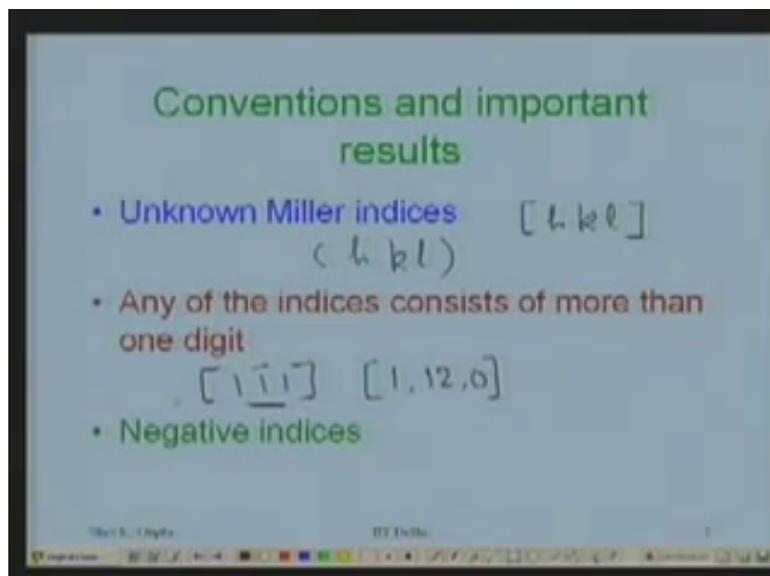
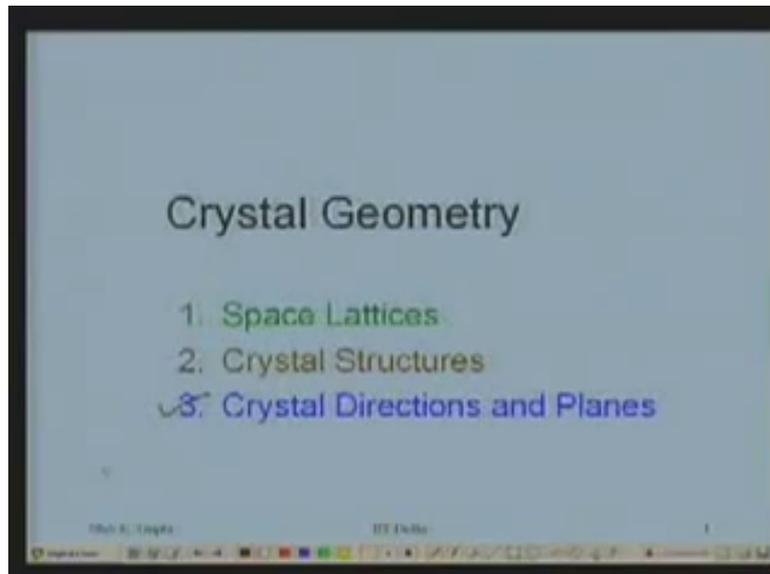


Material Science
Professor S. K. Gupta
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Lecture No 5
Crystal Geometry

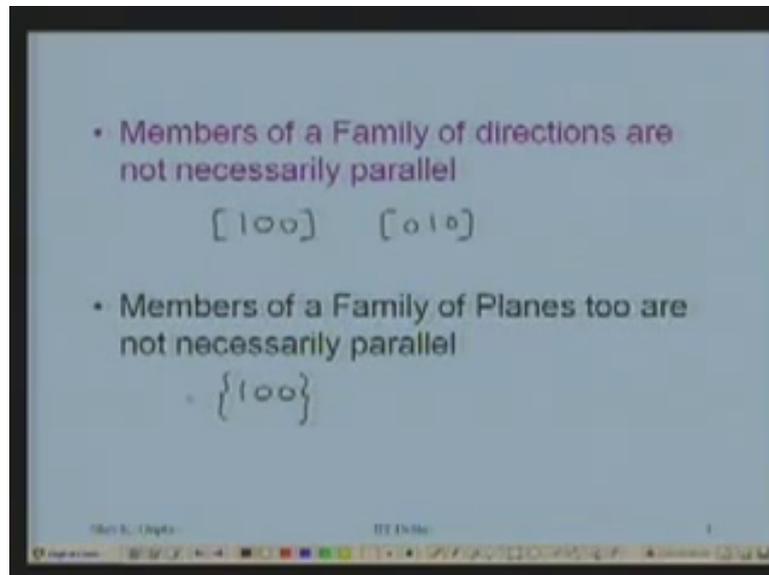
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Well in the last class we were talking about the crystal direction and planes and what we named them as Miller indices of directions and Miller indices of planes. Well just to say what we talked about we said the unknown Miller indices are used for directions as hkl and for planes we can write hkl and I told you that we do not use xyz. Any of the indices which consist of more than one digit we need to have a separator otherwise we do not use separator this is very important, so for example direction $1\bar{1}1$, I do not have to use a separate but if

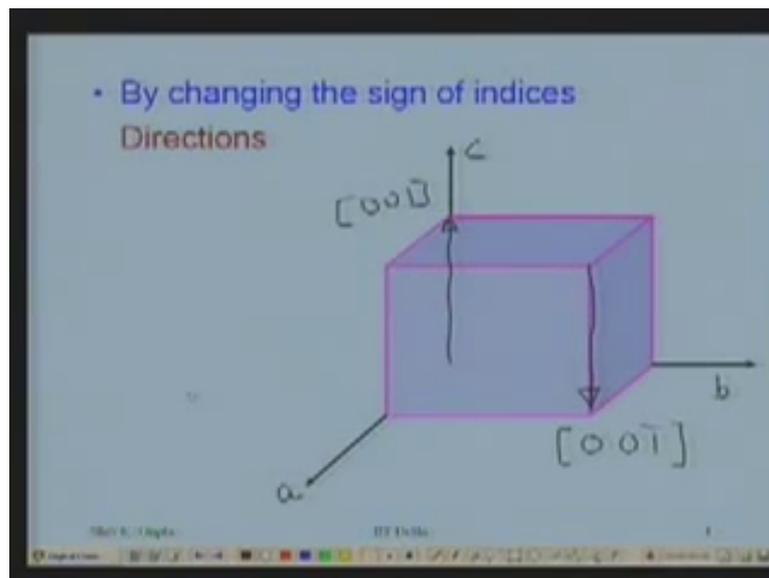
it is a direction $1\ 1\ 0$ I need to put a separator, right then if the indices happen to be negative the bar is placed on top of the index like here and it is read as $\bar{1}$.

