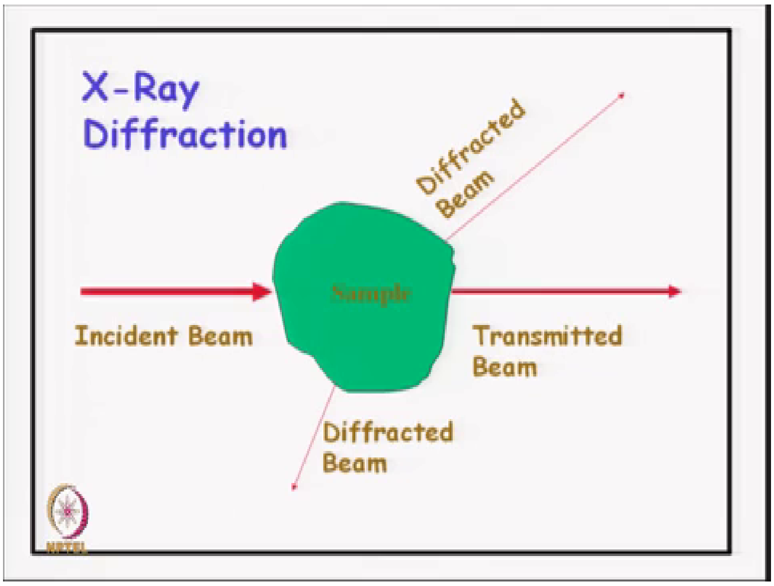
Introduction to Materials Science and Engineering
Prof. Rajesh Prasad
Department of Applied Mechanics
Indian Institute of Technology, Delhi

Lecture – 15
Bragg's Law

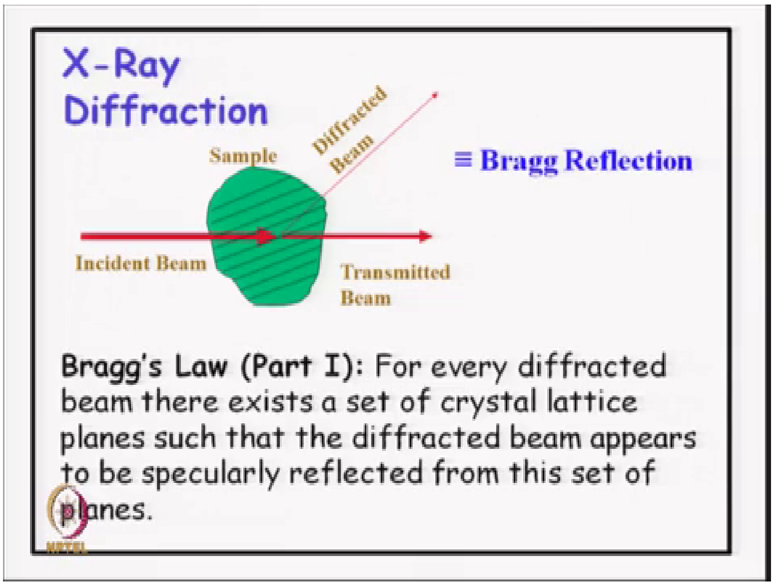
Hello and welcome, in the last lecture, we saw how lovey solved the mystery of X-Rays and the crystal structure by demonstrating that X-Ray crystals diffract X-Rays. This demonstration solved 2 big questions in science about the internal structure of crystals and about the nature of X-Rays. It demonstrated that crystals are periodic arrangement of atoms and it also demonstrated that X-Rays are waves. This important discovery then put a tool in the hands of crystallographer by which they can actually explore the atomic structure or the periodic nature of crystalline material. This follow up of work of using X-Rays as a tool to solve crystal structures was done by Bragg's and there is a famous Bragg's law which we will now cover in this lecture.

