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Lecture-23
Materials Characterization
Fundamentals of X-ray diffraction

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Hello everyone. Welcome to this material characterization course. In the last class, we started discussing the, the fundamentals of X-ray diffraction and then we just emphasize the basic physics of X-rays and how it is generated and so on. And we in this class, we will continue to look at the properties of X-rays. And since we have some basic understanding of this X-rays as an electromagnetic radiation which we have discussed in the fundamentals of the optical as well as scanning electron microscopy, the electromagnet characteristic also will exactly fit with the X-rays. But since we are going to talk about only the X-ray diffraction, we will recollect some of the concepts and the basic physics behind this. And we will also look at the properties and then move on to the concept of diffraction in much more detail. So, today what I am going to do is just X-ray waves.

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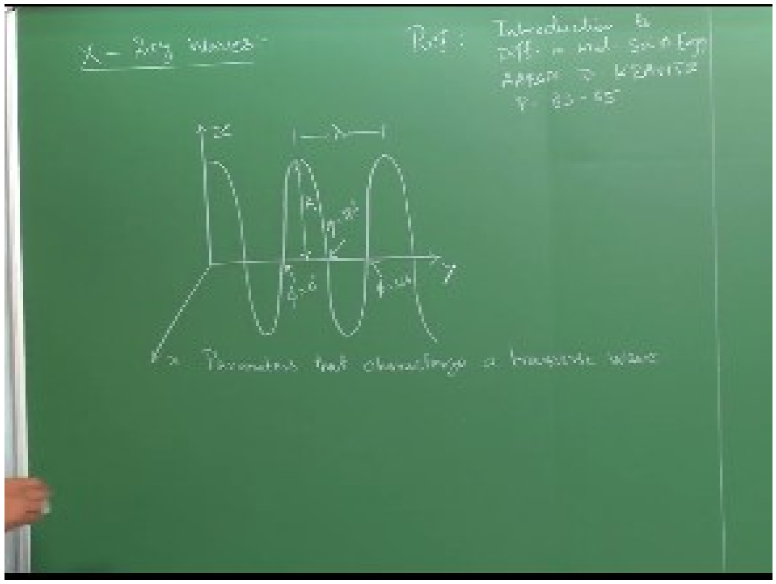

So, we are looking at the X-rays as a wave. So, we will look at the some of the fundamental aspects or parameters which describes the X-rays as waves. And what are the things we have to look at? This is what I just introduced. Then we will discuss the, the property is much more detail.

So, the schematic which have drawn to describe X-rays as transverse waves. A transverse wave are the waves where they have the oscillation in one plane and you have the direction propagation direction is this. So, their oscillation direction as well as the propagation directions is mutually perpendicular. They are all called a transverse wave and then you have the amplitude ‘A’ and you have the wavelength ‘λ’. And what I have marked here is, it is a phase angle. For a complete one cycle of the wavelength the Φ is about 360° that is 2π. So, we will just define these things, so that when we use these parameters for explaining the wave properties this will be more handy. And this is the reference, a book from where I have taken this “Introduction to buy fractioning material science and engineering by Aaron d Kravitz”. So, now we will see that will write few remarks.

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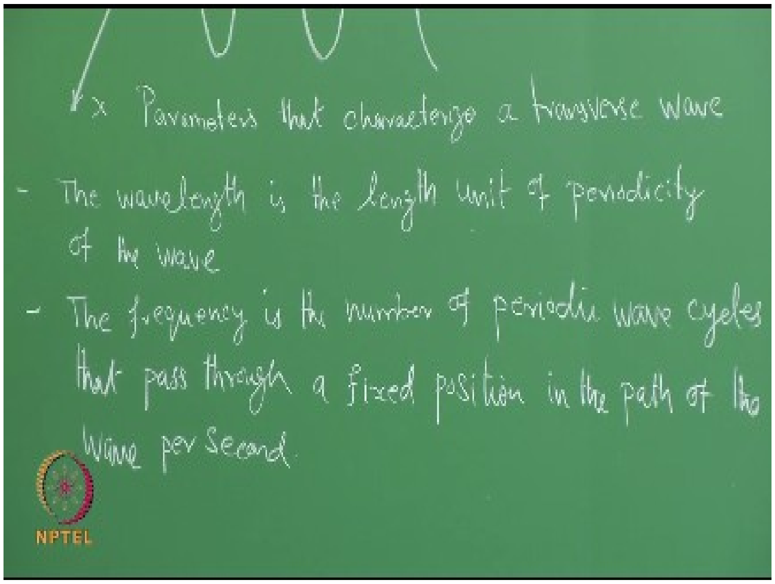

