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NPTEL
NATIONAL PROGRAMME ON TECHNOLOGY ENHANCED LEARNING

Lecture - 25
Materials Characterization
Fundamentals of X-ray diffraction

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Hello everyone. Welcome to this material characterization course. In the last class we just discussed about the properties of X-rays in terms of phase relations and then how this phase relation influences the diffraction and then we just looked at little bit elaborately how we understand the Bragg's law and then how it explains the diffraction intensity and so on. And then we have, let us recall that what we have discussed in the Bragg's law. It is we just said that, it is not that the diffraction intensity is coming from the first layer of the atomic plane and also the subsequent planes which is underneath the surface also contribute to these diffraction intensities through constructive interference. And then we have seen that how this contribution from each atom in the planes below the surface and how the overall diffraction intensity is envisaged.

So, and subsequently we looked at writing this Bragg law in a different form and then how it can be used to analyze the crystal system. And then we will continue in that line today. And before that I would like you to make a brief a description on the reciprocal lattice. Formally we have not introduced this concept so far but in the fundamentals of this course, I mean the lectures we discuss little bit about this reciprocal lattice. However, we will be using this concept throughout this course and not only this X-ray diffraction and also only now after this, we will discuss about electron diffraction in transmission electron microscopy. There also we will use this extensively and what I request you to do is you should go through for all the mathematical treatment of this concept which is really out of the scope of this course. You should refer a physics of materials which is also there in this NPTEL portal where you have a detailed mathematical treatment is given.

And also, specifically there is a 10-hour course is being offered by Professor Pratap Haridoss, where exclusively on the reciprocal lattice. What I request all of you to do is go through that physics of materials lecture notes or videos as well as the 10-hour course exclusively on the reciprocal lattice. Then if you follow this it will be very easy. In order to save time I am avoiding all this basic mathematical relations but then I will briefly talk about it.

In fact, we will be dealing with more practical aspects of this reciprocal lattice concept and we will be actually seeing in practice how we can visualize a reciprocal lattice in reality. So, in our course we will look at more the application part of it and not the basic mathematical part of it but nevertheless I will keep on referring this concept and then I will try to make you understand as much as possible in terms of physical phenomenon.

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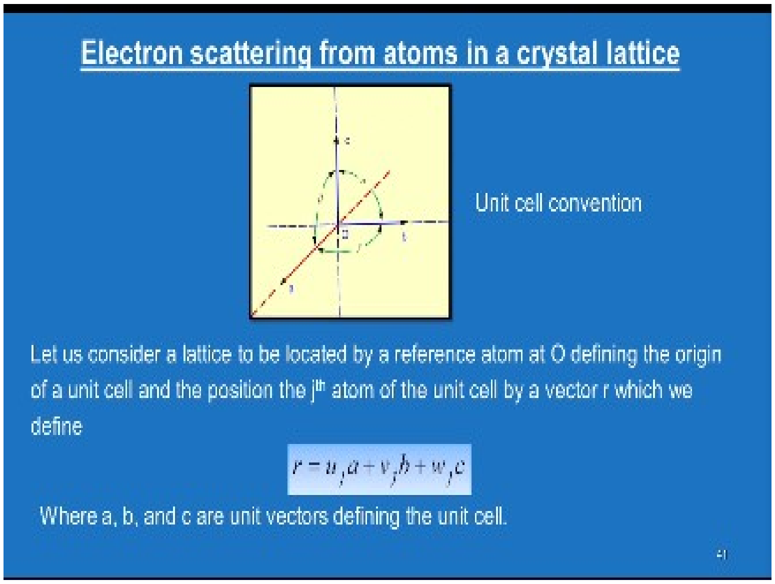

Electron scattering from atoms in a crystal lattice

Unit cell convention

Let us consider a lattice to be located by a reference atom at O defining the origin of a unit cell and the position the j^th^ atom of the unit cell by a vector r which we define

$$r = u_j a + v_j b + w_j c$$

Where a, b, and c are unit vectors defining the unit cell.

So, if you look at the suppose if you want to talk about electron scattering from atoms in a crystal lattice, first we have to talk about the crystal lattice and this is how we define any unit cell, a conversion is where you have this a, b, c; all are vectors and then the angle between them are α, β, . So, this is a called unit cell convention. So, let us consider a lattice to be located by a reference atom at ‘O’ defining the origin of unit cell and the position the jth of the unit cell by a vector ‘r’ which we define normally $\mathbf{r = u_j a + v_v b + w_j c}$ **,** where a, b and c are unit vectors defining the unit cell.

This is, I am saying because we will be referring this a vector, this is a vector in the real lattice which we will be using it extensively in the X-ray diffraction intensity expressions as well as when we talk about reciprocal lattice. So, this is the convention and it is a vector in a real lattice. You have to remember that is very important.

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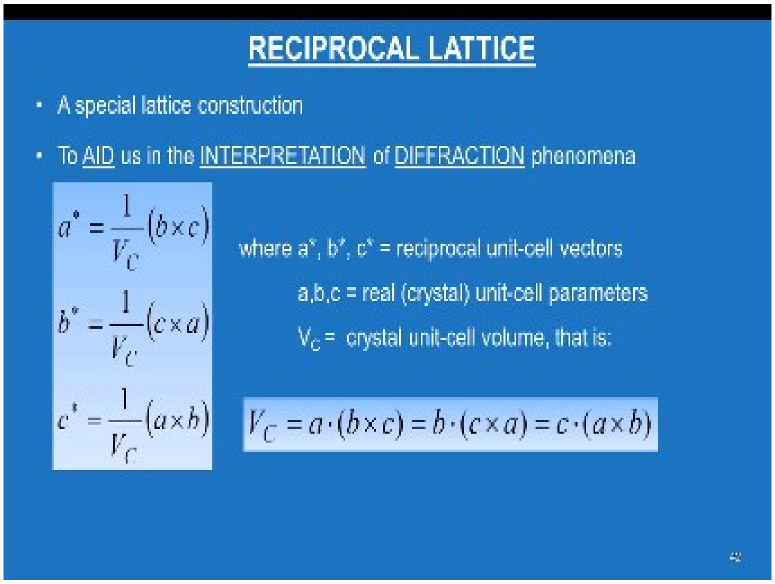

RECIPROCAL LATTICE

- A special lattice construction
- To AID us in the INTERPRETATION of DIFFRACTION phenomena

$$a^* = \frac{1}{V_C}(b \times c)$$

$$b^* = \frac{1}{V_C}(c \times a)$$

$$c^* = \frac{1}{V_C}(a \times b)$$

where a*, b*, c* = reciprocal unit-cell vectors

a,b,c = real (crystal) unit-cell parameters

V_C = crystal unit-cell volume, that is:

$$V_C = a \cdot (b \times c) = b \cdot (c \times a) = c \cdot (a \times b)$$

And excuse me what is reciprocal lattice? It is a special lattice construction to aid us in interpretation of the diffraction phenomena. So, this is the fundamental aspect of it and how this lattice parameters are reciprocal unit vectors are defined which is $\mathbf{a^* = 1/V_c\,(b \times c),\ b^* = 1/V_c\,(c \times a)}$ **and** $\mathbf{c^* = 1/V_c\,(a \times b)}$ where a*, b*and c* they are all reciprocal unit cell vectors where a, b, c they are all real crystal unit cell parameters and V_C is the crystal unit cell volume that is $\mathbf{V_C = a\ .\ (b \times c) = b\ .\ (c \times a) = c\ .\ (a \times b)}$. So, these are all be fundamental expressions which you might have already studied are must have come across much before that.

