Basics of Materials Engineering
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Lecture - 10
Crystal Structure - 8 (X-Ray Diffraction and Determination of Structure)

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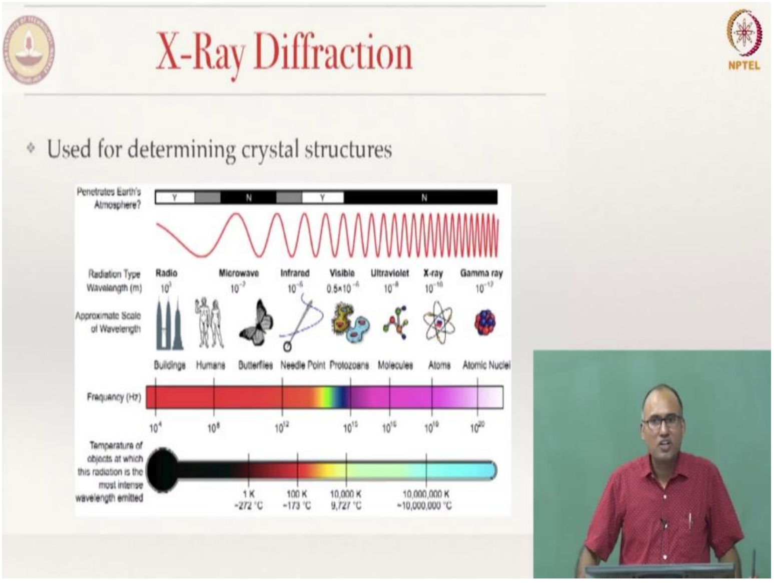

Let us assume you are given a material and you are not told what the material is and you are required to identify the material. How do you do that? Because the slide is there, so you do not say X-ray diffraction but, you can actually do by using the diffraction of light.

So, this slide is very informative and talks about resolutions that you can obtain by using different rays. The reason why X-rays are used is because the resolution that you will get is at the angstrom level. So, you can actually measure, resolve the distances at the interatomic planar sizes and that is why X-rays are used.

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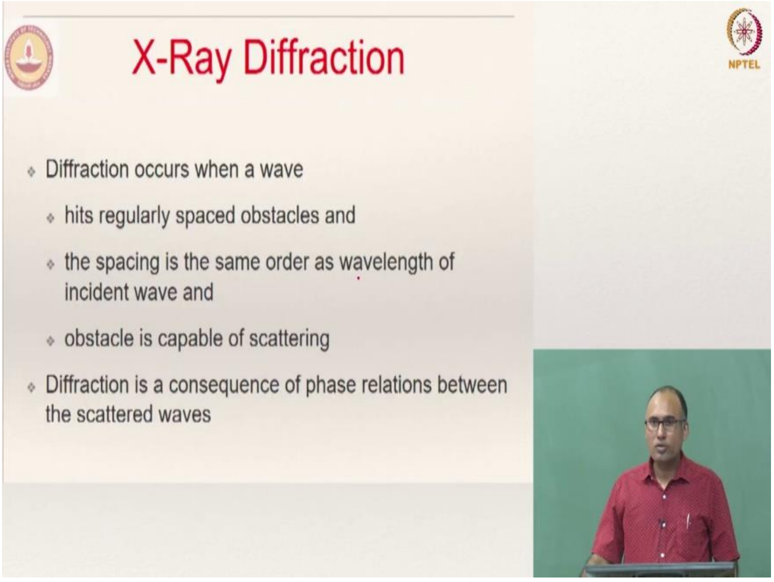

We can use diffraction of light or here X-ray diffraction and we know how diffraction occurs, right? Diffraction occurs when the wave hits regularly spaced obstacles. If the spacing is the same order as the wavelength of the incident wave and when the light is hitting, if the obstacle is capable of scattering the light only then you will have the diffraction.