(Refer Slide Time: 01:19)



So, let us look at X-Ray diffraction, we have an incident beam we falling on a sample we expect a transmitted beam which is in the same direction as the incident beam. If all of the X-Rays is not absorbed there will be a transmitted beam this is what is used in normal medical use of X-Rays when you when we have X-Ray photographs, but if the sample is crystalline then you can expect beams other than the transmitted beam; beams in direction other than the transmitted beam direction. These beams are the diffracted beam you can have more than one such a diffracted beam from the same crystal under same condition.

(Refer Slide Time: 02:14)

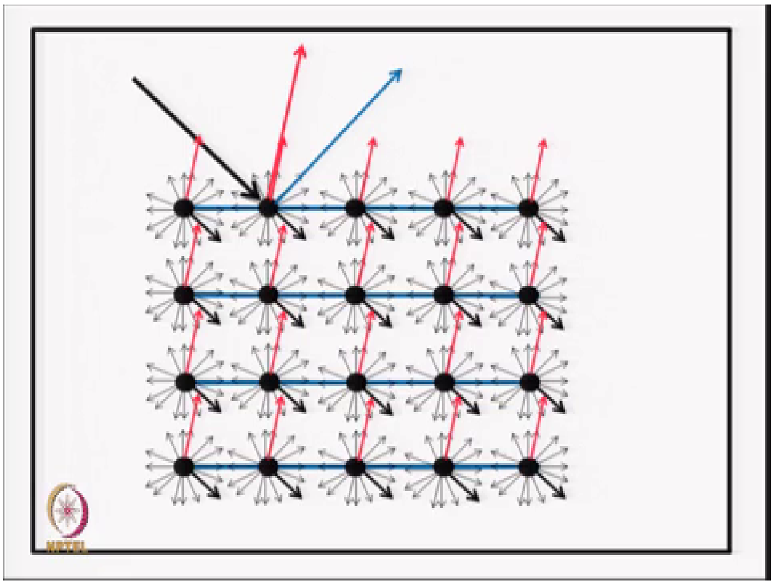


Now, these diffracted beam from the sample if analyzed properly can be used to solve the structure of the crystal because the direction and intensity of these beams depend upon the crystal structure. Bragg simplified this analysis of crystal structure by a very important observation, what he saw is what I have claimed what I have written as Bragg's law part one because this is something sometimes not paid attention to. So, this is the first part of the Bragg's law that for every diffracted beam there exists a set of crystal lattice planes such that the diffracted beam appears to be specularly reflected. Specularly reflected means reflected like a mirror. So, although atoms are interacting with the X-Ray incoming X-Ray and creating a diffracted beam, but the end result can be interpreted according to the according to bragg the end result can be interpreted as a reflection from a crystal lattice plane.

If I introduce a set of planes in this sample, these parallel lines are indicating the set of planes and with respect to this plane I can imagine that incident beam is simply reflected from this plane to create the refracted beam. So, looking at the diffracted beam as a reflection from a crystal lattice plane was the first important step taken by Bragg's and this is the famous Bragg's law. That is because of this interpretation many times the diffracted beam is named as bragg reflection the diffracted beam is also called a reflected beam instead of being called a diffracted beam.

But we should keep in mind that the way although we call it reflection although we interpret it as a reflection actually it is diffraction of X-Rays from the interaction of all the atoms in the crystal.

(Refer Slide Time: 05:36)