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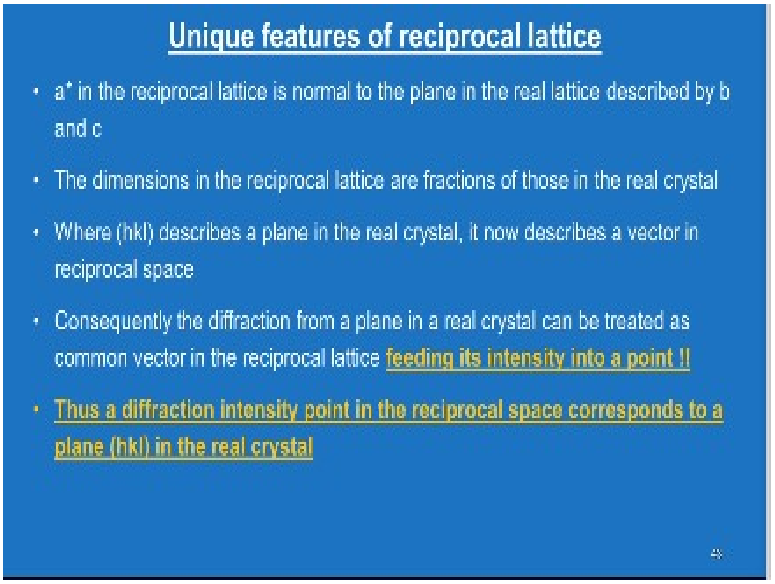

Unique features of reciprocal lattice

- a^* in the reciprocal lattice is normal to the plane in the real lattice described by b and c
- The dimensions in the reciprocal lattice are fractions of those in the real crystal
- Where (hkl) describes a plane in the real crystal, it now describes a vector in reciprocal space
- Consequently the diffraction from a plane in a real crystal can be treated as common vector in the reciprocal lattice feeding its intensity into a point !!
- Thus a diffraction intensity point in the reciprocal space corresponds to a plane (hkl) in the real crystal

Let us now go through some of the unique features of a reciprocal lattice. a^* in the reciprocal lattice is normal to the plane in the real lattice described by b and c. The dimensions in the reciprocal lattice are fractions of those in the real crystal, where (hkl) describes a plane in real crystal, it now describes a vector in the reciprocal space. Consequently the diffraction from a plane in a real crystal can be treated as common vector in the reciprocal lattice feeding its intensity into a point. Thus, a diffraction intensity point in a reciprocal space corresponds to a plane (hkl) in the real crystal.

You see these are all the some of the basic features of the reciprocal lattice. Infact we will be talking about this, the reciprocal point in an in a real system, in a practical situation as a electron diffraction pattern, well where we will try to interpret for its complete accountability. What it means that we will do it detailed study. And what is said here is, in fact it is it is not just one plane here, not necessarily one plane here. It could be a set of planes. It is always referred as a set of (hkl) planes, which I mean for which correspond to each reciprocal lattice points. So, that we will see it in a appropriate time.

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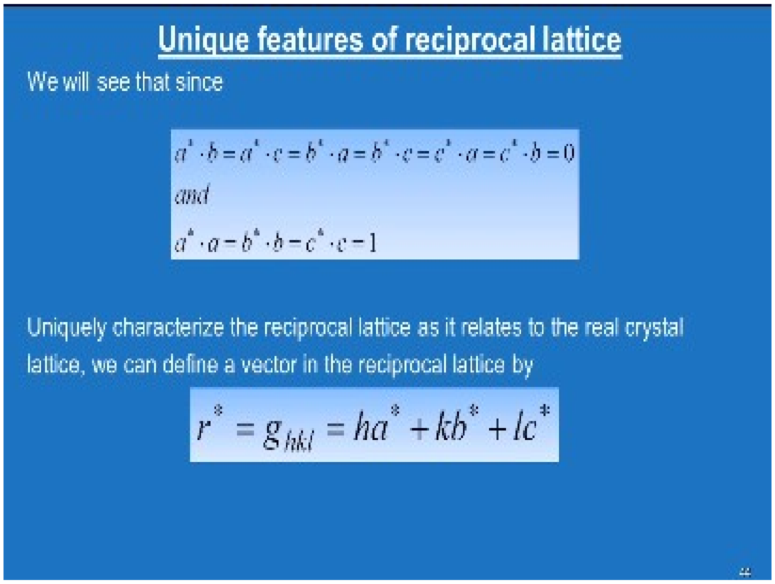

Unique features of reciprocal lattice

We will see that since

$$a^* \cdot b = a^* \cdot c = b^* \cdot a = b^* \cdot c = c^* \cdot a = c^* \cdot b = 0$$

and

$$a^* \cdot a = b^* \cdot b = c^* \cdot c = 1$$

Uniquely characterize the reciprocal lattice as it relates to the real crystal lattice, we can define a vector in the reciprocal lattice by

$$r^* = g_{hkl} = ha^* + kb^* + lc^*$$

We will also see some of the other relations. that a.b I mean $\mathbf{a^*.b = a^*.c = b^*.a = b^*.c = c^*.a = c^*.b = 0}$. These are all some basic relations. And very importantly now, we will see the uniquely characterize the reciprocal lattice as it relates to the real crystal lattice, we can define a vector in the reciprocal lattice by

$$\mathbf{r^* = g_{hkl} = ha^* + kb^* + lc^*}$$

So, this is a reciprocal lattice vector. So, you just compare this with the real. Do not confuse this with the real lattice vector. This is a reciprocal lattice vector. It is also called a ‘g’ vector. We will see in appropriate time what is the meaning of this ‘g’ and how do we interpret those notations. So, right now you have you have to keep in mind how a vector in the real lattice is represented and how the vector in a reciprocal lattice is represented and then what is the relationship mathematically.

