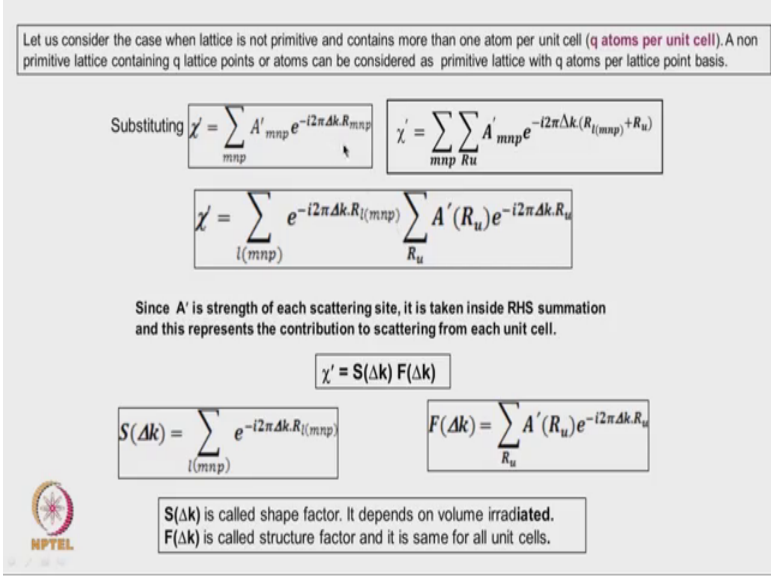

Let us consider the case when lattice is not primitive and contains more than one atom per unit cell (q atoms per unit cell). A non primitive lattice containing q lattice points or atoms can be considered as primitive lattice with q atoms per lattice point basis.

Substituting $\chi = \sum_{mnp} A'_{mnp} e^{-i2\pi \Delta k . R_{mnp}}$ $\chi' = \sum_{mnp}\sum_{Ru} A'_{mnp} e^{-i2\pi \Delta k . (R_{l(mnp)} + R_u)}$

$$\chi' = \sum_{l(mnp)} e^{-i2\pi \Delta k . R_{l(mnp)}} \sum_{R_u} A'(R_u) e^{-i2\pi \Delta k . R_u}$$

Since A′ is strength of each scattering site, it is taken inside RHS summation and this represents the contribution to scattering from each unit cell.

$\chi' = S(\Delta k)\, F(\Delta k)$

$S(\Delta k) = \sum_{l(mnp)} e^{-i2\pi \Delta k . R_{l(mnp)}}$ $F(\Delta k) = \sum_{R_u} A'(R_u) e^{-i2\pi \Delta k . R_u}$

S(Δk) is called shape factor. It depends on volume irradiated.
F(Δk) is called structure factor and it is same for all unit cells.

Then if we substitute for R, R u is essentially the position of the base say basis vectors in the lattice.

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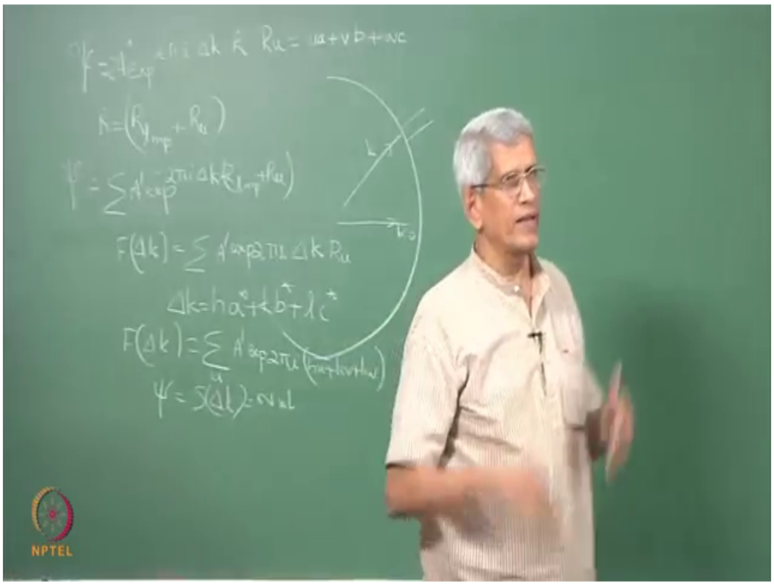

Then what will happen to be their size there will be two? This will be essentially this is what will turn out to be correct and then this can be return in term into 2 summation; correct one corresponding to the lattice position, another corresponding to the basis atoms which are there around each of the lattice point correct and so this factor is essentially nothing, but since we are considering it is a primitive lattice, each lattice has got on one layer that is each unit cell has got only one lattice point corresponding to it, this summation is essentially going to give the sum of scattering amplitude from each of the lattice points. So, if the beam is falling on common number of lattice points it is going to fall then that summation gives.

So, this is what we call it as the shape factor correct, and this factor is what we call it as the corresponding to atoms which are there within the unit cell or the number of atoms which are there around each lattice point, this is what we normally call it as the structure factor, correct.

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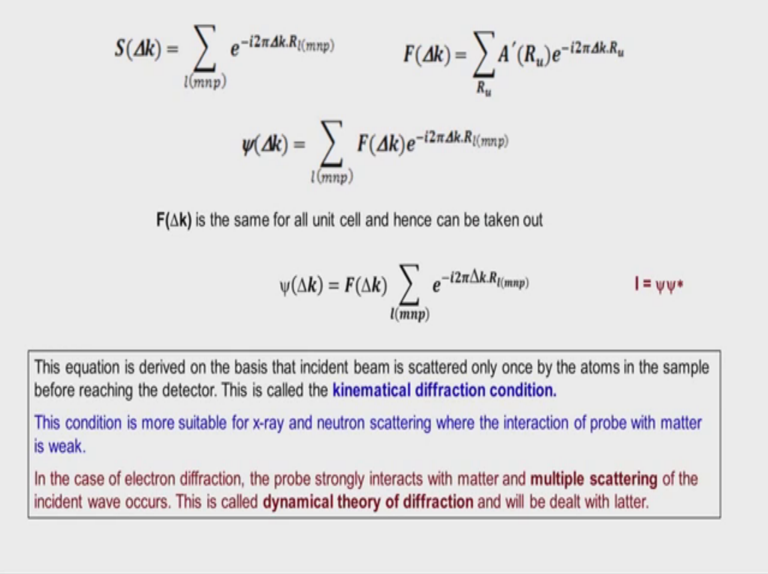

$$S(\Delta k) = \sum_{l(mnp)} e^{-i2\pi\Delta k.R_{l(mnp)}} \qquad F(\Delta k) = \sum_{R_u} A'(R_u)e^{-i2\pi\Delta k.R_u}$$

$$\psi(\Delta k) = \sum_{l(mnp)} F(\Delta k)e^{-i2\pi\Delta k.R_{l(mnp)}}$$

**F(Δk)** is the same for all unit cell and hence can be taken out

$$\psi(\Delta k) = F(\Delta k) \sum_{l(mnp)} e^{-i2\pi\Delta k.R_{l(mnp)}} \qquad I = \psi\psi^*$$

This equation is derived on the basis that incident beam is scattered only once by the atoms in the sample before reaching the detector. This is called the **kinematical diffraction condition.**

This condition is more suitable for x-ray and neutron scattering where the interaction of probe with matter is weak.

In the case of electron diffraction, the probe strongly interacts with matter and **multiple scattering** of the incident wave occurs. This is called **dynamical theory of diffraction** and will be dealt with latter.