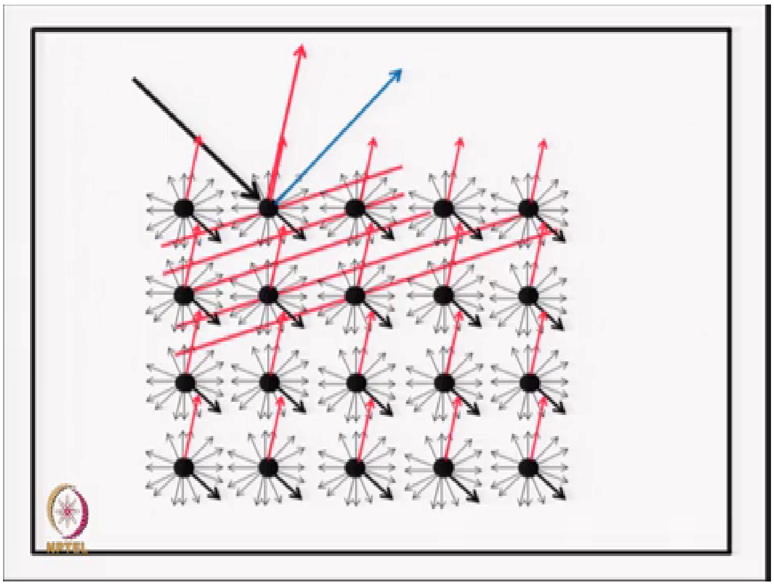
I have tried to show this in this slide where you can imagine these little black circles as atoms and let an X-Ray fall on it. So, X-Ray is coming in this direction this is showing an incoming direction now of course, I have shown only one arrow on one atom, but the X-Ray beam will fall on all these atoms in this direction, and once the atoms interact with this x incoming X-Ray beam they diffract in all directions. So, X-Rays is scattered from a single atom in all possible direction I have shown by these little arrow that this atom is interacting with the incoming X-Ray and is sending X-Rays in all other directions.

This will happen with all the atoms. So, all the atoms are receiving X-Rays in this direction and then sending out scattered X-Rays in all possible directions. If we then pick up a given direction, let us say the blue direction and see how the waves coming from different atoms in this direction add up they may add either constructively interfere or they may destructively interfere. If there is a constructive interference in this blue direction we will get a strong beam and that will be the diffracted beam from the crystal. So, here we have not yet introduced any crystallographic plane. So, the phenomenon of diffraction is actually interaction of all the atoms with the incoming X-Ray. That is what; that is what gives result or results in this diffracted beam. So, incoming beam falls on all the atoms and they interact with the incoming beam and create scattered radiation in all possible direction, then only in some specific direction they constructively interfere and those specific direction are the directions of diffracted beam.

So, far so good this is what was discovered by lovey. Bragg's contribution came in as the next step what he said that we can now interpret this blue diffracted beam as a reflection from a set of lattice plane. Now I have introduced these blue planes which a parallel set of planes containing the atoms and the diffracted beam an incoming beam are inclined at equal angles to this plane so that the diffracted beam appears simply a reflection from this blue set of plane this is the first part of Bragg's law.

As I have said that this may not be the only diffracted beam coming in this setting this experimental setting. So, let us assume that there is another direction the red direction in which also there is a constructive interference. So, if we have a constructive interference in this red direction we will again get a strong beam in that direction now. This strong beam of course, now the incident beam the black incident beam and the red diffracted beam do not appear to be reflected from this blue set of planes, but Bragg's law assures that we will be able to find another set of plane from which this red diffracted beam also will appear to be reflected.

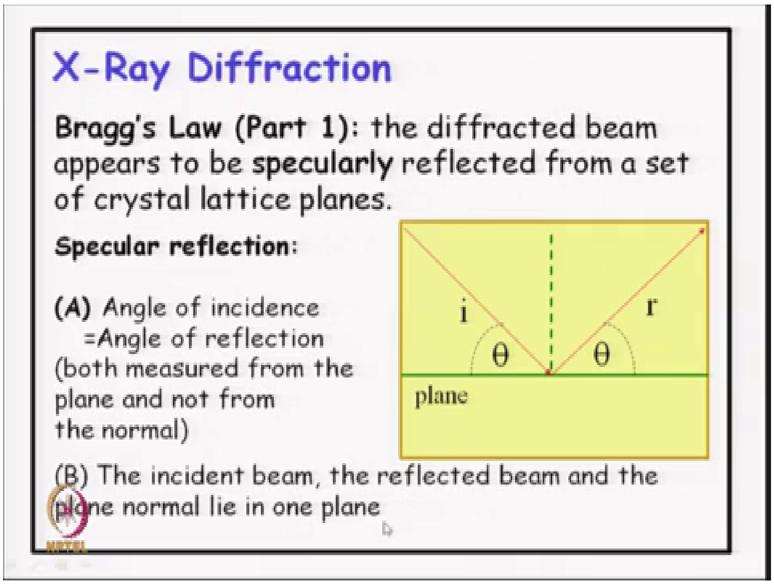
(Refer Slide Time: 08:28)



So, let us try that. So, I remove the blue planes now and draw a new set of planes the red plane from which again the incident beam and the red diffracted beam make equal angles.

