Physics I: Oscillations and Waves

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Lecture - 24
X-Ray Diffraction

We have been discussing diffraction and we saw that if we have a periodic arrangement of sources. For example, we consider the diffraction grating where there was a periodic arrangement of slits and we saw that when we have a periodic arrangement of sources. We get a diffraction pattern where there is conjugative set of bright and dark Freingers observed and the diffraction grating is essentially a 1 dimensional periodic arrangement of sources each slit acts like source and there is 1 dimensional arrangement. If you make the slit width and the length of the slit comparable, you then have a 2 dimensional situation. You could have a pattern of squares for example, which could act like dimensional periodic arrangements of sources.

And you would also get a diffraction pattern inside the situation today; we are going to discuss a very interesting situation. where we have a 3 dimensional arrangement of 3 dimensional periodic arrangements of sources. We all know that the distribution of atoms and molecules inside crystalline solids crystalline solids, it has a periodic arrangement. So, there are certain solids, which are crystalline for example, salt NACL has a crystalline structure or diamond and the distribution of the atoms or the sodium chloride molecules inside these solids. It is known that, it has a periodic structure and this periodic structure, this periodic distribution of atoms or this periodic distribution of molecules could act like a some sought of a diffraction grating. So, this is a situation that we are going to discusses in today's lecture.

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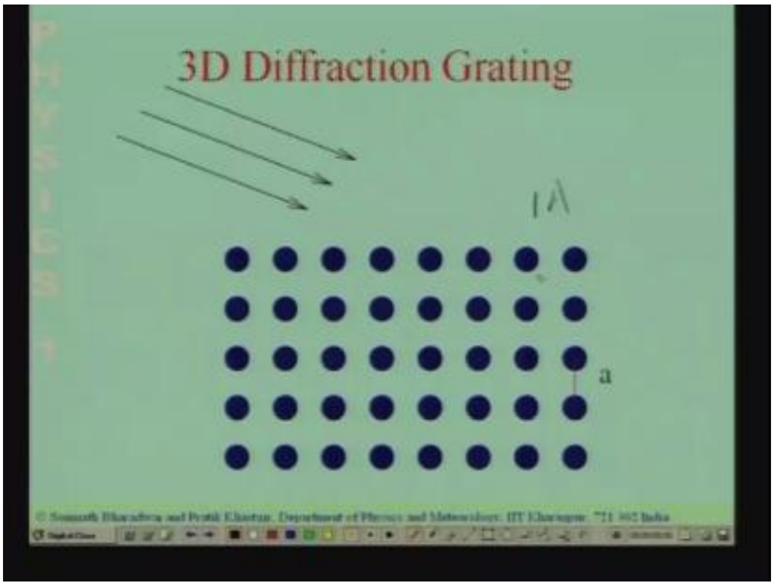

So, this shows you schematic diagram of the distribution of atoms or it could be molecules inside a crystalline solid. And we are going to discusses situation, where this is going to act like a diffraction gratings each of these atoms, each atom is going to act like sources of radiation coherent source. So, radiation from all of these atoms is going to coherent and we are going to consider a situation, where there is diffraction. So, you super pose the coherent emission from all of the sources and we get a diffraction pattern. Now, we know that the, inter atomic spacing is of the order of Armstrong's.

So, the inter atomic spacing, which I show by a over here a is the triberty (refer time: 03:53) use a to denote the inter atomic spacing are the unit cell. The spell the cell spacing and this is the order of 1 Armstrong this is known. The atomic the distance typical distance between atoms inside crystalline solids is of the order of 1 Armstrong's. And we saw that the diffraction, when we consider grating for example, the diffraction condition for the maxima is d sin theta is equal to m lambda either Maximas at different angles theta provided, this formula is satisfied.

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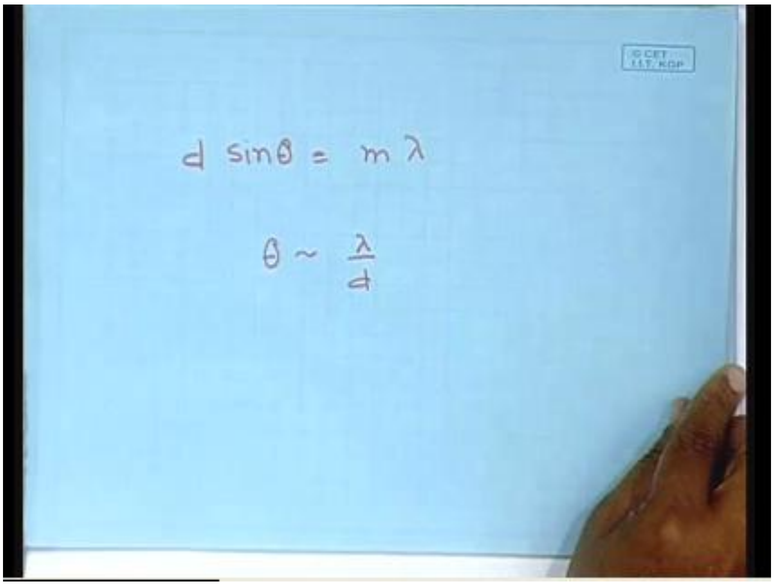

So, the Maximas the angular spacing between the Maximas is of the order of lambda by d. And where d is the spacing between the sources right in this case, we are going to consider situation were these interatomic spacing is the, is d so, you saw the order of 1 Armstrong.

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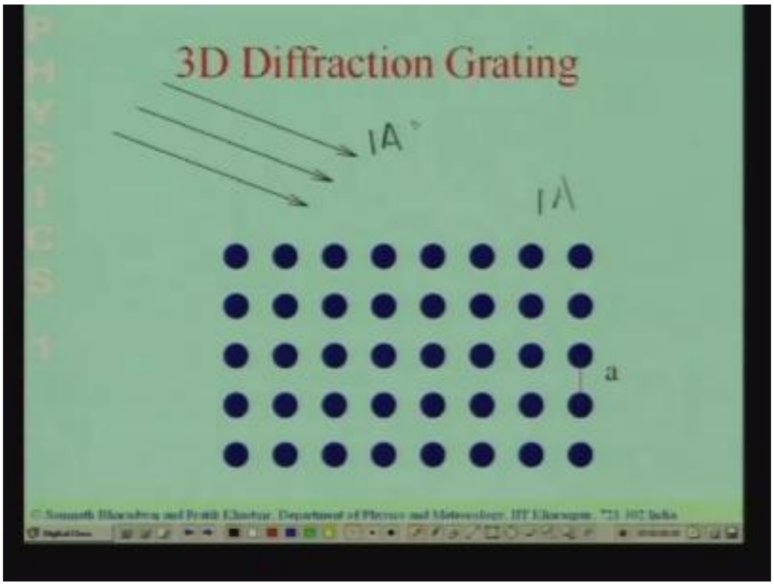

So, we have to what is tells us is that, we have to consider some kind of radiation some kind of a wave, where the wave length is of the order of 1 Armstrong. So, we have to consider a situation, where the wave length of the radiation is of the order of 1

Armstrong. So, and the wave length, which we are going to use is of the order of 1 Armstrong and we have discussed the electromagnetic spectrum and we saw that 1 Armstrong is x ray. So, the wave length range around 1 Armstrong corresponds to x-rays. So, we are going to consider a situation, where there is a x ray incident on crystalline solid and this is what is shown over here.

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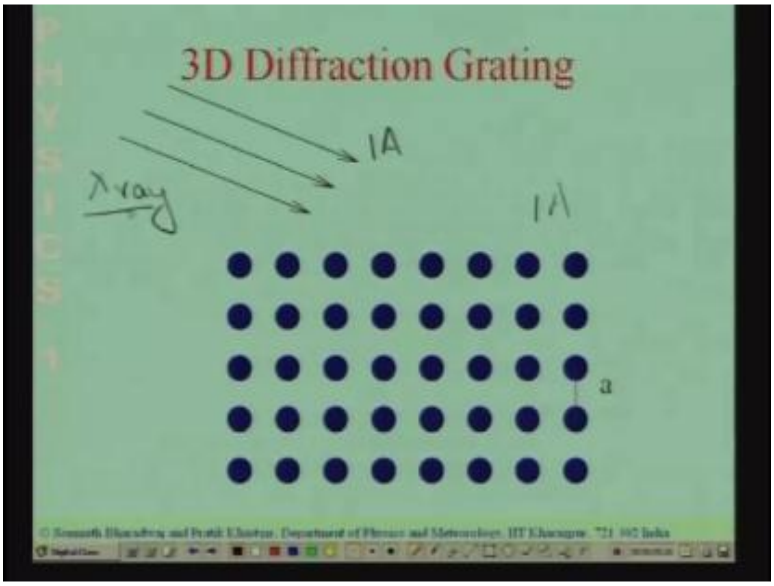

You have x ray, which has a wave length of the order of 1 Armstrong, which is incident on a crystalline solid. Now, what is going to happen? When you have x ray radiation x ray remember is an electromagnetic wave, which is incident on a solid on some crystalline solid. Now, electromagnetic radiation, we have discussed several number of times, that electromagnetic radiation is an oscillating electric field. So, the way you think of this incident electromagnetic.

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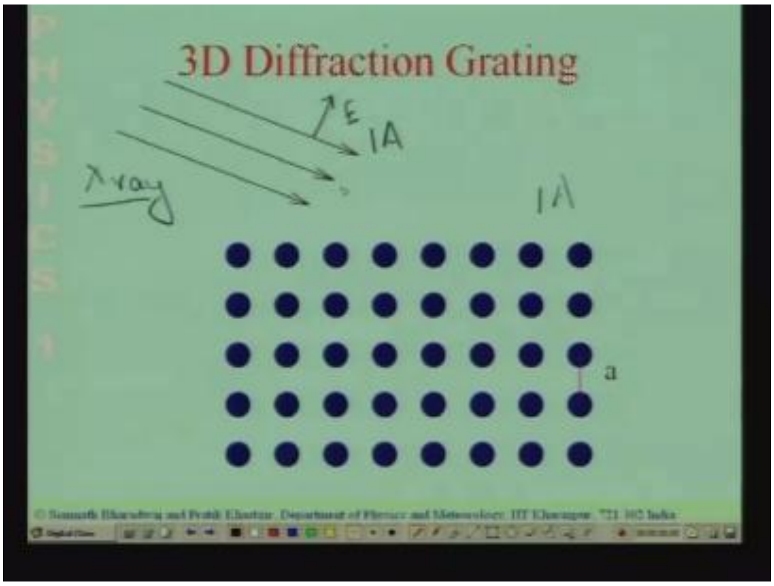

Radiation is actually, in terms of a wave and this wave has an oscillating electric field. So, this is the electric field let us, say hypothetically and there is going tobe an incident wave of electric field, which is oscillating they will also be a magnetic field. Now, you have these electric, so, you have this electromagnetic wave, which is incident on this solid and this picture show, you that is the atoms, which are range periodically inside the solid. Now, the atoms, we know have a nuclei and they also have electrons, now, when these atoms, when an individual atom is under the influence of the external oscillating electric field.

So, we have an atom under the influence of an external oscillating electric field. The electric field is oscillating electric field is the x-ray electromagnetic wave. And the atom is under the influence of this external oscillating electric field both the nucleus and the electrons are going to experience this oscillating electric field. Now, the acceleration of the nuclear is going to be much smaller, because the acceleration is the acceleration of any particle in a under the influence of an electric.

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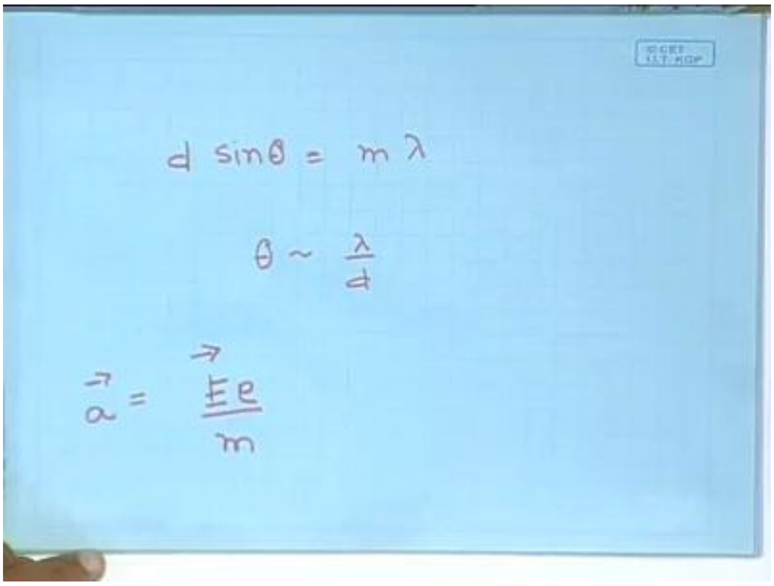

Field is E the electric field in to the charge divided by the mass the mass is this is the acceleration. On the particle and the nucleus is much heavier than the electrons. So, the acceleration of the electrons is going to be much larger than the acceleration of the nuclear so, the electrons in this atom.

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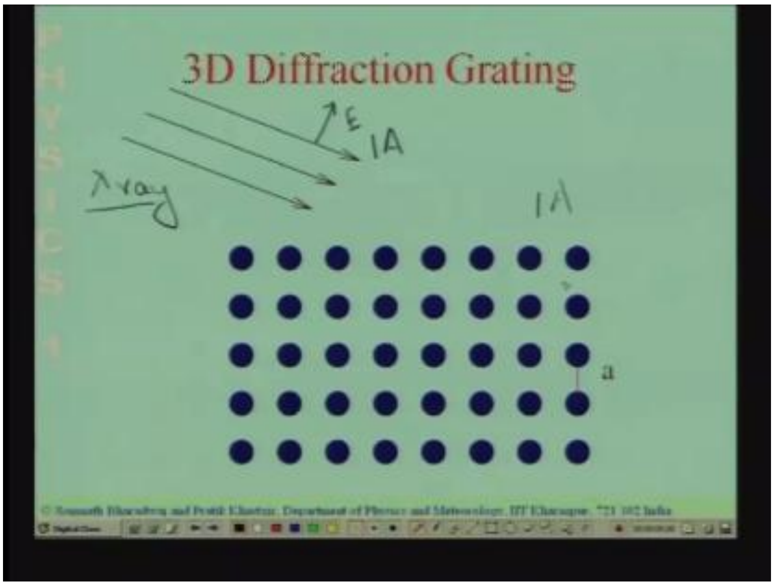

The electrons in this atom are also going to accelerate in response to this external electric field, there are going to experience an external force. Now, we can think of this the electrons has being bound to the nuclease electrons are actually, bound to the nuclease and we can think of this in the external disturbance is small. I have told you that, you can think of the response has that of a simple harmonic oscillator. So, we can think of the electron has been bound to the nucleus by a some kind of a simple harmonic by a simple harmonic oscillator potential by a spring. And there is an external force, which has a frequency the external the frequency is the frequency of the x-ray radiation. So, we have a simple harmonic oscillator the electron bound to the nucleus, which is under the influence of an external force the external force is, because of the electro x x ray, which is incident you have this oscillating electric field.

And we saw that the electron, if you look at the large time behavior the oscillator is going to oscillate at the frequency of the external force is going to oscillate at the frequency of the external force. So, the electron inside the atom is going to oscillate at the same frequency as the x ray. And we also saw that, when an electron oscillates it emits electromagnetic radiation an oscillating electron emits electromagnetic radiation and this radiation, again is at the same frequency at which the electron is oscillating. So, let me recapitulate, what I have told, you when I have x-ray of some frequency incident on the atom. It is going to set the electrons into oscillation with the same frequency and the electrons are going to emit radiation at the same frequency.

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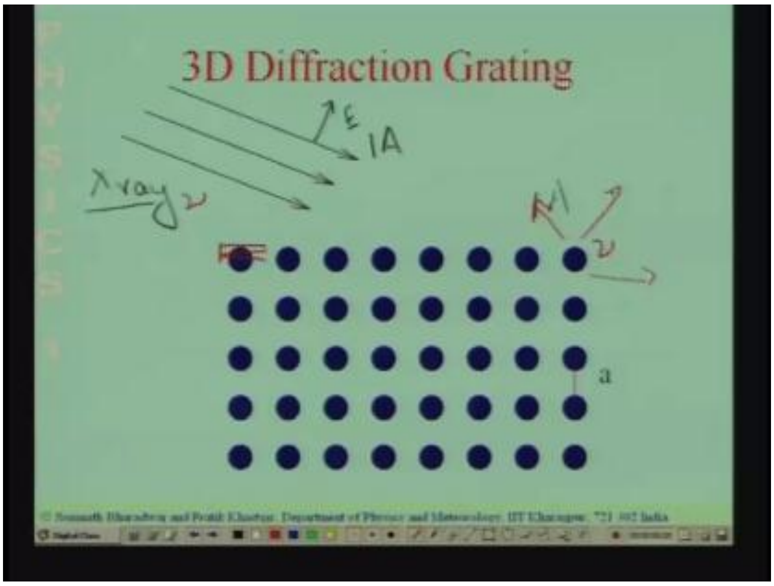

So, if I have electromagnetic radiation of frequency nu incident on this solid on this crystal the electrons, inside this are going to radiate. And the frequency nu the electrons inside here are going to radiate at the frequency nu and the radiating the oscillating electron are going to ah. The electron inside are going to oscillate at the same frequency has the x-ray and the oscillating electron is a dipole oscillation is going to emit radiation in various direction.

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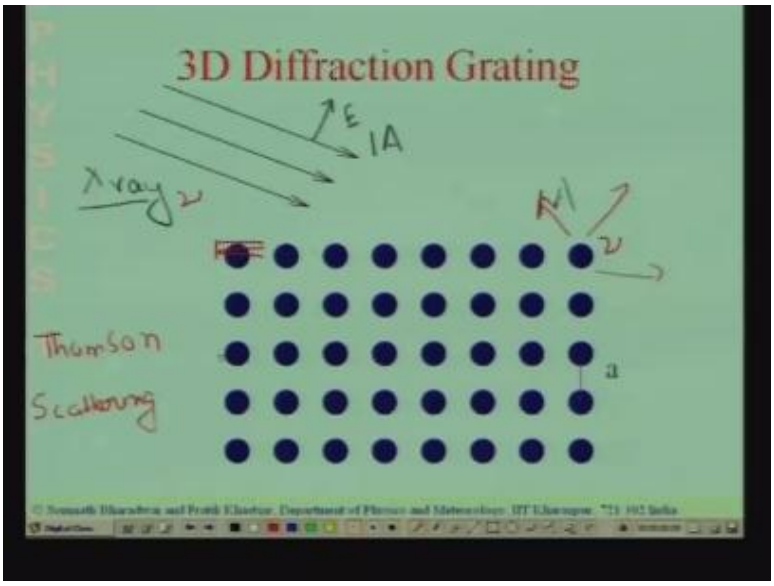

So, this going to radiate emission at the same frequency nu in the various directions and we have discussed the direction dependence of the dipole radiation. So, each atom the bottom line is that each atom over here, each atom over here is going to act like, source of radiation at the frequency nu and all of these sources is are going to be coherent. So, we are going to have coherent radiation coming out from each of these atoms. And this radiation is going to be at the same frequency as which as the incident x ray the incident x-ray is there only in 1 direction. Each of these atoms is going to scatter, it out this is called Thomson scattering Thomson scattering Thomson. So, you are going to have this radiation coming out and to determine.