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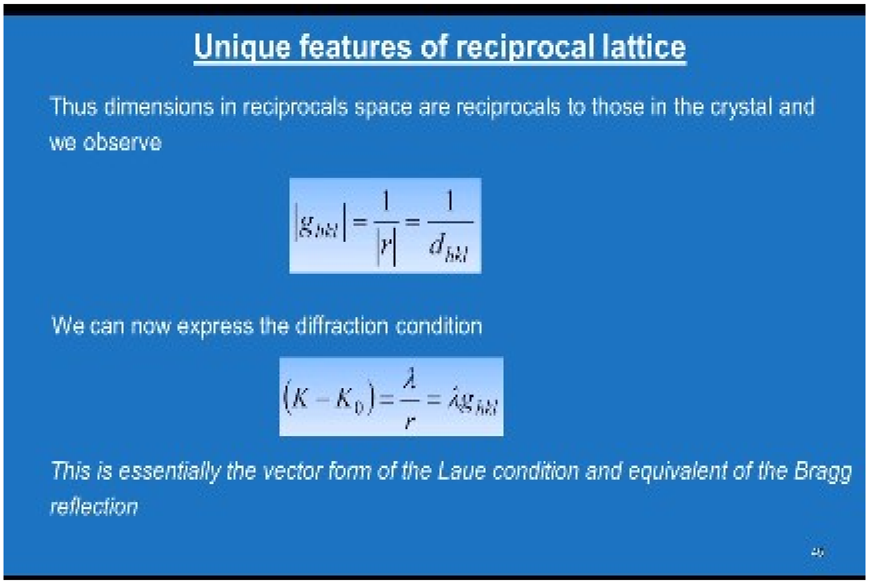

Unique features of reciprocal lattice

Thus dimensions in reciprocals space are reciprocals to those in the crystal and we observe

$$\left|g_{hkl}\right| = \frac{1}{|r|} = \frac{1}{d_{hkl}}$$

We can now express the diffraction condition

$$\left(K - K_0\right) = \frac{\lambda}{r} = \lambda g_{hkl}$$

This is essentially the vector form of the Laue condition and equivalent of the Bragg reflection

And if you can see further, the dimensions in the reciprocal space are reciprocals to those in the crystal and we observe $|g_{hkl}| = 1/|r| = 1/d_{hkl}$ We can now express the diffraction condition in a vectorial form $K- K_0 = \lambda/r = \lambda g_{hkl}$ This is essentially a vector form of Laue condition and is equivalent of the Bragg diffraction. Just for the completion I have brought this relation. This is a I would say it is a vectorial form of a Bragg condition.

For example, Bragg law describes the diffraction in terms of scalar equation. What you see $n\lambda = 2D \sin \theta$ is a scalar equation. We can also define the diffraction condition by a vector equation. So, this is one of the forms. We will now see it in much more detail in two three slides later, how this law a condition our vectorial form of representation of diffraction equation.

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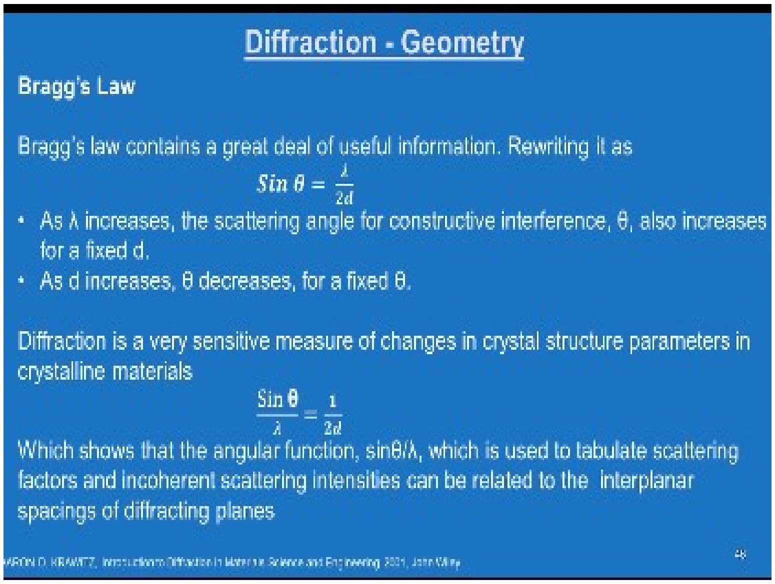

Diffraction - Geometry

Bragg's Law

Bragg's law contains a great deal of useful information. Rewriting it as

$$Sin\ \theta = \frac{\lambda}{2d}$$

- As λ increases, the scattering angle for constructive interference, θ, also increases for a fixed d.
- As d increases, θ decreases, for a fixed θ.

Diffraction is a very sensitive measure of changes in crystal structure parameters in crystalline materials

$$\frac{\text{Sin}\,\theta}{\lambda} = \frac{1}{2d}$$

Which shows that the angular function, sinθ/λ, which is used to tabulate scattering factors and incoherent scattering intensities can be related to the interplanar spacings of diffracting planes

RON D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering 2001, John Wiley

So, in the last class we just looked at a Bragg law and how it can be used in analyzing the crystal system. There are few more points we will see about this Bragg law. So, Bragg's law contains a great deal of useful information we can write **sin θ = λ/ 2d**. There are two things we have to keep in mind. As λ increases, the scattering angle for a constructive interference θ also increases for a fixed d. As d increases θ decreases for a fixed λ.

So, diffraction is a very sensitive measure of changes in the crystal structure parameters in the crystal line materials. Hence **(sin θ) / λ = 1/ 2d** ,which shows that the angular function (sin θ) / λ which is used to tabulate scattering factors and incoherent scattering intensities can be related to the inter planar spacing of diffracting planes.

So, the diffraction is very sensitive measure of changes in the crystal. So, this that is why this particular parameter is used as an angular function to identify the changes in the crystal structure which we will see in the subsequent slides.

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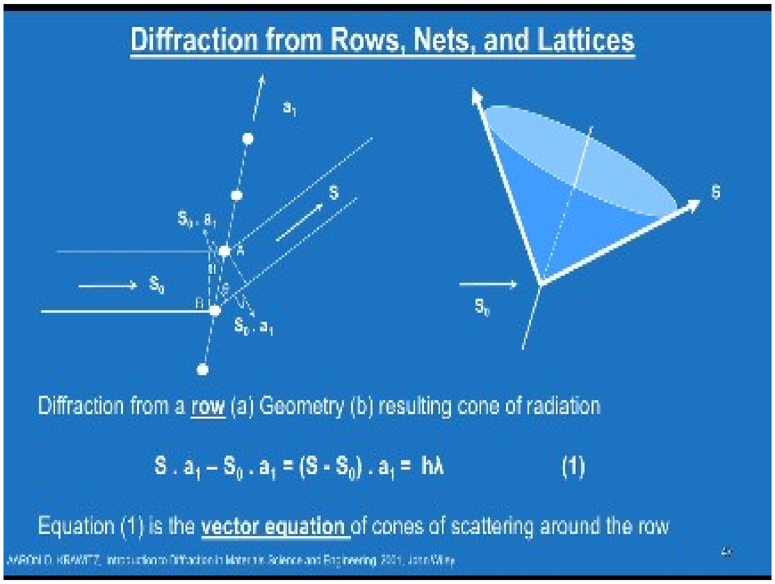

Diffraction from Rows, Nets, and Lattices

Diffraction from a row (a) Geometry (b) resulting cone of radiation

$$S . a_1 - S_0 . a_1 = (S - S_0) . a_1 = h\lambda \qquad (1)$$

Equation (1) is the **vector equation** of cones of scattering around the row

ARNOLD D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering, 2001, John Wiley

Now, as I just mentioned before, what we have seen so far as a diffraction condition in terms of Bragg law, I would say Bragg's law, it is in a scalar form. There we just try to use a parallel plane one after the other. So, the all that we have showed in the form of animation is only the rays which are subjected to constructive interference or a diffracting beam. But we have not seen a diffraction condition for an individual atom, such as rows or a 2D or 3D lattice.