So, these 2 together is going to decide the intensity of each of the diffraction spot and with this derivation essential assumption are the main assumption which we have made is that the wave which is coming is being scattered by one lattice point, the wave which is scattered before it reaches the detector we do not assume that it is being scattered again. So, when such an assumption is being made this type of scattering the theory which is developed is called as the kinematical theory of diffraction. Most of the x-ray diffraction it is assumed that it is only one scattering even which is taking place. There are some conditions where even in x-ray multiple diffraction do multiple scattering do take space for which the dynamical theory was derived, in fact that extension of that what is being used in the electron microscopy. The other one which we have to consider it is that, since it is a primitive each atom that is each lattice point represents one unit cell and then if we consider that is the summation which is going to a shape factor that we will deal with later.

Let us look at the structure factor. Suppose the sample contains gets a primitive lattice only one atom per unit cell, then each atom is going to be at the origin correct the atom is going to be only at the origin of the unit cell, then what will happen to that is the c F of k, R u, correct. If it contains one atom per unit cell R u will turn out to be 0 0 0, correct otherwise what will be the value it can be any general vector which we can take this R u will be equal to h u plus k v no; u into a plus v into b plus w into c that is what R u. If you consider diffraction is taking place in a particular direction, the diffraction vector we represented with h k l. So, this vector delta k essentially can be written as h into a star plus k into b star, plus l into c star. So, if we substitute this will turn out to be k v plus l w this is what this equation will turn out to be, correct.

If it contains it is a primitive lattice the lattice point is at the origin, that u v w will turn out to be 0 0. So, this factor will all turn out to be only 1. Suppose n n lattice points are there in that sample, then what is going to be the total intensity of the total scattered amplitude that will be equal to because s of delta k right for the primitive lattice if n atoms are going to be there this number is n, n into 1, that is what is going to be the amplitude, the size starts is why at the intensity is that will turn out to be n square.

Student: one.

Huh if it is one and only thing which we have to consider here is that by into that amplitude this a star will also come into the picture. This amplitude part I said that we will come back later. Suppose we assume that the lattice contains it is a b c c lattice, b c c can be considered as a simple cubic lattice with 2 atoms per each lattice point and the position at which the atoms will appear R 1 will be R u 1, u 1 is at 0, 0, 0, another R u 2 will be half, half, half, correct with respect to unit cell this is the position at which it is going to come.

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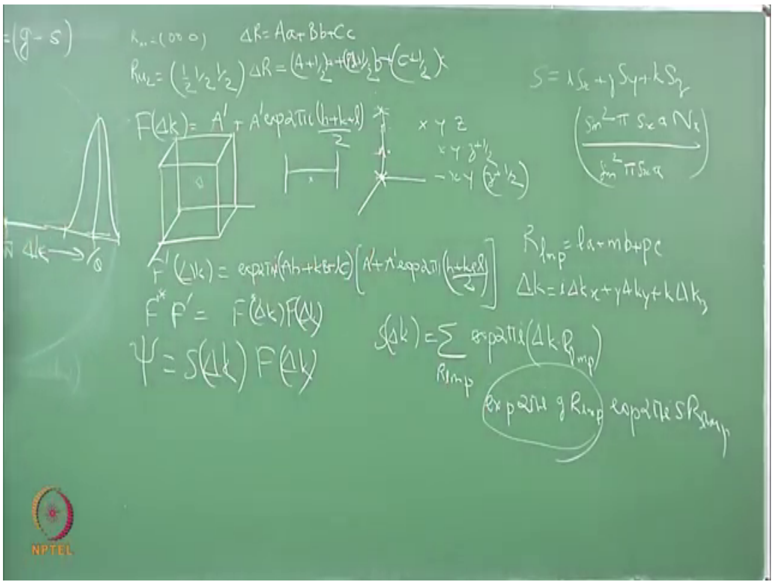

Then if we substitute for this here in this, what it will turn out to be? Then F of delta k will turn out to be 1 is A dash plus another is A dash into exponential 2 pi i, h plus k plus l by 2. This is what it is going to turn out correct this is going to be the scattering from each of the lattice point, this multiplied by the number of lattice points which are there which are contributing to a the intensity of the diffracted spot then we can find out the total amplitude and the intensity we can get that information.

This automatically tells us what is the selection rule for visibility or invisibility of the diffraction spots; here what it has to be h plus k plus l by 2 has to be h plus k plus l has to be an even number correct. If it is even then it is always going to be that max intensity maximum will be there when it is odd you get minus. Then since the scattering intensity because we are considering 2 atoms per unit cell and they are of the same type since we are considering b c c as a crystal, this scattering amplitude is going to be the same. So, it turns out to be 0 correct what one should remember here is that with respect to a unit cell we have considered the position of this atoms, correct.

So, essentially we have all the diffraction spots whatever we do all these calculations are valid for the lattice. Either; one atom can be there here and then another atom can be here at the center that is what this condition is. Suppose I keep the position of the atom this position is shifted by some distance some vector delta R, then this atom will also be shifted by the vector delta R, the position of atom in the unit cell is not unique; even if we till the position shift the atom position, the intensity of the diffracted spot is not going to change now the position where they are going to come. What will essentially happen is that suppose this delta R turns out to be at A into a, B into b plus C into c where a b c are some constants. So, by which all the atom positions are shifted; now what will happen to this expression when we write it.

Student: (Refer Time: 17:46).

Substitute it then.

Student: (Refer Time: 17:47).

Similarly, this will become delta R will become what it will become A plus half into a correct plus B plus half into b plus C plus half into c correct this is what it will turn out to be. So, finally, if we substitute this f of delta f dash of delta k, before the new position will turn out to be exponential of 2 pi i A into h l into c into it will turn out to be A dash plus A dash into exponential 2 pi i h plus k plus l by 2. This is how this expression will turn out to be, this you can substitute and see that.

This is only a phase factor, intensity when we write it we write F dash star into F dash, then this factor will turn out to be one right then it will turn out to be nothing, but F star delta k d F of delta k; this is the way it will turn out to be that means, that the diffraction intensity is not really dependent upon what is exactly the position at which the atom is placed in the lattice is it clear? Only thing is that the atom is all displaced by the same amount each of the position because the relative distance has to be kept that same then the intensity just does not matter because whatever we get it in intensity is corresponding to the lattice is what we are getting it lattice point, the basis the contribution of the basis is essentially to the intensity and that does not change by changing the position of the atom like this.

Now, f c c can be considered as a simple cubic lattice with 4 basis atoms correct similarly diamond can be considered as a simple cubic lattice with 8 basis atoms, only thing is that the position of the basic atoms which we fix it is corresponding to the lattice position of the position in the f c c, that way also we can consider. Similarly diamond cubic can also be considered as an f c c and with respect to that with 2 atom positions for each of the lattice point of f c c lattice point that way also we can consider it. Using these concepts one can calculate the amplitude of the diffracted spot from the unit cell. Now I would expect you to do this as an exercise and workout and check for yourself and normally what we see in the diffraction pattern is not the amplitude, but the intensity.

So, when we try to find out the selection rules there is the formula for the intensity and then try to find out what are the conditions under which it will be present or absent that way I would expect you to do that. There is for various structures, there is different you can consider lattices with either you can consider different Bravais lattice with one atom per unit cell or it can be considered as a primitive lattice with some number of basis atoms corresponding to each of the lattice point whichever way you want you can consider it, but when you find out the selection rules are the intensity which you wanted to find out, it has to be done taking psi that is F of star that way you try to find out; that way one can find out what all the factors which it is going to be.

