Texture in Materials

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Module - 03
X-ray diffraction phenomena
Lecture - 06
Diffraction and Bragg's Law

Good afternoon everyone. This is the 6th lecture of Texture in Materials. And we are starting module 3 that is X-ray diffraction phenomena, and this lecture is all about diffraction and Bragg's law.

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The concepts that are covered in this lecture are X-ray diffraction, understanding constructive interference, diffraction principles, Bragg's law.

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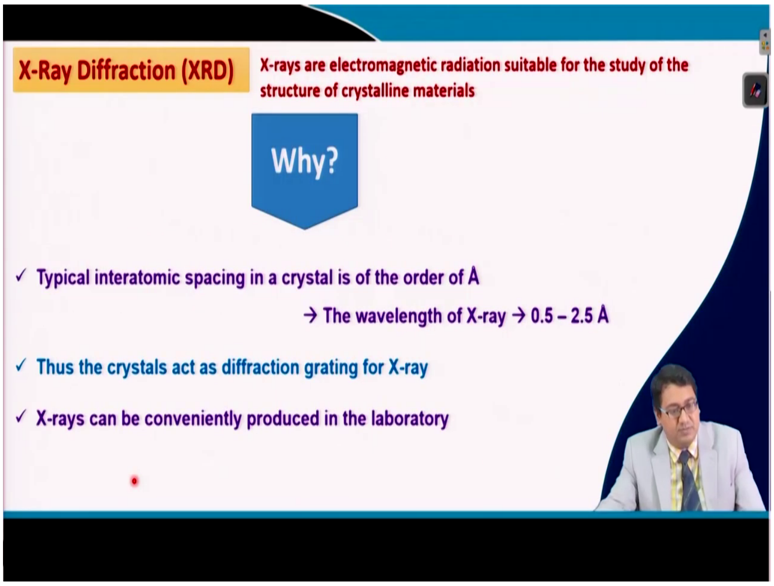

X-ray diffraction is generally known as XRD. X-rays are electromagnetic radiation suitable for the study of the structure of crystalline materials. It is suitable to study the structure of crystalline material using X-rays because the typical interatomic spacing's in the crystals is of the order of Armstrong, which is almost in the same range as the wavelength of the X-rays, which is of the order of 0.5 to 2.5 Armstrong. Thus the crystals act as a diffraction grating for the X-rays. X-rays can be conveniently produced in the laboratory. Therefore, X-rays are the most easily available electromagnetic radiation for diffraction activities.

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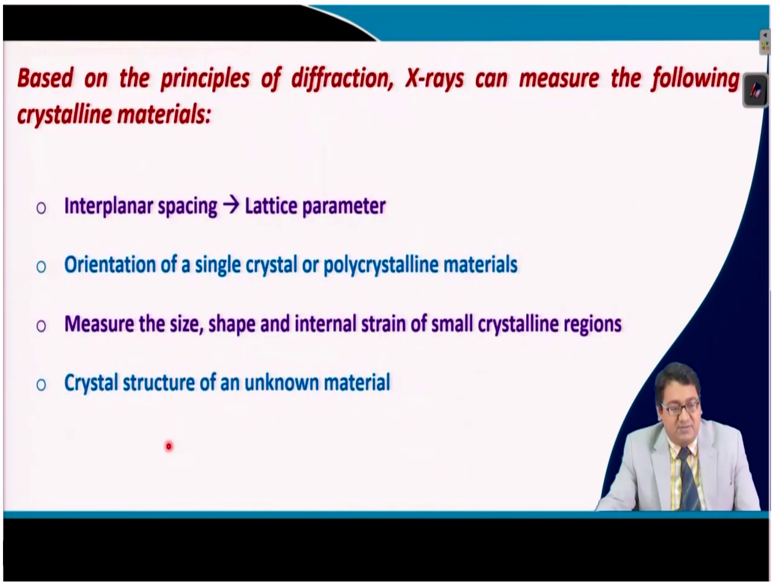

Based on the principles of diffraction, X-rays can measure the following in crystalline materials. They can measure the interplanar spacing that is they can measure the lattice parameter; orientation of a single crystal or a polycrystalline sample. They can measure the size, shape and internal strain that is dislocation densities of small crystalline regions of the polycrystalline material. They can also be used to find out the crystal structure of an unknown material.