So, they appear to be reflected. So, this is the claim of Bragg's law that for every diffracted beam I can always find a crystal set of crystal lattice planes from which the diffracted beam appears to be reflected.

(Refer Slide Time: 08:55)



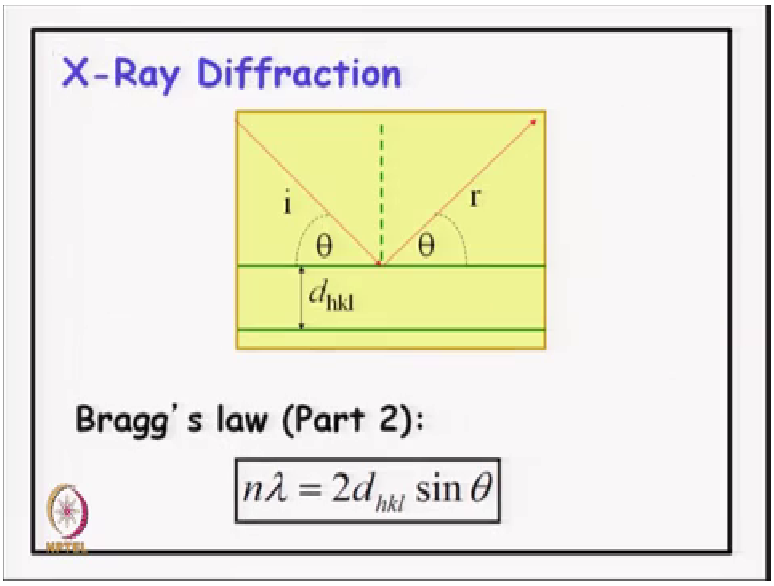
So, this is the first part appears to be specularly reflected.

Let us make it clear what is the specular reflection we all know, that a specular reflection means reflection from a mirror which follows the law of reflection all of you are familiar with laws of reflection. So, the incident beam the first law of reflection is that the incident beam the and the reflected beam make the same angle with the plane or the plane normal. So, the angle of incidence is equal to angle of reflection only difference here from normal physics nomenclature is that in X-Ray reflection or X-Ray diffraction we take the angle from the plane instead of plane normal.

So, this has to be kept in mind, but of course, if the angle with the plane normal is equal, angle with the planes also will be equal. So, angle of incidence is equal to the angle of reflection and the second part which is also important in reflection from mirrors we know that the incident beam the reflected beam and the plane normal also lie in 1 plane this is true for X-Ray diffraction also.

Now, let us look at the second part or the mathematical or the numerical part because the second part is the mathematical or mathematical in nature.

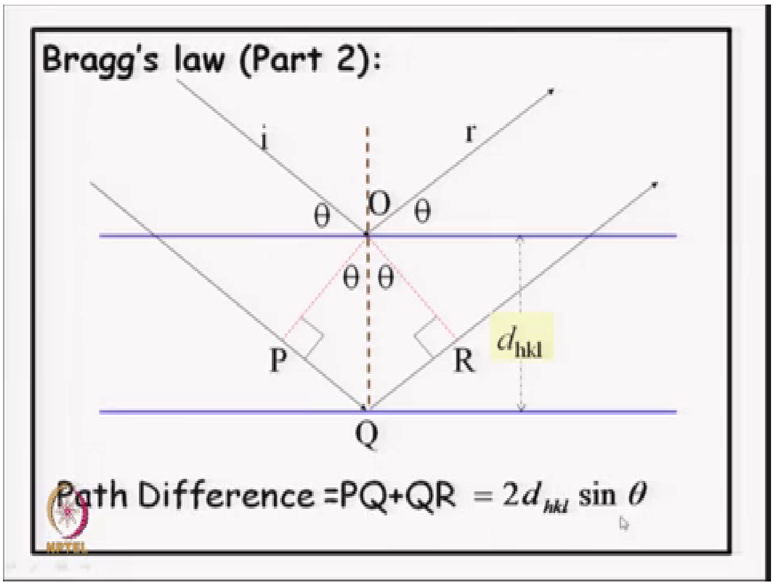
(Refer Slide Time: 10:22)