So, the wavelength which we have marked this tells the length unit of periodicity of the wave, that is one full cycle which is the periodicity. And that we also talked about the frequency of this waves. The frequency is the number of periodic wave cycles that pass through a fixed position in the path of the wave per second. So, we use these terms quite frequently. So, it is better always to put it very clearly the, the basic meaning of this parameters. That is why we are going through this. Now we will write an expression for the since the electromagnetic radiation travels with the speed of light, so, we can write this well-known in expression

$$\lambda = c / \nu$$

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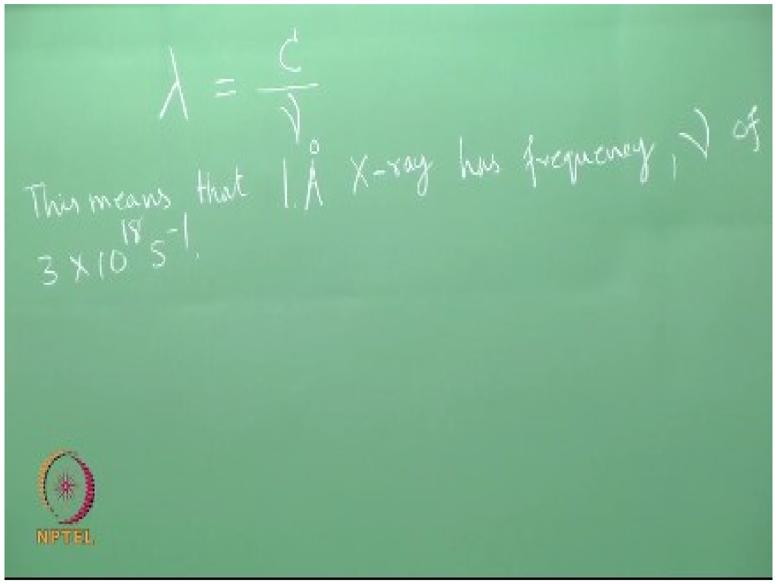

c by ν is the frequency and the wavelength of the X-rays. They are related like this and 'c' you the speed of the light. That means, one angstrom X-ray have a frequency ν of $3 * 10^8$ per second. So, few more points about this wave. During one full cycle, the wave amplitude oscillates through 360° are 2π radians of the phase angle Φ. The phase angle for a wave travelling along the Y-axis is given by

$$\mathbf{\Phi = 2\pi y / \lambda}$$

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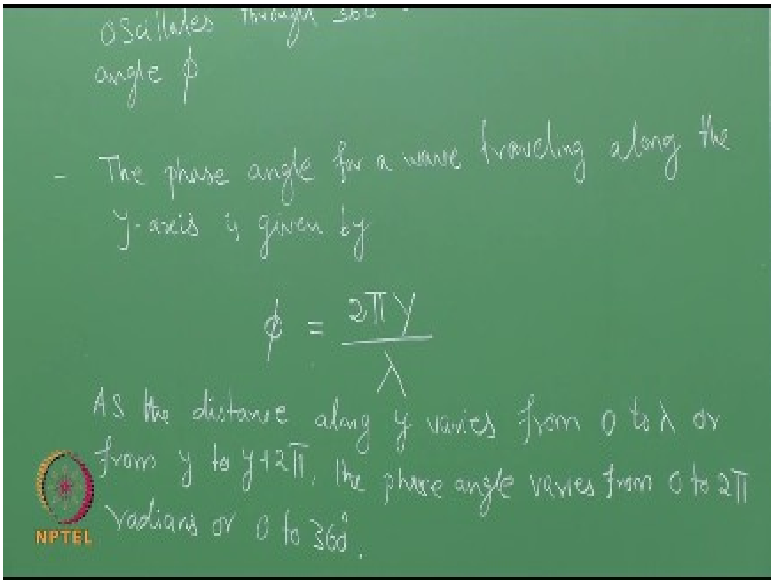

So, this particular information we have already discussed in the phase contrast microscopy when we looked at the light optical system. The similar thing we are doing here, just for reinforcing the understanding. And because we will be using this all the concept related to diffraction and imaging and so on, not only here in electron diffraction as well. Everything is common here.