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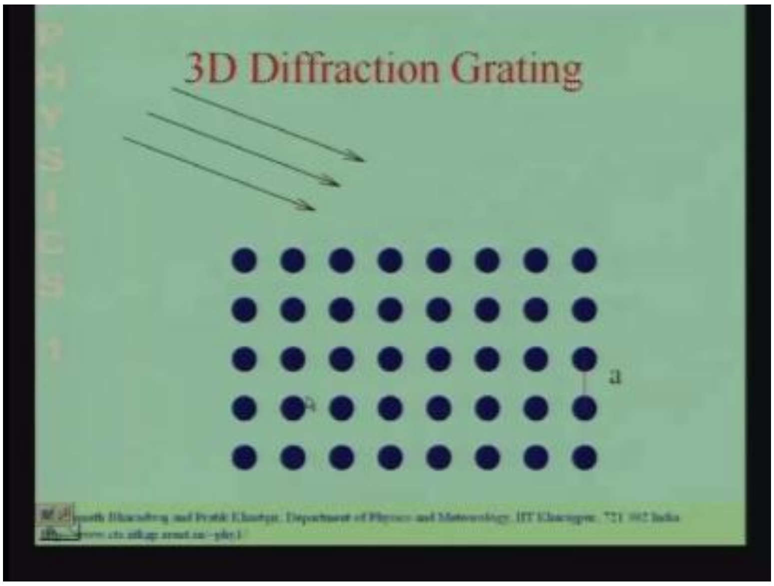

The intensity pattern in different directions, you have to add up the radiation from each of these from these from this periodic arrangement of sources. And we have seen, that if you have a periodic arrangement of sources, which are radiating coherent all of them are radiating this same the coherent radiation. So, the radiation from here and here they all they are coherent. Then you are going to get diffraction pattern.

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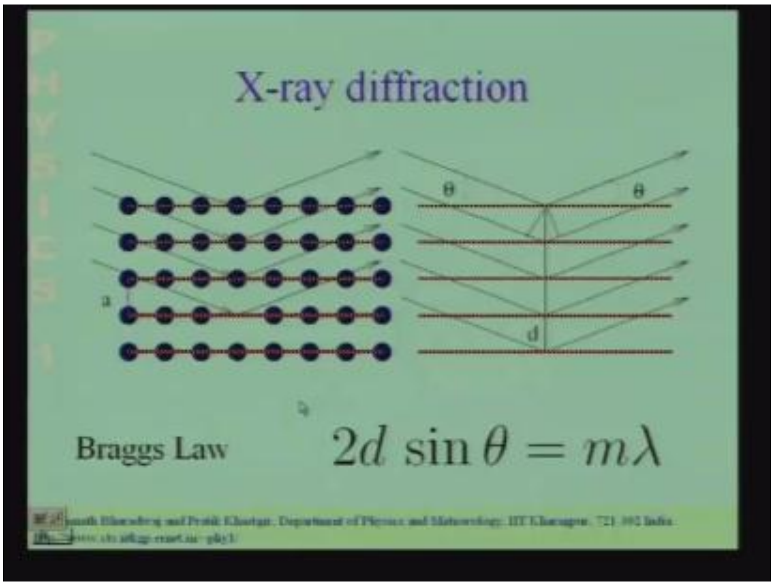

So, what we have over here is x-ray diffraction pattern that is going to produce by the radiation from this periodic arrangement of sources, each atom is going to scatter out radiation in all direction. And if you look at the intensity in a particular direction, you are going to get the sum of the radiation from all these atoms with different phases; this is quite complicated situation, because now, you have a 3 dimensional situation. When you get with slits in diffraction grating, you had just a 1 dimensional distribution here. You had have a 3 dimensional distribution of sources. So, it gets a little complicated, but there is a simpler way of thinking about, it which was pointed out by Bragg.

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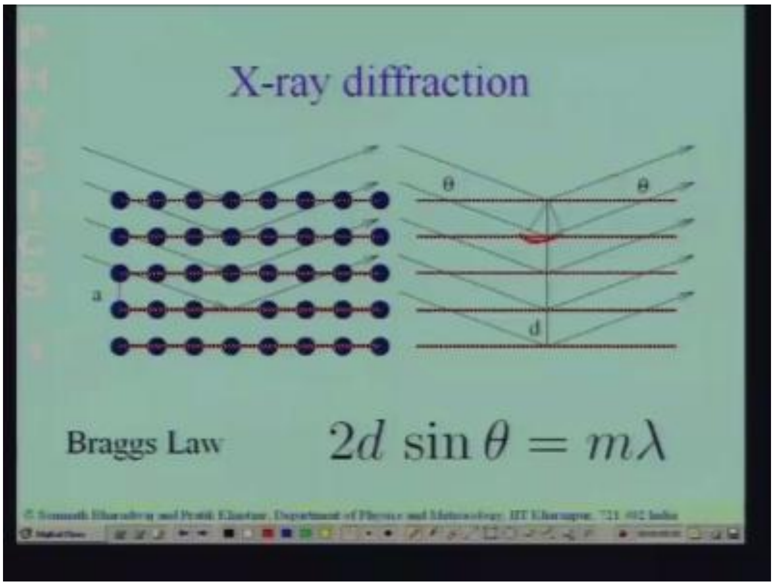

And the way you think about, it is that you can think of this scattering from these atoms in terms of plains. So, this is the crystal the same crystal lattice the atoms spacing atomic spacing is a the inter atomic spacing is a. And each of these atoms sends out radiation and we are interested in the resulting diffraction pattern. So, what Bragg said was that, you can think of this has in terms of plain, this is the crystal. I can draw plains, this is 1 plain, I can draw sets of different sets of plain, this is 1 set of plain. So, here I have 1 particular set of plains and these are the plains draw in red. And this scattering, I can think of as follows the this is incident radiation, it gets reflected over here from each of these plains.

And if I am interested, if I consider a situation, where the light is incident at a grazing angle theta…. So, the light is at grazing x-ray is at grazing angle theta and we want to see, what is going to be the incident the intensity of the radiation that is scattered out. Rather reflected out from these plains and so, it is going to be reflected out at the same angle theta. And the one the wave that is reflected from the first plain is going to be at a phase difference with respect to the wave reflected from the second wave, which again is going to be at a phase difference with respect to the radiation reflected from the third plain.

And the phase difference corresponds to this path difference, because this has to travel a larger distance. So, there is an extra path and this is the extra path, so, you will have a set of waves, if I look at the radiation in this direction in the reflected direction. I will have a set of waves, but these waves are going to have a phase difference. So, there is going to be a phased difference between this and this and this. And this phase difference corresponds to this path difference and if you work out the condition. That they should all be in the same phase you will get the condition that 2 d.

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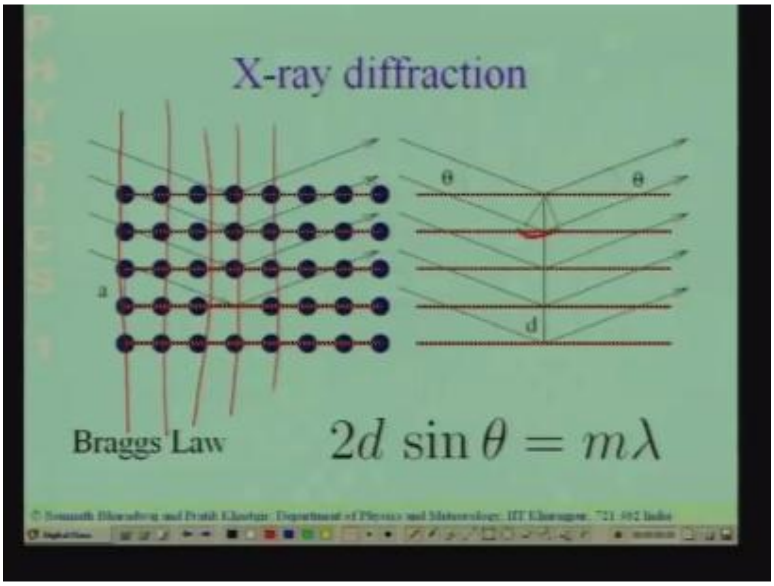

Sin theta is equal to m lambda 2 d sin theta by lambda is the path difference between 2 conjugative the waves reflected from 2 conjugative plains. And if this is a integer multiple of the this is, this is an the path difference is an integer path difference is 2 d sin theta. If the path difference is an integer multiple of the wave length, we know that this is there go to be in phase and that is the condition for a maxima. So, what Bragg proposed this is called Braggs law is that, we can think of this complicated situation in terms of reflection from a set of plains. Drawn thorough the crystal and this is a particular set of plains, you can have many set of plains this is 1 possible set of plains, you could also have plains. Like this and you have to consider all such possibilities, this is one possibility which I have shown here.

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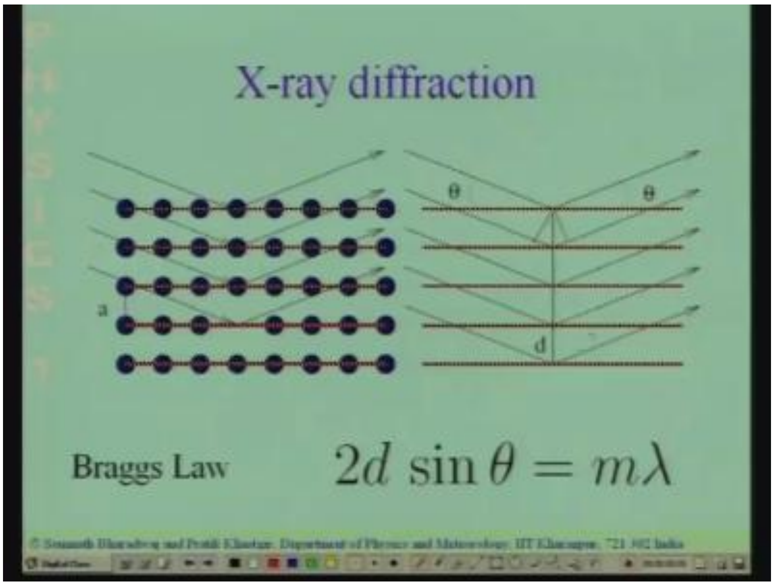

So, we are considering only one possibility and if you will get a Maxima, if this condition 2 d sin theta is equal to m lambda. Let me show you another possible set of plains.

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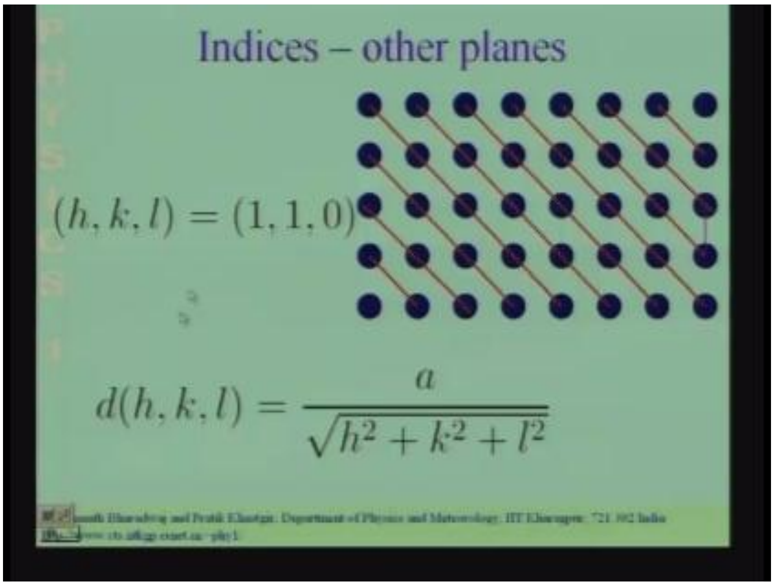

So, this shows, you another possible set of plains, which can be drawn thorough that crystal. And you have to consider when you have a x-ray incident on this lattice and you want to find out, where the maximas will occur. You have to consider reflection from all such plains and the maximum will be, you will get maxima, if the condition 2 d sin theta is equal to m lambda.

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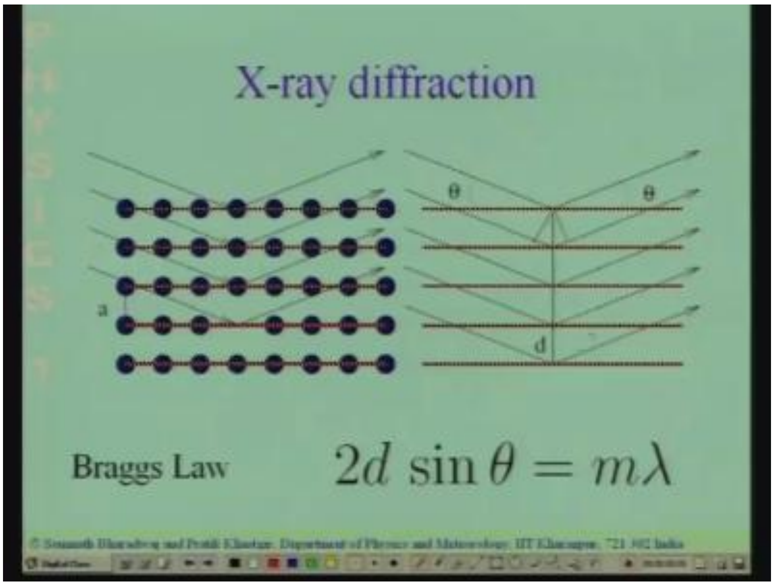

If this condition is satisfied for any of these plains, now, there are 3 indices call the miller indices, which are used to quantify to label these plains. So, there are 3 indices call the miler indices, which are use to label these plains and the set of plains drawn over here. Correspond to miller indices h k l. So, the miller indices are call a liper (refer time: 18:04) the symbol used for the 3 miller indices are h k and l and these particular plains correspond to h k l values 1 0 0. Let me spend a few minutes and explain to you do what we mean, very briefly by these miller indices. So, let me draw a picture in to dimension again.

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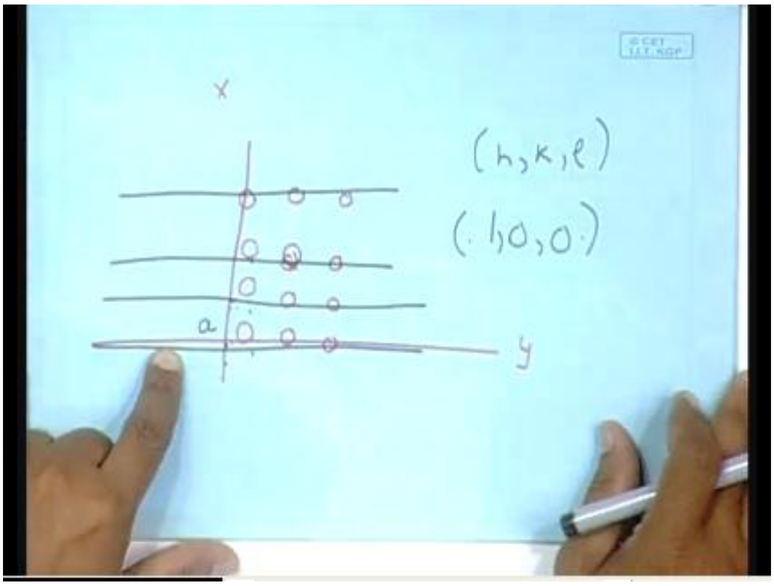

So, this is my crystal, this should be here like, this let me draw another set, then we can start the discursion. So, this is my crystal let us, say let me call this the x axis and this the y axis. And I have also have the z axis now, I can draw a plain through this crystal, which set of plains, which go like this. And these plains have intercept unity in terms of the spacing (refer time: 19:15) inter atomic spacing; they have a set a intercept unity along the x axis. So, h k and l refer to the intercepts of these plains with the x y and z axis so, the intercept the distance between the intersections of these plains on the x axis here. Is 1 the plains never interest the y axis or the z axis. So, h k l equal to 1 0 0 label these set of plains.

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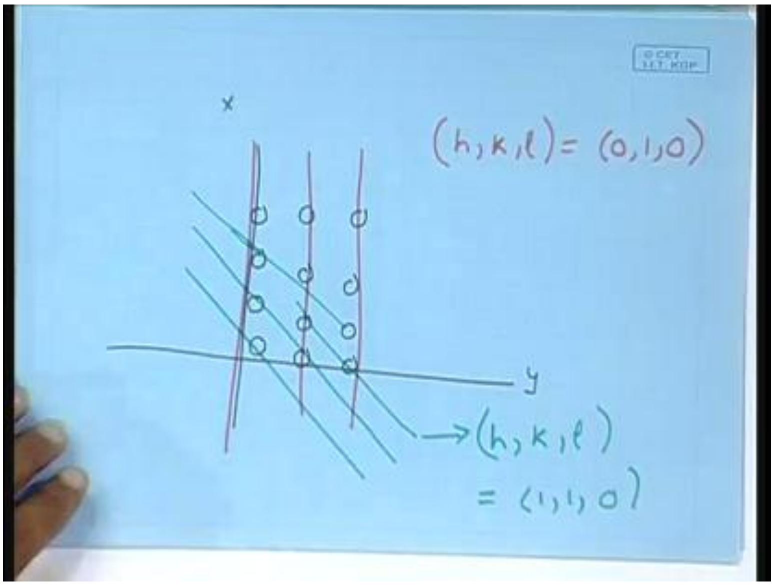

I could also consider a situation the same let draw the same lattice the same crystal, I again I have the x axis over here and the y axis over here and I could have plains, which have vertical now. Now, these plains, they never intersect the x axis, they never intersect the z axis, but they intersect the y axis and the separation between this intersections is 1. So, h k l have values 0 1 0 for these plains again, I could have another set of plains, which are like this. And these, the green once have h k l values 1 1 0, because they intersect both the x axis and the y axis and the spacing is 1 the spacing is also 1. So, corresponding to different set of integers h k l n h k and l, I will get different plains, which can be drawn through this crystal and this crystal that we are consider is cubic.

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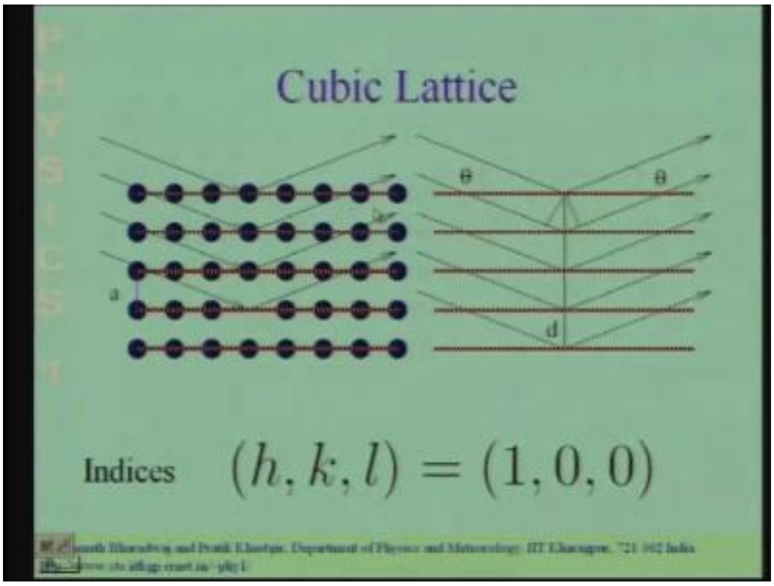

Lattice I have shown, you only a section through the cubic lattice, but the along this is the x axis this they axis along the z axis also the arrangement is exactly the same. So, we are considering a cubic lattice and in this cubic lattice, I can have different kinds many different plains. And the inter plainer distance d is what is refer to as d inter plain distance is what is refer to as d. So, let me show you another example.