If you apply that condition what it will happen for a primitive lattice? There is no extinction condition correct that is all the diffraction spots are going to be visible, it does not matter whether it is a triclinic lattice or a whether it Is an orthorhombic all that planes will give raise to diffraction, then if it say a centered or b centered or c centered depends if suppose it is an a centered lattice.

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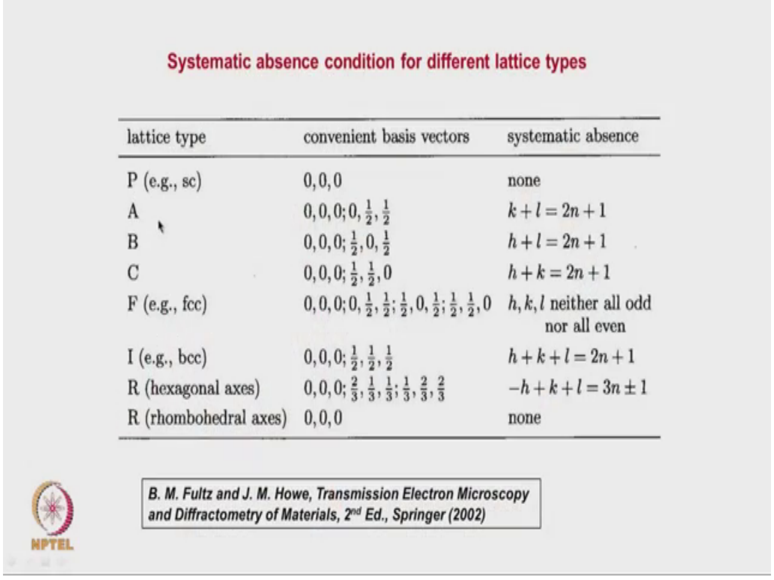

Systematic absence condition for different lattice types

| lattice type | convenient basis vectors | systematic absence |
|---|---|---|
| P (e.g., sc) | 0,0,0 | none |
| A | $0,0,0;0,\frac{1}{2},\frac{1}{2}$ | $k+l=2n+1$ |
| B | $0,0,0;\frac{1}{2},0,\frac{1}{2}$ | $h+l=2n+1$ |
| C | $0,0,0;\frac{1}{2},\frac{1}{2},0$ | $h+k=2n+1$ |
| F (e.g., fcc) | $0,0,0;0,\frac{1}{2},\frac{1}{2};\frac{1}{2},0,\frac{1}{2};\frac{1}{2},\frac{1}{2},0$ | $h,k,l$ neither all odd nor all even |
| I (e.g., bcc) | $0,0,0;\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | $h+k+l=2n+1$ |
| R (hexagonal axes) | $0,0,0;\frac{2}{3},\frac{1}{3},\frac{1}{3};\frac{1}{3},\frac{2}{3},\frac{2}{3}$ | $-h+k+l=3n\pm1$ |
| R (rhombohedral axes) | 0,0,0 | none |

B. M. Fultz and J. M. Howe, *Transmission Electron Microscopy and Diffractometry of Materials*, 2nd Ed., Springer (2002)

The orthorhombic a centered; so the positions of the basis vectors will be 0, 0, 0, 0, half, half, then with respect to this the systematic absences will be seen when k plus l is equal to 2 n plus 1 where n is an integer. I would expect all of you to derive all this because only the final expression is being given then you will understand it much better.

Similarly, like f c c when we do it, we get the condition whether h k l are all odd or even; similarly for hexagonal axis if you use for Rhombohedral system, then we get the condition that minus h plus k plus l equals 3 n plus 1, these various conditions this is just using this formula ok choosing the basis vectors for the different atom positions, and then trying to find out what all the conditions under which the intensity will add up what all the conditions under which the intensity will be becomes 0. This happens because all atoms we assumed to be the same type of an atom, but suppose there is glide and screw axis which is present.

Let us consider the glide. What is a glide mean that is in between the point there is one more in a intermediate position where there is an atoms are there right. So, in that direction where we consider as the glide essentially it is half the distance some plane is going to be there, and what will be the effect of any position initially it was not there. If at half position if it comes what it will happen the condition which will happen with respect to that, the reflection corresponding to all the even odd ones will not be present in that direction only even reflections will be present. You consider a simple cubic lattice simple cubic lattice that is 1 0 0 plane is the one which gives rise to a fundamental diffraction correct there is no absence is there. In between if I put an atom at the middle then it becomes body centered, then what is going to be the separation between the planes now it becomes to 0 0, that is the one which gives rise to a diffraction, the other one which is a distance which is going to be exactly half of that that interferes with it and the intensity of 1 0 0 becomes 0 correct; 1 0 0 reflection is not permitted in we see it simple cubic and no b c c as well as f c c.

Similar to that here also initially from here to here is the lattice translation vector, so, these are all the planes which are giving raise to diffraction, now because we have a glide along this one, there is a row of atoms are coming in this particular plane the effect of that is what is going to be is that, if it is in the direction a direction. So, h will represent the diffraction plane index corresponding to that correct and h should be equal to 2 n that is what essentially. So, the systematic absences you will have a differences which will come here that is what the; for the glide which it is going to be there. The presence and absence you will find that 2 n plus one is absent the 2 n when you take it will be present that is 2 0 0 reflection will be there one 0 0 will be absent 3 0 0 reflection will be there. This is for absence for h k 0 you know why this term h k 0 we consider it.

Student: (Refer Time: 26:54).

How do you represent a position of a atoms in the unit cell for a mirror? Suppose it is x y e z.

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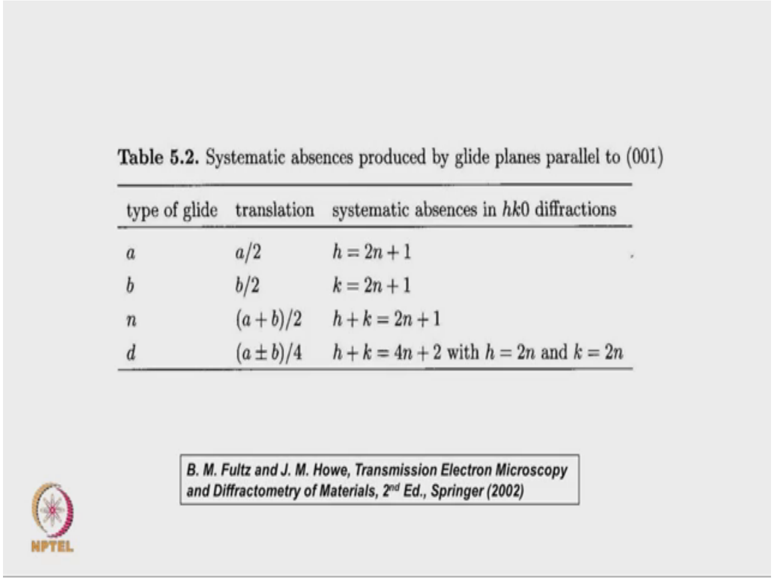

**Table 5.2.** Systematic absences produced by glide planes parallel to (001)

| type of glide | translation | systematic absences in $hk0$ diffractions |
|---|---|---|
| $a$ | $a/2$ | $h = 2n + 1$ |
| $b$ | $b/2$ | $k = 2n + 1$ |
| $n$ | $(a + b)/2$ | $h + k = 2n + 1$ |
| $d$ | $(a \pm b)/4$ | $h + k = 4n + 2$ with $h = 2n$ and $k = 2n$ |

*B. M. Fultz and J. M. Howe, Transmission Electron Microscopy and Diffractometry of Materials, 2nd Ed., Springer (2002)*

The mirror plane is along assume that 0 0 1 if the mirror is there are the glide plane is there, glide is along 0 0 1 if you take it then what will happen? So, if the glide then this is first x y e z plus half from any position it will be brought to this position correct, then the reflection will be taken of this one.