Usually this is what is quoted as Bragg's law and the first part is forgotten, but the real intellectual jump in Bragg's use of X-Ray diffraction was the first part of interpreting or assuring that the diffracted beam can always be interpreted as reflection, but once it is interpreted as a reflection we have a set of parallel lattice planes with some spacing dhkl and there is an incident angle theta with respect to that plane. So, the second part of Bragg's law connects the incoming wavelength lambda. Lambda is the wavelength of the incoming X-Ray. N is a number which is the order of diffraction dhkl is the inter planar spacing and theta is the angle with the plane is the same and as we have said because of the specular reflection nature the incoming angle incident angle and the outgoing angle or the reflection angle are all the same theta.

So, n lambda is equal to 2 dhkl sin theta is the second part of the Bragg's law this can be proved very simply it is not a very difficult to prove this.

(Refer Slide Time: 11:50)



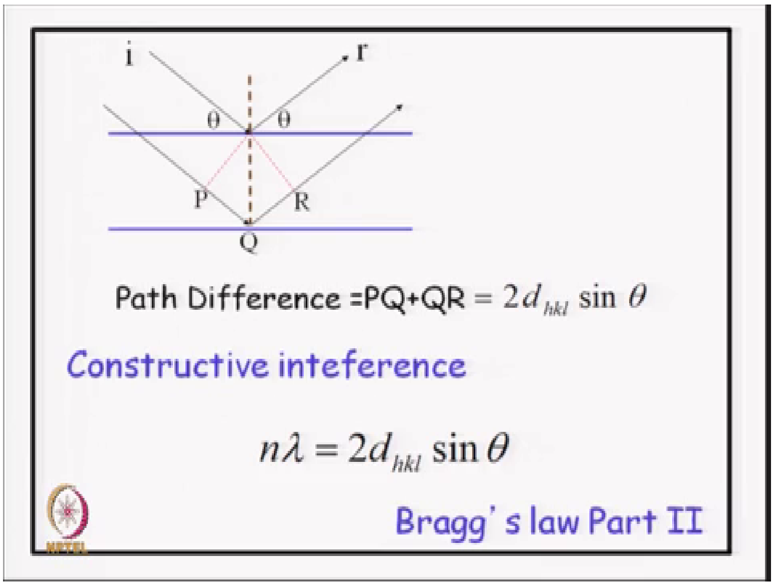
So, we take up this proof here. So, the blue line shows the first the top crystal plane which is receiving the incomingX Ray eye and is reflecting it or diffracting it in the direction r the incident angle theta is equal to the reflection angle theta let us introduce now the second plane at a distance dhkl.

Now, the x-rays will also go onto the second plane and reflect we want to find out we want to construct this path difference let us complete the geometry. So, we drop perpendicular from o on the second beam OP and again on the reflect second reflected beam OR. So, OP and OR are perpendiculars on from O onto the x-ray beams coming and reflected from the second plane.

The path difference, by path difference we mean the difference in the total path length covered by the top beam and the bottom beam. You can see that the incoming X-Rays will travel the equal distance before OP, before OP they are parallel and they are covering equal distance. Similarly, after OR again they are traveling equal distance. So, the extra distance which the bottom beam goes through is the distance PQR. So, if we find this distance PQ plus QR that will be the path difference that is the extra path or extra path length which the second beam has to travel. This of course, can be easily solved by looking at this right-angle triangle OPQ or OPORQ.

