Chemical Crystallography
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Lecture - 45
Data Reduction-Lorentz and Polarization Correction

Welcome back to the course of Chemical Crystallography. In the previous lectures, we started understanding what is called data reduction. So, we discussed about initially the method of data collection. And we understood that a set of data means, it is a set of raw images, which are recorded using some area detector, it can be a CCD, it can be a CMOS or it can be any other area detector. And then it is our job to extract the intensities out of those diffracted beams. And then scale them and apply a certain number of corrections, which are then applied to all the reflections.

And we then generate the final hkl file which is the intensity file for all the reflections that were recorded during the experiment. So, in the previous class, we talked about absorption correction, and how one can utilise different types of absorption correction using set of packages, using set of methodologies most of them are theoretical. And how to reduce the problem of absorption by choosing an a crystal of appropriate shape and size.

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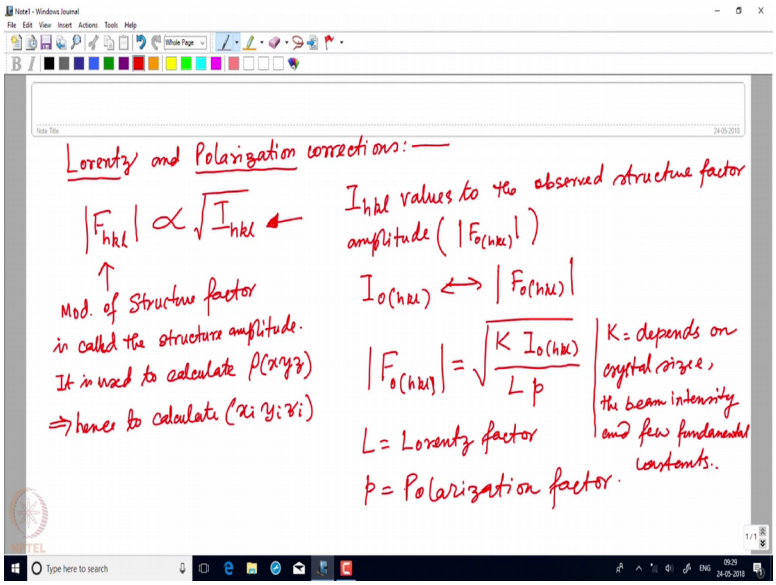

So, today we will try to understand two more correction problems, correction terms, which are incorporated, they are called the Lorentz and polarization corrections. These two corrections are simultaneously applied on each and every data collection, and then the corrected intensities are extracted. So, as we know the modulus of structure factor for every reflection F hkl is proportional to the square root of I hkl that is the structure that is the intensity that is absorbed. So, this modulus of structure factor is called the structure amplitude. And this structure amplitude, it is used to calculate rho x y z, which means the electron density associated with different locations of atoms in the unit cell. And hence to calculate x i y i z i for all the atoms present in the unit cell.

And what is measured is I hkl the intensity that comes out of every lattice plane designated as h k and l. So, what we need is to convert the I hkl values to the observed structure factor amplitude that we write as F o of hkl. So, what we need is a relationship between I observed for every hkl width the mod of F observed hkl. So, the relationship is that is used in a data reduction program is written as F o hkl that is the modulus of observed structure factor is equal to the square root of a constant K multiplied by I o hkl divided by two terms Lorentz and polarization factors. So, this L is called the Lorentz factor, and p is called the polarization factor. When this constant K depends on the crystal size, the beam density and few fundamental constants.

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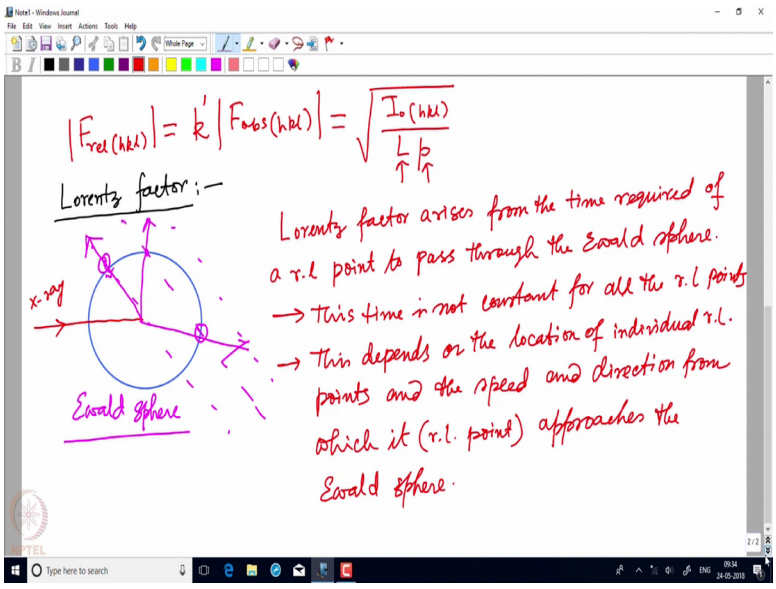