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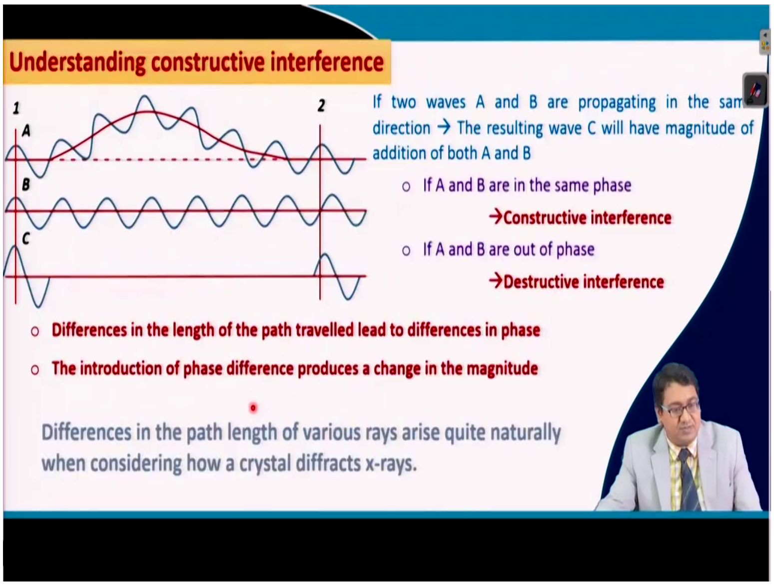

Now, while we understand how the diffraction phenomena work, we should know and understand the constructive and destructive interference between two or more waves. Say for example, if two waves wave A and B are travelling or propagating in the same direction, the resultant wave C will be having the magnitude of the sum of both wave A and wave B.

So, if A and B are in the same phase, say in this position 1 – if A and B are in the same phase, then the C will be the addition of both this wave will be in terms of constructive interference. Whereas, if at point B the A and B are not in the same phase or out of phase, then also the addition of these two waves will give the value of the amplitude of the wave C right. So, if A and B are out of phase, then it will give a destructive interference right. In point 2 the A and B have given, a destructive interference is because the travel of wave A is different from the travel of wave B. Therefore, the distance travelled by wave A is larger than that of B. These differences in the length of the path travelled by wave A as compared to wave B results in a change in the phase or difference in the phase between these two. This introduction of the phase difference between A and B produces a change in the magnitude of the resultant wave C. The differences in the path travelled of various rays electromagnetic rays including X-rays arise quite naturally when considering how the crystals diffract these rays right and in this case these are X-rays.

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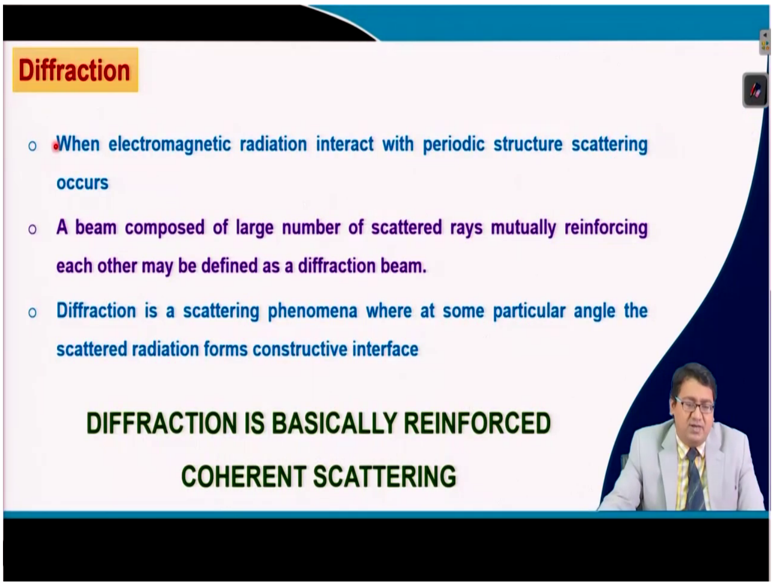

So, if we find out what is diffraction, what is the definition of diffraction? When electromagnetic radiation interacts with a periodic structure, then scattering phenomena takes place, which means, the electromagnetic radiation scatter in all possible direction. A beam composed of a large number of scattered ray mutually reinforce each other and may be defined as a diffraction beam. So, when an electromagnetic radiation falls on the periodic structure, the electromagnetic radiation is scattered in all directions. The scattering principle is that the electromagnetic radiation scatters in all directions at 360 degrees, but that the material is having a periodic structure.

Therefore, some of the scattered radiation at a certain angle will be able to come out with reinforcing each other, and some of them will be hindered because of the positions of the atom. So, diffraction is a scattering phenomenon where at some particular angle the scattered radiation forms a constructive interference, whereas, in other positions other angles it gives a destructive interference. So, diffraction is basically reinforced coherent scattering.