You can see that this angle is theta OQ is the inter planar spacing dhkl. So, PQ is nothing but dhkl times sin theta and similarly QR is also dhkl times sin theta. So, the total path difference as shown here is 2 dhkl sin theta, and from elementary physics we know that the path difference

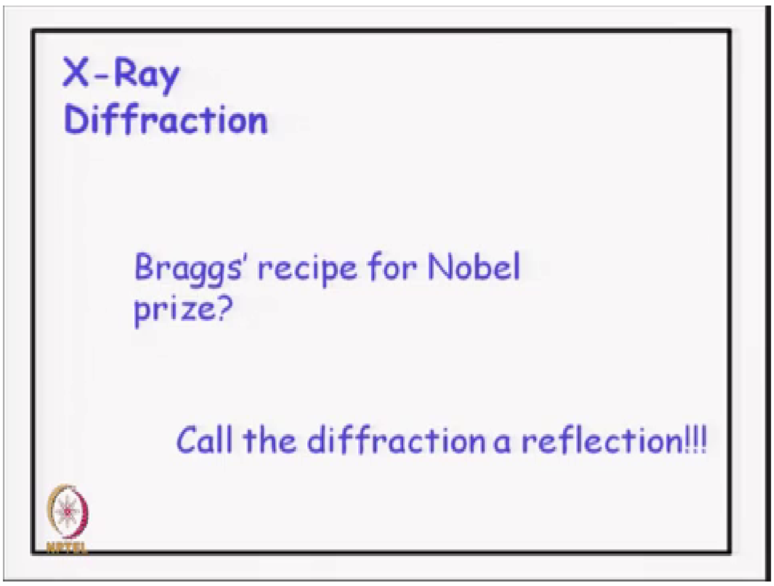
(Refer Slide Time: 14:28)



So, for constructive interference path difference should be an integral multiple of the wavelength. So, this is what gives you in the final Bragg's law that the path difference is integral multiple times the wavelength and lambda is equal to 2 dhkl sin theta. This completes our derivation and description of Bragg's law.

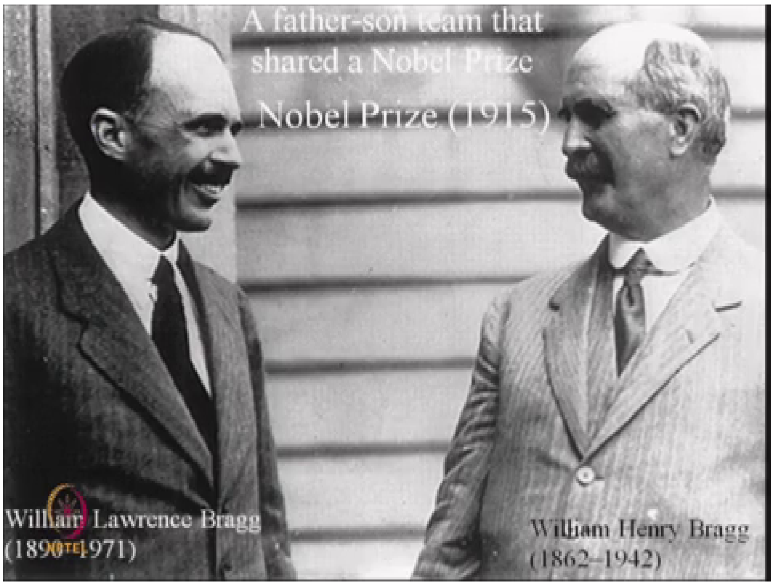
In the next lecture we will use Bragg's law for as an example to solve some crystal structure.

(Refer Slide Time: 15:04)



But before we do that let us look at the history little bit of history of Bragg's discovery. So, as I told you the Bragg's the first part of the Bragg's law was the real quantum jamming. So, Bragg's recipe of Nobel Prize wall to call the diffraction a reflection. This interpretation is what really simplified the solution of crystal structures now we also had an interpretation for his diffraction experiment, but using that interpretation it was more difficult to solve the crystal structure. So, the real contribution of Bragg's was interpretation of diffraction beam as a reflection.