So, this will turn out to be minus x y e z plus half this is going to be the position of one of the atoms correct is it not? So, the 2 positions are going to be there if we substitute for this in the same expression, we will be getting this sort of. Similarly let us like if it is a diagonal glide it is going to be there, then h plus k it will turn out to be if it is going to be a diamond glide then it is going to be h plus k equals 4 n plus 2, these sort of this one only the table which is being given, I would expect you to work out all these things and check this table whether it is correct or not, then you will understand also how it comes ok there is no point in spending time and deriving all these.

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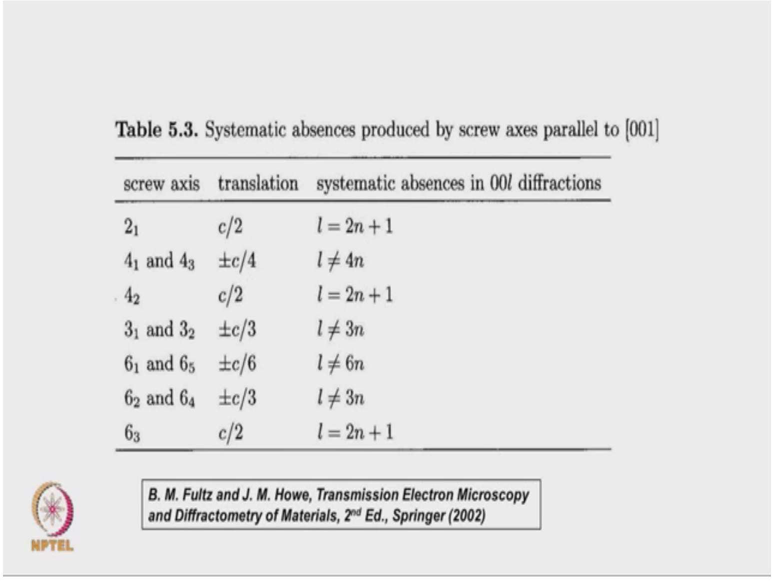

**Table 5.3.** Systematic absences produced by screw axes parallel to [001]

| screw axis | translation | systematic absences in $00l$ diffractions |
|---|---|---|
| $2_1$ | $c/2$ | $l = 2n + 1$ |
| $4_1$ and $4_3$ | $\pm c/4$ | $l \neq 4n$ |
| $4_2$ | $c/2$ | $l = 2n + 1$ |
| $3_1$ and $3_2$ | $\pm c/3$ | $l \neq 3n$ |
| $6_1$ and $6_5$ | $\pm c/6$ | $l \neq 6n$ |
| $6_2$ and $6_4$ | $\pm c/3$ | $l \neq 3n$ |
| $6_3$ | $c/2$ | $l = 2n + 1$ |

B. M. Fultz and J. M. Howe, Transmission Electron Microscopy and Diffractometry of Materials, 2nd Ed., Springer (2002)

What will happen in the case of a screw also? Suppose we say that there is a threefold screw along c axis; that means, that initially with respect to this axis an atom was here, that is maybe 3 atoms here maybe some 3 atoms are there threefold symmetry, now atoms are not in this plane and in this plane now one in this plane another at one third of the distance another at one third of the distance correct then at.

Student: (Refer Time: 29:28).

Full distance one lattice point it comes similarly like this along all these axis it is going to be there. So, essentially if you look in that direction we have 2 more planes which have come in between, correct.

So, now what is going to happen is that initially this 1 0 0 plane which was responsible for it with respect to this now the closest distance is going to be one third of that. So, 3 0 0 planes are the ones which are going to be the planes which are present, others are going to be absent, that is what essentially is given with this condition that is with respect if it is 2 1, l is equal to here 3 1 and 3 2, l is not equal to 3 n it is absent and these conditions follow exactly the same whether using the symmetric condition we can derive what all the reflections which will be absent.

So, what you can make out from this that is a almost all the symmetry elements which we are considering, what will be the effect on the diffraction pattern that is given by these relations. Indexing a pattern we can get some information about with respect to a lattice, what all the types of groups to which it can this crystals can belong, but we can get information about exact atom positions because the phase of the atom position is lost when they we take the intensity of the diffracted spot. Is it not whether the crystal contains a twofold rotation a twofold screw or 4 1 screw, all these types of screw axis whether they are present or not that information is contained in the diffraction pattern itself is this clear.

So, regarding screw we have regarding glide also we have that information then regarding the atom positions in the lattice which positions they are occupying, we are getting conditions for the presence or absence of a diffraction spots for various types of Bravais lattices correct? These are all the information which is available from this structure factor calculation is this clear. So, when we have to find out the intensity the total intensity is part it depends upon the delta k, and we have to take f of delta k. We have now just considered f of delta k how it is going to they are depending upon the type of a crystal structure how f of delta k gets affected s of delta k depends upon how many atoms are going to be there, correct.

Here what is the expression for this the expression for this is correct this is the expression to find out the total amplitude of the scattered wave from each of the individual lattice position, how do we define this? This definition we define it as correct this is how we defined that vector R at each of the lattice point right, delta k we can define as this way we can define it is it not what it will happen? This is the sort of an expression which will turn out here m n p is written I think I have taken l m p.

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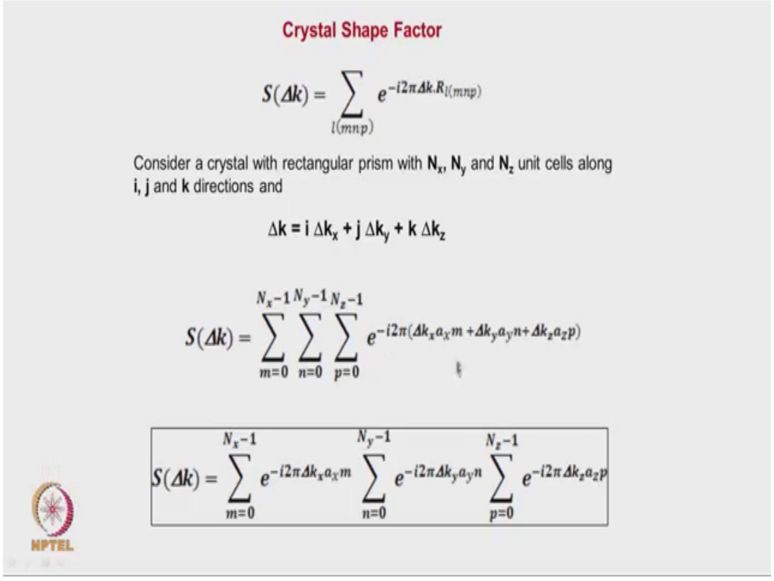


**Crystal Shape Factor**

$$S(\Delta k) = \sum_{l(mnp)} e^{-i2\pi \Delta k . R_{l(mnp)}}$$

Consider a crystal with rectangular prism with $\mathbf{N_x}$, $\mathbf{N_y}$ and $\mathbf{N_z}$ unit cells along **i**, **j** and **k** directions and

$$\Delta \mathrm{k} = \mathrm{i}\, \Delta \mathrm{k_x} + \mathrm{j}\, \Delta \mathrm{k_y} + \mathrm{k}\, \Delta \mathrm{k_z}$$