So, the as the distance along y varies from 0 to λ or from y to (y + 2π), the phase angle varies from 0 to 2π radians or 0 to 360°. So, you have to keep this in mind, the wavelength here we are measuring, which is going to be related to the, the phase difference as well as the path difference like we discussed in the light optical microscope, which is going to be discussed and quantified when we talk about diffraction and so on. So, that is why we are introducing this again. Though we have already gone through it but it is better to have a clear idea about these parameters and another thing is I want to draw a plane polarized light or plane polarized wave.

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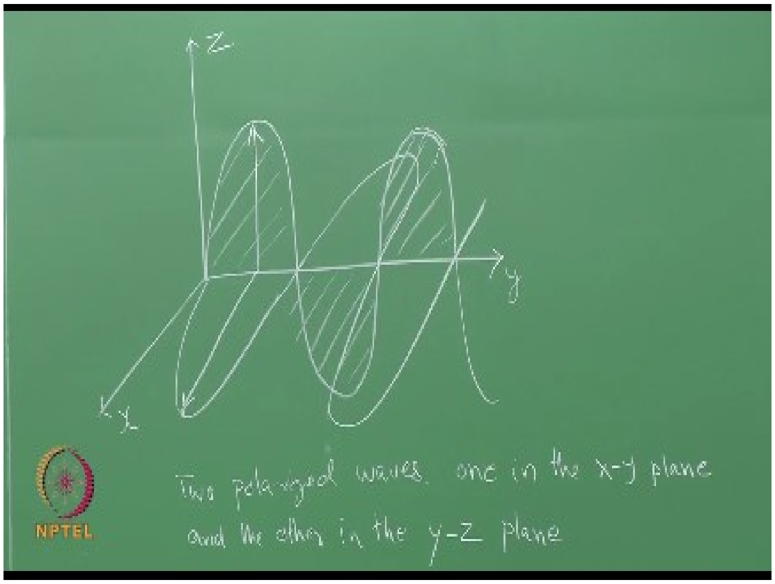

What I have drawn, the schematic is, two polarized waves one is hatched, the other one is which is there in the I mean the hatched wave is in the YZ plane. And the other wave which is perpendicular to this oscillation, oscillation plane perpendicular to this plane is in XY plane. And this is un-polarized light. I mean like we have already discussed this or in this case we are talking about X-ray waves not light. The amplitude vectors for a series of un-policed waves traveling down the Y-axis so that is how it is going to look like.

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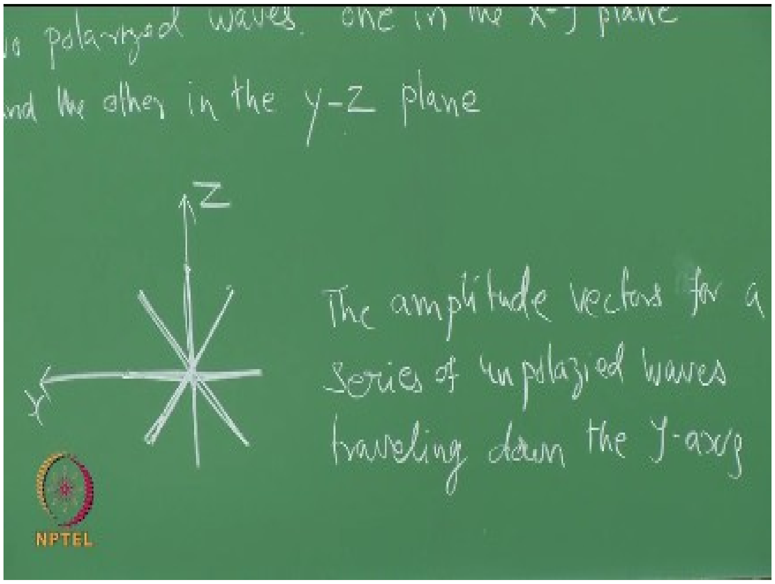

So, for the that means what of what we are trying to show here is, for an un-polarized light the amplitude vectors of the wave will be in the all over the all the directions compared to the plane polarized light like this what we are saying here.