So, now we will get into that I mean discussion where we will try to arrive at a diffraction condition in an one dimension, two dimension and then three dimension and see what is the difference between, what we have seen in a in a Bragg's law condition and what we are going to see in this discussion. So, look at the schematic. I have just drawn here a scatters. I would say it is a repeat distance in a 1D lattice or rows of atoms.

The repeat distance is described and the direction is described by the vector a_1, and then you have the incident X-rays S_0, which is falling on this row and S is the scattered rays. We will say that it is a deflected ray as well, provided it follows some condition. And in order if you look at the in order to define S as a diffracted beam, we need to look at the condition whether it obeys the a kind of diffraction, I mean a condition or whether it obeys a diffraction condition or whether it facilitate the diffraction condition interms of its geometry. So, now what you can see here is, you see, the atom A and B which scatters and then this is the θ and this is the θ from this side and this is a perpendicular I have drawn for this line and this is a perpendicular drawn for this line. Now, in order to be in the same phase of S and S_0, they should have a path difference should be having some certain conditions. What is that condition?

Suppose, if you look at this atom and then look at this ray after scattering, this is the path difference. And similarly, if you look at this ray, which hits on the atom A and then it scatters this way, and this length, this is the path length. So, there is a difference. These two rays are having two different path length. So, mathematically if you see, what is this length? This length is nothing but $S_0 . a_1$. Similarly, here this length is $S . S_0 . a_1$.

This is S_0 is an incident wave vector and this is the lattice repeat distance that is also in vector and this distance is $S_0 . a_1$. Similarly, this distance is $S_0 . a_1$. And that is how the path length differs. So, now we have already seen that in order for the S rays, that is the scattered ray, to be in the on the same phase of S_0, the path length or path differences should be a integral multiple of a wavelength. So, that is what we have written here.

$$\mathbf{S . a_1 - S_0 . a_1 = (S - S_0) . a_1 = h\lambda} \qquad \mathbf{(1)}$$

So you see that $S . a_1$ that is this minus $S_0 . a_1$, that is the path difference between these two should be equal to an integral multiple of wavelength hλ. And equation (1) is a vector equation of cones of scattering around the row. So, what actually we are seeing is, this there is a intensity cone which is spread like this. So, this is an incident intensity and this is scattered intensity. Actually this kind of a cone of intensity is generated or around the row.

And we will now see one example how this cone is related to the angle of incidence θ and then how it changes with the angle and the wavelength and the inter-atomic distance and so on. So now, you remember that this particular equation accounts for a diffraction in atoms lying in a row. So, now we are just said that if this path differences are in the integral multiple of λ, then these two waves, that is, incident wave as well as diffracted beam will be in the same phase and then constructive interference takes place so the diffraction happens. So, this is a condition for that. Now, we will look at one example to look at the effect of the angle.

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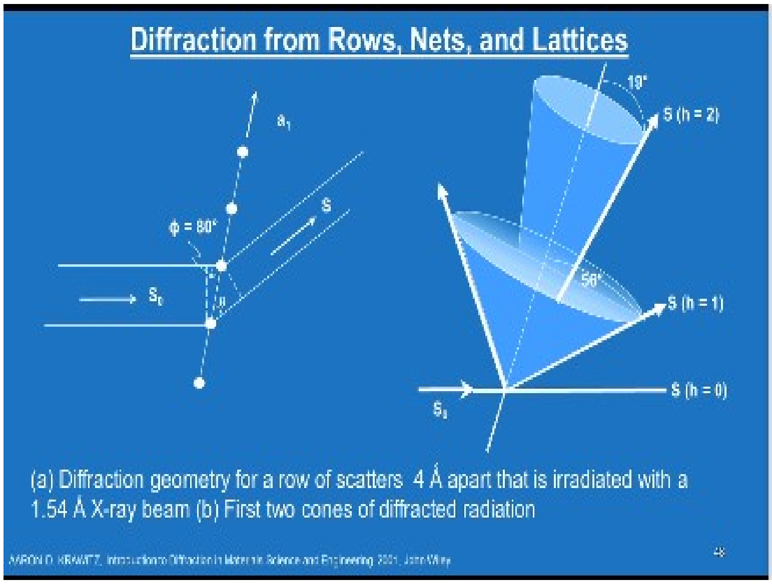

Diffraction from Rows, Nets, and Lattices

(a) Diffraction geometry for a row of scatters 4 Å apart that is irradiated with a 1.54 Å X-ray beam (b) First two cones of diffracted radiation

AARON D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering 2001, John Wiley

Similar schematic, where the incident angle is about 80. And then let us assume that the defection geometry for a row of scatter, this is a row of scattering row of scatter is 4 A^0, that is irradiated with the 1.54 A^0 X-ray beam. So now, you see that the value for λ is equal to I mean θ is equal to 80, 56 and 19 corresponding to h=0, h=1 and h=2 and so on. And how this intensity cone going to be different? You see that when the h=0, you can see that incident beam is almost on the same direction of the diffracted beam. And as the value of the H increases, you can see that the angle decreases. You can see that it is 56 and 19. And you can also see that, are the h=0, the cone is completely opened up. You can you can assume that it is completely opened up and as the h value increases, you can see that how the θ is decreasing. So, this is another one example to visualize the How this the intensity cone varies with the different values of θ.

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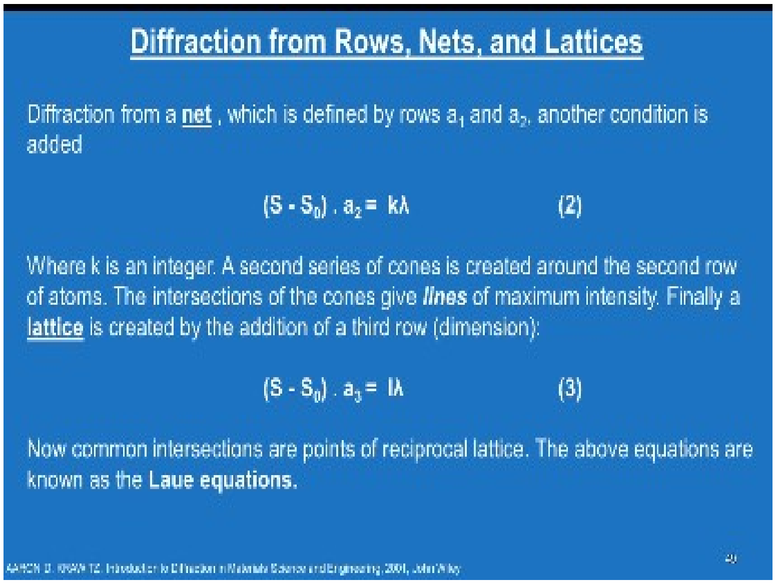

Diffraction from Rows, Nets, and Lattices

Diffraction from a **net**, which is defined by rows a_1 and a_2, another condition is added

$$(S - S_0) . a_2 = k\lambda \qquad (2)$$

Where k is an integer. A second series of cones is created around the second row of atoms. The intersections of the cones give ***lines*** of maximum intensity. Finally a **lattice** is created by the addition of a third row (dimension):

$$(S - S_0) . a_3 = l\lambda \qquad (3)$$

Now common intersections are points of reciprocal lattice. The above equations are known as the **Laue equations.**

Now, we will move on to the two-dimension. So, diffraction from a net that means two dimension which defined by rows a1 and a2. Another condition is added to the previous condition. That is, the

$$\mathbf{(S - S_0) . a_2 = k\lambda} \qquad \mathbf{(2)}$$

that is, a path difference is also should also be equivalent to multiple I mean multiple of integral multiple of λ; kλ where k is an integer. A second series of cones is created around the second row of atoms. The intersections of the cones give lines of maximum intensity.