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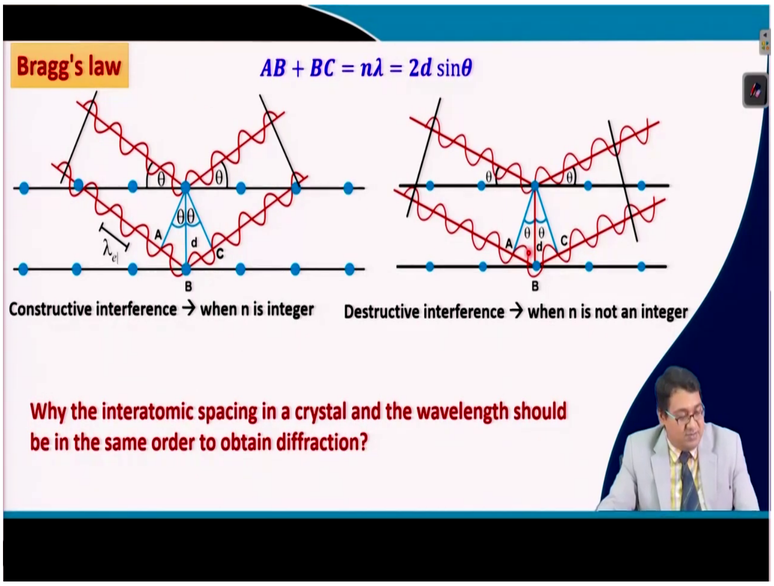

Now, we come to Bragg's law that we have given an example of two hkl planes at a distance of d – separated by a distance d. So, the distance between the two hkl plane is d right. And now the incident X-ray electromagnetic beam is falling from this direction as I am pointing it with the help of my pointer, and it is falling on the first plane. So, it is falling on the first plane and it is diffracting.

It is falling on the next plane, and it is diffracting. Now, that the path length travelled by the second electromagnetic X-ray radiation is higher by A B plus B C as compared to the first radiation during the diffraction. But if in this case, a constructive interference takes place because the path length extra path difference travelled by the second wave is equal to A B plus B C is equal to 1 lambda, 2 lambda, and therefore, A B plus B C is equal to 2 lambda. Whereas, if you calculate d, then d is basically sorry the path length A B plus B C in terms of d, then A B is equal to d times sin of theta, whereas B C is also equal to d times sin of theta. Therefore, in this case it is 2d sin theta equal to 2 times of lambda.

Thus, we can find out that from Bragg's law a 2d sin theta that is a, equal to A B plus B C is equal to an integer of times of lambda, then the path difference leads to a constructive interference when the electromagnetic radiation comes out of the sample towards the detector. So, if you look here both the rays the ray 1 and the ray 2 have a maximum at the same position and the minimum at the same position. So, the addition of these two will lead to constructive interference.

On the other hand, if we look at the second figure, we can find out that the electromagnetic radiation incidenting on the first plane, and another one – second one incidenting on the second plane, the path difference A B plus B C is equal to half of lambda half of lambda and half of lambda. So, it is 3 times half of lambda – 3 by 2 of lambda. So, in this case, 3 by 2 of lambda is basically equal to 2d sin theta.

So, 3 by 2 is not an integer. And when the electron beam diffracted X-ray beam sorry not the electron beam, the diffracted X-ray beams comes out of the sample, then that in case of beam 1 if the diffraction has a minima, then in case of beam 2 the diffraction has a maxima. Addition of these two will become 0. And therefore, there will be destructive interference when the n of multiplied by lambda n is equal to 3 by 2.

So, if n is not an integer, then you will get destructive interference. When n is an integer, we get constructive interference, and that is what is known as Bragg's law. And now while we understood the Bragg's law, we can understand that why the interatomic spacing in the crystal and the wavelength of the X-rays should be of the same order in order to obtain a diffraction in a periodic crystal structure.

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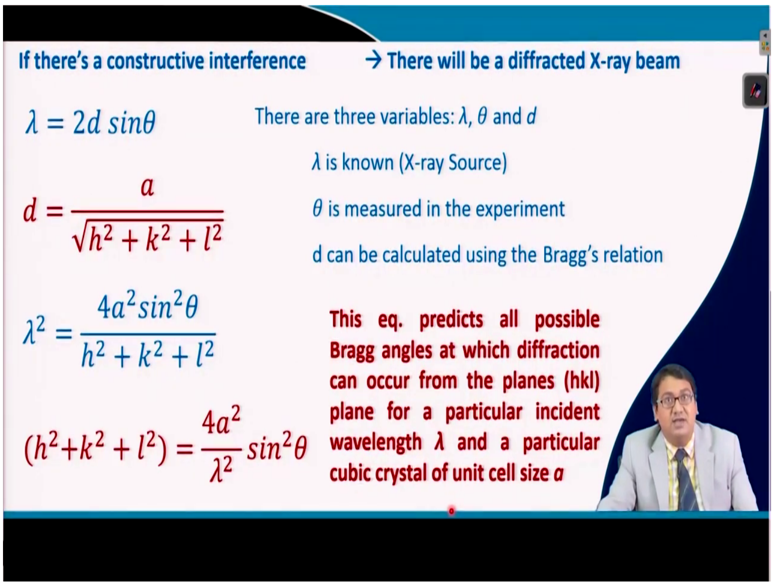