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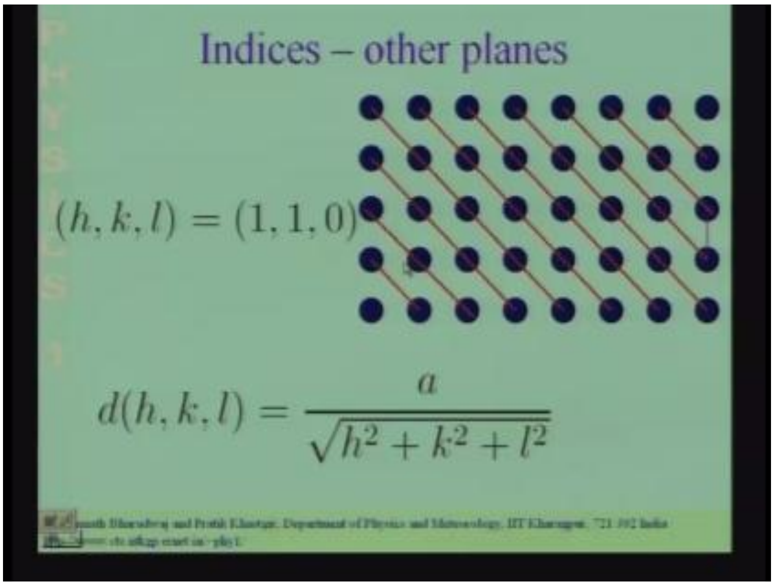

Through the same crystal now, I have drawn these plains at 45 degrees, these plains also go through atoms and they are. So, the arrangement of the atoms looks a same on this on these plains. And these plains have indices will indices 1 1 0, because that is where they interesect the x and y axis they do not interest the z axis at all. That is why, they have miller indices 1 1 0 for different values of the miller indices, I will get different plains to this solid. And there are different possible integers, which are allowed they will all different integers, will give you different plains. Now, the next question is what is the inter plainer spacing corresponding to these plains.

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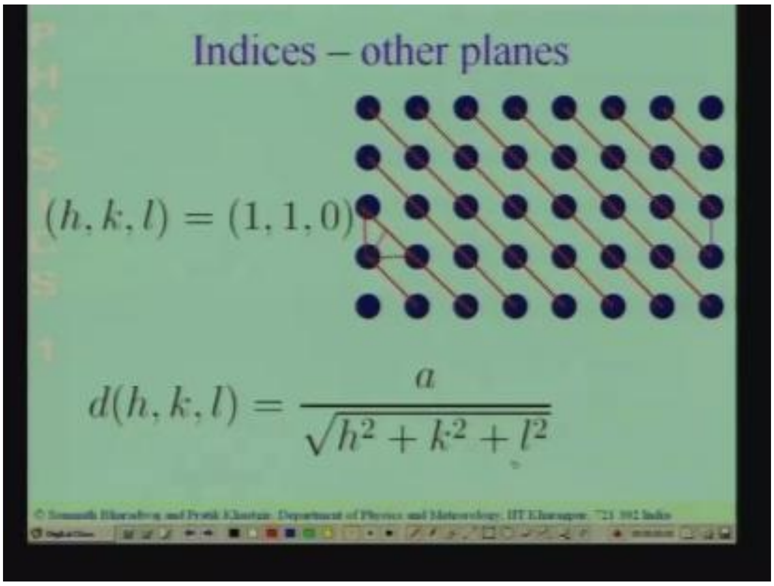

So, what we these plains the, inter plainer spacing is exactly the same as the, inter atomic spacing it is a. For these spacing's these plains, you can see that the, inter plainer spacing is, if you have apply Pythagoras theorem the, inter plainer spacing. You can calculate it for these plains and it is going to be, you can this is the, inter plainer spacing. And you can see, then it is 1 by square root of 2 of times the, inter atomic spacing. So, in general the inter plainer spacing d which is dependent on h k l the 3 indices, which label the plains is going to be the inter atomic spacing a divided by the square root of h square plus k square plus l square, so, we going to have maxima.

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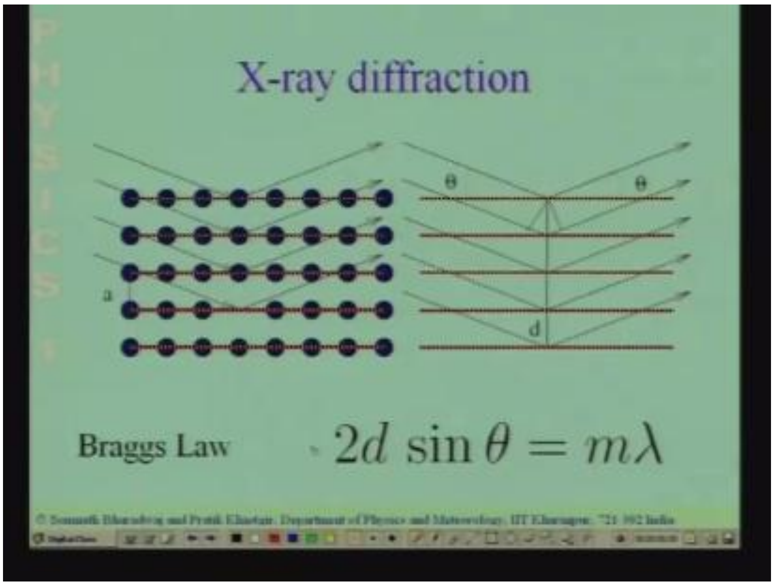

For corresponding to theta, theta remembers is grazing angle not the incident angle. Which, we have been using earlier in diffraction, it is the grazing angle it is a angle with reference to the plain and not with reference to the normal. So, whenever the condition 2 d sin theta is equal to m lambda, whenever this condition is satisfy, you are going to get a maxima in the intensity pattern. So, I have explained to you over here and told you the I have told you the basic idea and also the condition under, which you will get a maxima in the diffraction pattern. When you use x-ray, when x-ray is incident on a crystal now, let me next discuss a device call the x-ray.

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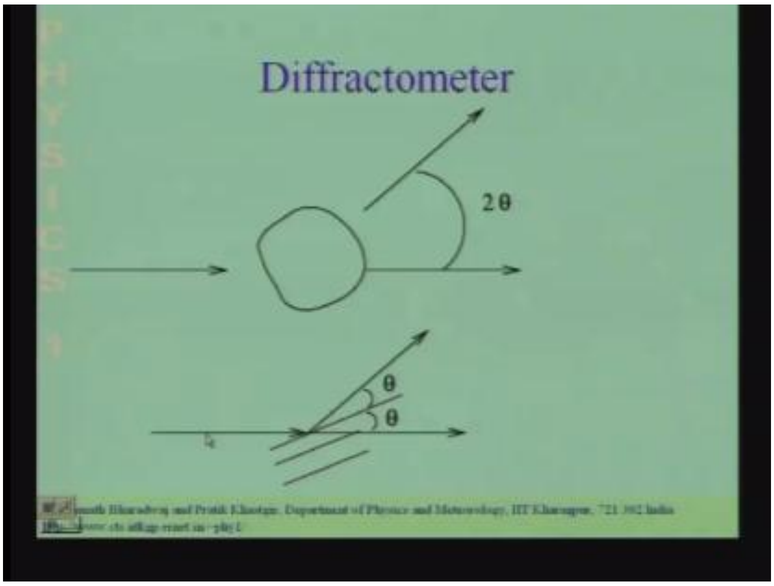

Diffractometer x-ray diffraction incidentally is very useful technique to determine the structure of materials. If I give you a crystal and I do not know, it is inter atomic spacing I do not know, how the atoms are arranged. I can use the diffraction pattern to determine the inter atomic spacing and the structure the arrangement of the atoms inside this crystal.

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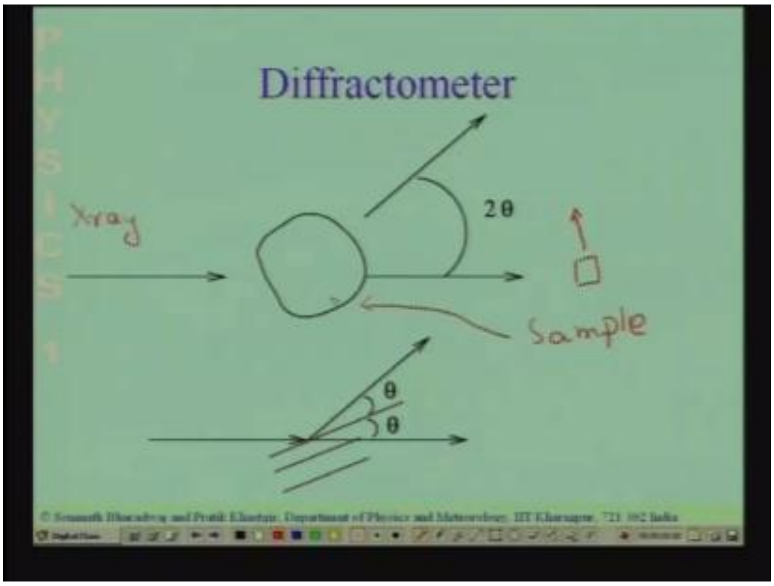

So, there is a device called X-ray diffractometer and let me briefly explain this x-ray diffractometer, so, we have x-ray incident. So, there is x-ray, which is incident on the sample so, this is my sample, so, there is x-ray incident on the sample. And the sample is a crystal or it could be the sample is a crystal over here or it could be many single crystals. Whichever be the case there is going to be x-ray scattered in all directions the intensity of the scattered x-ray is going to vary with the direction. And what happens? In this x-ray diffractometer is there, is a x-ray camera or x-ray some a device, which can measure the intensity of the scattered x-ray and this device is move to different angles. And it measures the intensity of the scattered x-ray as a function of this angle of the function of this angle over here. Now, let us just see, what is the relation between the angle over there and this theta the angle the grazing angle made with a plains inside the crystal.

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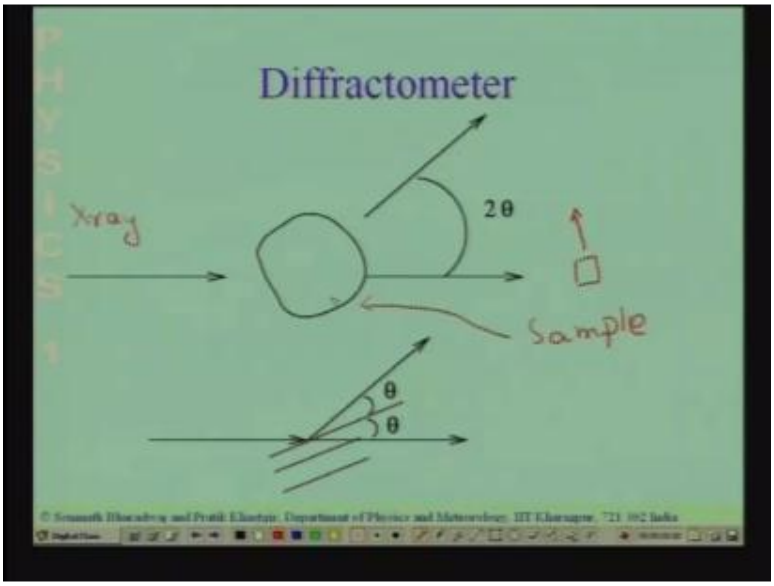

So this sample over here is a crystal, it has let us take a crystal inside the sample and inside the crystal. We can draw plains. So, let us consider a set of plains.

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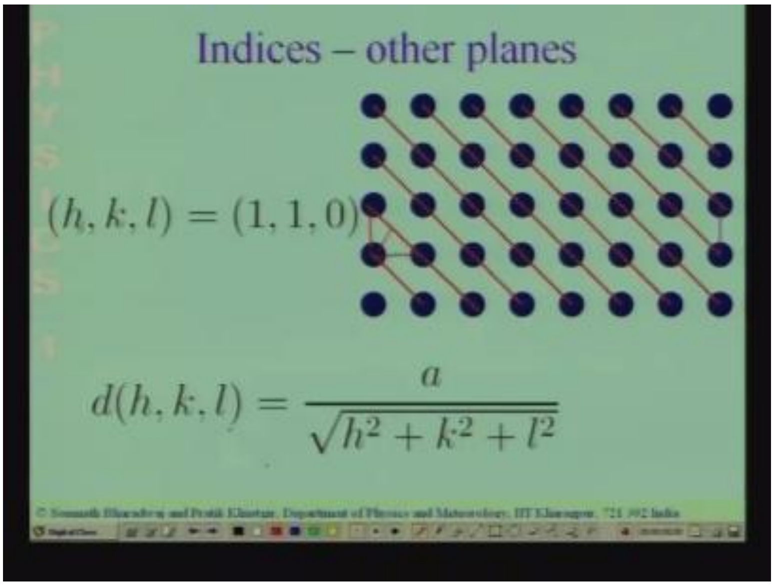

Plains could the plains could corresponds to any of these miller indices, but let. So, there could be some plains inside.

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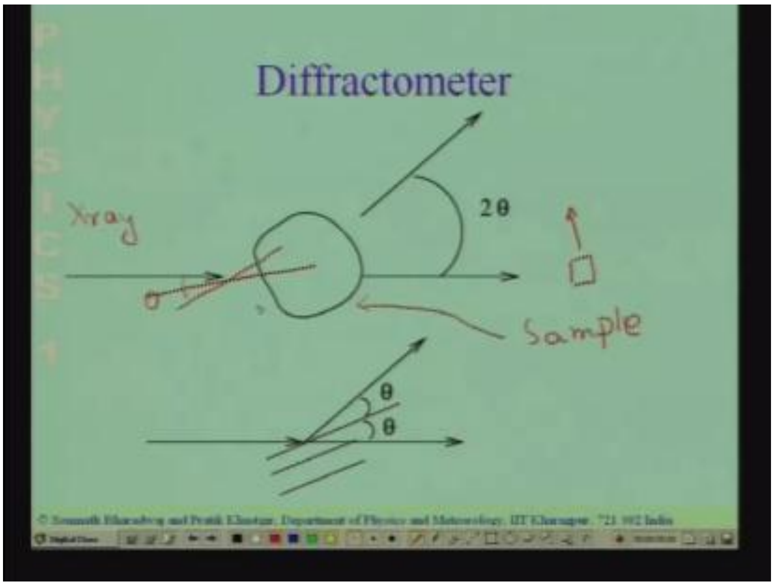

That crystal, so, let us say that, these are the plains. So, x-ray incident like this and these are the plains inside the crystal, which is a part of the sample. Now, if the plains are like, this if the plains orientated like this, then this grazing angle is theta. which is also the angle over here and the angle the reflected angle over here is also theta the reflected grazing angle. So, you can identify this angle that the scattered the angle of the scattered x-ray with reference to the incident x-ray has been twice theta, where theta is the grazing angle with respect to the plains. If you measured the intensity in this direction then, it would have made this x-ray scattered in this direction has been scattered by plains, which make a grazing angle theta. If this angle is 2 theta then this plains the plains, which are scattered the x-ray in this direction are under grazing angle of 2 theta.

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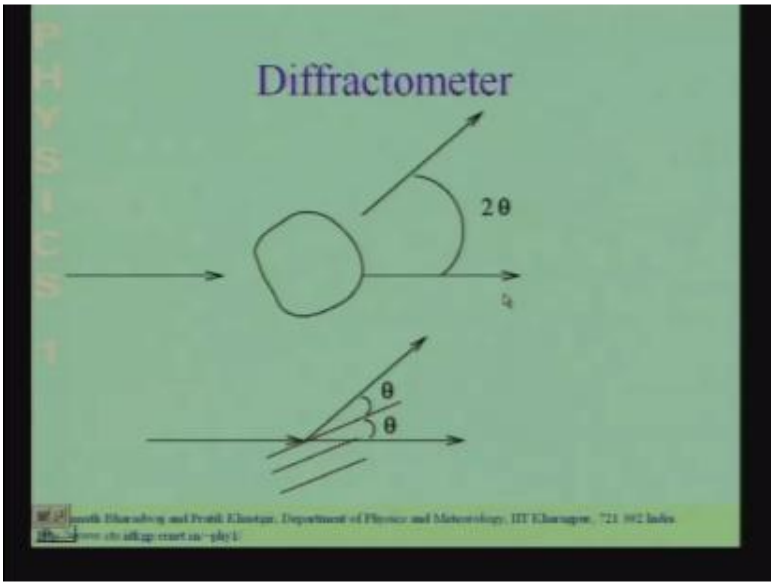

So, you can measure the intensity of the scattered light as a function of this angle, which you can interpret, has been twice the grazing angle with respect to the plains, which have the scattered x-ray in this direction. And what you get is the intensity pattern has a function of this 2 theta from them x-ray diffractometer.

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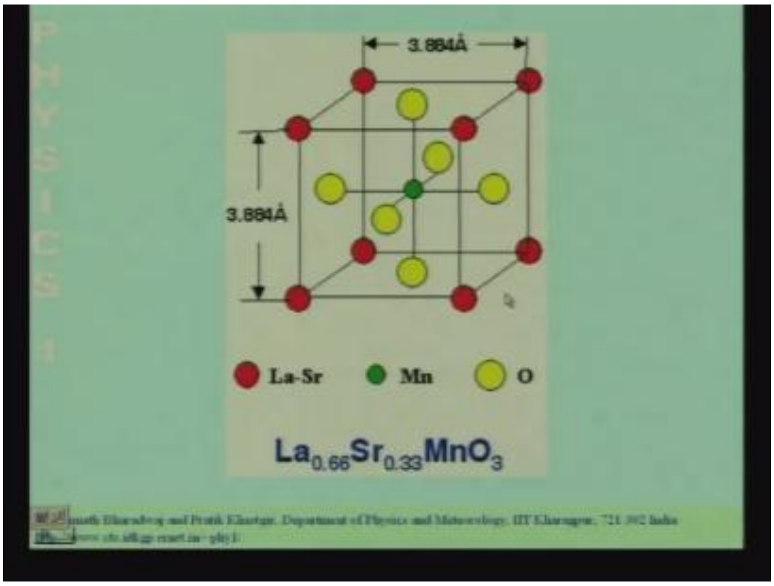

Let me consider an example, over here. So, I am going to show, you a particular example and the example, which we are going to consider.

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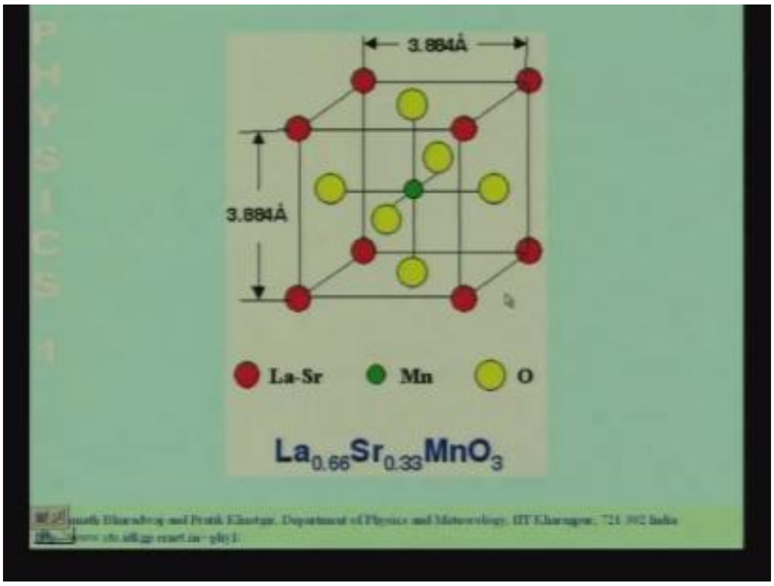

We have lanthanum strontium manganese oxide, so, we have a crystal it, which has a crystal structure which is known. So, the crystal structure of this solid is shown over here in this solid. The solid is essential lanthanum manganese oxide, but over here strontium has replaced some of the lanthanum atoms and the lanthanum atoms which have or the strontium atoms there shown in red. So, the red once are the lanthanum atoms some of the lanthanum have been replaced by strontium. The green over here is the manganese and the yellow atoms are the oxygen. So, this lanthanum (refer time: 30:14)) strontium manganese oxide is one cell of the crystal. So, we are going we are considering a crystal we are considering a crystal.