So, this is where you have to be a little bit careful. We are now talking about intersections of cones from the two different rows. First, we talked about a single row. Now, we talked about at two dimension that means, one more row is added and then where that repeat distance is a_2 and this also is going to produce a cone of radiation for a given θ, around each scatter that is here lattice positions, you can say or atoms, whatever it may be.

Each one is going to produce a cone around it and these two cones are going to intersect. So, all the cones are going to intersect and that they are going to form a line of maximum intensity.

Finally, a lattice is created by addition of a third row that is, one more dimension where the path difference necessarily to be

$$(S - S_0) . a_3 = I\lambda \qquad (3)$$

which is another dimension. So, this is again has to be satisfied for the diffraction to be occurring.

Now, common intersections are points of reciprocal lattice. So, now we talked about one point and from there we talked about a line of maximum intensity and then now the line has become a point of intersection where we will have a maximum intensity. That is where the reciprocal lattice point comes. All these equations (1), (2), (3) are known as the Laue equation. Please understand, in the Bragg diffraction schematic, we were talking about only a parallel plane and then we said that the diffraction intensity comes from each of the rows or in fact all the atoms which are in phase or in other ways contributing to the constructive interference then account for the diffraction intensity. But in a Lava equation, it is in a vectorial form of I mean concept mathematically, where we talk about an individual atom where in the form of a row or a 2D lattice as well as 3D lattice and then how each one is contributing to the diffraction or I would say that the each of the equation derives a condition for the diffraction to take place.

So, there is a difference between the concept discussed in a Bragg's law or a condition for a diffraction through Bragg equation as well as conditions for the diffraction to take place through a Laue equation. So, in fact Laue equation is much more general and you can talk about an individual scatters in the 2D or 3D lattice.

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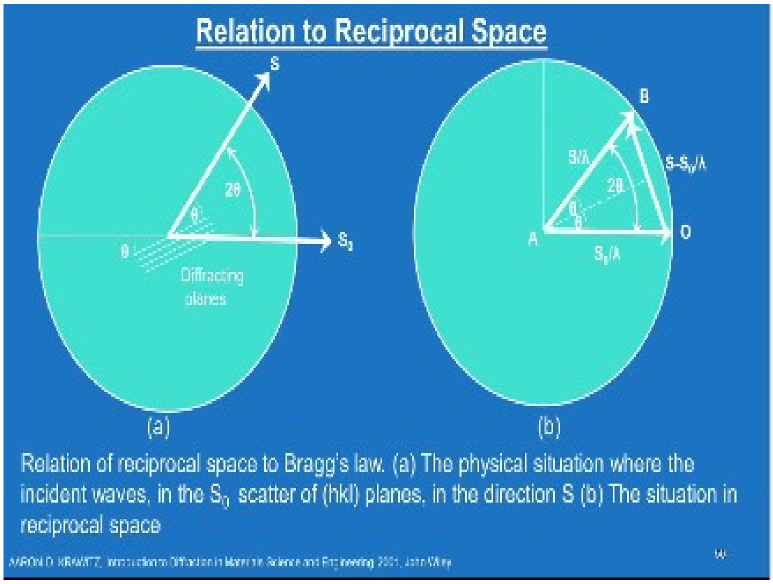

Relation to Reciprocal Space

(a) (b)

Relation of reciprocal space to Bragg's law. (a) The physical situation where the incident waves, in the S_0 scatter of (hkl) planes, in the direction S (b) The situation in reciprocal space

AARON D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering 2001, John Wiley

Now, we will try to relate this reciprocal space I mean as well as the Bragg law. Look at this schematic. I have just drawn a cross-section of a solid sphere. that is why the inside of the circle is shaded. That means a cross section of the sphere, where inside you are seeing that at a plane and then this is incident ray and this is a diffracted ray and then you have the 2θ angle is shown like this. And let us now look at the remarks. Relation of reciprocal space to Bragg's law. How we can relate to the Bragg law.

The Bragg law is related to reciprocal space through Ewald sphere. Another concept, similar to reciprocal concept for a diffraction. It in an Ewald sphere. So, what you are now seeing on the schematic is, a cross-section of Ewald sphere. So, that is what you are seeing. Let us see 'A' is the physical situation where the incident waves in the S_0 scatter of hkl planes in the direction S. 'B' is the situation in the reciprocal space.

So, this is a real space like you have S_0 and S and what you are seeing is an actual condition for the diffraction through an Ewald sphere. You see that, let us assume this as A and this is B and this is O. From the geometry, we will be able to derive some expression based on which the diffraction condition can be arrived. So, suppose if you define this AO vectors S_0 / λ and AB vector S / λ and you can look at this is called a diffraction vector (S - S_0)/ λ by this relation.

You see that, the Ewald sphere radius is 1/ λ. So, that is something which you have to remember. The Ewald sphere radius is 1/ λ and then now we will see how this geometry can be related to a diffraction. So, from the figure (b), **$AO = 1/\lambda$ and $\sin\theta = (BO/2)/AO$** . So, let us see what is that. So, this is the triangle we are talking about. So, this is BO. So, BO/2 for sin θ ,we can write like this.