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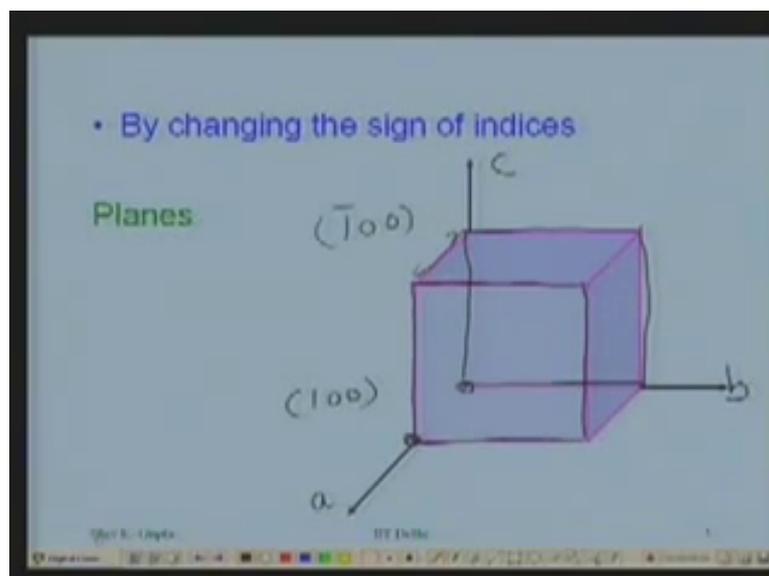
Members of a family of a directions as a told you they need not be parallel like I in a cube I showed an example of edge of a tube which is parallel to the a axis is $1\ 0\ 0$ parallel to the b axis is $0\ 1\ 0$ they look alike physically but they are perpendicular to each other in a cube, okay. Similarly members of a family of plane that is those planes physically look identical like the front face and the back face in a cube. The top face and the bottom face right hand side face and the left-hand side face they look alike they form a family. These planes again belong to the family $1\ 0\ 0$ right they are not parallel because we said that all parallel equidistant planes are given one index they are call the same thing because they will be looking alike absolutely and their location in space is also parallel in the same way in the crystal.

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By changing the sign of indices is possible in case of directions to reverse the direction, say for example we talked about this direction before that its name this axis a b and c this direction is 0 0 1 but if I put this direction here you can name it the way I told yesterday it will be 0 0 bar 1 they are parallel but the sense is opposite, right that is how by changing the signs 0 if I change the sign there is no need we do not the change the sign for 0 and 1 the sign change becomes bar 1 direction is reversed you can try for any other direction for that matter.

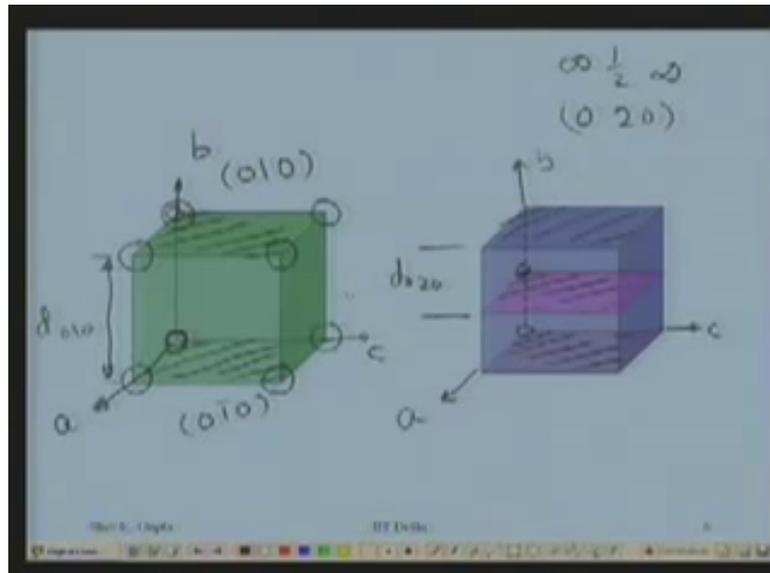
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Similarly in case of planes as I told you that by changing the sign of indices I go to a plane opposite side of the origin, okay say for example in this case let me take a plane and name my axis as a b and c you will name this plane as 1 0 0 and I have taken my origin there, if I take

my origin here and try to find the name of the plane which is here, the back you would name this as $\bar{1} 0 0$. I change the sign and one is the back of the means this origin is here plane is at the back, origin is here the plane is in front it is $1 0 0$ this is the same set of planes actually and distance between them is here that is what we shall see next.

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Alright next we talked about as I said the set of parallel equidistant planes are given one name, okay that is what I want to show you here what happens when the distance between the plane changes they are still parallel. Let us talk about the bottom face and the top face of crystal unit cell let me name this as a b and c the top face if I name you will find out will become $0 1 0$ and the bottom face when I work out by taking the origin here you know that it is $0 \bar{1} 0$, so the set is this top plane here and this bottom plane there and the distance between them is given by this let us call that $d_{0 1 0}$ alright, now let us locate in a unit cell same unit cell maybe let us name this as c here, a here and be there, this plane in the middle if I start with this origin it is parallel to a parallel to c and makes an intercept of half on b.

So intercepts are infinity half and infinity, reciprocals of this intercept would become $0 2 0$, so this pink plane here is $0 2 0$. If I take the origin on this $0 2 0$ let me find out what is the top plane that will also be $0 2 0$ another word now the set of $0 2 0$ plane is 1 the top here, this pink and the one in the bottom here these constitute the set of $0 2 0$ and the set of $0 1 0$ is the bottom and the top, can you see the difference? You are I have and interleaving plane between the two $0 1 0$ planes, the spacing between them what I call $d_{0 2 0}$ is half of what is $d_{0 1 0}$. In other words you can also say that a $0 1 0$ set of planes is a subset of $0 2 0$ but only

thing is that sometimes 0 2 0 plane may not exist in a crystal means there are no physically no atoms are lying on that, so for example simple cubic crystal.

Simple cubic crystal the atoms are only at the 8 corners of the lattice point how much is the unit cell? Lattice points are only at the corners, there is no atom going to be there in the middle, physically that is not a plane, right. That is the only thing it is possible but this 0 2 0 set is going to be top plane, the bottom plane and the interleaving middle plane in their and 0 1 0 is the bottom and the top, is this clear? That is what we started with that equidistant parallel planes given one name, this set of 3 planes here will be called 0 2 0 this will be called 0 1 0 and I said if they are parallel only distance is different they are related relationship you can see that 0 2 0, 0 1 0, 1 and 2. One has become 2 there, right. We shall also see further now this relationship in terms of numbers and expression.