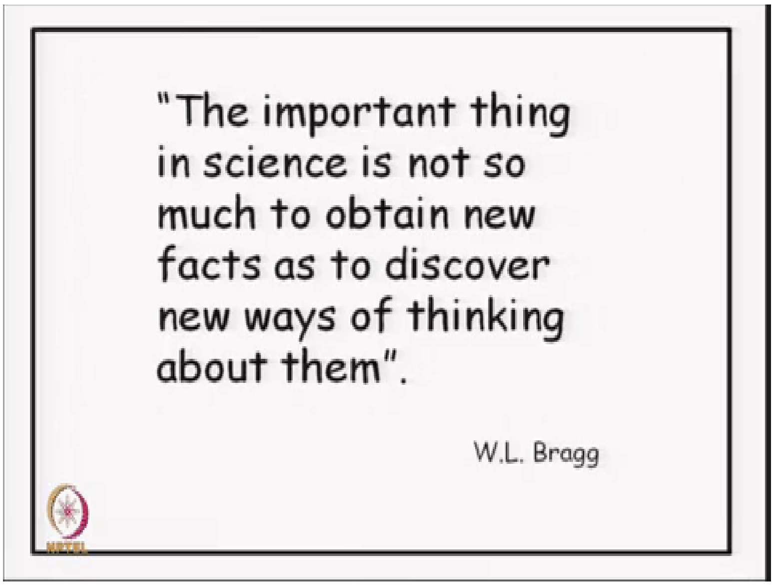
(Refer Slide Time: 15:49)



And it was not 1 Bragg but 2 Bragg's. Lawrence Bragg the son and for Henry Bragg the father and it was a father son team. It is the only father son team who has shared a single nobel prize in the history of Nobel Prize. So, they got Nobel Prize in 1915 for using X-ray diffraction for solution of crystal structures.

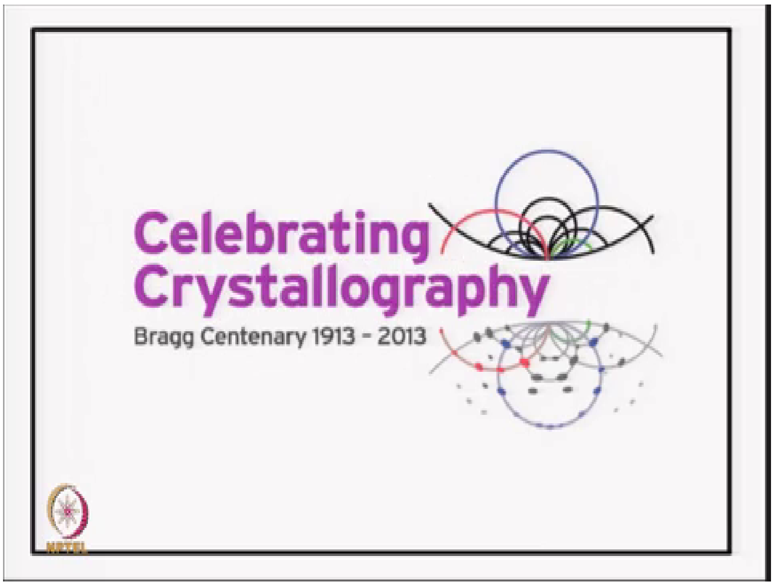
So, when we now were very comfortably say let us say that copper is face centered cubic all these knowledge began with the crystal structure solution of Bragg the first crystal structure they solved was in 1913. So, before that it was only an assumption or hypothesis that crystalline materials have this kind of periodicity. So, the actual solution required this x-ray diffraction and Bragg's for the master of this technique and solved various crystal structures in the beginning using this tool.

(Refer Slide Time: 16:59)



Here is a quotation from son Bragg that the important thing in science is not so much to obtain new fact as to discover new ways of thinking about them. So, Bragg's thinking of diffraction as a reflection was the real step here.

(Refer Slide Time: 17:22)



And because they solved the first crystal structure in 1913 international union of crystallography celebrated Bragg's centenary in 2013. So, there was a lot of conferences and celebration in 2013 to mark this important landmark in the history of science.