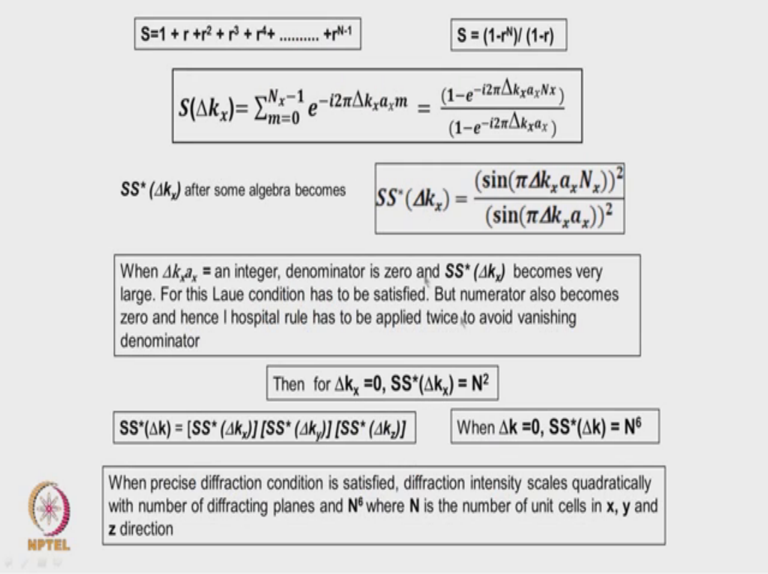
$$S(\Delta k) = \sum_{m=0}^{N_x-1} \sum_{n=0}^{N_y-1} \sum_{p=0}^{N_z-1} e^{-i2\pi(\Delta k_x a_x m + \Delta k_y a_y n + \Delta k_z a_z p)}$$

$$\boxed{S(\Delta k) = \sum_{m=0}^{N_x-1} e^{-i2\pi \Delta k_x a_x m} \sum_{n=0}^{N_y-1} e^{-i2\pi \Delta k_y a_y n} \sum_{p=0}^{N_z-1} e^{-i2\pi \Delta k_z a_z p}}$$

So, this can be written essentially in this form because since it is an exponential function. So, essentially summation corresponding to one corresponding to this one product of 3 terms one in the x direction, one in the y direction, and another in the e z direction. This summation is over in the particular direction with respect to delta k x, the atom position from m equals 0 to N x minus 1 that is essentially from N x atom positions are there, correct.

Similarly, on the other direction because we are choosing a Cartesian coordinate. If anyone of this term if we take it how we can write this? This is 1 minus I into e to the power of 2 pi delta k x this if you take it within bracket the whole to the power of m.

(Refer Slide Time: 35:16)



S=1 + r + $r^2$ + $r^3$ + $r^4$+ .......... +$r^{N-1}$

S = (1-$r^N$)/ (1-r)

$$S(\Delta k_x)= \sum_{m=0}^{N_x-1} e^{-i2\pi\Delta k_x a_x m} = \frac{(1-e^{-i2\pi\Delta k_x a_x Nx})}{(1-e^{-i2\pi\Delta k_x a_x})}$$

**SS* (Δk$_x$)** after some algebra becomes

$$SS^*(\Delta k_x) = \frac{(\sin(\pi\Delta k_x a_x N_x))^2}{(\sin(\pi\Delta k_x a_x))^2}$$

When $\Delta k_x a_x$ = an integer, denominator is zero and **SS* (Δk$_x$)** becomes very large. For this Laue condition has to be satisfied. But numerator also becomes zero and hence I hospital rule has to be applied twice to avoid vanishing denominator

Then for **Δk$_x$ =0, SS*(Δk$_x$) = N$^2$**

**SS*(Δk) = [SS* (Δk$_x$)] [SS* (Δk$_y$)] [SS* (Δk$_z$)]**

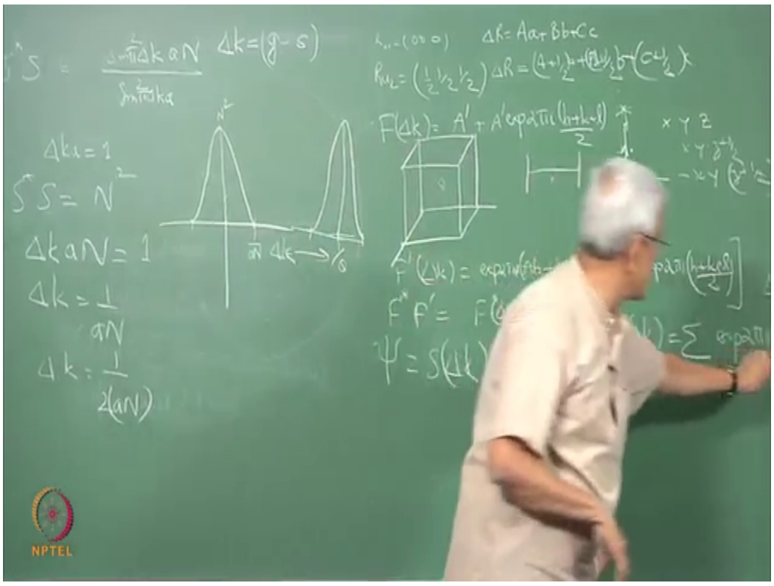
When **Δk =0, SS*(Δk) = N$^6$**

When precise diffraction condition is satisfied, diffraction intensity scales quadratically with number of diffracting planes and **N$^6$** where **N** is the number of unit cells in **x, y** and **z** direction

We can write it right is this nothing, but if I put this as R this sigma is one R to the power of m this summation will turn out to be one plus R plus this is how we can write it, this is a geometrical series.

So, what is the sum of a geometrical series 1 minus R to a power of n, this is what this value will turn out to be for each of them this is just the mathematics.

(Refer Slide Time: 35:50)



So, finally, if you substitute SS star, we will be getting a term like this. This is essentially 2 sin terms are there because the this is the intensity which we are considering it right and this is what it turns out to be how will this function look like if you try to plot in this is when delta k into a equals now pi has to be there, is equal to 1 what will happen to this term this will become 0 correct, but at the same time this also will become 0.

Student: (Refer Time: 36:36).

When such similar functions that are hospital rule you remember that with which we try to find out that has to be applied, then what will happen is that S star S will turn out to be N square. This part of it you can whatever the differentiation which you have studied earlier part of that that you have to apply and you will get this, this is corresponding to at delta k equals 0, correct.

So, there are 2 conditions which are coming suppose delta k into a into N equals 1 then what happens? Then also this function will become 0, but these need not become 0. So, there are many secondary maxima. So, one maxima that is corresponding to this becomes 0 means that first 0 comes as delta k equals 0 if you try to plot it maximum is n square it (Refer Time: 37:44) and where is the first minimum comes for delta k equal to one by a into N where N is the number of atoms in that direction.

So, if this is the delta k which we are trying to plot it focus here. So, for a delta k value which is corresponding to 1 by a N the intensity will drop down to 0 correct or this delta k value at which this side also you will be getting it. So, if you look at this width that gives information about the number of atoms in a particular direction which is contributing to diffraction.

If the number is going to be infinite in all the directions then this will turn out to be almost like a point here the delta k value will become smaller and smaller is it not; that means, that the number of atoms in a row can be equivalent to number of planes which are perpendicular to that also we can take that to be. So, depending upon how many planes which are going to scatter contribute to scattering, the intensity more the number of planes the intensity of the diffracted spots become the width becomes smaller and smaller it becomes very sharper.