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Problems

- In a cubic crystal $[hkl]$ is perpendicular or normal to (hkl)
- In a crystal system having orthogonal set of axes

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

d_{hkl} is the spacing between two consecutive (hkl) planes or the distance of the (hkl) plane from the origin

Well this is a problem I shall leave out for you to work it is very simple to do that, only it is true in a cubic crystal that a direction hkl is perpendicular to the plane hkl . In other words you would notice that is 0 1 0 direction is perpendicular to 0 1 0 plane but it is true in a cube only you may not find this to be true in any other crystal system and secondly when you are doing that you will also be able to show this that in crystal systems where the 3 axis a b and c are orthogonal to each other, what are such crystal systems? Cubic, tetragonal and orthorhombic alright, so there is the distance between an hkl plane d is related to the indices of the plane hkl and the lattice parameters a b c like this.

While in orthogonal system can use to solve this problems you can use the (12:30) set of axis because they are orthogonal to each other and distance a b c unit distance you can convert into angstroms knowing the value of a length, b length, c length convert them into Angstrom and use the knowledge that some of the squares of the direction co-sine is one, okay to use that you will be able to get 1st and 2nd both these solutions. Now we shall use this formula for cubic systems, in a cubic system notice that a becomes equal to b becomes equal to c on the right-hand side I have a common denominator and therefore one upon the square becomes equal to h square plus k square plus l square divided by the square which I make reciprocal I can write it like this.

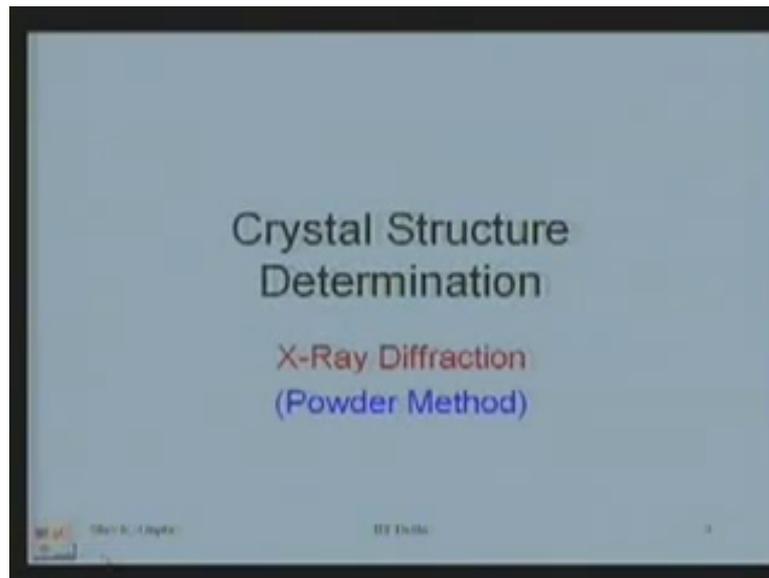
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The image shows handwritten mathematical derivations for the interplanar distance d in a cubic system. At the top, the general formula is written as $d^2 = \frac{a^2}{h^2 + k^2 + l^2}$. Below this, two specific cases are worked out:

- For Miller indices (010), the derivation shows $d^2 = \frac{a^2}{0^2 + 1^2 + 0} = a^2$, leading to the boxed result $d = a$.
- For Miller indices (020), the derivation shows $d^2 = \frac{a^2}{0^2 + 4 + 0} = \frac{a^2}{4}$, leading to the boxed result $d = \frac{a}{2}$.

I can write it like this d square equal to a square divided by h square plus k square plus l square, now you can see I just showed you about 0 1 0 and 0 2 0 let us see for 0 1 0 the d would be a square divided by 0 plus 1 square is 1 plus 0 that becomes a square or in other words d is equal to a . Let us do the same thing for 0 2 0 which I showed you is an interleaving plane between 2 0 1 0 let us see what does do we get for d , d square is equal to a square divided by 0 plus 4 plus 0 becomes a square by 4 and d becomes a by 2 it is half the distance between the planes that is why 0 2 0 is an interleaving plane between 0 1 0 planes, right.

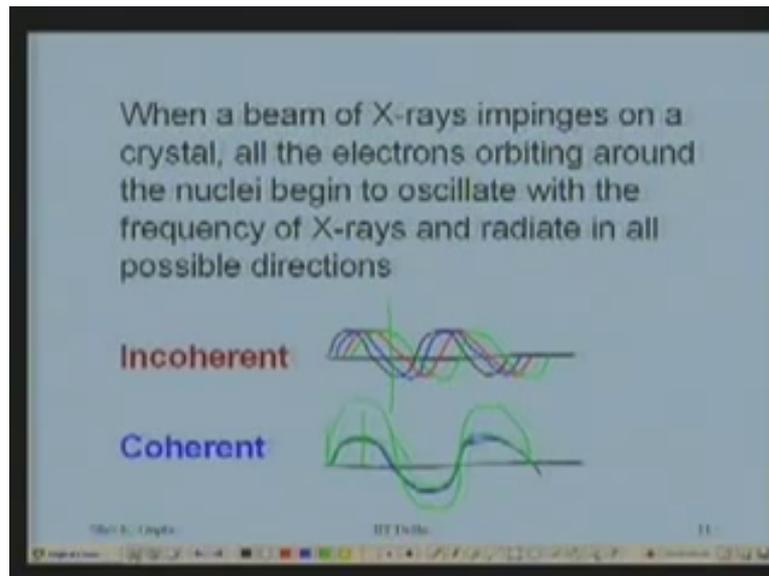
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Alright with this we move on to do the determination of a crystal structure and we shall be showing you something for very simple structures, complex structures are involved, however it is possible and we have been able to identify and list these are available in the literature thousands of crystals already known and there are very some of them are very complex structure but in this course the 1st course we shall look at very simple structures like let us say space lattices body centred cubic and motif or the basis was only one atom of iron sitting on the BCC it is a BCC iron crystal.

How do we determine the crystal structure of such a crystal or FCC space lattice one copper atom sitting on it or one nickel atoms sitting on each lattice point becomes either FCC copper or crystal or it becomes FCC little crystal how do we identify these crystal structures? How do we determine this? For this we use axial diffraction or electron diffraction or neutron diffraction procedure used is basically diffraction. Whether I use x-rays, electromagnetic radiations or I use high energy particles like electron or high-energy neutrons which can also behave like waves, so we shall study the axial diffraction using the x-rays we shall look at the diffraction.