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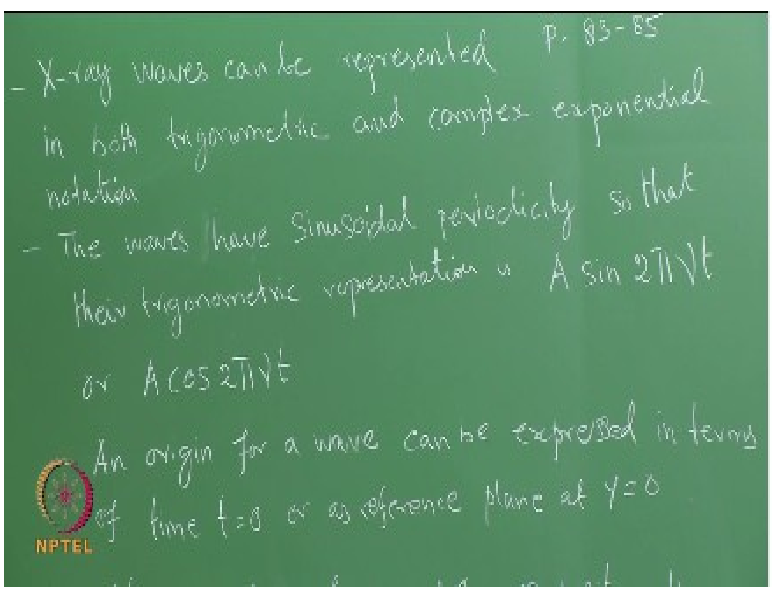

Now, okay few points we have to remember. X-ray waves can be represented in both trigonometric and a complex exponential notation. The waves have sinusoidal periodicity so that their trigonometric representation is a sine **$A \sin(2\pi\nu t)$** or **$A \cos(2\pi\nu t)$** . We can keep an origin for the wave can be expressed in terms of time that is t=0 or a reference plane at y=0. At a point y_1 from a reference position there will be a "phase shift" given by **$2\pi y / \lambda$** that is the wave at y_1 is described by a sign **$A \sin 2\pi (\nu t - (y_1 / \lambda))$**

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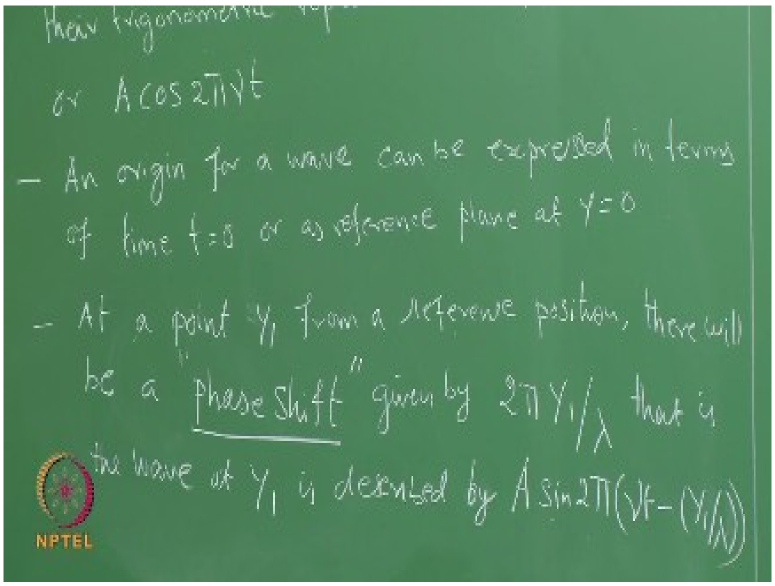

So, in order to understand the phase relations this is very important in, in the some of the concepts like diffraction imaging. So, these fundamental parameters and their notations and how they are described are very important. And normally people have lot of difficulty in getting these concepts. That is why we are going little slowly and also you should remember this parameters like phase shift and then how they are represented for a given wave property. So, now we will look at another property okay.