If it contains only 2 spots which are going to be there then what will happen you know if it contains only 2 planes, then what will happen? It is only that it is like a sin function that is one between the first order diffraction and the second order diffraction the intensity will be continuously dropping down in between it will become 0 and then it will go to a maximum, the separation between the peaks will not come. Normally in the x ray diffraction peak when you get it the first order diffraction to the second order diffraction if you look at it the peak width is very small n a and you have studied that using the peak width or the full width at half maximum which you measured (Refer Time: 39:59) that is also another measure of the peak width, that you can talk about the size of the grain this is the reason why in a diffraction spot when more spots which are arranged in a periodic wave (Refer Time: 40:14) lattice points which are arranged in periodic way, they give rise to they contribute to diffraction then we get peaks at only some specific position and in between positions there are some intensities are there, but that intensity is too small compared to the peak height that we are not able to see it.

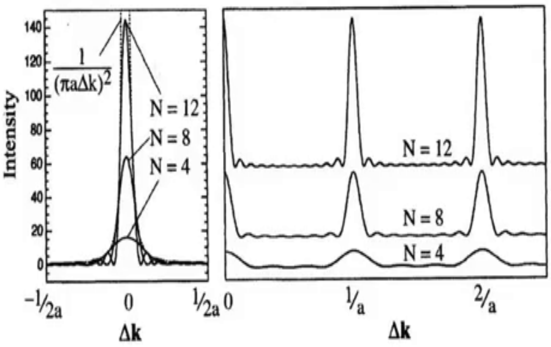
So, this is the general condition which we can derive to find out when the maxima will take place when the minima will take place, that is essentially depends upon what is the value of N because this gives the condition for minimum of the peak right the intensity becoming 0, the intensity becoming maximum intermediate peaks what it will happen 1 by 2 into a N, correct if this value becomes if we substitute then this term will turn out to be pi.

Student: (Refer Time: 41:12).

Finally it will turn out to be pi by 2 correct then the maximum intensity will come. So, that is what is shown here for various peaks, that is the reason why we call this term as a shape factor; because depending upon how many atoms in each of the direction contribute to diffraction, the width of the diffraction peak in that direction depends on that.

And another important information comes is that though the maximum of the intensity we get it at corresponding to delta k equals 1 by a or delta k equals 0 or multiples of delta k, that delta k equals n by a you can write it for that value will be getting that all peak positions. For delta k values away from it also there is some intensity some contribution to intensity right is it not? It is not that only at the exact g value you are getting the intensity, see this will correspond to a position which is on 0 another it may come somewhere like this a position will come, but away from this particular value this will come first 1 by a, away from this also up to a particular width we are getting some intensity. So, that is the effect of finite size of the sample which is diffracting what will be the other way also this can be considered.

(Refer Slide Time: 42:53)

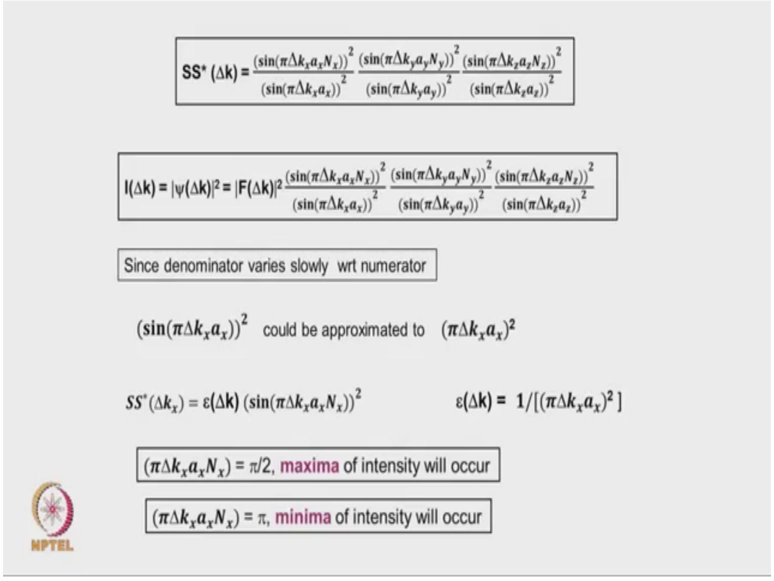


***B. M. Fultz and J. M. Howe, Transmission Electron Microscopy and Diffractometry of Materials, 2nd Ed., Springer (2002)***

Here we have written suppose we wanted to represent this deviation from the exact delta k value this value when it corresponds to 0 or corresponds to this value this is what we call it as a reciprocal lattice vector, and some deviation from the reciprocal lattice vector also we get it. So, that is what we write it as a general delta k. So, this delta k can be represented as g minus s we can write it, s is the deviation from the exact brag position that way we can do it.

So, if we substitute this value here then this will turn out to be exponential 2 pi I, g dot R l n p into S dot R l n p will come correct. This term is going to be one now this term is going to be S of delta k is going to depend upon summation over l n p over this term correct. What is S? S is deviation from the brag position that can also be in a vector notation we can write it S equals I into S x plus j into S y plus k into S z. If we write like that then what will happen is that this expression is there n a, all the delta k x will be replaced by S x this will be replaced by S y, this will be replaced by s z that is what it will turn out that you can derive that part of it though.

(Refer Slide Time: 44:39)



$$\boxed{SS^*(\Delta k) = \frac{(\sin(\pi\Delta k_x a_x N_x))^2}{(\sin(\pi\Delta k_x a_x))^2}\frac{(\sin(\pi\Delta k_y a_y N_y))^2}{(\sin(\pi\Delta k_y a_y))^2}\frac{(\sin(\pi\Delta k_z a_z N_z))^2}{(\sin(\pi\Delta k_z a_z))^2}}$$

$$\boxed{I(\Delta k) = |\psi(\Delta k)|^2 = |F(\Delta k)|^2\frac{(\sin(\pi\Delta k_x a_x N_x))^2}{(\sin(\pi\Delta k_x a_x))^2}\frac{(\sin(\pi\Delta k_y a_y N_y))^2}{(\sin(\pi\Delta k_y a_y))^2}\frac{(\sin(\pi\Delta k_z a_z N_z))^2}{(\sin(\pi\Delta k_z a_z))^2}}$$

Since denominator varies slowly wrt numerator

$(\sin(\pi\Delta k_x a_x))^2$ could be approximated to $(\pi\Delta k_x a_x)^2$

$SS^*(\Delta k_x) = \varepsilon(\Delta k)\,(\sin(\pi\Delta k_x a_x N_x))^2$ $\varepsilon(\Delta k) = 1/[(\pi\Delta k_x a_x)^2]$

$(\pi\Delta k_x a_x N_x) = \pi/2$, maxima of intensity will occur

$(\pi\Delta k_x a_x N_x) = \pi$, minima of intensity will occur

Student: (Refer Time: 44:57).

When you expand this;

Student: (Refer Time: 44:58).

This term will turn out to be sin squared I will write for a x, sin squared pi S x into a into N, x divided by sin squared pi S x into a this, you will look at these 2 these 2 are similar correct exactly that is what it is going to turn out to be. So, this can be express in terms of how much is the deviation from the brag angle up to which we are able to see some intensity in the diffraction spot correct. Where is the first minimum occurs for what deviation that way also we can represent it the width, correct.

Student: Sir (Refer Time: 45:53) we s y into (Refer Time: 45:54).