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The x-rays we use are characteristic radiations of certain metals. This is when an electron from the K shell is knocked off by some high-energy electron. The metal target is made a cathode and electrons from the anode at high velocity come and impinge on the metal target. The knock off of electrons from the lattice K shell. Electrons from the L shell will try to drop into the K shell and lose its energy. That radiation is what is called characteristic radiations and it gives a maximum intensity produced for this K alpha radiation. There are the different metal targets and here are their wavelengths.

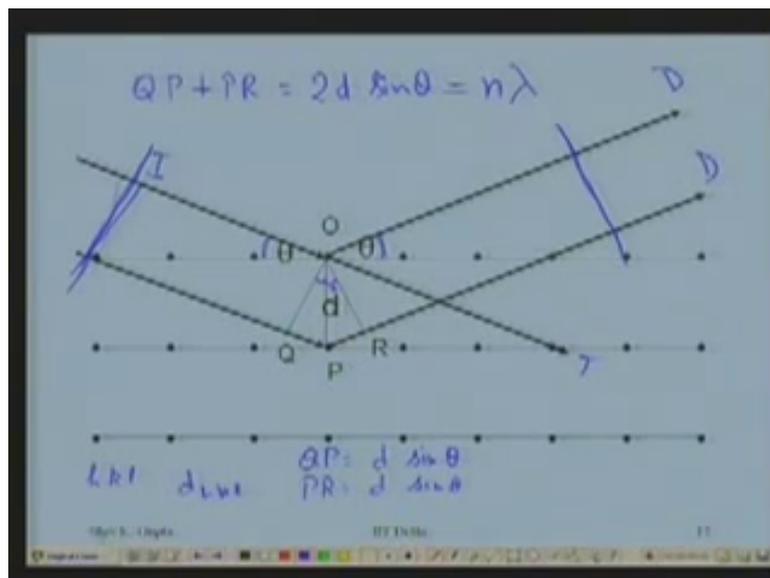
You see these wavelengths all these wavelengths are in the range of 1 to 2 Angstrom. This is the range in which atomic diameter exist and in other words the wavelength which we are using to study the windows in the crystal, windows will be of the size of the atomic diameters spaces between the atoms you know, so diffraction occurs like in the slit experiments you have done in school so diffraction is also done by these 3 dimensional crystals which have three-dimensional windows or you can call them three-dimension slits therefore the radiation use is of the same order of magnitude in wavelength as the spacing between them alright.

Now what happens actually when these x-rays are impinged on the crystal for which are trying to study the crystal structure their electrons orbiting around nuclei of nuclei of every atom they are just orbiting around. When this x-ray fall on them they start additionally oscillating the same frequency as the frequency of the x-rays as a result these electrons in turn start radiating x-rays because they are oscillating, all oscillators are going to radiate but in most directions these radiations come out in the incoherent fashion, what is the meaning of the incoherent fashion? Let us say one oscillator gives out in this direction radiation like this,

there is another one which gives out radiation like this there is a 3rd one gives out like this so on and so forth.

Well if you now keep adding more and more waves coming from...there are going to be electrons in the range of (20:44) 24 26 and they are all radiating and they are radiating in different directions with different phase, so they at any point you want to see the net intensity is 0 net amplitude positive amplitude, negative amplitude and net intensity, net amplitude is 0. These are the incoherent radiation which occur in most of the directions but there are very few directions which they meet in a coherent fashion that is they are all in face one, 2nd one, 3rd one so what is going to happen at any point the amplitude would be 3 times it will be increasing, so net amplitude would be very high and we will be able to see the intensity coming out in that direction there are very few directions are of those directions errors what we shall see the next.

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Here I show you a picture where I have 3 planes taken in a crystal these are the atoms placed on these planes and this is the incident ray of x-rays coming from that direction that is the wave front it is coming and we will consider one ray this is one incident ray in the BM this is the 2nd incident ray one falls under this plane and makes this angle Theta what I call incident angle this is different from what you have defined incident angle in reflection, okay it is the angle made not with the normal to the plane angle made with the plane, right and this is the incident ray that is the transmitted ray.

Most of the x-rays what we impinged on to the crystal from which we are trying to understand the crystal structure they just get transmitted most of it. A fraction of the intensity is the one which gets diffracted and that diffraction let us say it is taking place in this direction and this one from here is diffracted in that direction that is called the... I will be able to observe these provided they are in face here that is what I talked about the coherent, if one is coming out coherently with the other I will be able to observe this otherwise I shall not be able to observe this.

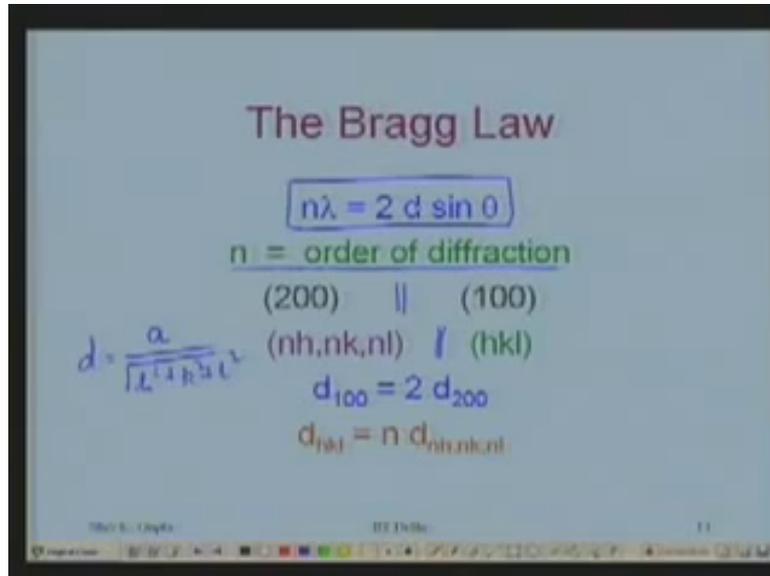
Now considering the Bragg law we consider this process as what we have considered in school in reflection in the similar fashion that is this angle of incident is Theta here the angle of diffraction is also Theta, okay diffracted is going there. Now if they are in starting from here the wave front goes here and it is in face the distance travelled by the wave front here and the distance travelled by the wave front here. If either they should be same if they are not same the difference between them should be integral multiple of the wavelength then only they will be face the difference between them is one wavelength they were again been faced.