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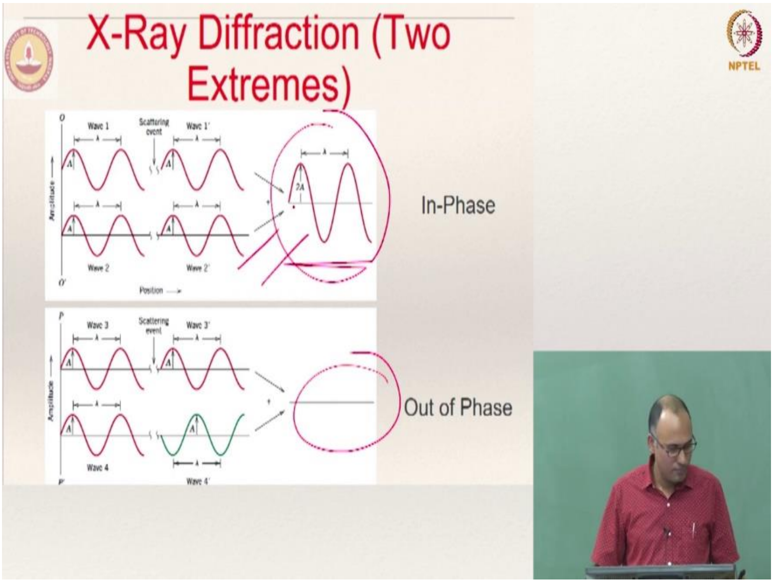

This picture gives you a little bit more information. So, when you have 2 waves: wave 1 and wave 2 which are in phase, their interference causes some amplification and you get a resultant wave like that. This is a constructive interference and this is a destructive interference. So, diffraction occurs when you have something like that.

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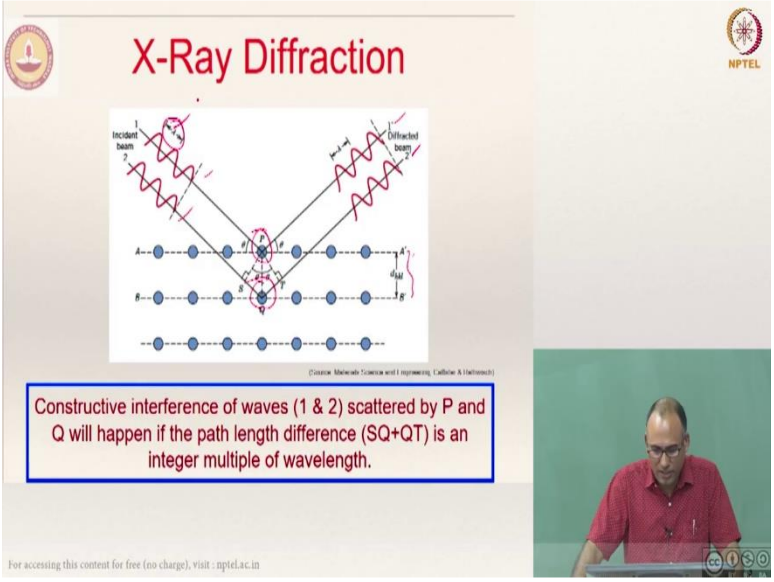

Let us say these are your atomic planes. So, the two planes of atoms are separated by a distance d_{hkl}, where (hkl) are the indices of your plane. They are two parallel planes. Let us say you are shining light and the X-ray is incident. This is incident wave 1 and incident wave 2. Depending upon this distance the diffraction happens, so this is the diffracted beam 1 and diffracted beam 2. And this is the wavelength λ.

Wave 1 is scattered by atom P and wave 2 is scattered by atom Q. The path length difference between wave 1 and wave 2 is ($SQ + QT$) because, wave 2 is traveling more distance than wave 1, and the additional distance is ($SQ + QT$). If that distance happens to be an integer multiple of the wavelength lambda, only then you will have constructive interference, otherwise it will be out of phase and then you will not have constructive interference.