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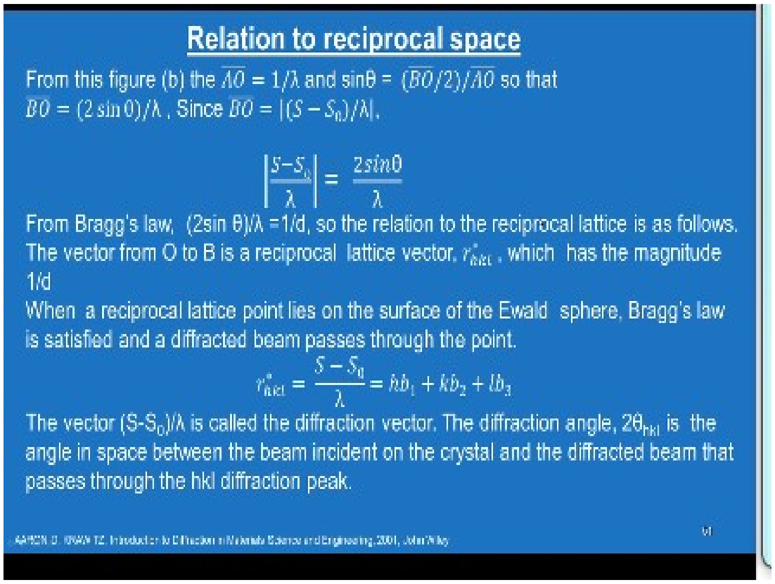

Relation to reciprocal space

From this figure (b) the $\overline{AO} = 1/\lambda$ and $\sin\theta = (\overline{BO}/2)/\overline{AO}$ so that $\overline{BO} = (2\sin\theta)/\lambda$, Since $\overline{BO} = |(S - S_0)/\lambda|$.

$$\left|\frac{S-S_0}{\lambda}\right| = \frac{2\sin\theta}{\lambda}$$

From Bragg's law, $(2\sin\theta)/\lambda = 1/d$, so the relation to the reciprocal lattice is as follows. The vector from O to B is a reciprocal lattice vector, r^*_{hkl} , which has the magnitude 1/d

When a reciprocal lattice point lies on the surface of the Ewald sphere, Bragg's law is satisfied and a diffracted beam passes through the point.

$$r^*_{hkl} = \frac{S-S_0}{\lambda} = hb_1 + kb_2 + lb_3$$

The vector $(S-S_0)/\lambda$ is called the diffraction vector. The diffraction angle, $2\theta_{hkl}$ is the angle in space between the beam incident on the crystal and the diffracted beam that passes through the hkl diffraction peak.

BO/ 2 divided by AO so that BO can be written as **$(2\sin\theta)/\lambda$** and then since **$BO = |S - S^0|/\lambda$** by λ which is nothing but this distance. Which is which can be rewritten like this **$|(S - S^0)/\lambda| = 2\sin\theta/\lambda$** . From Bragg law $(2\sin\theta)/\lambda$ can be written as 1 / d. So, the relation to the reciprocal lattice is as follows. The vector O to B is a reciprocal lattice vector r^*_{hkl} which has the magnitude 1/ d. When a reciprocal lattice point lies on the surface of the Ewald sphere, Bragg's law is satisfied and a defector beam passes through the point. So, now you write the reciprocal lattice vector

$$r^*_{hkl} = (S - S^0)/\lambda = hb_1 + kb_2 + lb_3$$

the vector $|S - S^0|/\lambda$ is called a diffraction vector, which is nothing but r^*_{hkl} in a reciprocal lattice space. The diffraction angle $2\theta_{hkl}$ is the angle in the space between the beam incident on the crystal and the diffracted beam that passes through the hkl diffraction peak. So, you have to remember this how this is related to a diffraction condition through this diagram.

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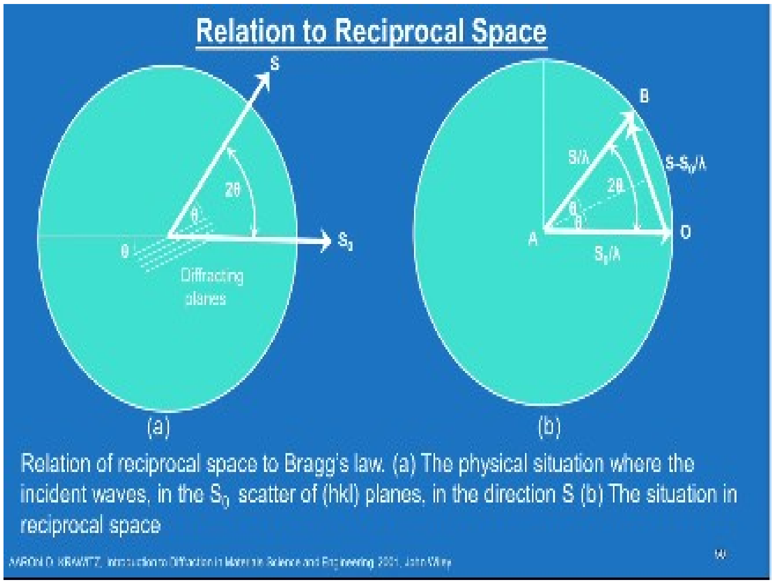

Relation to Reciprocal Space

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So, what it says is this is the diffraction vector S, which is nothing but r^*_{hkl} in a reciprocal space. So, whenever this point hits on the surface of this sphere, then the diffraction condition is satisfied and that is what is stated here.

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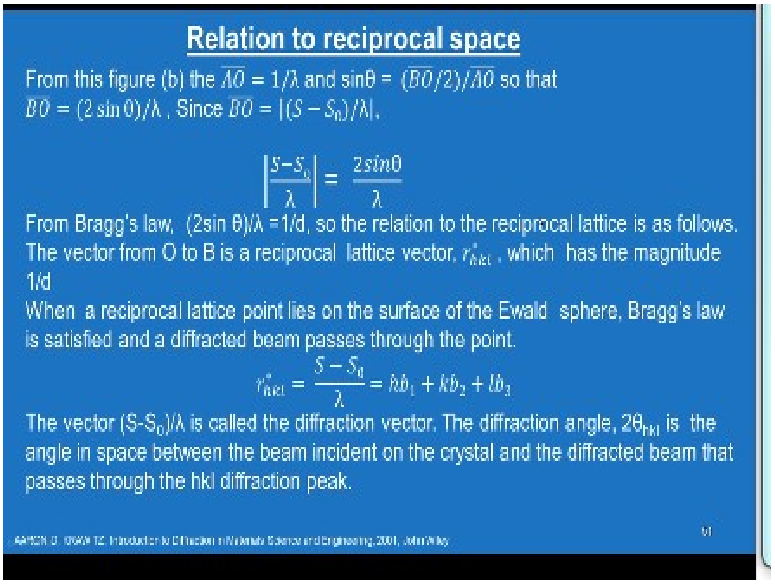

Relation to reciprocal space

From this figure (b) the $\overline{AO} = 1/\lambda$ and $\sin\theta = (\overline{BO}/2)/\overline{AO}$ so that $\overline{BO} = (2\sin\theta)/\lambda$, Since $\overline{BO} = |(S - S_0)/\lambda|$,

$$\left|\frac{S-S_0}{\lambda}\right| = \frac{2sin\theta}{\lambda}$$

From Bragg's law, $(2\sin\theta)/\lambda = 1/d$, so the relation to the reciprocal lattice is as follows. The vector from O to B is a reciprocal lattice vector, r^*_{hkl} , which has the magnitude 1/d

When a reciprocal lattice point lies on the surface of the Ewald sphere, Bragg's law is satisfied and a diffracted beam passes through the point.

$$r^*_{hkl} = \frac{S - S_0}{\lambda} = hb_1 + kb_2 + lb_3$$

The vector $(S-S_0)/\lambda$ is called the diffraction vector. The diffraction angle, $2\theta_{hkl}$ is the angle in space between the beam incident on the crystal and the diffracted beam that passes through the hkl diffraction peak.