The difference between them is to wavelength they will be in face of the difference between them is a fraction of the wavelength of will not be in face it will be like what I showed you in incoherent fashion they will be meeting in incoherent fashion and that is what is happening in most of the directions this is the direction which they are meeting currently let us see what is the path difference between them, can draw a perpendicular from here onto this 2nd ray here, right and similarly I can drop perpendicular from there, so what happens is this path travelled here this part travelled here is the same and similarly this part from the source up to this point and part of the source up to here is the same.

So part differences is QP plus PR if I say the risk the distance of separation between 2 consecutive planes in the crystal let us say this plane is hkl then d I am talking about is d_{hkl} this is the d so it is possible for me to find out the distance QP if this angle is Theta this angle is also Theta and therefore QP is equal to $d \sin \Theta$ similarly this angle is also Theta so then PR is also equal to $d \sin \Theta$ and the total difference in the path is QP plus PR is able to $d \sin \Theta$ plus $d \sin \Theta$ is $2 d \sin \Theta$, so if these 2 rays have to be in same face or it have to be coherent, the path difference QP plus PR must be $2d \sin \Theta$, is this clear? And if these are means if $2 d \sin \Theta$ must be integral wavelength right that is if they are coherent, I did not make the complete statement. If these 2 rays are coherent they are in same face is

path difference must be equal to integral number of wavelength then they are in phase and this gives me the Bragg law.

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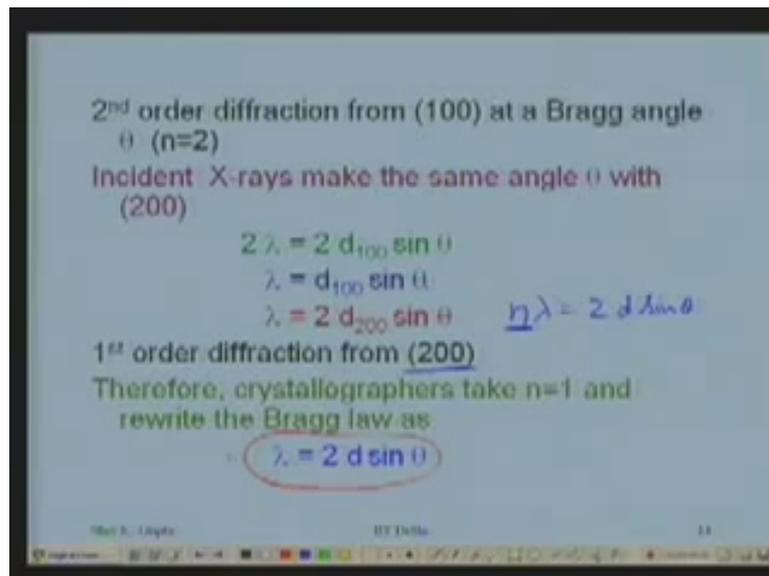


This gives me the Bragg Law which I have written here that $n\lambda$ is equal to $2d \sin \theta$. In this there are number of parameters in this expression n is 1 parameter it is an integer λ is the wavelength which radiation I am using that is the value of λ d is the spacing between the consecutive planes there could be more than one sense of plane in a crystal like 1 0 0, 1 1 0, 1 1 1, 2 0 0, 2 1 0 and so on and so forth there could be variety of these spacing then θ values at which this will diffracting will be different, so there are so many parameters let us try to fix some of them and see what we can get out of it. 1st of all we concentrate on the n what we call the order of diffraction n we refer to as the order of diffraction.

Now to understand this order of diffraction which is an integer and the path difference between the diffracted rays which are coming from 2 consecutive planes differ by that you know their paths they have travelled by that much distance, so we shall have already seen that a plane hkl like 0 1 0 I showed you is parallel to 0 2 0 and 0 2 0 plane is interleaving 0 1 0 as a matter of fact is a subset of 0 1 0 similarly I say 2 0 0 is parallel to 1 0 0 that I can say about any plane nh, nk, nl where n is constant integer is parallel to any plane hkl . (())(30:28) if h is 1, k is 2, l is 1 it is I can say 1 2 1 plane is parallel to 2 4 2 plane right similarly it is parallel to 3 6 3 plane right that is the meaning of it.

Also from the formula of d which I write again for you, d is equal to in a cube a divided by under root h square plus k square plus l square I can also that d 1 0 0 is equal to twice d 2 0 0 which I can generalise d for hkl is equal to n times d of nh, nk, nl can get it from here n square h square plus n square k square plus n square l square and from the under root login always take-out n, so d of hkl will be n times the d of nh and k nl. If we know these listenership what we have done let us see what happens is to this Bragg law.

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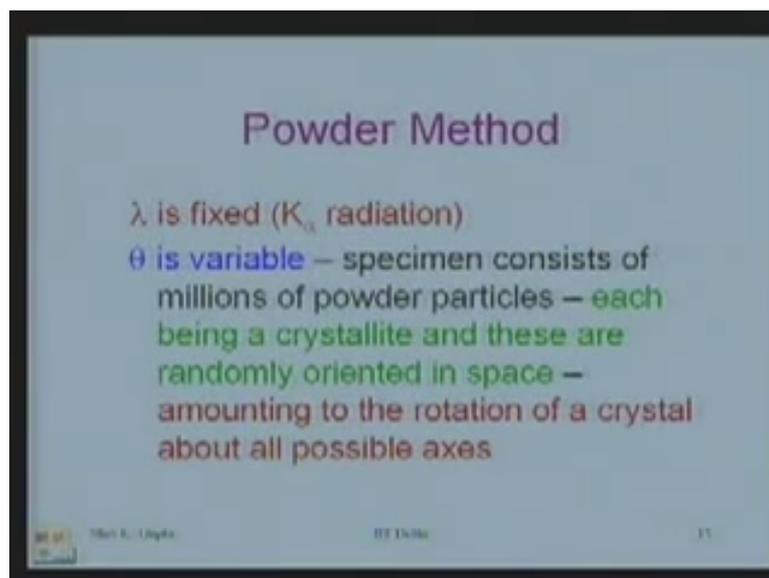
Now let me consider to look at the Bragg law 2nd order diffraction that means n is equal 2 because n I said is the order of diffraction. In other words the path difference between the 2 consecutive diffracted rays from the 2 consecutive planes is 2 wavelengths. 2nd order diffraction from 1 0 means 2 consecutive 1 0 0 planes at a Bragg angle is Theta at which it is happening 2nd order means n is equal to 2. Now incident x-rays make the same angle Theta with 2 0 0 as they make with 1 0 0 why it is so? They are parallel that is what I just shown therefore let us rewrite the Bragg Law which is 2nd order from 1 0 0. 2 lambda this is 2nd order 2 d 1 0 0 sin Theta it is satisfied if I simplify this 2 cancels with 2 it becomes a lambda is equal to d 1 0 0 sin Theta, d 1 0 0 I have already seen is equal to 2 d 2 0 0 if I rewrite this it becomes lambda is equal to 2 d 2 0 0 sin Theta.