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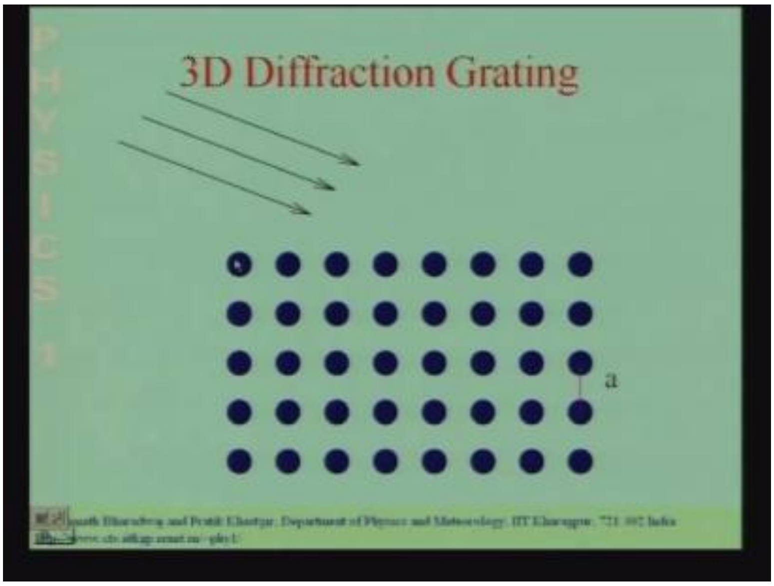

Like this and the unit cell of the crystal a unit cell is one such lanthanum strontium manganese oxides.

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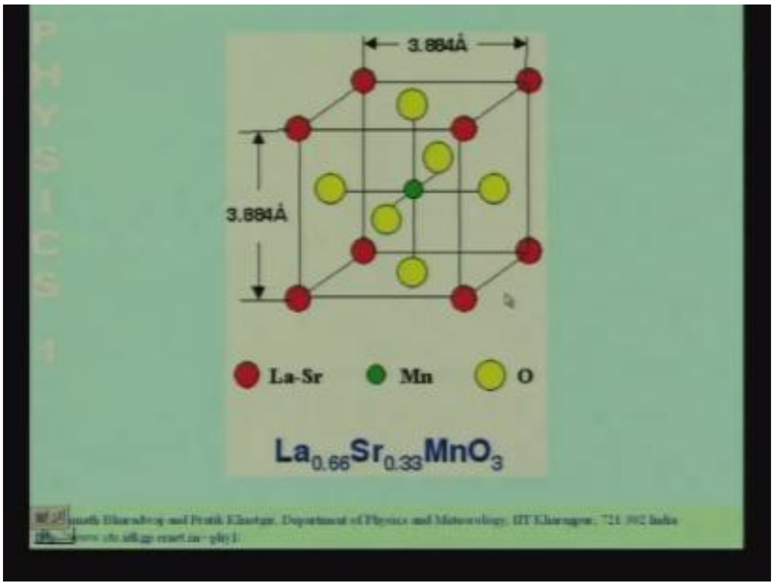

So, you have a periodic arrangement of such lanthanum, manganese, strontium, lanthanum, strontium and manganese oxide.

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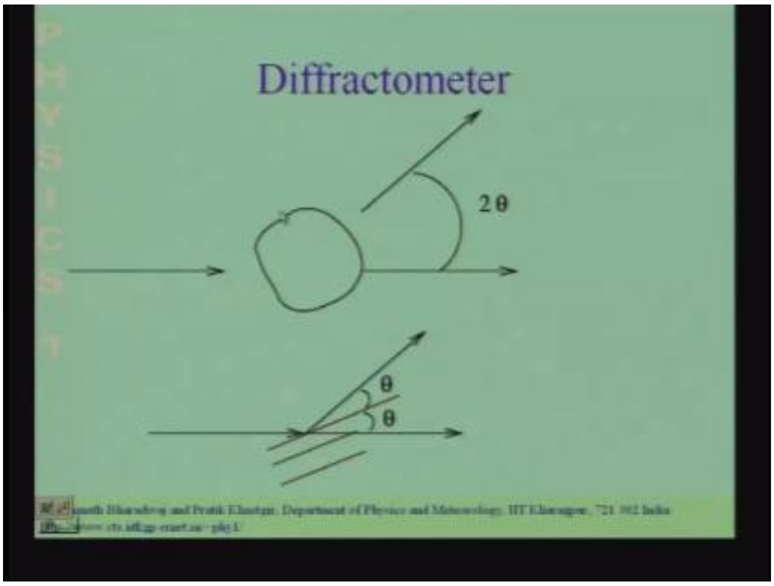

And so, you have now, a sample made up of that lanthanum strontium manganese oxide on which you have x-ray. And what you have done is what the diffractometer does is it, measures the intensity of the scattered x-ray. As a function of this angle which is called 2 theta.

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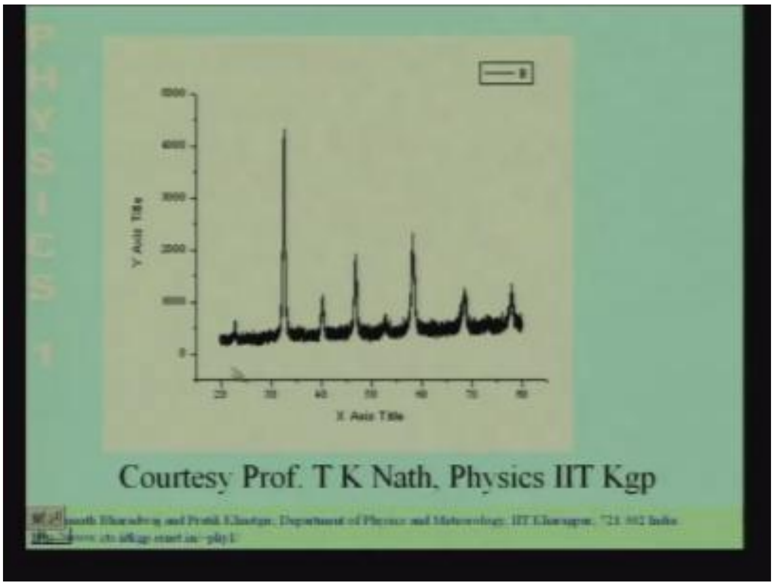

And this shows, you the intensity which is measured at different angles 2 theta. So, x axis as 2 theta, the y axis as the intensity and notice that as you vary the angle.

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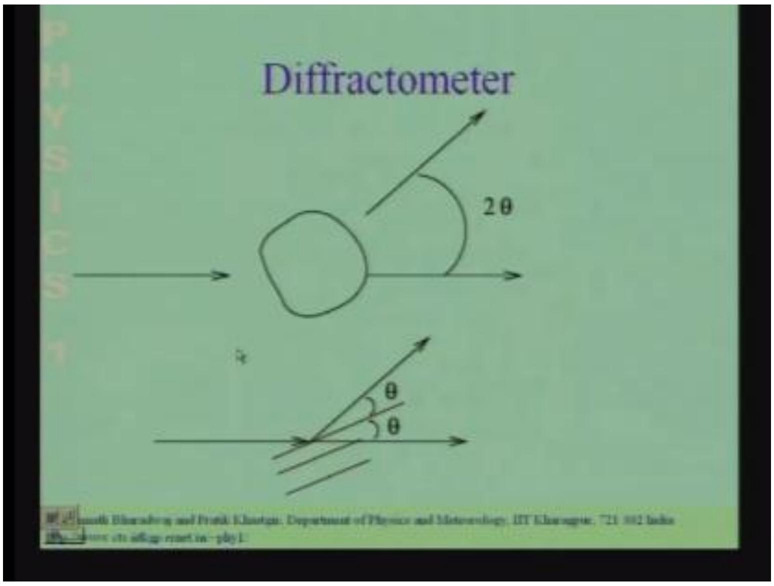

As you vary this angle 2 theta.

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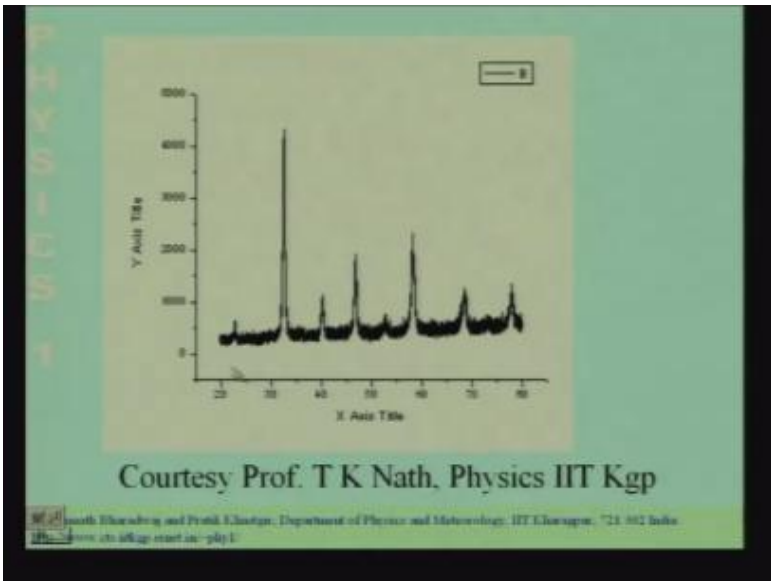

You find that there are Maximas in certain directions. So, in certain directions the x-ray scattered x-ray as a very high intensity. And these you can interpret has being the Maximas of the diffraction pattern.

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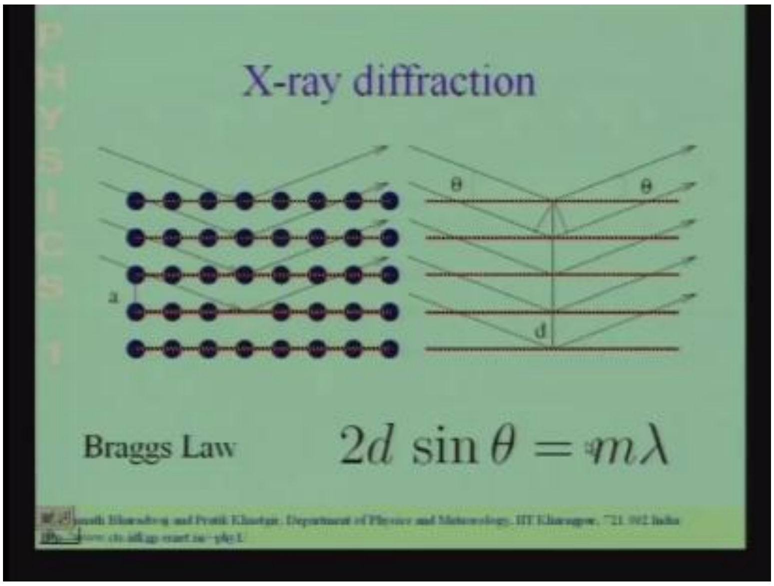

so, these are direction where this formula 2 d sin theta is equal to m lambda is satisfied.

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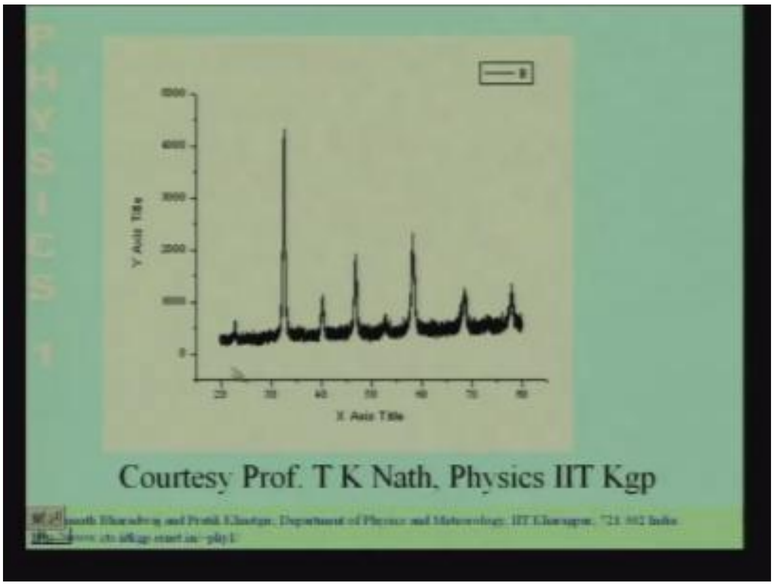

So, in this picture these lines are the x-ray Maximas and what you can get from the x-ray diffractometer. Is the intensity the angle where you have the different Maximas.

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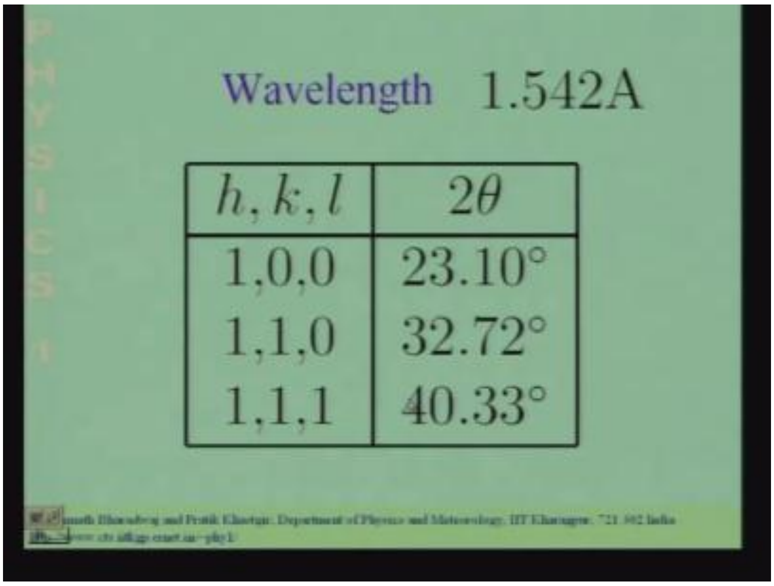
Wavelength 1.542A

h, k, l	2θ
1,0,0	23.10°
1,1,0	32.72°
1,1,1	40.33°

This table shows, you the angles where you have the different Maximas the wave length of this radiation of the incident x-ray, there is 1.5 4 2 Armstrong.

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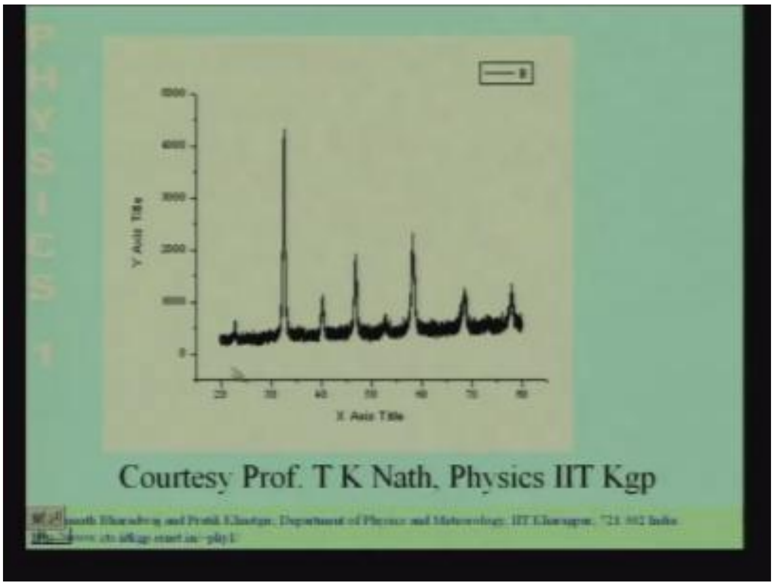

And what has been done here is we taken this graph and measure the angle corresponding to these Maximas.

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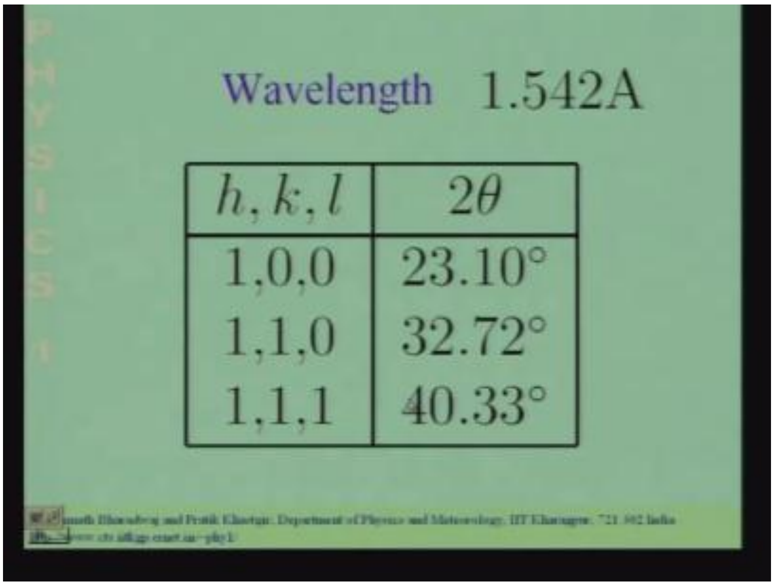

So, the smallest angle, where you have a maxima is corresponds to 2 theta being 23.10 degrees.

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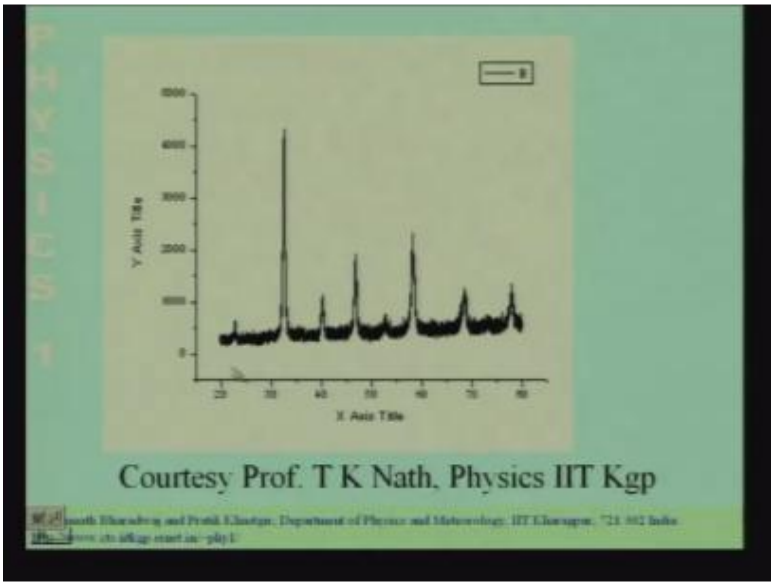

So, this is at 23.10 degrees remember that this.