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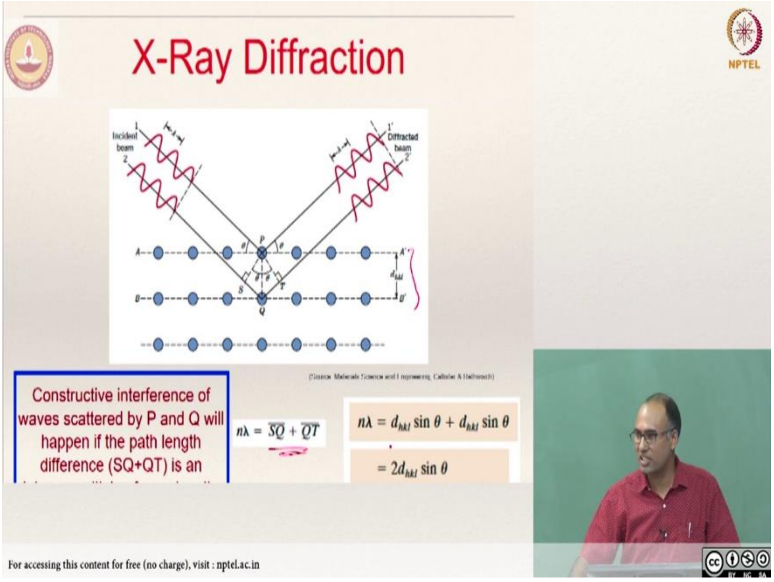

$$n\lambda = \overline{SQ} + \overline{QT}$$

$$n\lambda = d_{hkl} \sin\theta + d_{hkl} \sin\theta$$

$$n\lambda = 2d_{hkl} \sin\theta$$

You know what is your incident wave wavelength λ, right? And, hence you can calculate d_{hkl}. What is d_{hkl}?

Student: Interplanar spacing.

Interplanar spacing. If you can find out that, then you know what is the interplanar of spacing and then from there you can actually calculate what is the lattice structure that is we are talking about. I will show you one diffraction pattern and people will usually use that to identify what is the lattice.

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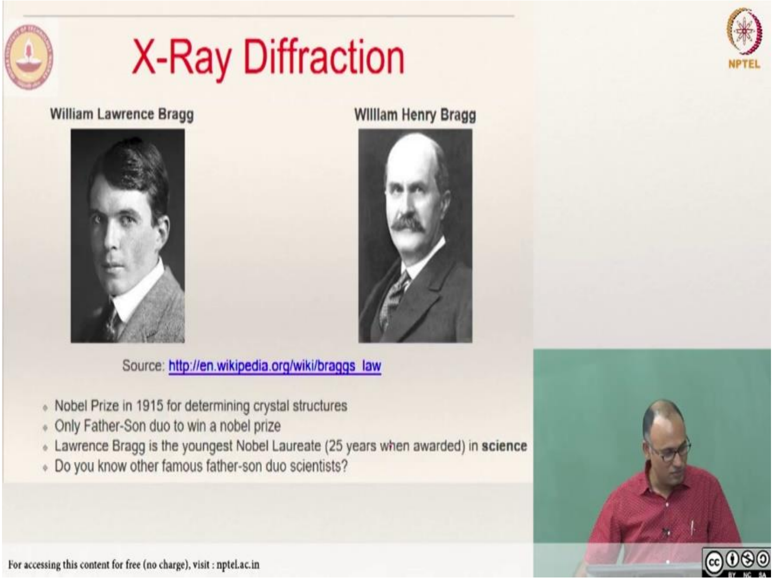

So, these are the two guys responsible for this knowledge Lawrence Bragg and Henry Bragg, both of them have same first name and last name, their middle names are different. They both were given Nobel Prize for determining crystal structures in 1915. Both are father and son and till date I think he is the youngest Nobel laureate at the age of 25. Yeah?

So, you guys still how many years? 3 more years.

Yeah? You guys have 3 more years to become youngest if you want. Do you know other farther son duos in science? Wife and husband duos?

Student: (Refer Time: 05:35).

Yeah.

Student: (Refer Time: 05:37).

Curies and how about son Curie? You do not know?