Now let us compare this with the Bragg law and lambda is equal to 2 d sin Theta if I compared it, it is a 1st order diffraction n equal to 1 from a 2 0 0 plane and it is coming in the same direction the words if I am observing a 2nd order diffraction from a set of 1 0 0 planes that is also the ray or the beam coming 1st order from 2 0 0 what part of the intensity is the 1st order from 2 0 0? What part of intensity is 2nd order from 1 0 0 it is not possible for me to

distinguish they are superimposed, so we consider that order of diffraction is 1 unity n is taken to be 1 and therefore the Bragg law can be rewritten by taking n equal to 1 λ equal to $2d \sin \theta$. How does the parameter n λ d and θ I have fixed up one n equal to 1 and λ is equal to $2d \sin \theta$ then how do I resolve...what I am getting is a 2nd order from 1 0 0 or 1st order from 2 0 0.

I just showed you in a simple cubic crystal there is no 2 0 0 plane and if I observe a 2 0 0 diffraction from such a crystal I would know that it is merely a 2nd order form 1 0 0 because physically 2 0 0 is not a plane but if it is a body centred cubic 2 0 0 is a physical plain there is a body centred item sitting there and therefore it could be 1st order from 2 0 0 it could be 2nd order from 1 0 0 so that much we have to understand, right that will be a tacit understanding once I take n to be unity or the order diffraction to be unity in the Bragg law and modify the Bragg law to read λ is equal to $2d \sin \theta$, is that right?

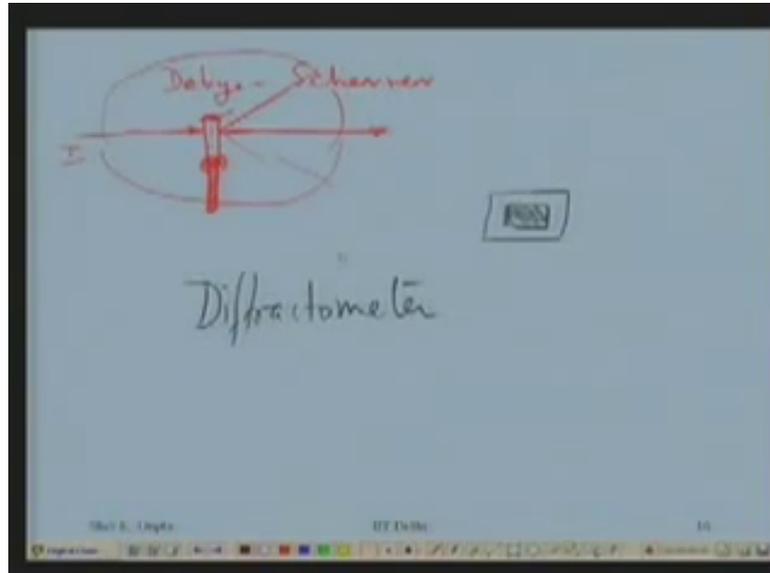
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Well generally powder method is used and it is very simple to work with in here we fixed the value of λ that is we use monochromatic radiation, characteristic radiation K alpha which we refer to in the beginning of the class and then θ becomes a variable because I am using powder, powder means millions of crystallites each powder particle is a crystal by self a crystal has been ground to a powder and it is a very small powder particle and each one is a crystallites. When in an ensemble of this powder where it is kept in a cavity or in a tube or someplace these powder particles will be all are randomly oriented in space that means each crystal is randomly oriented in space. It (())(36:48) saying that crystal has been rotated about all possible axis in all possible orientations once I have millions of such particles that is

one advantage which we get using the powder method. The Theta is becomes all possible combinations all variables Theta is a variable and this what it (())(37:11) rotating the crystal about all possible axes in space.

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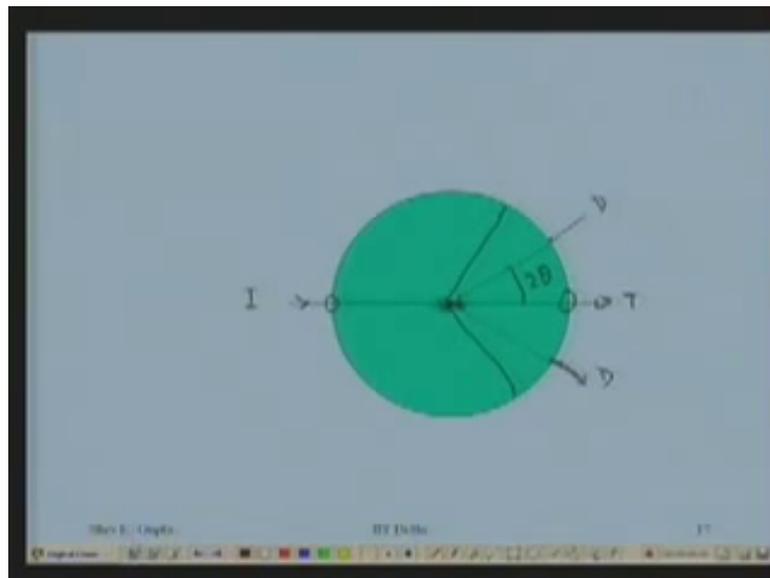


The powder particles or powder specimens which are used and be used either in a camera, camera is a Debye scherrer camera the geometry of which we shall discuss. In here the specimen is in form of a tube, this plastic tube which is non-crystalline is mounted over a wire of metal and this tube you can seal these ends with the help of a material like quick fix and tube is filled with the powder particles and then on top you can again seal it with the quick fix, fix non-crystalline, plastic tube here is non-crystalline they will not give rise to diffraction and the metal wire of course for rigidity we are using that, it can give rise to diffraction but it is not allowed to come in the beam of x-rays, right that kind of specimen is put in the middle of a or in the center of a camera which is a cylinder basically, alright.

I will show you the geometry of the cylinder from one side there is a hole made and a collimator is placed x-rays come like this, incident x-rays of the specimen and they get transmitted like this and diffracted rays goes in different directions, okay. So that is the powder specimen used or if you are in a great hurry can use the glass fibre, on the glass fibre you can put some quick fix or glue and roll it in the powder so that again you get a cylindrical specimen of the powder which can be kept again in the middle of the camera and x-rays come from one side get transmitted out and diffraction is...On the cylinder we are putting the film all around the cylinder, cylinder is like that because this in the middle of the camera.