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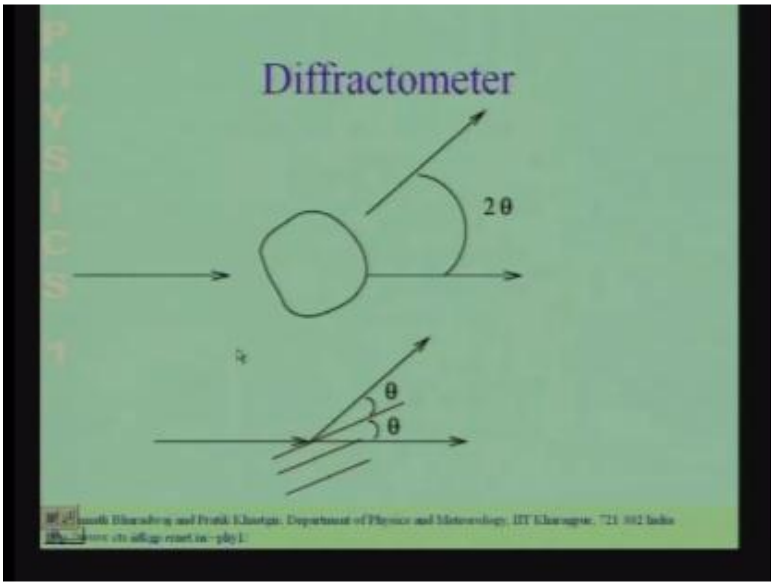

Angle is actually 2 theta is the total angle between the incident direction and this scattered direction.

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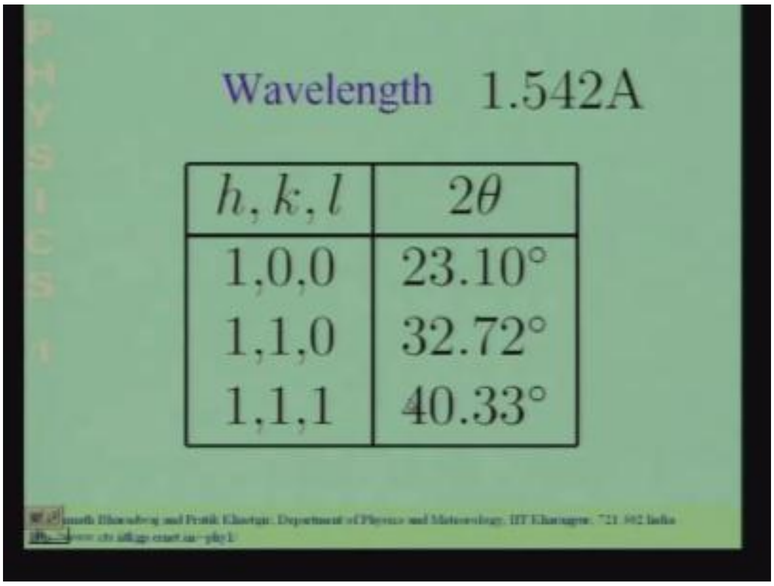

So, the first the smallest angle at which you have a maxima is 23.10 degrees then you have an maxima at 32.7 2 degrees which is this 1.

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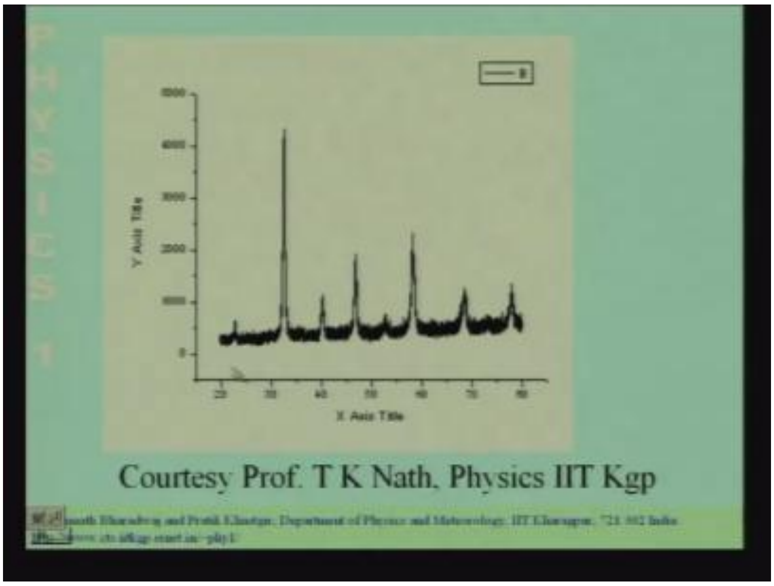

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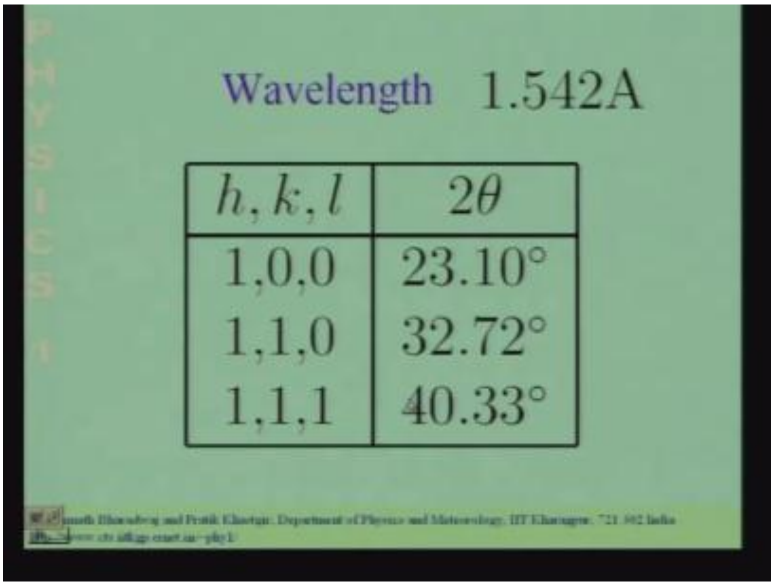

And then you have a Maxima at 40.3 3 degrees which is the 1 over here and I have not shown, you the values corresponding to these other Maximas.

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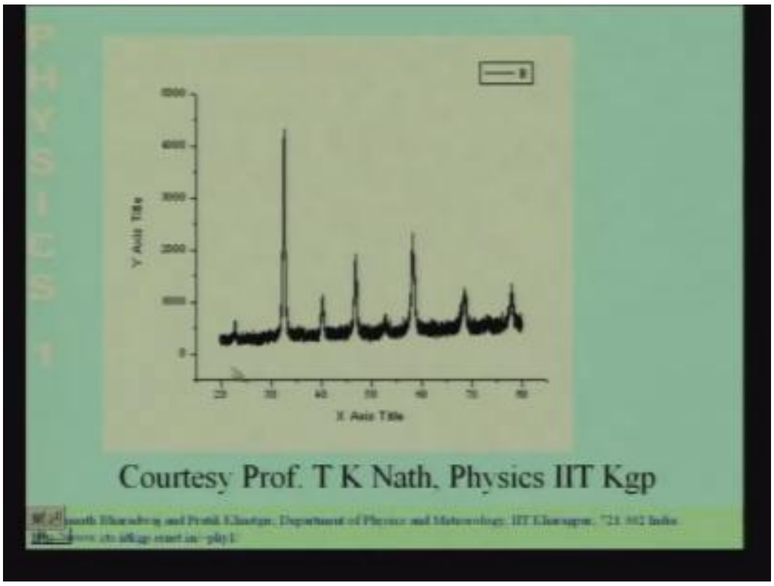

Now, the question is that we have to interpret these different Maximas.

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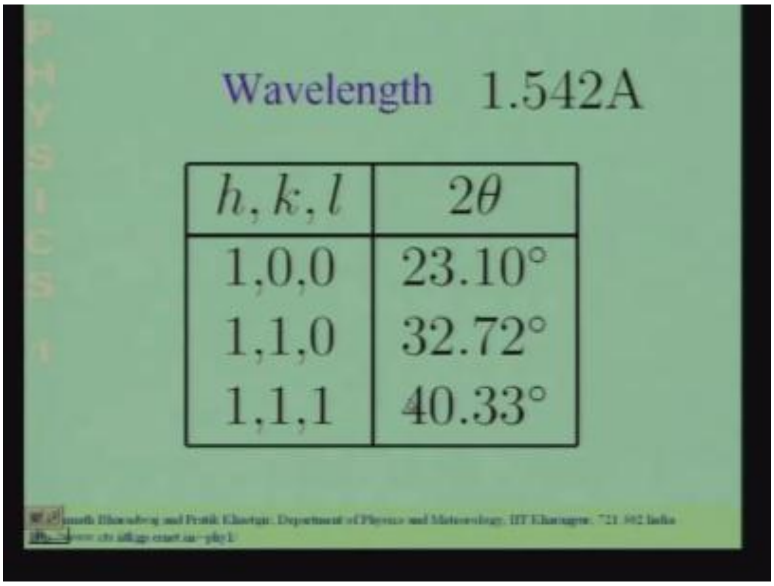

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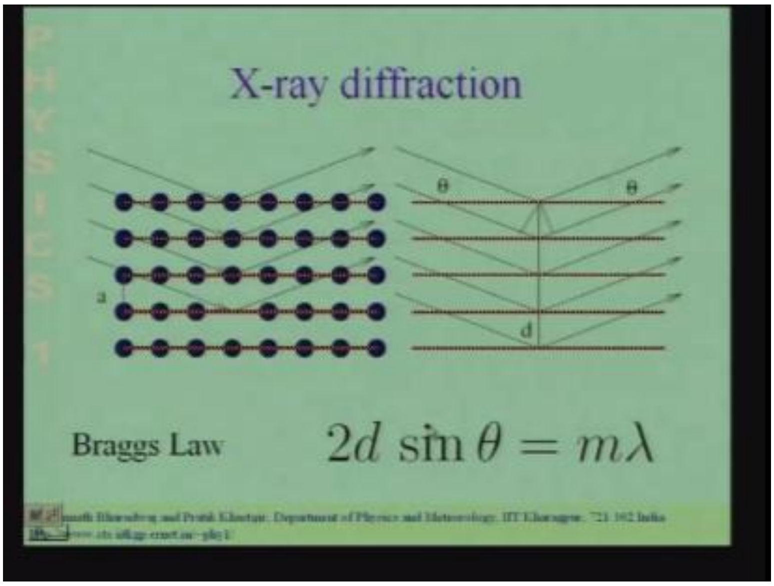

So, there are two things, which could change the first thing that could change is the value the order of the maxima m or this value of d d is the spacing between the plains.

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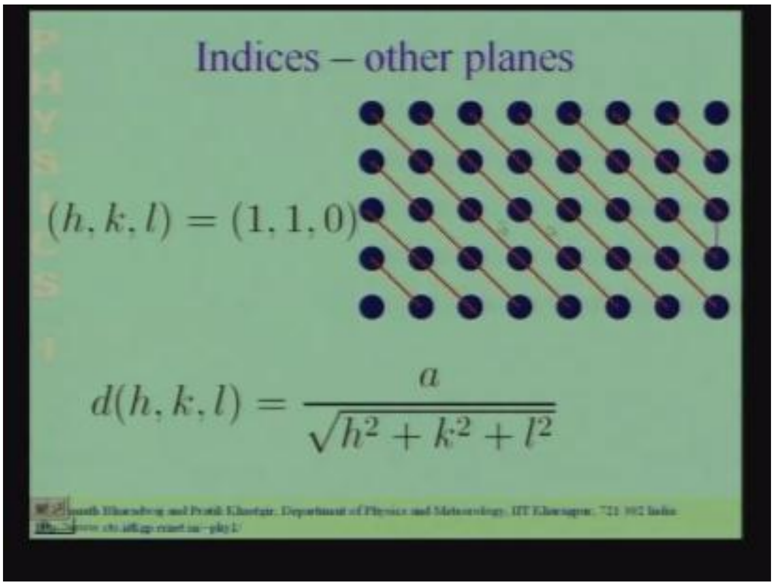

And if I change the plains, there are many possible plains through the crystal, if I change the miller indices the value of d is going to change.

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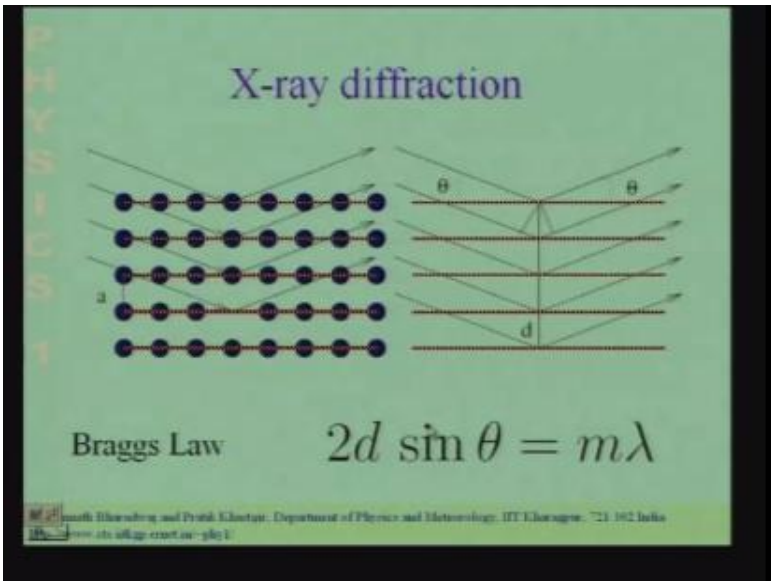

Also the order of the maxima could be different; you could have a first order maxima second order maxima third order maxima etcetera. The zeroeth order maxima corresponds to sin theta equal to 0 theta equal to 0, which is the direction of the incident radiation itself and that we are not interested in. So, now, people who do x-ray they know, that the intensity of the higher order Maximas m equal to 2 3 4 5 etcetera is much smaller than the intensity of the first order maxima, so, m equal to 1.

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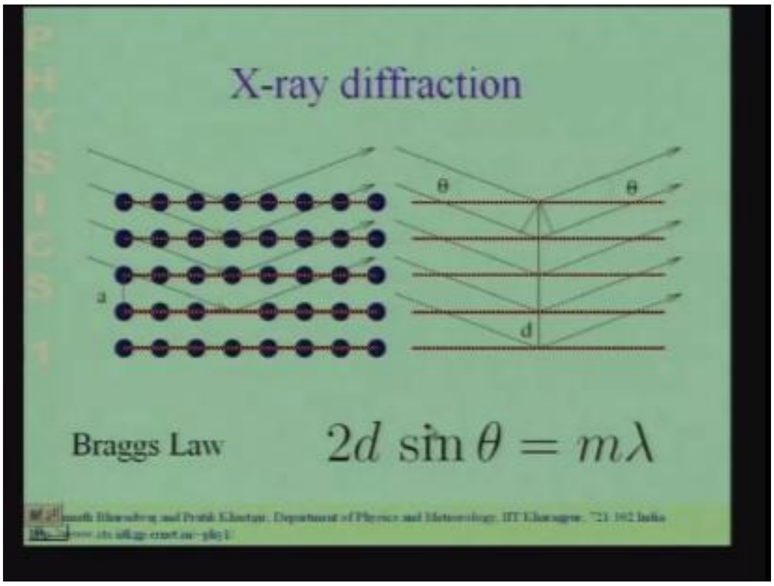

It is known that m equal to 1.

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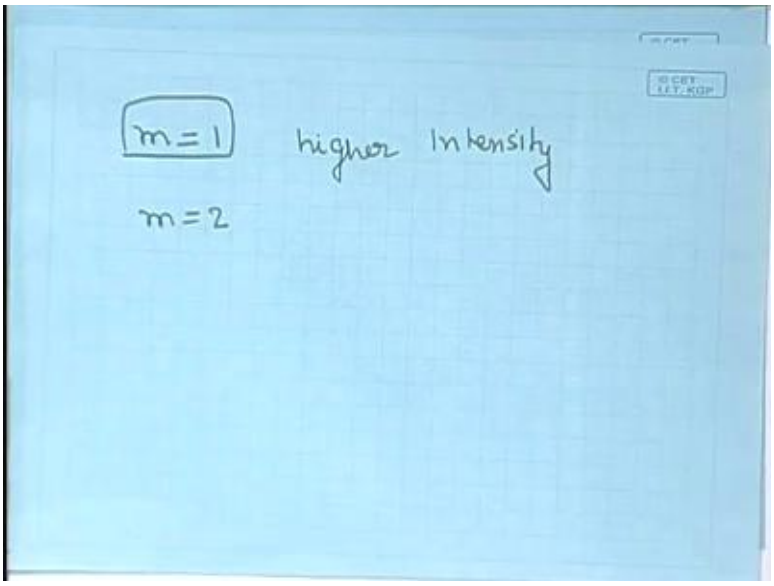

As a much higher intensity, compare to m equal to 2 and higher order. So, in our discussion, so, typically when you interpret these x-ray Maximas. The diffraction pattern the x-ray diffraction pattern, you can interpret the bright lines has been m equal to 1 which is what we are going to do over here.

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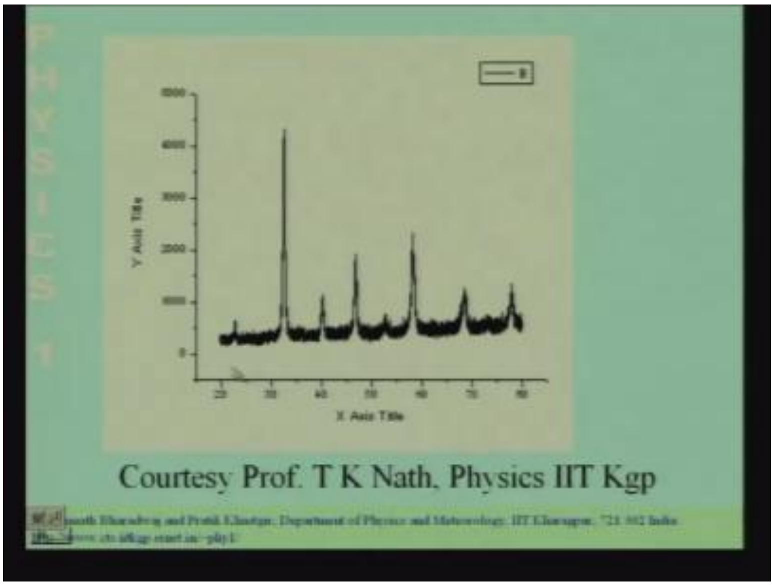

So experience with x-ray basically, tells us that you are going to see mainly be first order maxima and you can interpret all of these lines has been due to the first order maxima.

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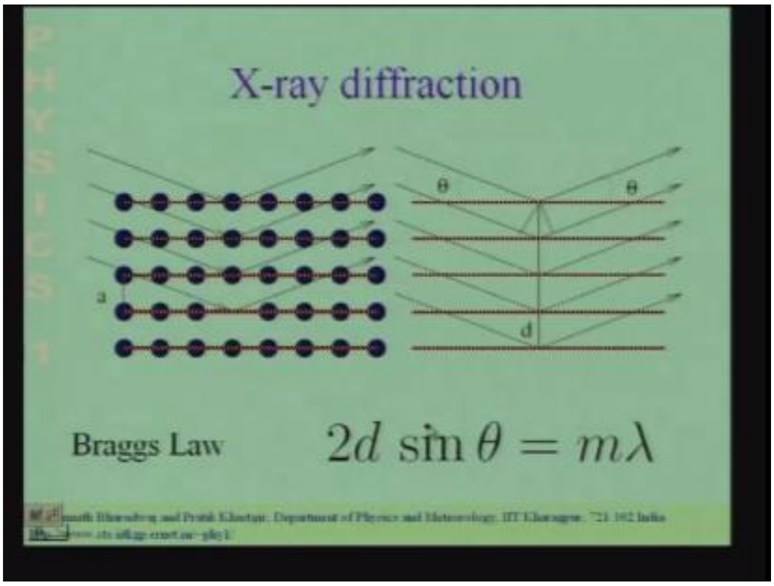

So, we are inter take m equal to 1, so, we are going to restrict a attention to M equal to 1.