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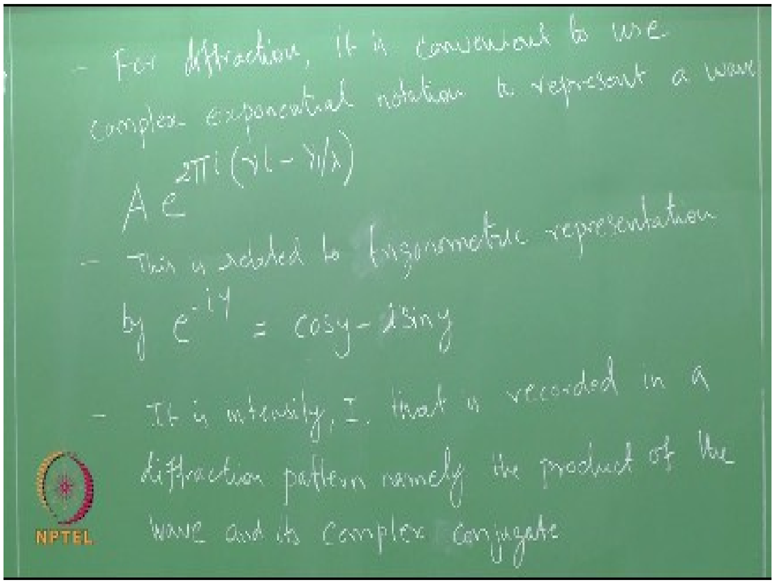

What I have written is, for a diffraction, it is convenient to use complex exponential notation to represent a wave in the form $\mathbf{A\ e^{2\pi i\ (vt - (y1\ /\ \lambda))}}$ So, this is what same thing. So, what we are now trying to do here is, look at the other notations which we will be using in the concept of diffraction. Something like an exponential notation like this. And this is related to trigonometric representation by $\mathbf{e^{-iy} = cos\ y - I\ sin\ y}$. However, it is an intensity, I, that is recorded in a diffraction pattern namely the product of the wave and its complex conjugate. So, to appreciate that part, let us consider a small volume of material scatters in an incident X-ray wave. If the volume is divided up into n point sources a wave from the point K is given by $\mathbf{E_k = A_k\ e^{2\pi i\ (vt - (y1\ /\ \lambda))}}$. So, this is the wave from the point k from the n sources. So, that means if you want to sum up all the waves coming from n sources, we will modify this expression accordingly. We can write,

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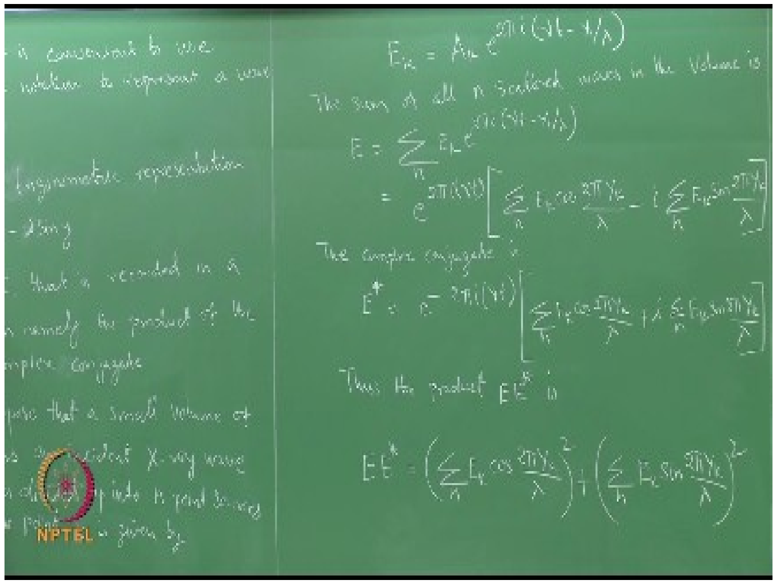

So, what we have done here is, you have represented the wave from the point k from the material which has got n point source. And we are now summing up all the scattered n scattered waves in the volume of the material that is

$$\mathbf{E = \sum_n E_k\, e^{2\pi i\, (vt - (y_1 / \lambda))}}$$

$$\mathbf{= e^{2\pi i\, (vt)} \left[\sum_n E_k \cos (2\pi y_k / \lambda) - i \sum_n E_k \sin (2\pi y_k / \lambda) \right]}$$