AARON D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering, 2001, John Wiley

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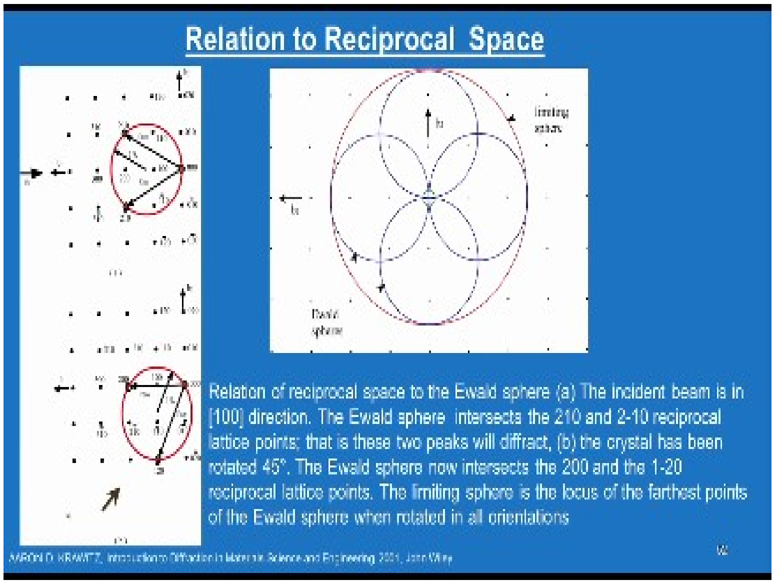

Relation to Reciprocal Space

Relation of reciprocal space to the Ewald sphere (a) The incident beam is in [100] direction. The Ewald sphere intersects the 210 and 2-10 reciprocal lattice points; that is these two peaks will diffract, (b) the crystal has been rotated 45°. The Ewald sphere now intersects the 200 and the 1-20 reciprocal lattice points. The limiting sphere is the locus of the farthest points of the Ewald sphere when rotated in all orientations

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And now in order to visualize this concept little more we will look at some more a schematic. What we are seeing here is, in a schematic (a) and (b) a relation of reciprocal space to the Ewald sphere here. (a) is the incident beam is in 100 direction. suppose this is the S_0. The S_0 is in the

100 direction. So, the Ewald sphere intersects the red markers in Ewald sphere which intersects 210 and 2-10 reciprocal lattice points, that is here as well as here. That means these two peaks will diffract. these two reciprocal points are diffracting set of planes.

And what we are seeing in the schematic (b) is now the crystal has been rotated to 45°. So, the crystal has been rotated to 45°, then what happens is, the Ewald sphere now intersects 200 and 1-20 reciprocal lattice points. You can see that 1-20 and 200 reciprocal points which are coming on the intersecting the Ewald sphere. So, between these two rotations, no other points are possible for the diffraction. That is what it means.

So, if you look at the diffraction spots 2-1 0 and 210 after rotating to 45°, you have a new plane 200 or 1-20. And between these two rotations there are no other possibilities for the diffraction. That is what it means. So, this is one way of interpreting the whole sphere concept. And what is this schematic shows? This is also a set of Ewald sphere but it says the limiting sphere. What do you mean by limiting sphere? The limiting sphere is the locus of the farthest point of the Ewald sphere when rotated in all orientation. So, right now we have seen that rotating into two directions and suppose if you rotate another 45°another 45° another 45°, what are all the points will intersect in the reciprocal lattice? That is this is the reciprocal lattice, where all it will intersect. That is a maximum possible planes which will contribute to the diffraction are the planes maximum number of planes that will intersect the Ewald sphere that is called limiting sphere.

So, that is what shown here in a in a plane of b_1 and b_2 lattice and this defines the limiting sphere like this. And another very interesting example I would like to show

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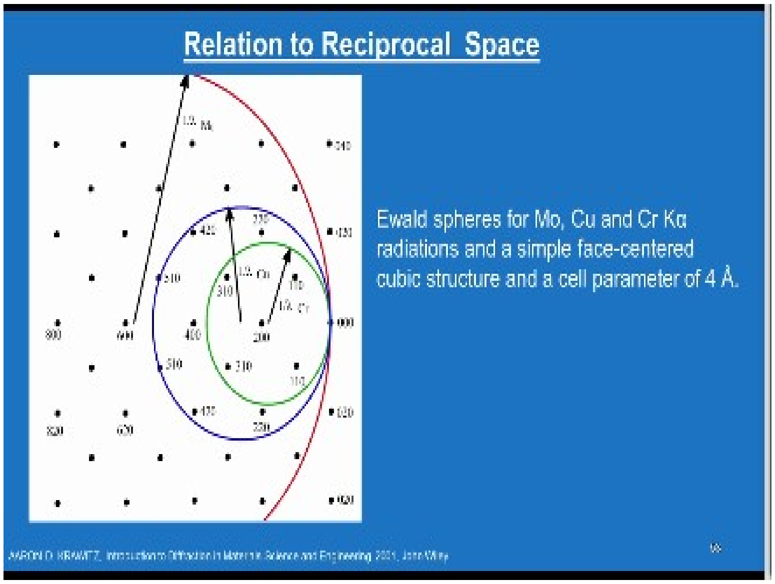

Relation to Reciprocal Space

Ewald spheres for Mo, Cu and Cr Kα radiations and a simple face-centered cubic structure and a cell parameter of 4 Å.

AARON D. KRAWITZ, Introduction to Diffraction in Materials Science and Engineering 2001, John Wiley

where the Ewald sphere for molybdenum copper and chromium Kα radiations. In analyzing the simple face centered cubic structure with the cell parameter $4A^0$. Suppose if you use one of this radiation, for example, let us use a chromium radiation. So, which is 1/λ of chromium which forms the Ewald sphere around these lattice points I mean reciprocal lattice points which have only 110, 310, 200. Since your reciprocal I mean your Ewald sphere radius is 1/λ which is a function of a wavelength of a given radiation, it can explore the possibility of finding the reciprocal planes only in a limited number, that is 110, 310 and 200 type. Suppose if you use a copper radiation, then our radius increases, then you are a Ewald sphere becomes little bigger and now you see in addition to their 110 and 310 and 200 planes you are able to examine 510, 420, 220 etc.

So, as the λ changes you are able to incorporate large number of reciprocal lattice points, that means you are able to get into atomic planes more atomic planes which are satisfying the Bragg conditions. So, the one last one is a molybdenum radiation. You see that it covers quite a bit of reciprocal points. That means it forms a huge sphere Ewald sphere which will interest which will intersect through many reciprocal points including large number of planes.

So, there is this is what the Ewald sphere concept is readily visualized. So, what you are now seeing is the black spot is as I said it is a reciprocal lattice point. And then we will also look at this similar electron diffraction pattern and then again, we will come back with the Ewald sphere concepts to understand little more on the diffraction phenomenon. But to start with this is very nice example and schematic to understand the relation between the Bragg's law and reciprocal lattice and Ewald sphere.