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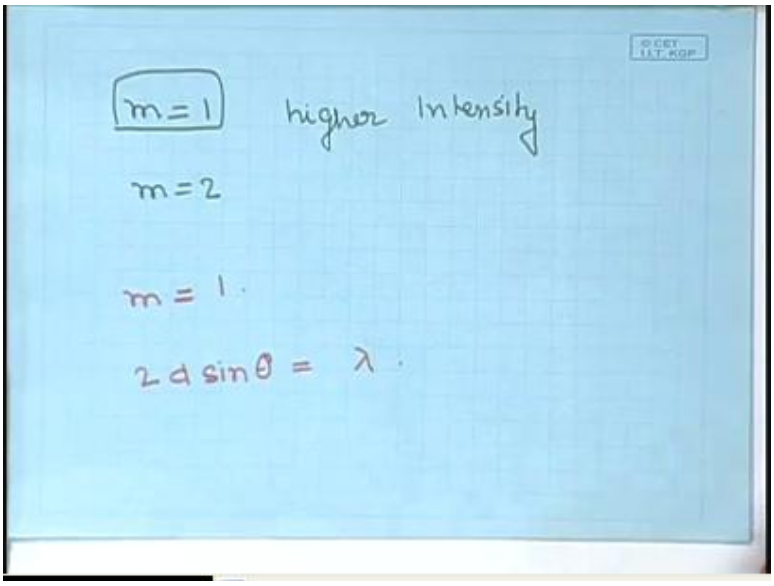

So, the condition for maxima is 2 d sin theta is equal to lambda, now, there are many possible plains which can be drawn through the crystal I have shown you?

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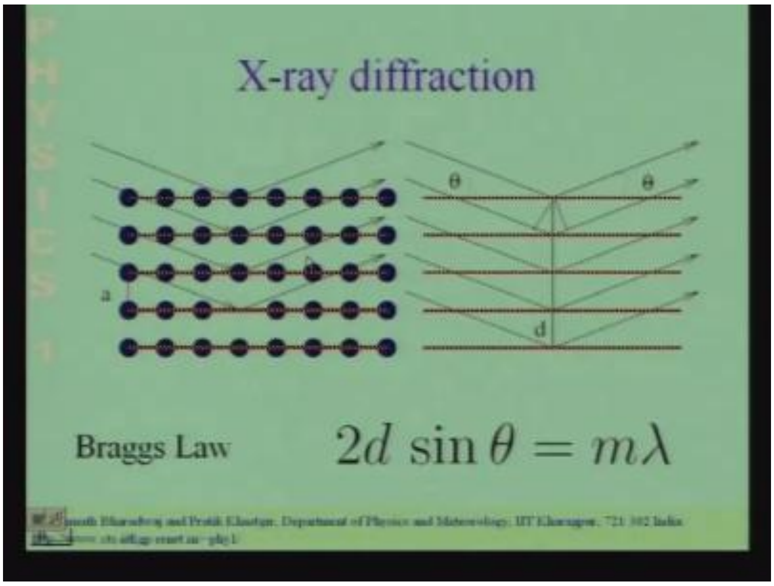

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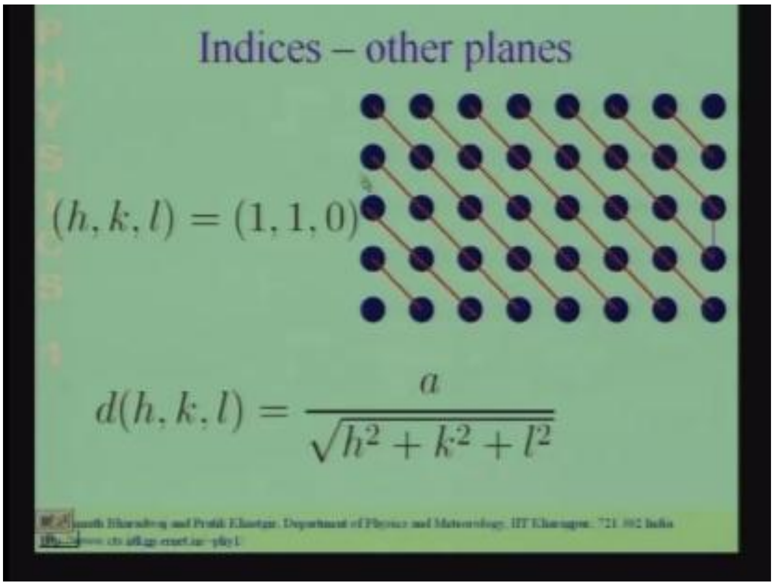

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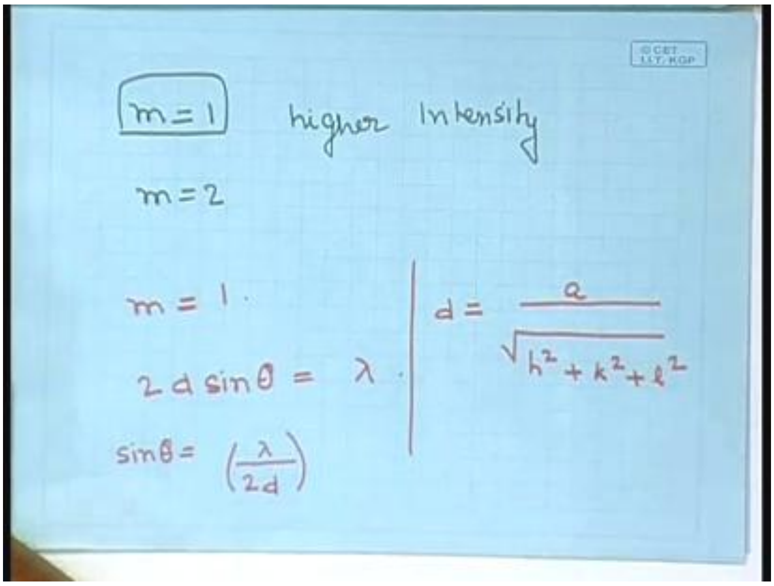

One example, but you could have many other plains and these plains d is going to be the, inter atomic is the inter atomic spacing divided by the square root of h square plus k square plus l square. And we can, write this as sin theta is equal to lambda by 2 d now, let us go back to the intensity pattern.

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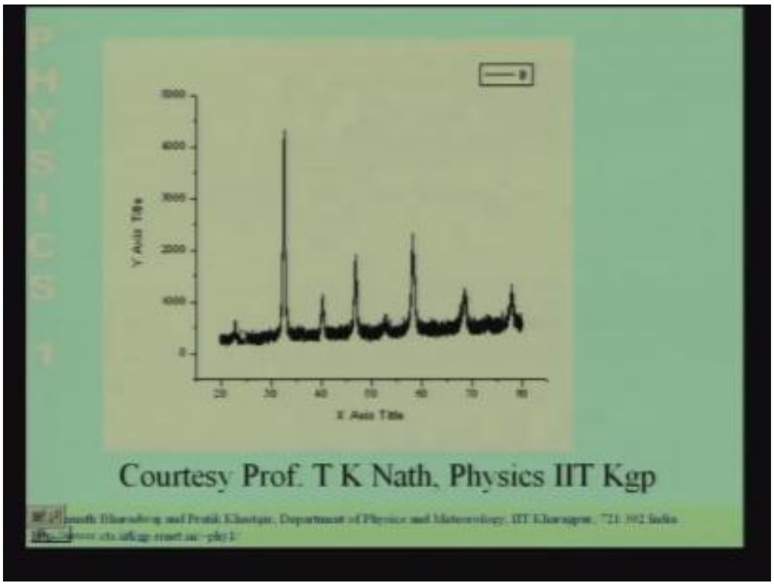

This is the intensity pattern and ask the question? That what does this smallest angle of theta what is this corresponds to.

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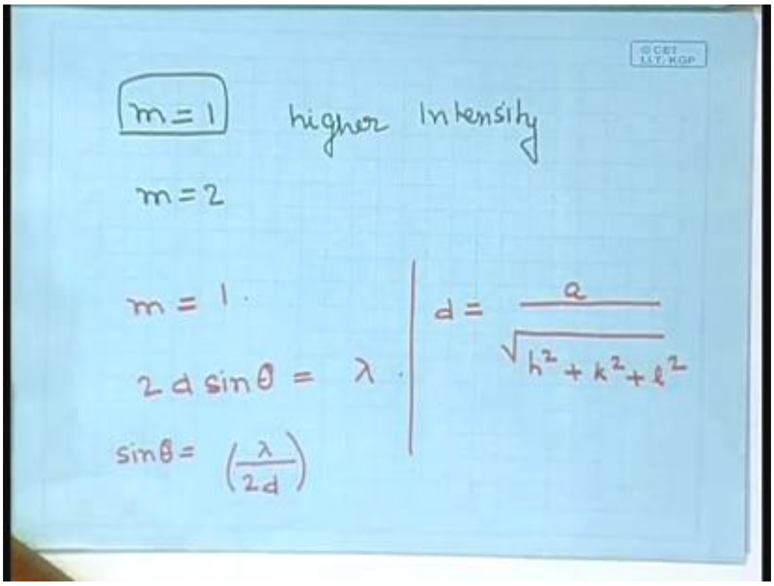

So, when theta is smallest, we can say that d see this only thing now, you can vary is d the plain the, inter plainer spacing theta and d. So, any change in theta, you can interpret has being a change in d so.

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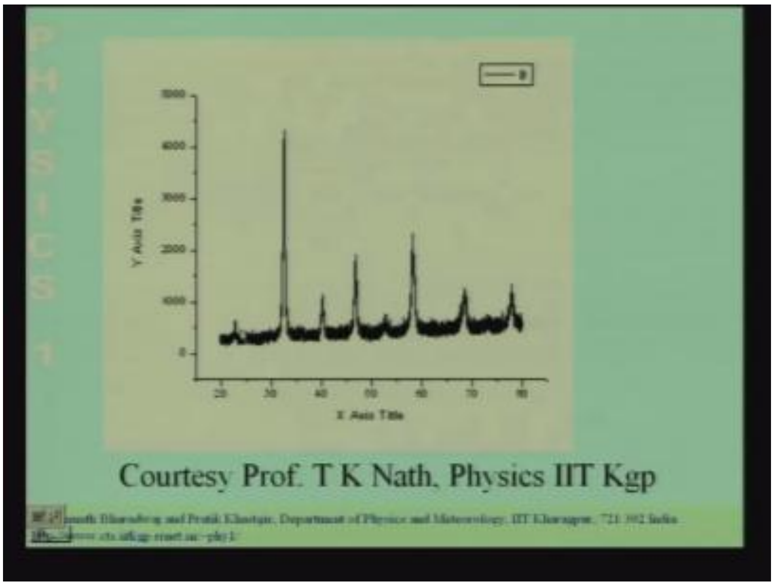

So, this maxima corresponds to a particular value of d this corresponds to under different value of d this corresponds to another value of d.

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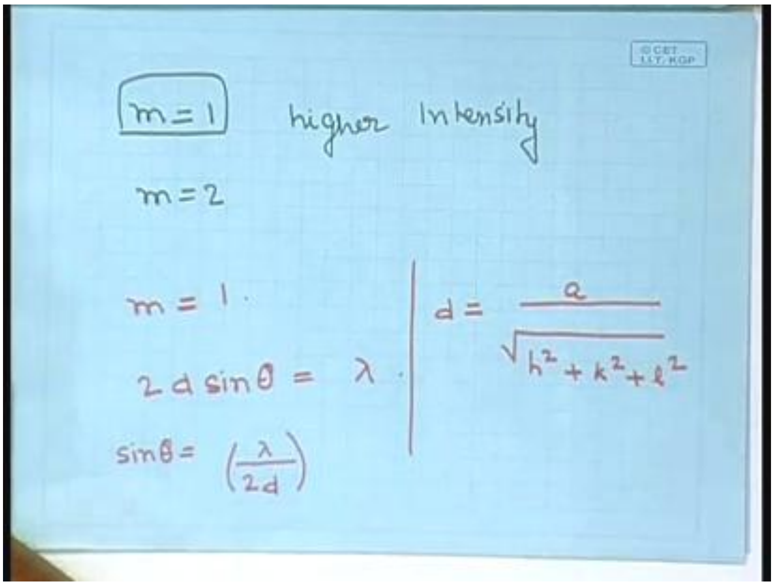

And D will change for the same the crystal for the crystal a is fixed that is inter atomic spacing the inter lattice, that a lattice constant or the periodicity of the crystal. So, d can change, because of the change miller indices. So, you can look at different possible.

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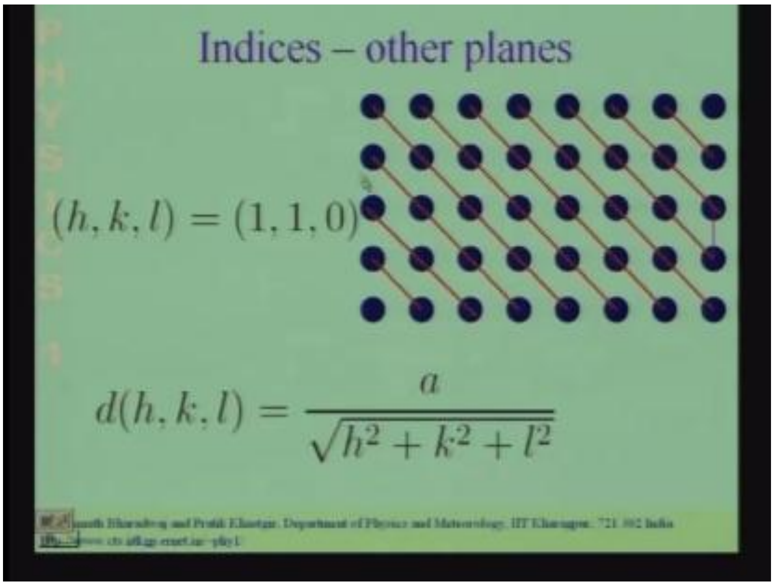

Plains you have this come possibility.

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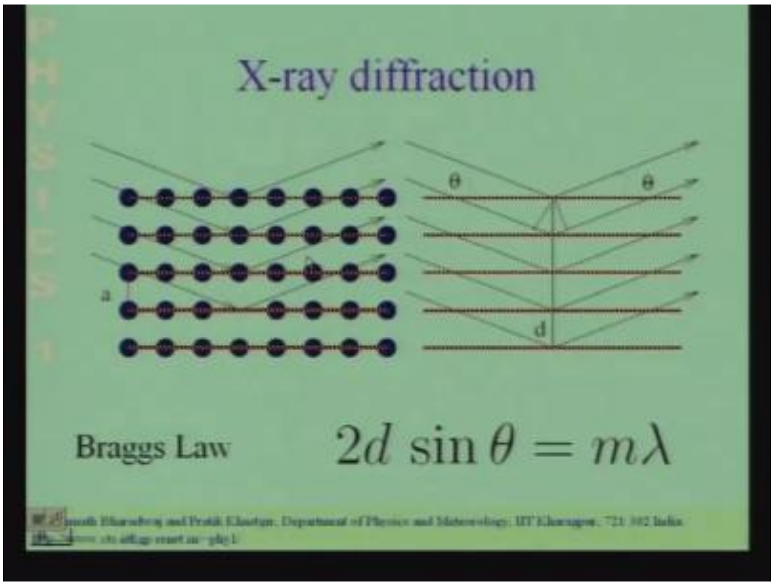

Or you have this possibility.

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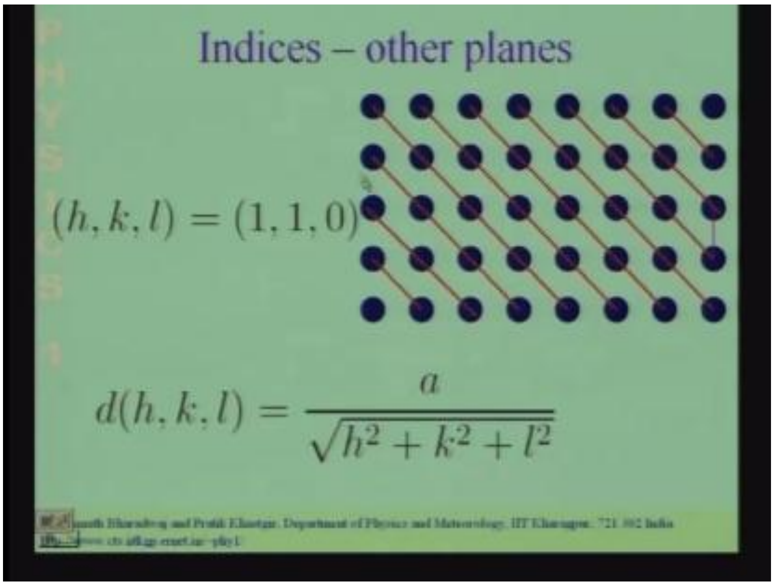

And this has a smaller value of d compare to this.

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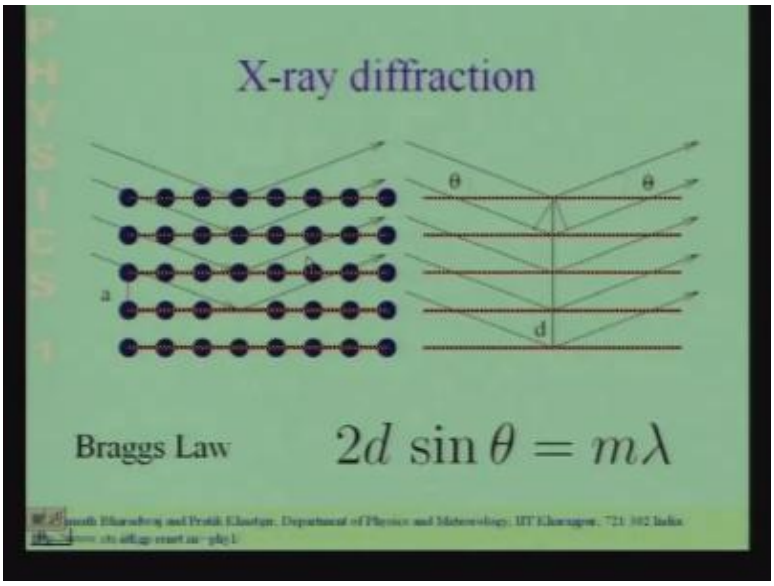

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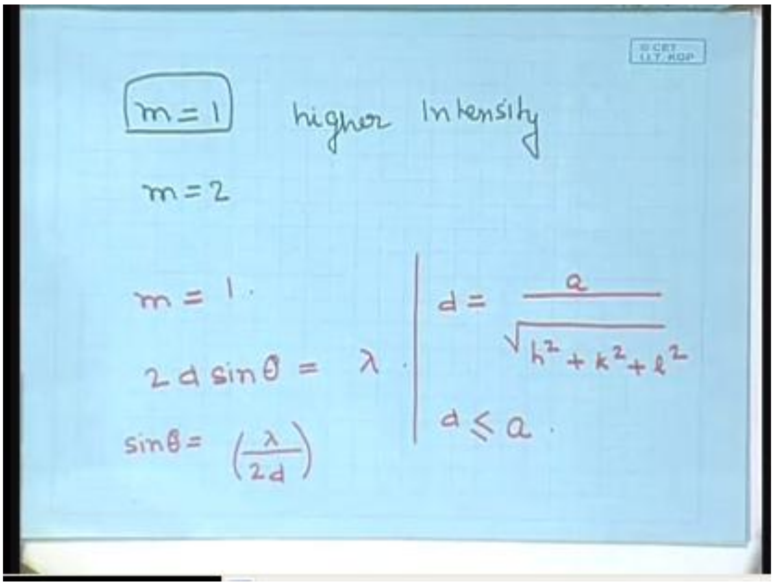

So, the largest value which d can have is d equal to a and d will be necessarily smaller than are equal to a now if you reduce the value of d if you reduce the value of d. This is going to get larger and sin theta has to be equal to this. So, theta also will have to be larger. So, smaller value of d means larger angle theta. So, we can interpret what this tells us that this we can interpret.