And you can express this exponential in terms of the trigonometric function like what we have just said here and it takes a form like this and then you can write the complex conjugate for this

$$\mathbf{E^{*} = e^{-2\pi i\, (vt)} \left[\sum_n E_k \cos (2\pi y_k / \lambda) + i \sum_n E_k \sin (2\pi y_k / \lambda) \right]}$$

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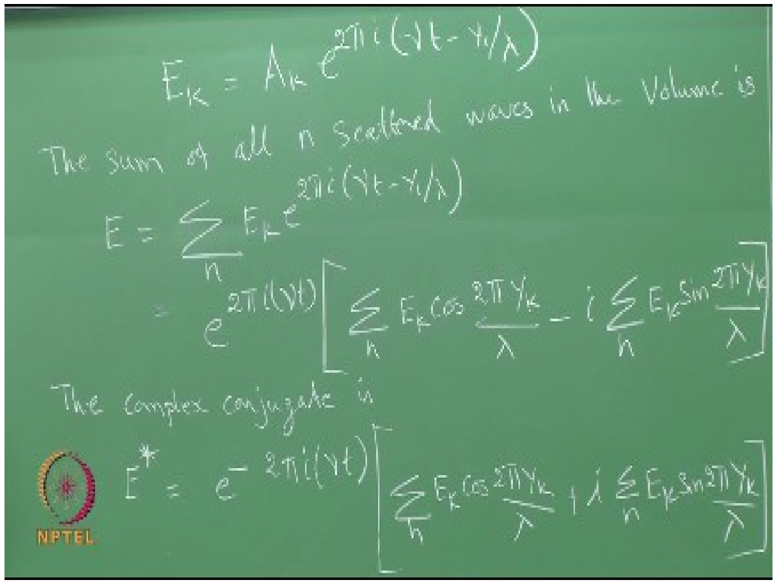

So, the intensity is the product of the.

$$\mathbf{EE^* = \{\textstyle\sum_n E_k \cos(2\pi y_k / \lambda)\}^2 + \{\sum_n E_k \sin(2\pi y_k / \lambda)\}^2}$$

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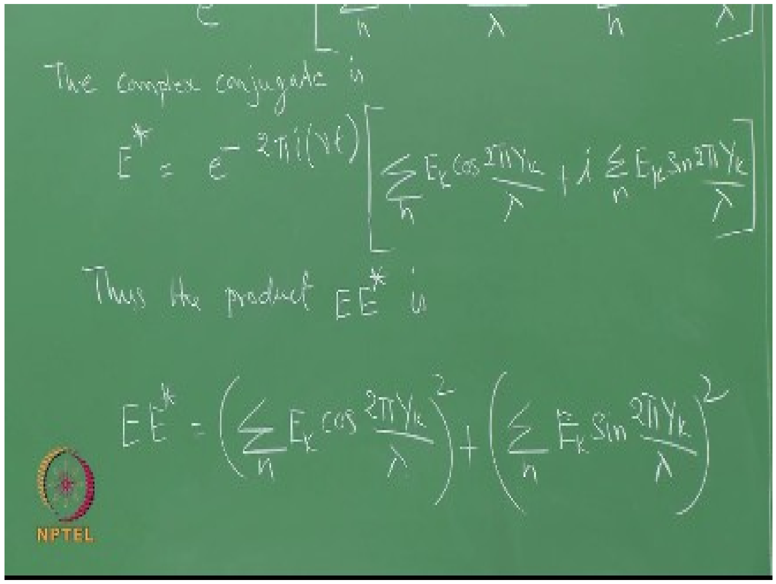

So, it is just to give you some idea how the waves are represented and how each expression is looking like when you consider the wave properties. So, we will be using some of this basic function when we talk about diffraction as well as the sum of the interference of these waves of X-rays. So, after this I will start discussing about the diffraction and my first attempt is going to talk about diffraction in terms of phase relations.

Since we talked about a phase and then I hope you have some idea about this phase and phase shift and we also have already seen the phase difference and path difference. They are all measured in terms of wavelength. So, we will relate this phase relations with diffraction and then we will try to give a complete explanation of how do we appreciate a diffraction in the I mean a diffraction of X-rays in the crystal lattice. That we will see in the next class. Thank you.

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