So, if there is a constructive interference, there will be a diffracted X-ray beam right. And this diffracted X-ray beam should follow the equation n lambda equal to 2d sin theta which indicates that lambda is equal to 2d sin theta. So, there are three variables here – lambda, theta, and d. Lambda comes from the X-ray source. So, we know what is the value of lambda. Lambda is the wavelength of the X-ray source.

Theta is can be measured from the experiment, and theta is the Bragg's angle. d can be calculated from the Bragg's relationship, that is lambda equal to 2d sin theta. Now, we know that d that is the distance between the two hkl plane is equal to the a that is the interatomic spacing divided by root square h square plus k square plus l square. And therefore, one can calculate lambda if we put the value of d in terms of interatomic spacing and the values of h, k and l of the plane.

So, lambda square can be given by 4 a square times sin square of theta divided by h square plus k square plus l square. Now, this is how we can calculate the value of h, k, and l. Because we know the inter atomic spacing of the polycrystalline material that we are measuring, we know the value of lambda from the X-ray source, and therefore, we also know the value of theta, which is the Bragg angle for which the intensities are coming. So, these equation predicts all possible Bragg's angle at which the diffraction can occur from the certain hkl plane or hkl planes for a particular incident wavelength lambda which belongs to a certain X-ray coming from a certain elemental source and a particular cubic crystal of a unit cell size a right.

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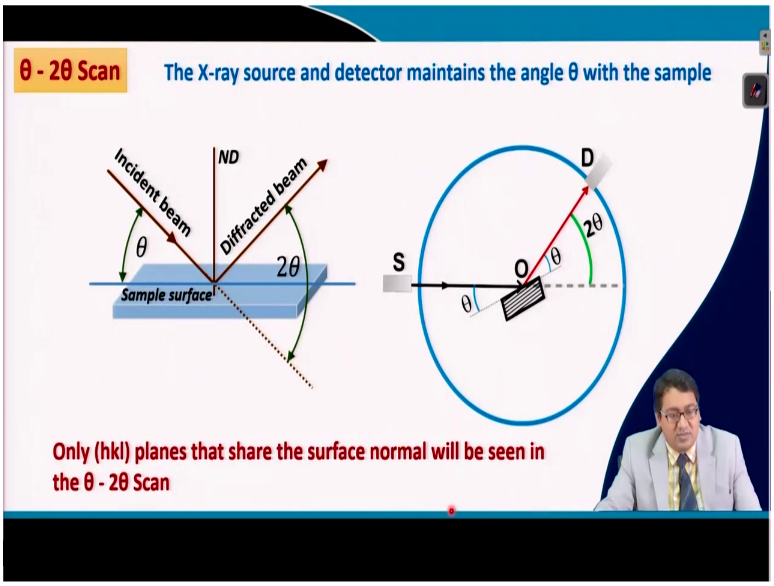

So, that once we have an X-ray source and a detector. In order to have a diffraction from a particular plane, a diffraction angle Bragg's angle of theta has to be kept constant. And in order to know how this n lambda equal to 2d sin theta has to be maintained, one should know the value of lambda which is the wavelength of the X-ray source. And thereby if we do a theta-2 theta scan, and we fix the value of theta for a particular incident X-ray beam, the diffracted beam will go at an angle 2 theta compared to the incident beam, and theta with respect to the sample surface. So, it will have the surface normal ND which will be bisecting both the incident beam and the diffracting beam.

So, that a theta-2 theta scan is done in such a way that if you look into the right side figure, a source for the X-ray beam gives the X-rays a monochromatic X-ray of a particular lambda. And the sample is rotated from 0 degree to any theta value from 0 degree to the X-ray beam means the sample surface is parallel to the X-ray beam, and then it is rotated from 0 degree to any theta value. And then there is a detector that is rotated by an angle 2 theta if the angle of deviation of the sample surface from the X-ray beam is theta. So, every time the sample is rotated by theta, the detector is rotated by 2 theta so that the diffraction beam can the diffracted beam can go into the detector.