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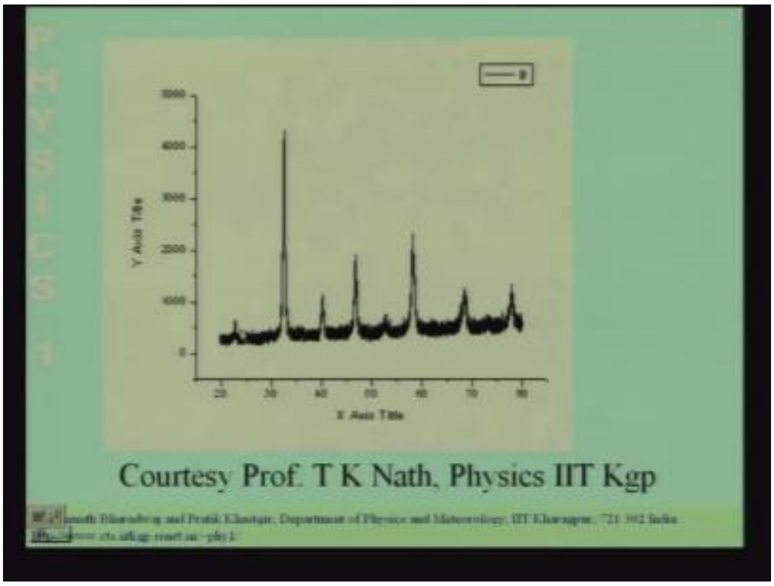

The smallest angle theta the smallest possible angle theta has arising due to the largest possible value of d.

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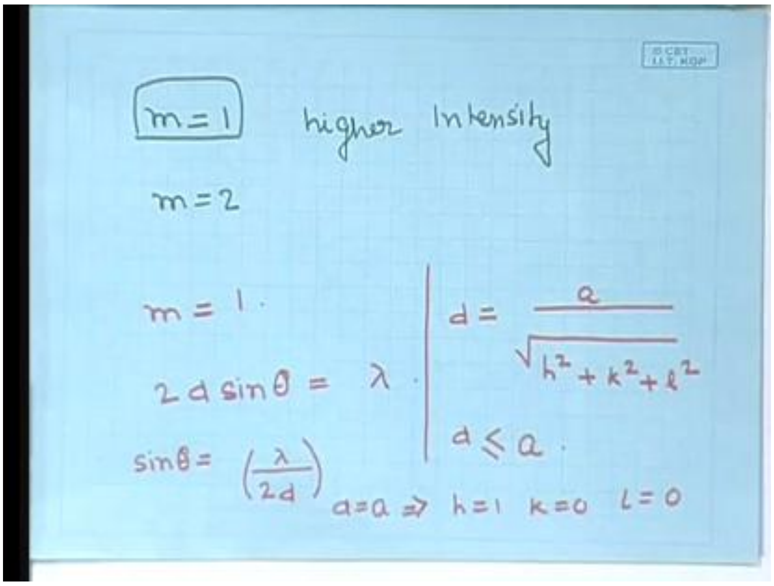

And the largest value of d is when h equal to 1 k equal to 0 l equal to 0 all you could also had h equal to 0 k equal to 1 l equal to 0 or h equal to 0 k equal to 0 l equal to 1. I all 3 of these will give you d equal to a. So, d equal to a is the largest possible or other d equal to a is the largest possible value of of d and this is going give you smallest angle theta. So, this is going to give the the maxima at the smallest angle theta.

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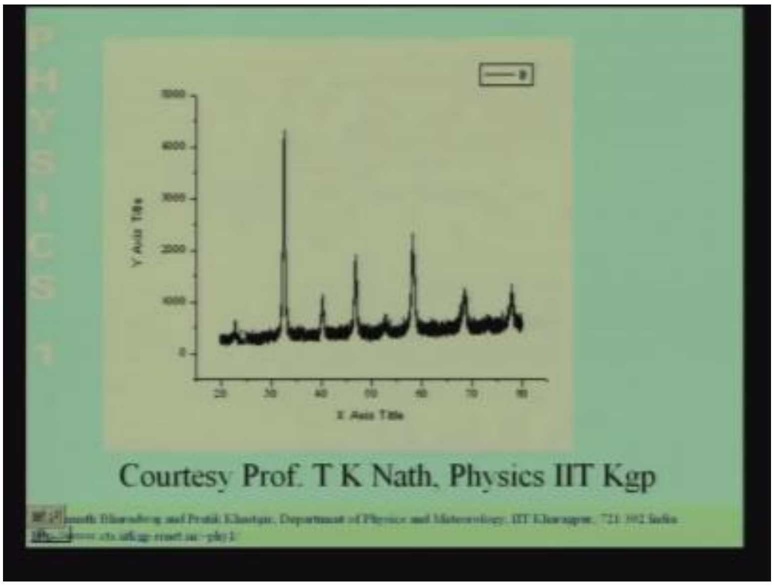

so, we can interpret this line as arising from d equal to a.

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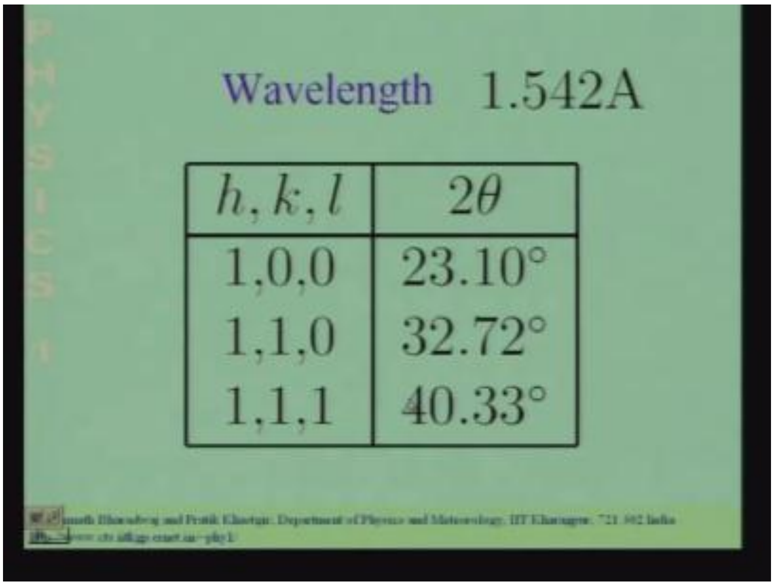

And the angle corresponding to that line is twenty 3 point ten degrees.

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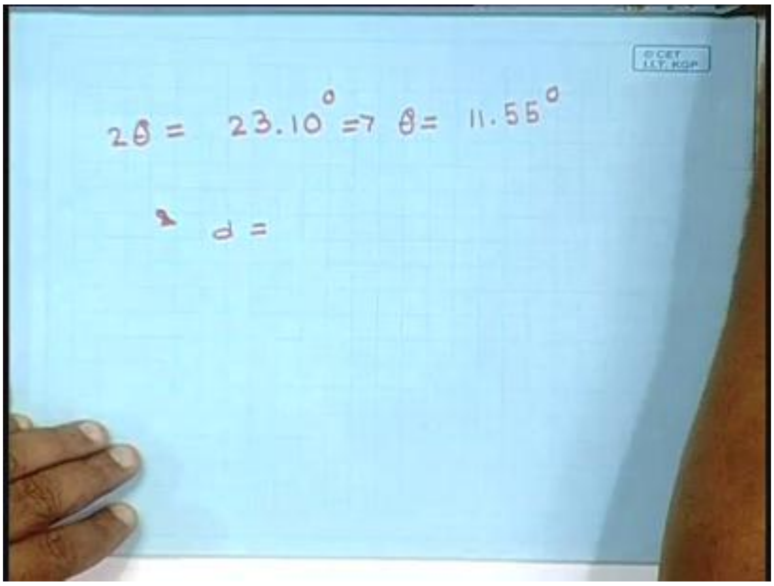

So, 2 theta 23.10 degrees which means that theta… So, we have to determine theta and theta is 23.1 divided by 2 which gives us 11.55. So, this is 11.55 degrees and 2 sorry d is equal to.

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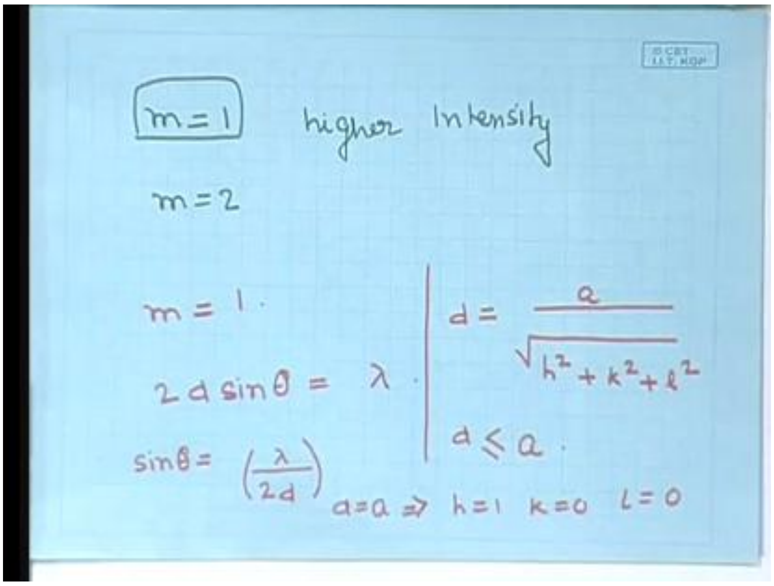

Let us determine d from here d is equal to lambda by 2 sin theta.

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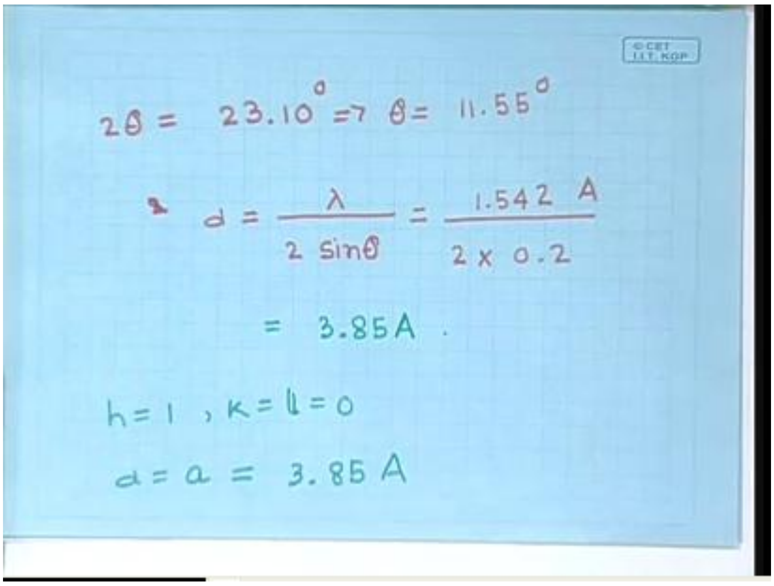

So, it is lambda by 2 sin theta and this gives us 1.542 divided by 2 into Armstrong 1 2 into sin of 11.55 let me calculate that. So, I have to take the sin of this which is point 2 0. So, this into 0.2. So, let me now do the calculation in to 2 equal to inverse of that into 1.542 and it gives me 3.85. So, it tells that the, inter the value of d for this 3.85 Armstrong. And the smallest angle theta we can interpret has been h equal to 1 and the other 2 which tells us that the d is equal to A which is 3.85 Armstrong. So, we can use the first the smallest angle theta to determine the inter atomic spacing and it comes out to be 3.85. Now, let us check if this gives us consistent results.

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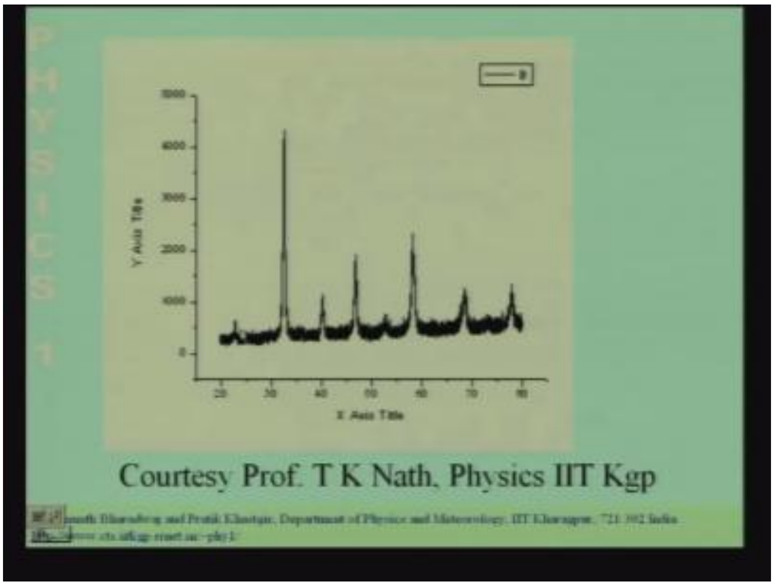

For the next one the next intensity maxima the next intensity maxima is found at an angle 2 theta.

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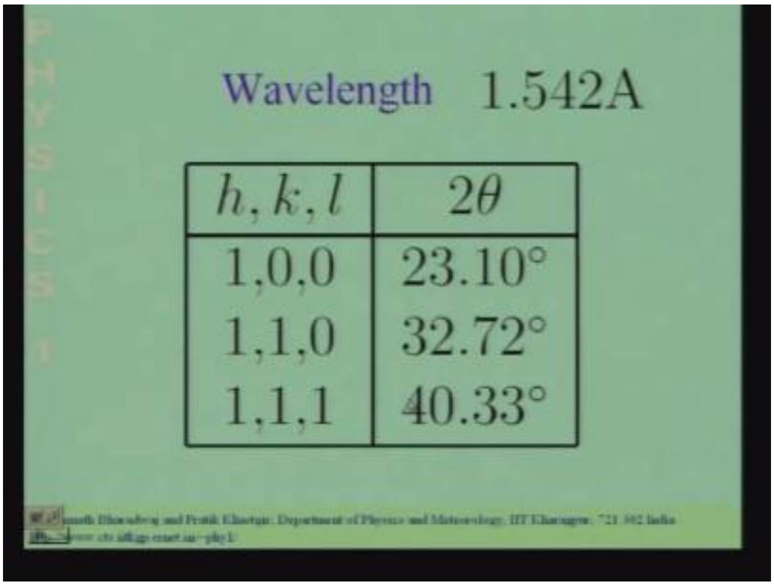

Equal to 32.72. So, let us check this.

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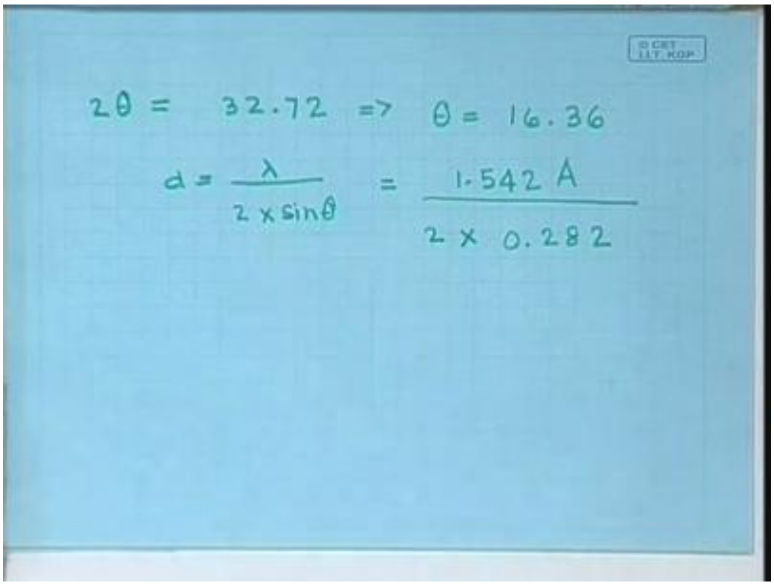

So, the next intensity maxima occurs at 2 theta is equal to 37 32 sorry 32.72 or theta is approximately equal to 16. Theta is equal to 16.36 and d is equal to lambda by 2 times sin theta which is the wave length of the x-ray is the same 1.542 Armstrong divided by 2 times the sin of 16.36. So, let me do that 16.36 the sin of that into 2 6 16.36.

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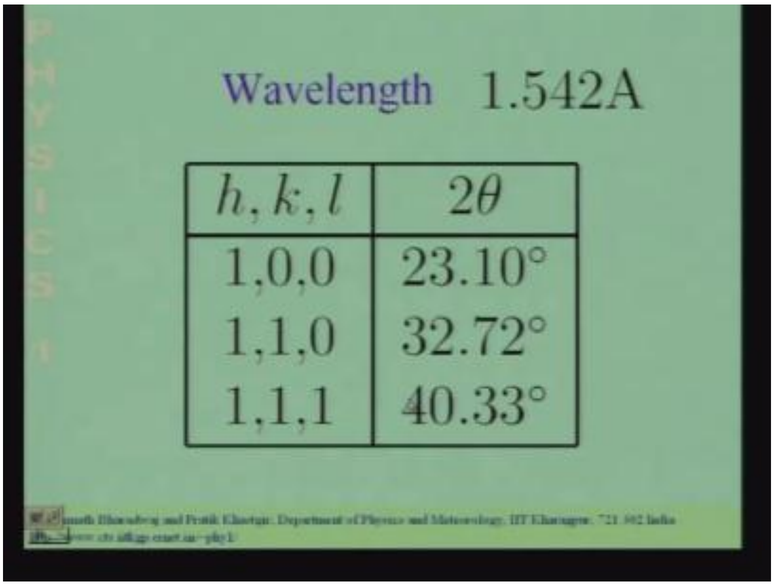

So, this is 0.28 1 2 82 actually, let me now do this calculation this into 2 into 1.542 which gives us doing the division 2.73 Armstrong.

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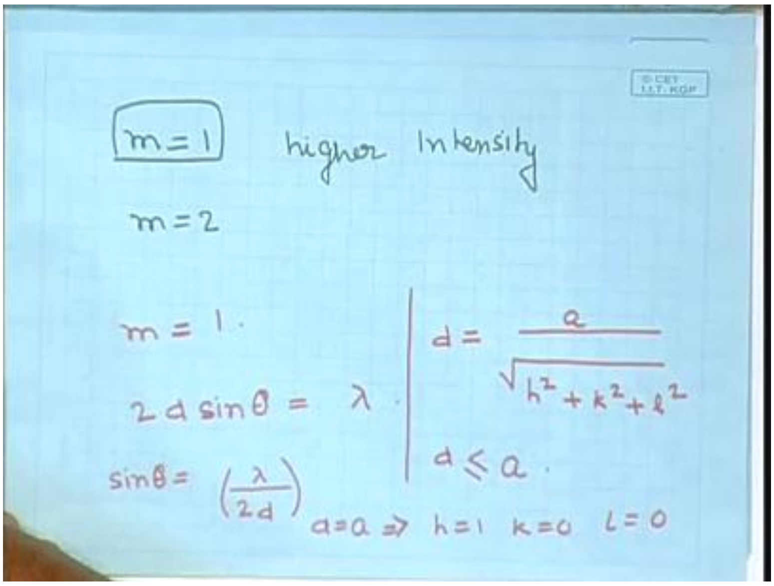

Now, I have told you that this corresponds to h equal to 1 k equal to 1 l equal to 0 that is the next set of miller indices and d is equal to a by in this case it is going to be a by square root of 2. Or we can use this calculate a square root of 2 into 2.73 Armstrong which comes out to be 3.87. So, we see that we can use the next line the line at the next value higher value of theta 2 also written with the unit cell. And we get exactly the same answer has we have done earlier.