Yeah, exactly;

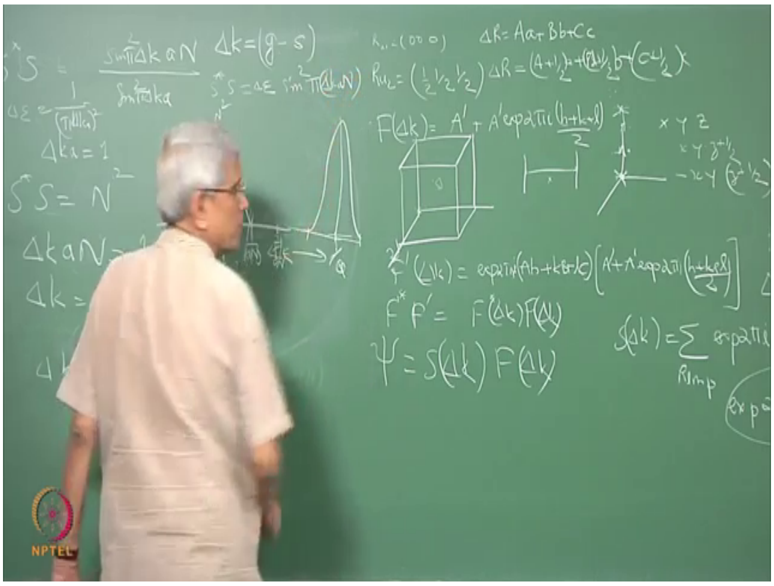
Student: Sir with beyond which also we should get some (Refer Time: 45:59).

Which one?

Student: Beyond (Refer Time: 46:02) also we can write and we get some (Refer Time: 46:05).

No intensity how we you will be getting it is essentially here this is what essentially one this is 1 by a correct and then 2 y a, 1 2 by a it will come like this it will go in this direction correct periodicity then you will be getting some intensity maxima corresponding to a by n right, then corresponding to in between then 1 by a by n, 2 by m by n like that it will come then some particular value of n by a by n will turn out to be this peak height. In between middle position corresponding to a value of equal to one by twice a by n you will be getting the maxima intensities; that maxima of intensity also if you try to look at it that intensity also will be changing it will be decreasing with, how we can look at it is that here if you see that how does it fluctuate between maxima and minima for a very large value correct compared to this here it is going to be a slowly varying function.

(Refer Slide Time: 47:34)



Student: (Refer Time: 47:24)

Which one?

Student: Upper one will vary every one by (Refer Time: 47:27).

Yeah, here;

Student: (Refer Time: 47:29) vary every one by (Refer Time: 47:30).

(Refer Time: 47:31). So, this can be approximated to essentially a function like delta psi equals 1 by pi delta k into a the whole square, this sort of approximation can be done it is a slowly varying function sin can be approximated to theta a theta that sort of a thing will come; compared to the upper one.

Student: (Refer Time: 47:54).

So, this intensity S star S can be written as something like delta epsilon into sin squared pi delta k into a into N it will turn out to be, this is what it can be used to find out how the intensity is going to vary.

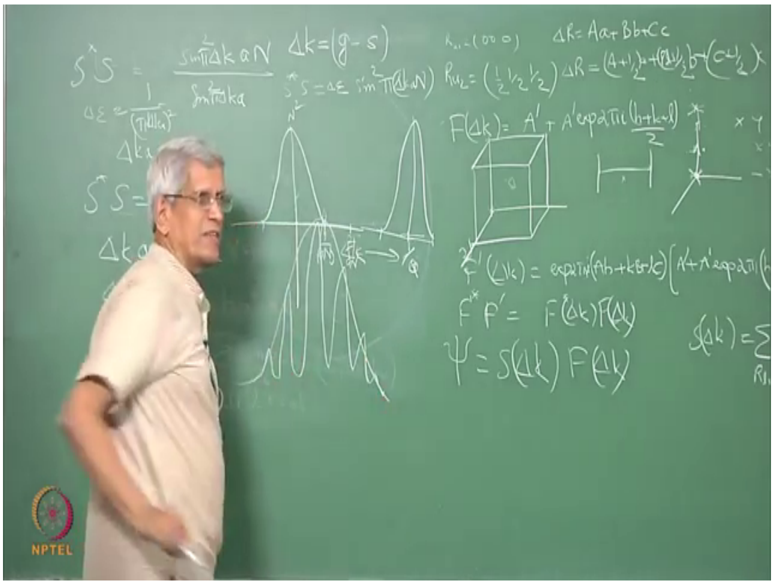
Student: (Refer Time: 45:15) so, delta epsilon means one by pi delta k (Refer Time: 48:18).

Yeah that is comes to on sharply compared to this one, compared to this is a slowly slowly varying function. So, this can be approximated to.

Student: (Refer Time: 48:27).

That is one by it will turn out to be pi delta k into a the whole square, this is what you call it as in the mathematics acts an envelope function no that does not matter essentially what is going to happen is that, suppose you have some one that is a peak is there in between you can have many peaks like, this it is be there.

(Refer Slide Time: 48:43)



These are all the fine peaks it is a overall intensity which comes, this function you call it as an because that is a slowly but that is also maybe a sin function, but the rate at which that is varying is going to be different.

No essentially what is important here is that intensity are the width of the diffraction spot if you look at it, that depends upon the dimension of the sample which is contributing to diffraction that is the effect of it is here for a crystal with 1 direction it is 12 atoms.

(Refer Slide Time: 49:28)

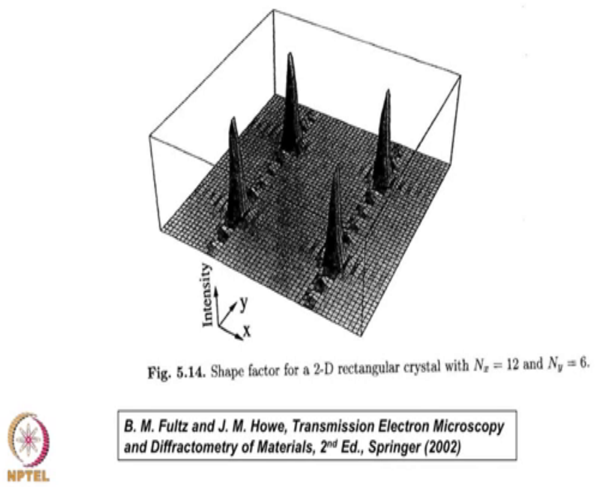


**Fig. 5.14.** Shape factor for a 2-D rectangular crystal with $N_x = 12$ and $N_y = 6$.

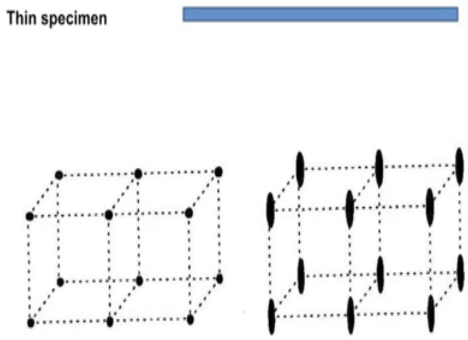
*B. M. Fultz and J. M. Howe, Transmission Electron Microscopy and Diffractometry of Materials, 2nd Ed., Springer (2002)*

And then another direction 6 atoms are there, this is how the peaks will look like in both these directions the intensity which is calculated which is being given. The direction in which the number of atoms have increased you can see that the height of this subsidiary peaks have come down, and here the subsidiary peaks are still prominent when it is going to be there.

Student: (Refer Time: 49:51).