Now, if such a situation exists, then if the sample is rotated from 0 to some certain theta and detector is rotated from 0 to some certain 2 theta, then one can obtain a theta-2 theta scan having diffraction intensities at certain thetas for different hkl planes right.

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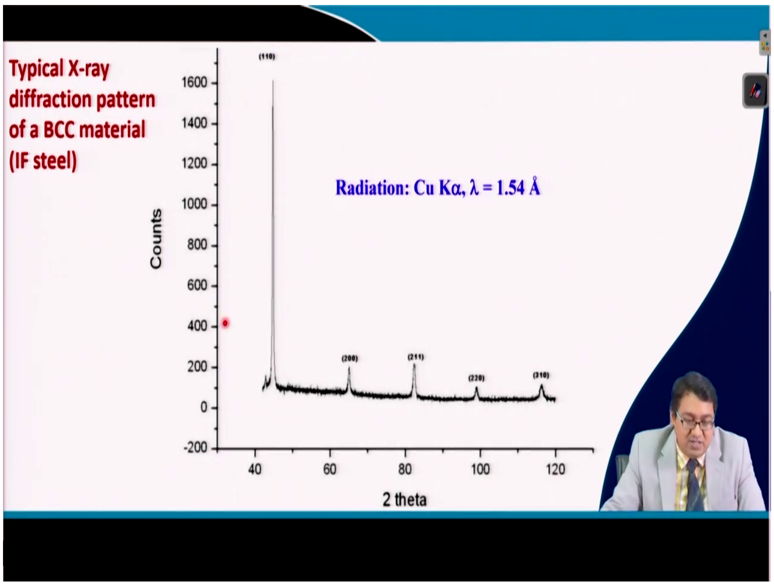

And therefore, here is an example of a typical X-ray diffraction pattern of a BCC material. And in this case, it is interstitial free steel and you can see that at a theta at a 2 theta, sorry, at a 2 theta which is in the x-axis, and the intensity counts at the y-axis at a theta of nearly 45 degree the high-intensity peak of the 110 plane could be obtained.

On the other hand, if we go if the scan is done and when the theta is increased at a certain theta greater than 60 degree which is maybe 63 or something, the 200 peaks could be obtained. And then 211 peaks and 220, and 310 peaks could be obtained at various theta which where the Bragg's law is satisfied. Now, this is for the copper K alpha radiation where the lambda is constant at 1.54 which means the lambda of the X-ray beam is kept constant. So, it's a monochromatic X-ray beam.

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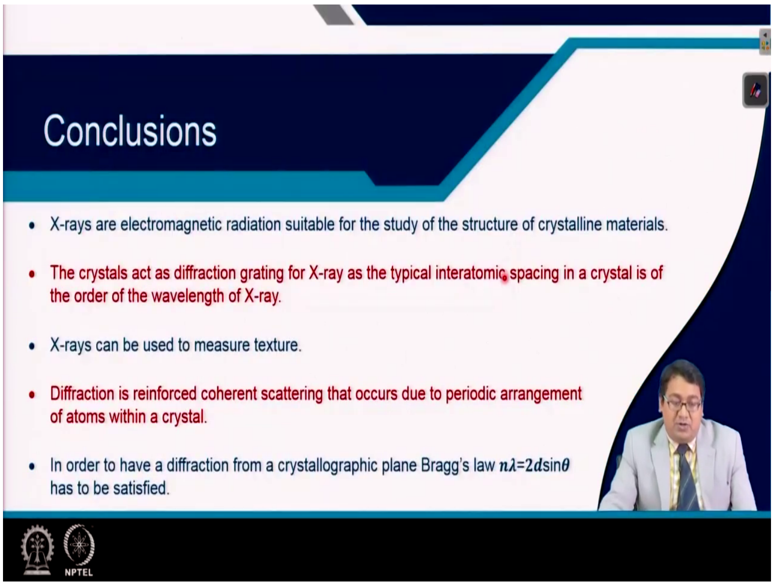

What do we learn from this lecture? We learned that X-rays are electromagnetic radiations that are suitable to study the structure of crystal crystalline material. The crystals act as diffraction grating for the X-rays as the typical interatomic spacing in the crystal is of the order of the wavelength of the X-rays. X-rays can be used to measure texture.

Diffraction is reinforced coherent scattering that occurs due to the periodic arrangement of atoms in the crystals. In order to have diffraction from the crystallographic plane Bragg's law n lambda equal to 2d sin theta has to be satisfied.

Thank you. That is it.