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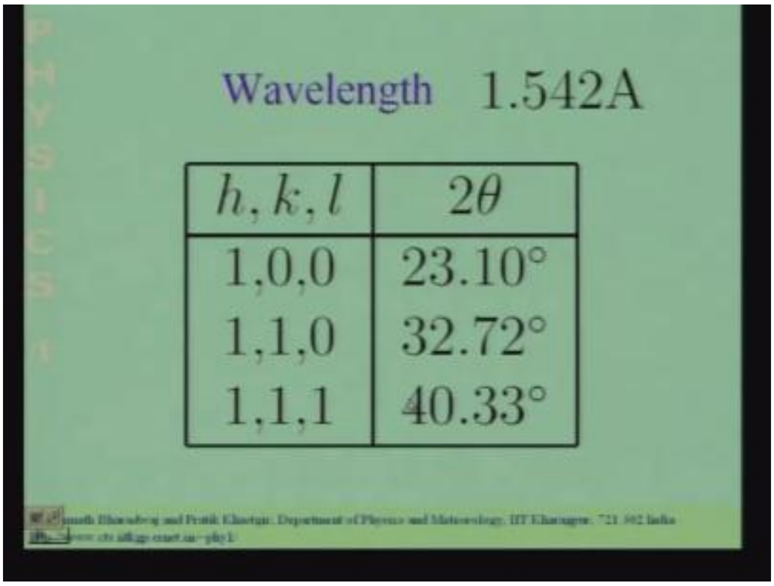

So, you can check I will leave it for you has a exercise to go through this. So, what you can do is you can check that all of these angles.

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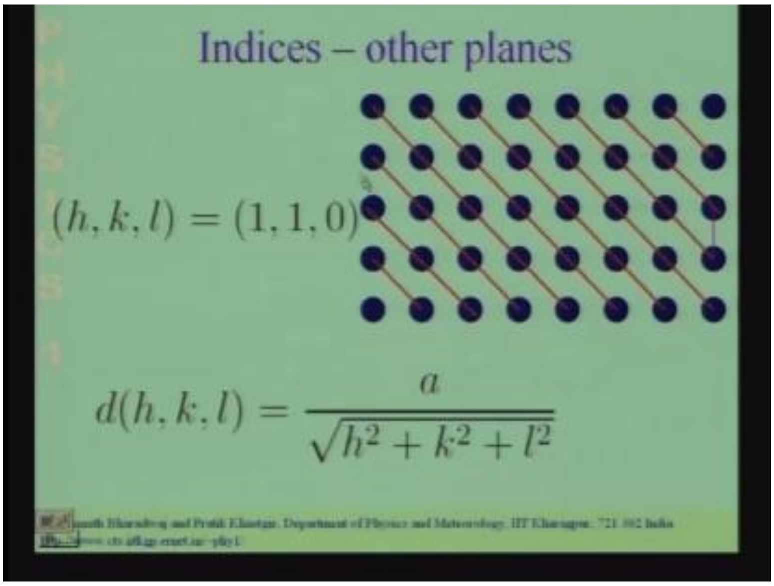

If you find the lattice constant by lattice constant we mean the spacing between these units cells and if you use all of these different lines that you have over here I have given you.

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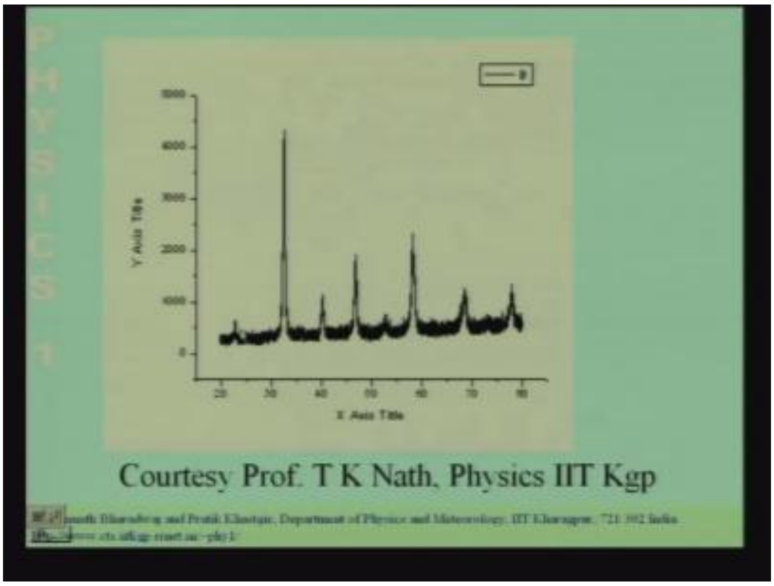

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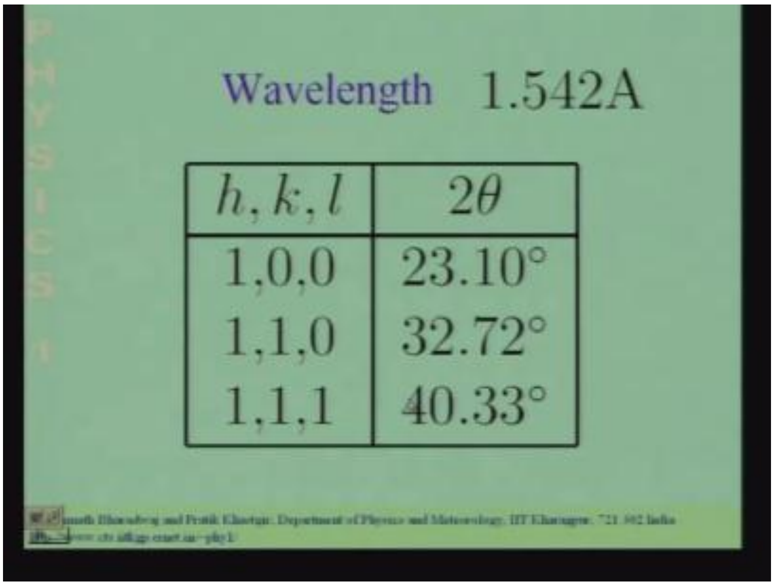

Three of the angles the angles corresponding to three of them and if you determine the you determine the the atomic inter atomic spacing using this data. Each of them you can interpret the first 1 has been as corresponding to h k l equal to 1 0 0. The second one has corresponding to 1 1 0 the third 1 as corresponding to 1 1 1 successively smaller larger and larger inter at inter plainer’s spacing.

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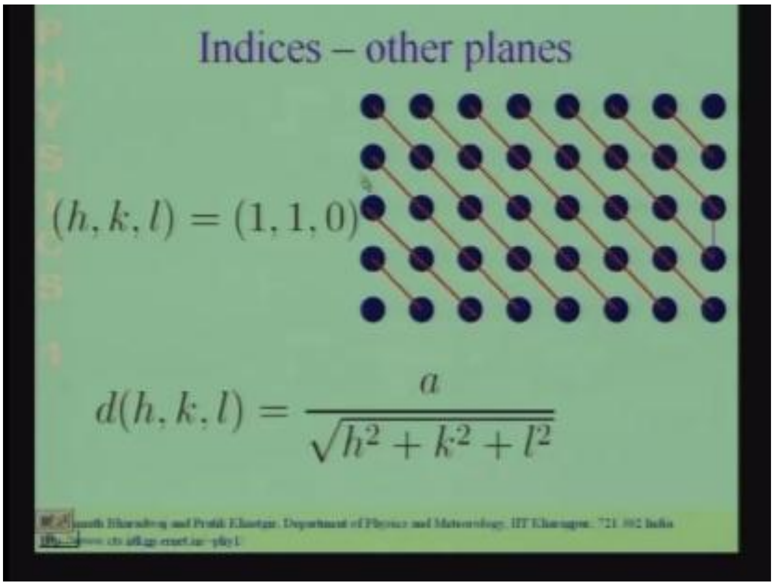

As you increase the values of h k and l the spacing between these is going to get smaller and smaller and has the spacing d gets smaller.

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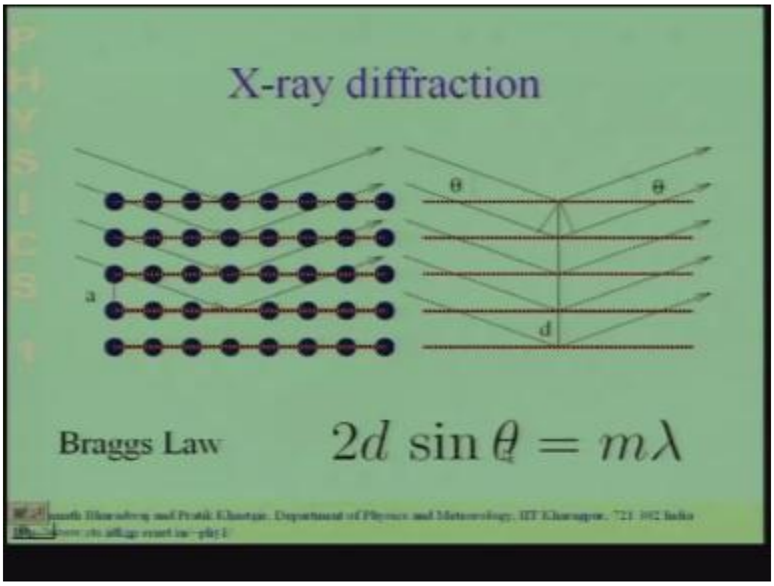

The angel theta over here as the spacing.

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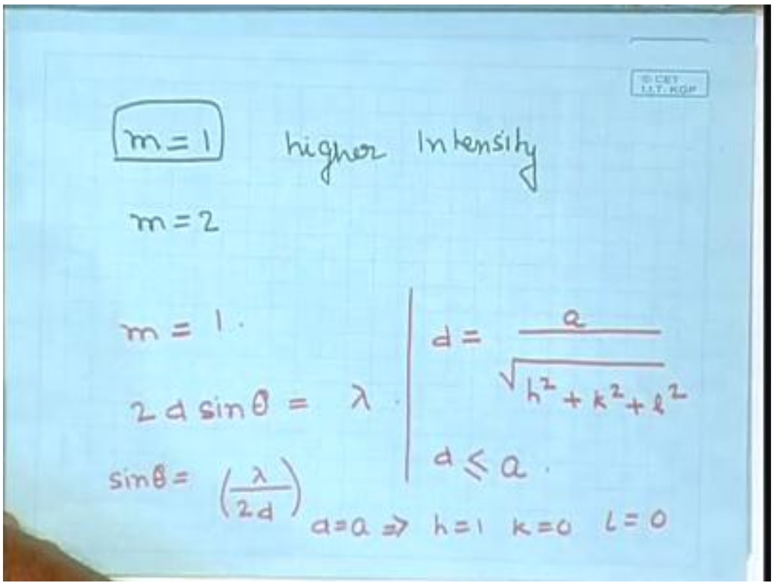

D gets smaller the angel theta as to increase and we can interpret these successive lines as corresponding to larger and larger values of h k and l.

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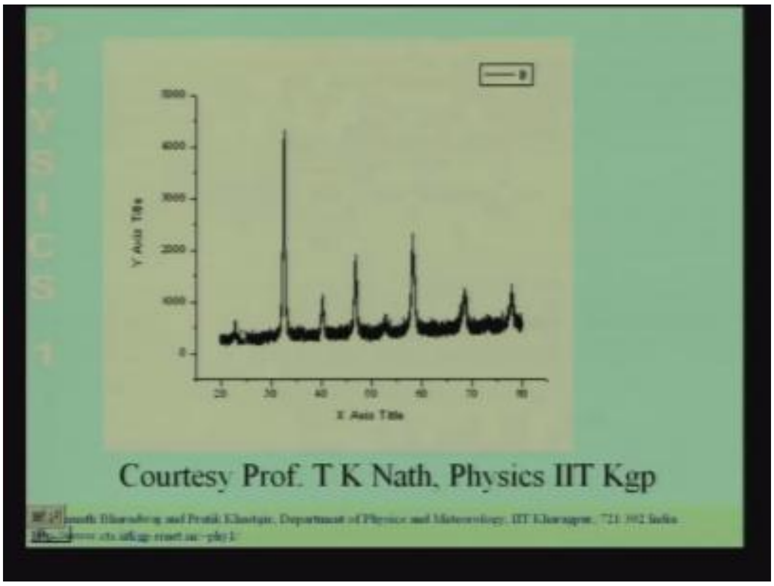

And we can use this to get the inter atomic lattice constant are the periodicity of this lattices. So, what I have try to show you here is a sum basic idea of x-ray diffraction x-ray diffraction the is a very useful tool to determine the knee structure of materials. The structure of materials and here I have shown you how you can use it to determine the lattice spacing of a cubic crystal. We have considered a simplest possible situation where you have a cubic crystal. There are more complicated situation where you have different kinds of crystal structures you could have tetra Hegel crystal various kinds rumba Hegel crystals different kinds of crystals. And the the subject of a x-ray diffraction is quite and involve subject it is I have try to give you only a glimpse of how the thing x-ray diffraction works. It is essentially a just an extension of the basic idea where each atom acts like a source and you have a periodic arrangement of these sources.

But it is a very the whole thing gets a little let get quite complicated as you go in to more and more complicated atomic structures. More and more complicated crystals, but it is a very useful tool and it has got wide applications in physics in metallurgy. Where you are interested in finding the structure of solids if you have a crystalline solid and you want to find how the atoms are arranged inside. Then you can use this tool of x-ray diffraction to determine this, the location of the diffraction the intensity Maximas in the x-ray diffraction pattern tells you about the structure of the atoms inside how the atoms are distributed inside. Finally I should also mention that this tool of x-ray diffraction has wide applications also in determining the structure of of living of biological materials. For example, of proteins of the DNA the structure of DNA was actually discovered.

A by using this tool of x-ray diffraction the the structure of proteins are also determine using x-ray diffraction they you have to problem there is you have to first crystallize the protein. And once you have a crystal you then bobhant with you send incident x-ray and you get a diffraction pattern the diffraction pattern. There is quite complicated and interpreting it is a very difficult exercise and that is where the challenge comes in interpreting the x the challenge is actually 2 places in crystallizing the substance and in it interpreting the diffraction pattern. So, in this lecture I have try to tell you about 3 dimensional situation where you have diffraction. And try to show you a application of of x-ray diffraction I leave the problem to you to actually work out.

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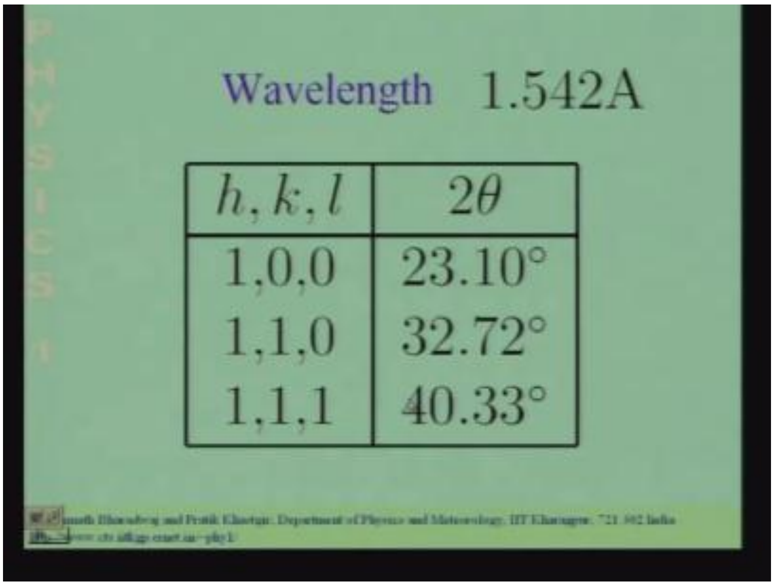

The lattices constant from this data. So, the data which I have given you let me just remind you again we have readings of 2 theta from the x-ray diffractrometer.

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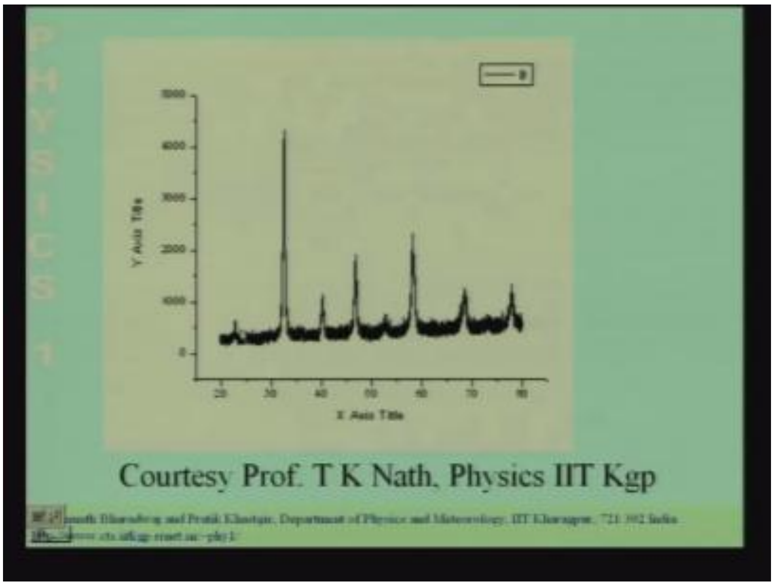

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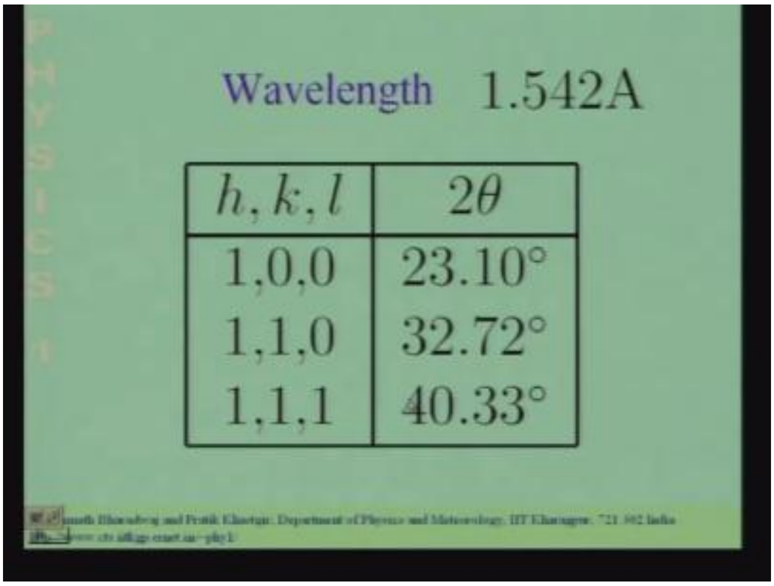

And I have told you that we can interpet the smallest value of 2 theta has arising from the miller indices plains with the miller indices 1 0 0. And the next maxima has arising from 1 1 0 and the next the one after that as arising from 1 1 1 and so, forth And I leaves it to you to check that if you calculate the lattices constant a using 3 of these you will get the same value of a And the main purpose of this exercise is to give you idea of how you can use x-ray diffraction to determine the structure of solids of crystalline solids. Here you can determine the lattice constant in more complicated solids where you have non cubic structures. You can also determine the kind of arrangement you have and various other things. So, let me stop here and continue in tomorrow’s lecture.