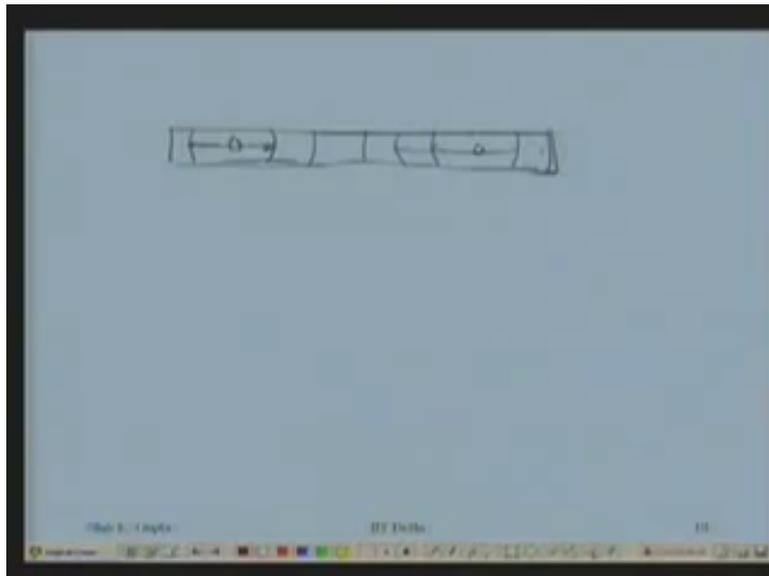
So cylinder is like that and around this we put an x-ray film on which this diffracted rays are observed or can be developed. We can see that or else we use a diffractometer. Again there is a powder specimen, this powder specimen is kept in a rectangular cavity made in a metal plate, in this cavity you fill the powder and then on top just simply spray some lacquer or any other plastic which will keep it together and not let it fall. At the same time it will not give rise to any diffraction, right. Now let us look at the geometry of this diffraction.

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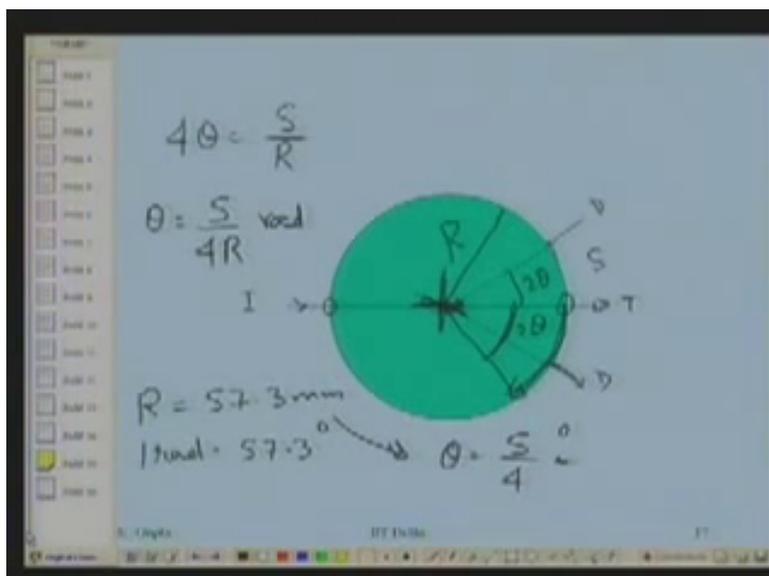
Geometry of the diffraction in the case of a camera here is my specimen, this is the incident ray that is the transmitted ray and that is diffracted ray. Between the diffracted ray and the transmitted ray the angle is always 2θ that you will see from the geometry of the (()) (41:51) which I made and the specimen here the particular plane which is diffracting let us say it is placed like this, so this angle is θ that angle is also θ but this angle becomes 2θ and this crystal or the set of plane in another crystal rotate it in this fashion give rise to diffraction in this direction and when this rotation is taking place like this the diffracted ray is really rotating about the incident ray and that performs a cone, this cone is intersecting the film here and there. Like that different set of crystal graphic planes will give rise to another cone may be let us say the corner somewhere here the next cone that gets recorded in the film here, so the film which has a hole here and a hole here so that x-rays can go through it is looked at.

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A narrow rectangular strip like this is a hole here and a hole there around the holes I have intersection of these cones this will go out and so on and so forth and maybe there are some more not (())(43:47) there now only thing this from this I should find out what is the diffraction angle or this what is the diffraction angle for this what is the diffraction angle for the other one so on and so forth this is what we have to find out. If I can find out these theta we can relate this Theta from the formula we have seen the lambda is equal to (())(44:08) data and d is equal to a for under root h square plus k square plus l square we can try to see how is this theta related to hkl.

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While we are doing this let us go back to the geometry of the camera, so this angle is 2θ and also this angle is 2θ the cone this intersecting at 2 places making 2 arcs with the film so I can relate this if I know the radius of the camera to the R then this spacing between them here to here let us say is S then I can say that 4θ is equal to S divided by R that is the definition of the angle and this angle is 2θ plus 2θ is 4θ , so for different pairs of arcs I have different value of θ and that can be measured, so θ can be taken as S upon $4R$. For simplicity this θ will come out in radian we take the value of R such that conversion to degrees becomes easy for us usually you take R to be 57.3 millimetre to take that you know that one radian is equal to 57.3 degrees, so converted into degrees you have to multiply by 57.3 and radius is there this cancels out.

So you get straightaway in such a camera you get θ is equal to S by 4 in degree, alright but when there is a diffractometer we use do not use x-ray film there we use the Geiger counters to measure how many packets of photons are coming, right. A Geiger counter is one of such counters here the specimen is kept in the center again and the Geiger counter moves this position goes in that direction and these are the incident rays, so the moment is such when it is moving from here to there it has moved at certain value of angle which is 2θ if there is a diffraction of the (hkl) that angle is 2θ but the specimen rotates by an angle θ only.

So that this angle is θ , so the machine is so synchronise the specimen rotates by an angle θ , the Geiger counter moves through angle 2θ by the time the Geiger counter we have moved to 180 degrees specimen would have just become perpendicular 90 degrees starting from this position the specimen would have gone there and Geiger counter would have moved here to there, again I am able to measure 2θ values directly and that gives me the θ values. Let us go back to see how can we use this θ to find out the hkl and from hkl how do we find out the...right.