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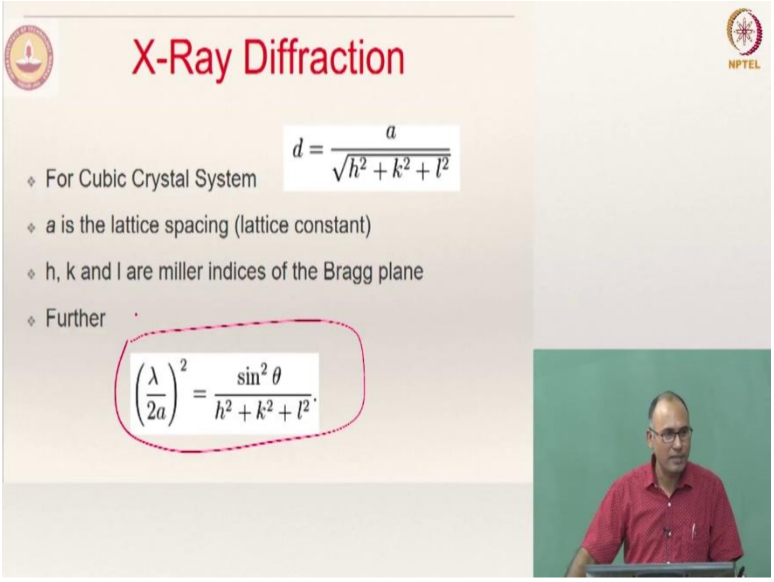

Alright. In mechanical engineering you know father-son duos? Have you heard of Bernoulli?

Student: (Refer Time: 05:58).

How many Bernoullis you are familiar with?

Only 2? Ok. Go back and read about Bernoulli in Google and then you will see at least 5. Okay, so, now you can use the formula that we have derived before.

$$n\lambda = 2d_{hkl}\sin\theta,$$

where (hkl) are the Miller indices of the crystallographic plane.

For a cubic crystal system, you know that

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

You substitute that in the previous formula and then you can actually derive this relation,

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

Where a is the lattice parameter.

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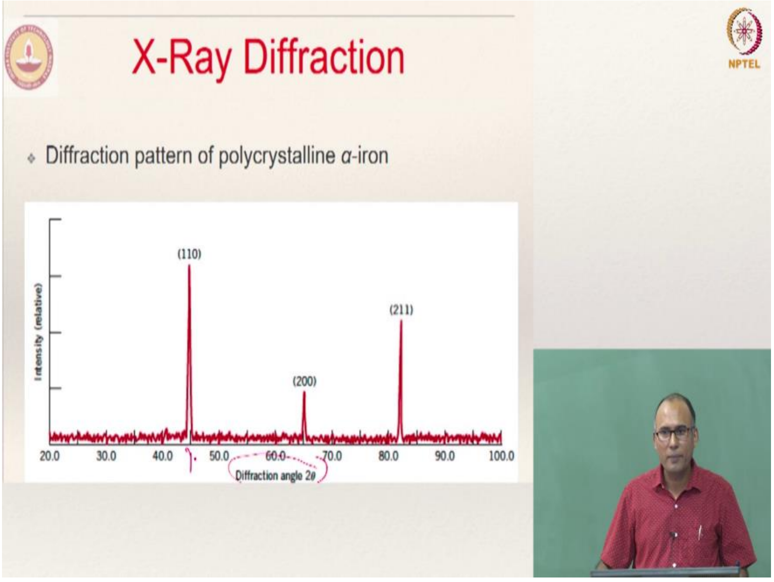

Alright. So, I will skip this, and then this is how a diffraction pattern looks like when we do the X-ray diffraction for a given powder sample. So, this is the X-ray diffraction pattern of the polycrystalline α-iron. By knowing at which diffraction angle you have peaks, you will be able to figure out which material you are looking at.

Suppose you have a new material; you do the experiment and get the diffraction peaks. And, then there will be a catalogue of diffraction peaks available in the literature because people before us have done that job for us, and then compare that and then see which one matches. And, then probably some of that is closely matching with the available diffraction peaks, ok? That is how you will identify crystal structure of a material.