So, the Ewald sphere actually links the Bragg law and the reciprocal lattice. That way we can consider. it is a very nice concept to appreciate the diffraction phenomena.

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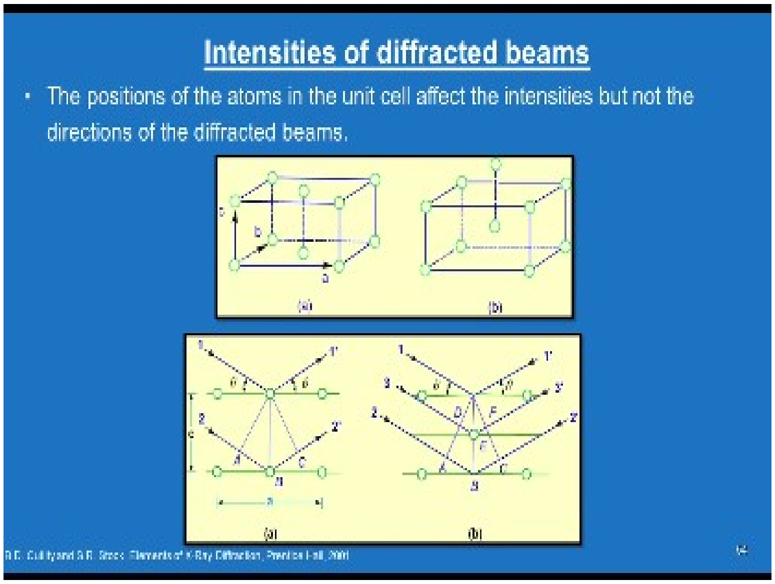

Intensities of diffracted beams

- The positions of the atoms in the unit cell affect the intensities but not the directions of the diffracted beams.

B.D. Cullity and S.R. Stock, Elements of X-Ray Diffraction, Prentice Hall, 2001

Now, we will move on to intensities of diffracted beam. At the end of the day, if you are interested in analyzing the crystal with X-ray diffraction, we are interested in intensities. And we will account for the intensity expressions and then we will see what are all the parameters which will influence the diffraction intensities, when it when it happens with the amorphous material, when it happens with the crystalline material or a single crystal or a poly crystal and so on. So, the intensities are important and their quantification is important but we should know what all the parameters which will control the diffraction intensities of X-rays. So, we will begin our discussion with this. Let us look at the two I mean crystal structures simple crystal structures. What you are seeing in the schematic (a) is a base centered unit cell and (b) is the body centered unit cell. The positions of the atoms in the unit cell affect the intensities but not the direction of the diffracted beings.

So, to prove this concept, how the positions of the atoms in the unit cell is going to affect the diffracted beam, we are going to illustrate through these two examples. One is a base centered unit cell another is a body centered cell. And if you assume that X-rays are coming and then diffracting through both the unit cells and then you will get the corresponding ray diagram like this (a) and then (b). I would like you to look at this ray diagram carefully. The Ray 11’ and 22’ and the distances c and these two diagrams we have already seen on the in the previous classes. You will recall when I talked about the importance of 200 planes. For example, if you see that what is the path difference between these two 11’ and 22’ ? They are out of phase by a one wavelength or I would say that the path difference **AB + BC** is equal to some **h λ** something like that.

So, but if you come to this unit cell the situation is slightly different. Suppose, if you assume that these two planes diffract the X-ray and then their face differences is about 1 * λ, here it is exactly half of that phase difference. For example, because we have the other plane which is inserted in between. So, the 3E3’ ray will have the phase difference exactly half of the the previous one.

So, that means, this phase difference is going to completely annul the intensities of the X rays diffracted by this ray 11’ as well as 2B2’. So, that means you are not going to get the intensities from 100 plane at all. So, I hope you get this idea. This has been already I had told you and the phase difference I also separately discussed, how you have to visualize the phase difference and how they annul each other or they contribute to the constructive interference.

So, in this type of a crystal, where you have this the path difference or the phase difference exactly half of this unit cell, they are going to lose the intensity from 100. So, that is what we are concluding.

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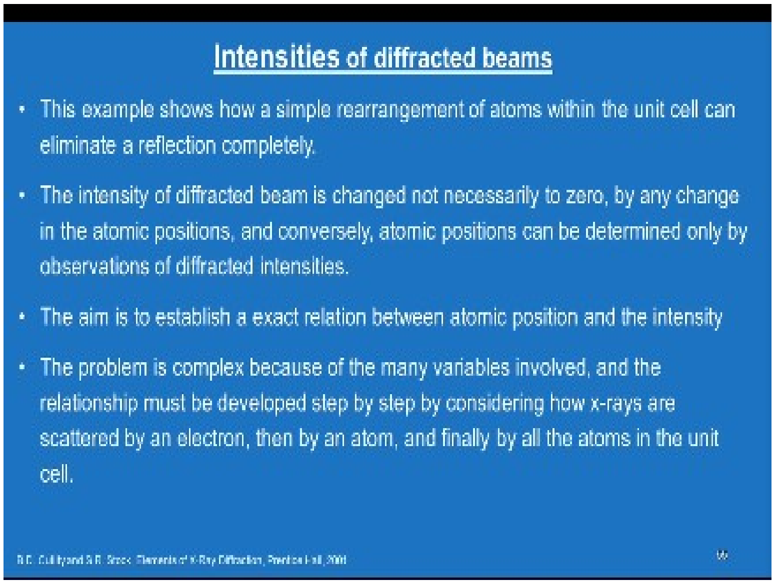

Intensities of diffracted beams

- This example shows how a simple rearrangement of atoms within the unit cell can eliminate a reflection completely.
- The intensity of diffracted beam is changed not necessarily to zero, by any change in the atomic positions, and conversely, atomic positions can be determined only by observations of diffracted intensities.
- The aim is to establish a exact relation between atomic position and the intensity
- The problem is complex because of the many variables involved, and the relationship must be developed step by step by considering how x-rays are scattered by an electron, then by an atom, and finally by all the atoms in the unit cell.

B.D. Cullity and S.R. Stock, Elements of X-Ray Diffraction, Prentice Hall, 2001

This example shows how a simple rearrangement of atoms within the unit cell can eliminate a reflection completely. The intensity of a diffracted beam is changed not necessarily to 0 but any change in the atomic positions and conversely the atomic positions can be determined only by the observation of diffraction intensities. So, the aim is to establish the exact relation between atomic position and the intensity.

The problem is complex because of the many variables involved. And the relationship must be developed step by step by considering how X-rays are scattered by an electron, then by an atom and finally by all the atoms in the unit cell. So, we would look at the how the diffracted intensities are changing by step by step first by scattering by the electron then by the madam and then by unit. Then we will look at the whole expression for the X-ray intensities diffracted by a crystal.

So, we will continue to look at this diffraction phenomenon and then we will in the next class we will start with the X-rays which when they are scattered by an electron, what are all the physical phenomenon we will go through. Those things we will look at in the next class. Thank you.

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