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In cubic crystals

$$\lambda = 2 d \sin \theta,$$
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$
$$\lambda^2 = \frac{4a^2 \sin^2 \theta}{h^2 + k^2 + l^2}$$
$$(h^2 + k^2 + l^2) = \left(\frac{4a^2}{\lambda^2}\right) \sin^2 \theta$$
$$(h^2 + k^2 + l^2) \propto \sin^2 \theta$$

In cubic crystal in cubic crystal well of course this is (48:56) what we talked about this is the d spacing related to the lattice parameter and the Miller indices of the plane hkl. If I substitute this d in here I can say that and square it lambda square is equal to 4 a square 2 is becomes 4 a square and divided by h square plus k square plus l square and sin theta also becomes square sin square theta, it is just (49:23) and made the square. Now from here what I do is I think that the denominator h square plus k square plus l square onto the left hand side and take the lambda square on the right-hand side and then I separate out these a and lambda like this, so h square plus k square plus l square is rewritten as equal to 4 a square by lambda square sin square theta, now for even if it is an unknown crystal what I have lattice parameter is a constant, right?

Lambda the characteristic radiations the x-rays I am using is also constant why I have separated this out is a constant, so now I see that h square plus k square plus l square is proportional to sin square theta that is a constant of proportionality 4a square by lambda square, so I have got different values of teacher and the sin square theta which I have obtained from there will be proportional to the h square plus k square plus l square, however this h square plus k square plus l square helpful to me to get the hkl.

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$(h^2+k^2+l^2)$	h k l
1	1 0 0
2	1 1 0
3	1 1 1
4	2 0 0
5	2 1 0
6	2 1 1
8	2 2 0
9	3 0 0 / 2 2 1

If $h^2 + k^2 + l^2$ is 1, hkl could be 1 0 0 or 0 1 0 or 0 0 1 is a question of family. If the $h^2 + k^2 + l^2$ is 2 it is 1 1 0, if it is 3 it is 1 1 1 if it is 4 it is 2 0 0, if it is 5 2 1 0, 6 it is 2 1 1, 8 there is no 7 you cannot find 3 integers if I square them and sum them the sum will be 7, so therefore I do not have $h^2 + k^2 + l^2$ as 7 I shall not have similarly 15, I shall not have 23, alright so on and so forth there will be number of them which I will not have. So 8 is 2 2 0 and 9 is 3 0 0, it can also be written as 2 2 1, 2 square plus 2 square plus 1 square, so that is how it is once I get the value of $h^2 + k^2 + l^2$ I shall be able to know the plane which has diffracted this.

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Extinction Rules

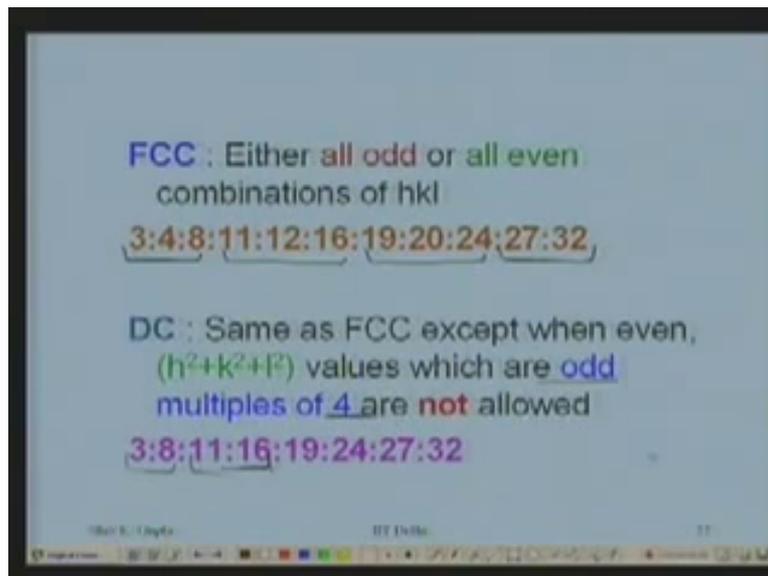
SC : All possible combinations of $(h^2+k^2+l^2)$
1:2:3:4:5:6:8:9:10

BCC : All even values of $(h^2+k^2+l^2)$
2:4:6:10:12:14:16:18:20

Now these rules which tell us for what values of $h^2 + k^2 + l^2$ I shall be observing a diffraction beam from the crystal, given crystal or from which plane I will not be observing that is for simple cubic crystal all possible combinations of $h^2 + k^2 + l^2$ are observed that means I observe 1, 2, 3, 4, 5, 6 and 7 is not there I observe 8, 9 and 10 and so on and so forth, right all now in a simple cubic crystal if there is only one atom on the lattice I do not have any 2 0 0 plane then what is the meaning of $h^2 + k^2 + l^2 = 4$ which is 2 0 0.

2nd order diffraction from 1 0 0 that is very good you understood that, now similarly in BCC we get all even values of $h^2 + k^2 + l^2$ that means I get 2, 4, 6, 8 is missing here 8 should also be there which you simplify this it becomes 1, 2, 3, 4, 5, 6 but this becomes 7 which is not there that is the distinction between this and this. If you get 7 will not be able to get hkl so you have to make it double call it 14 so that all others will also be doubled at is the distinction between simple cube and body centred cubic, alright.

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Now if I see the next one which is face centred cubic crystal in here but in here what we observe is the hkl values are either all odd or either all even this purpose 0 is taken as even and we get the combinations like 1 1 1 that makes it 3 then 2 0 0 which makes it 4 then 2 2 0 which makes it 8 and you see that it is the combination 3 4 8 which is repeating after that 11 12 16 on 8 I add 3 it becomes 11, I add 4 it becomes 12, I add 8 it become 16 like that but in here 28 is not possible again 28 is an integer where I cannot find this 3 integers and square them to get the sum equal to 28.

Then diamond cubic crystal is a crystal which we shall see in the next class but it is on the same space lattice FCC and here when the space lattices is observed because there are more than one atom sitting on the lattice point some more intensities are extinguished and those are whenever $h^2 + k^2 + l^2$ is even the odd multiples of 4 are missed out that is in 3 4 8, 4 is an order multiple of 4, 8 is an even multiple of 4, 8 is observed but 4 is not observed. Similarly 12 is an order multiple of 4, 16 is an even multiple of 4, 16 is observed 12 is not observed so on and so forth it goes on that is the diamond cubic crystal or crystals which crystallise like a cubic diamond they will be showing this and about the diamond cubic crystal we will talk about in the next class.