What will be the effect of this? The effect is that normally we assume that from a infinite the sample having infinite dimension when diffraction takes place we should get a spot pattern, correct.

(Refer Slide Time: 50:04)



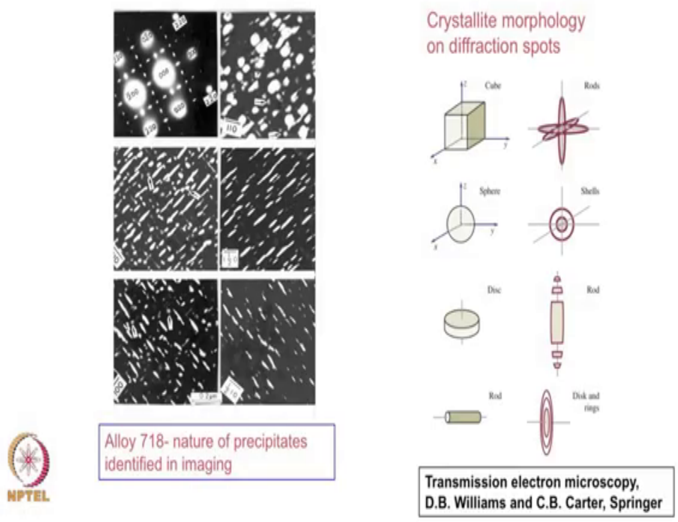
B. M. Fultz and J. M. Howe, Transmission Electron Microscopy and Diffractometry of Materials, 2nd Ed., Springer (2002)

Should be a dot which you should get it, but when the sample has got finite dimension, the reciprocal around to each reciprocal point we have an intensity distribution in k space is taking place, not only the intensity reaching maximum that is what is being shown here in this point and the others regions also there is an intensity distribution, this is in a t e m sample when we take it what is the thickness of the sample.

Student: (Refer Time: 50:41).

The thickness of the sample essentially is very small of the order of 100 nanometers or less, the other 2 perpendicular directions it is thickness is very large; because of that what is going to happen is that in the reciprocal lattice space along the e z direction, there is going to be a streaking of the diffraction spots. So, we will have intensity spots like this in the reciprocal lattice whereas, in these 2 directions x and y directions the streaking is not much.

(Refer Slide Time: 51:48)



Crystallite morphology on diffraction spots

Alloy 718- nature of precipitates identified in imaging

Transmission electron microscopy, D.B. Williams and C.B. Carter, Springer

What will be the consequence of this when you draw the award sphere?

Student: (Refer Time: 51:25).

The awards spheres cut some of this.

Student: (Refer Time: 51:27).

So, that is why you always get some intensity, that does not happen in x ray diffraction when the it is a large size of the sample more diffraction spots comes because of this reason, is this clear.

Student: Yes sir.

And this has a consequence also in the way the diffraction spots appear for different types of precipitate. Suppose we have a second phase particle, which are embedded in the sample. So, each of them has got a finite dimension it contributes to the scattering.

So, in the super lattice reflections corresponding to that second phase particle, the shape of the spot is determined by the shape of the precipitate itself. So, whichever direction it has got the less width.

Student: (Refer Time: 52:21).

In that direction the spread is going to be more in the diffraction spot right. So, here if you see this, this is a diffraction spot which is which you are seeing it there is a streaking which is there in this direction, this is the precipitates from which this diffraction spot has come. So, this direction if you look at it; this perpendicular direction width is less and that is where the streaking is more. In this direction it is length is large and you look at this.

Student: (Refer Time: 52:57).

The streaking is less. So, just by looking at the diffraction spot itself what the shape which it has you can tell this is what that shape are the morphology which the second phase particle has, just looking at the diffraction itself you do not have to go to an image. So, here what is being shown is that what all the morph are different types of morphology of the precipitate, what will be the size of the spot in the spherical space, this is essentially for a cube look at this (Refer Time: 53:28) these are called as (Refer Time: 53:29) this come, and it is for as sphere this is the way it will appear first second subsidiary maxima of that is what is being shown, if it is a thin disc you can see like this when you have a rod which is there like this, this is the way it will appear. This the type of shapes which they exhibit this can be observed in the recipro because of that you take a stacking fault; stacking fault is what is the dimension which a stacking fault will have what the width of the stacking fault.

Student: (Refer Time: 54:08).

Mostly one atomic layer what about the length can be large in both the dimensions right. So, when the width is small whenever stacking faults appear if you take a diffraction pattern from a region which contains a stacking fault, perpendicular to a fault you will be getting a line which is a streak which you will be observed. Similarly like g p zones when they form in aluminium that is nothing, but a one plane whereas, aggregation of a copper or silver which takes place in that particular plane.

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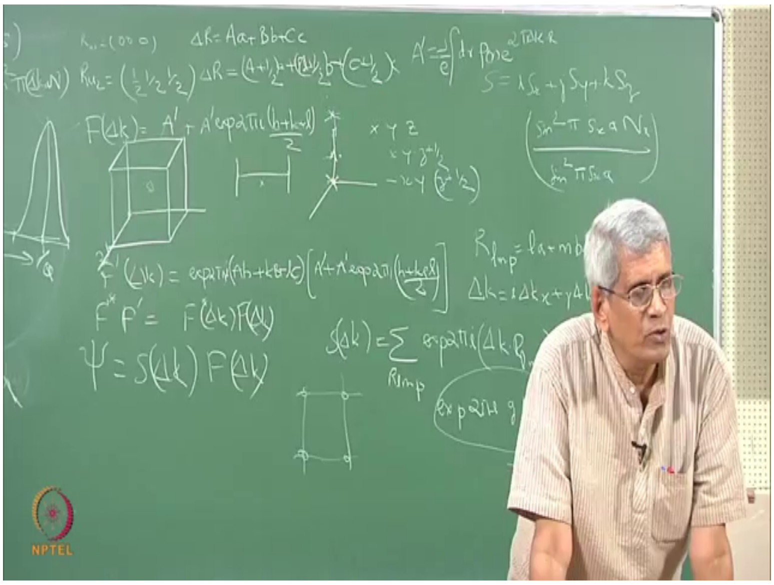

Perpendicular that you will be a, so there in the diffraction pattern which you get it in the t e m, you will be observed that there will be some streak which will be passing through this that depends upon that is what you will be observe. That is because that depends upon what is the direction in which they are there the; this streak tells us that the habit plane of them is 1 0 0 type, that will come to later.

So, essentially looking at the shape of the diffraction spot that is what I am coming to; that we can get a information about the morphology of the precipitate. This is exactly the same information you are doing it in x ray diffraction also there is no way it is different, they are also when you tell that when the gain size is very small you can find out from looking at the broadening of the peak this is exactly that same. They are what is going to happen is that a various corresponding various orientations all of them merge together correct because in a t e m when we say 1 1 1 reflection, you have to be very specific whether it is 1 1 1 or 1 1 bar 1 it is going to be it is totally distinct 2 directions their form that is not the way we get it in x r d.

So, we measure an average full width at half maximum and try to correlate it to the width of the grain. So, the information which we can looking at that shape we can get information about the morphology, and then the intensity of each of the reflection it is not only the shape factor in addition to it the intensity contribution comes from the each of the atom which are going to sit at that particular position, and the atomic scattering factor which this a dash which we have represented is just depends upon it is actually minus 1 e into k dot r it will turn out to be, a delta k dot r i should write it this is what it that we will come to later. In the next few classes we will come back to how this atomic scattering intensity comes for x ray electron neutron all these things we will discuss about it, what will do is we will stop here now.