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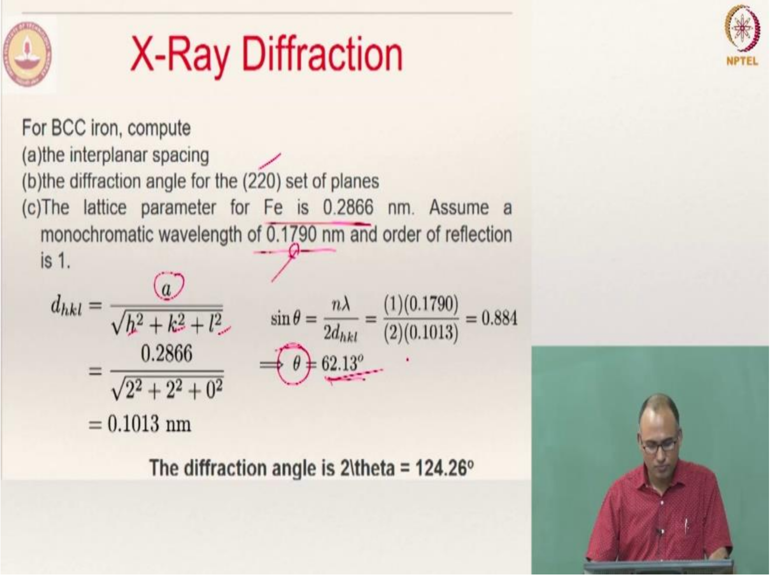

Alright. So, if you have a BCC iron, how do you go about computing the interplanar spacing, and the diffraction angle for the (220) set of planes? By knowing the lattice parameter of iron is 0.2886 nm and the monochromatic light whose wavelength is 0.1790 nm.

So, $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$, the lattice parameter $a = 0.2866$ nm, and (hkl) correspond to the (220) set of planes, then interplanar spacing is 0.1013 nm, right? And, then the diffraction angle will be 2*62.13 = 124.26°. So, when you do the X-ray diffraction experiment if the incident wavelength is this, then you will see a peak for (220) at diffraction angle of 124.26°.

That is how, we can actually back-calculate, and you will be able to identify the details of the crystal structure.

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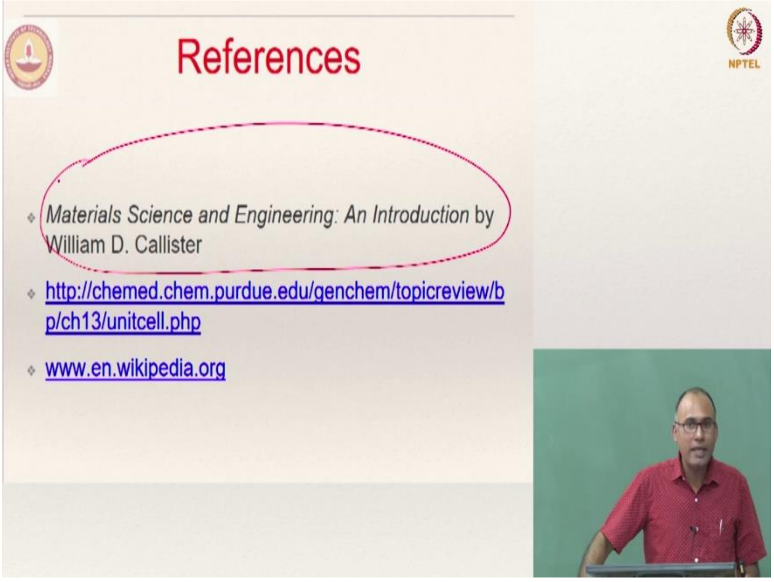

Alright. So, there is lot of information available online. One source is the Cambridge source that I have mentioned to you in the previous lecture. Wikipedia has several detailed instructions and the YouTube links that I have shown you please go through them and also of course, you should read the text book, right?

So, with that we will close the topic of crystal structure.