So, the result that one can write is the mod of F relative hkl. See now here, I am replacing the term observed with relative is equal to some constant K prime F observed hkl or F o hkl, which allow we may want to write is equal to square root of I o hkl I observed hkl divided by Lorentz and polarisation terms. So, now let us try to understand those two terms, which are incorporated here the term L and term p, the corresponding Lorentz and polarization factors.

Let us start with the Lorentz factor. The Lorentz factor arises due to the time required for a reciprocal lattice point to pass through the sphere of reflection. So, what we know is that, if this represents a the Ewald's sphere. And we have incident X-ray beam coming from this direction and meeting the crystal. Here the incident X-ray beam, we have reciprocal lattice points like that.

So, when a particular reciprocal lattice point passes through the Ewald's sphere, a diffraction occurs in that direction. So, when the reciprocal lattice point passes through this point, a diffraction occurs here. When a reciprocal lattice point passes like that a diffraction occurs there. So, each and every point in the reciprocal lattice has to pass through this Ewald's sphere to cause diffraction, this is what we understood in one of our previous lectures. So, the time taken for each of those reciprocal lattice points passing through the Ewald's sphere is different. And that time differ difference in time is dependent on where the reciprocal lattice point is.

So, the Lorentz term or Lorentz factor arises from the time required for a reciprocal lattice, I am writing it as r l reciprocal lattice point to pass through the Ewald sphere. This time is not constant for all the reciprocal lattice points, why? Because the reciprocal lattice points are spread over a region and depending on where the point is and what is the angular velocity of that point, while crystal is rotated based on that the amount of time that is required for this point to pass through the Ewald's sphere will be different. So, this depends on the location of individual reciprocal lattice points and the speed and direction from which it that is the reciprocal lattice point approaches, the Ewald sphere.

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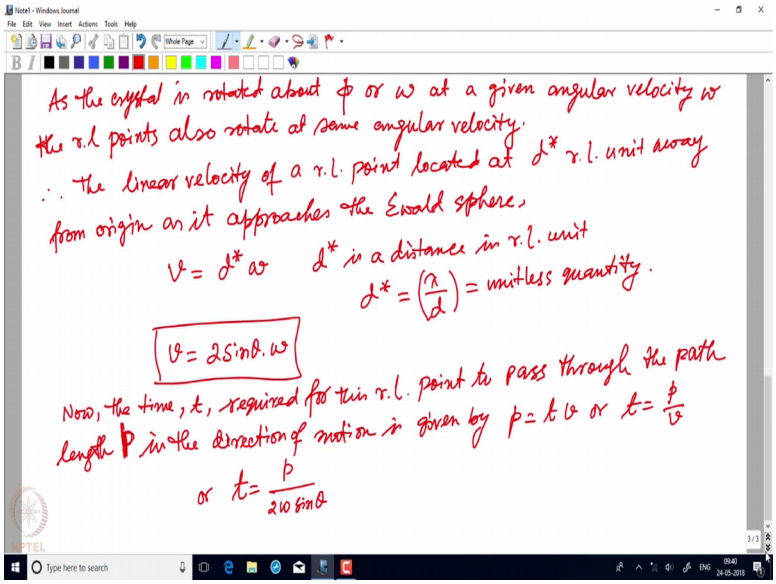

So, during a data collection a crystal is moved about phi or the crystal is moved about omega axis. So, when you are rotating it about phi, you are rotating the crystal at a given angular velocity or when you are moving the crystal in along phi omega, you are also moving it in even angular velocity. So, as the crystal is rotated about phi or omega at a given angular velocity omega. The reciprocal lattice points also rotate at same angular velocity.

So, the linear velocity of a reciprocal lattice point located at d star reciprocal lattice unit away from origin as it approaches the Ewald sphere, then we can write the linear velocity v is equal to d star omega. Remember d star is a distance in reciprocal lattice unit. So, here actually the d star means lambda by d. So, one can write this v is equal to 2 sin theta into omega following Braggs law. This lambda by d is an unitless quantity. So, now the time that is t required for this reciprocal lattice point to pass through the path length p in the direction of motion is given by p equal to this lower case p, this p equal to t v or t equal to p by v or t equal to p by 2 omega sin theta.

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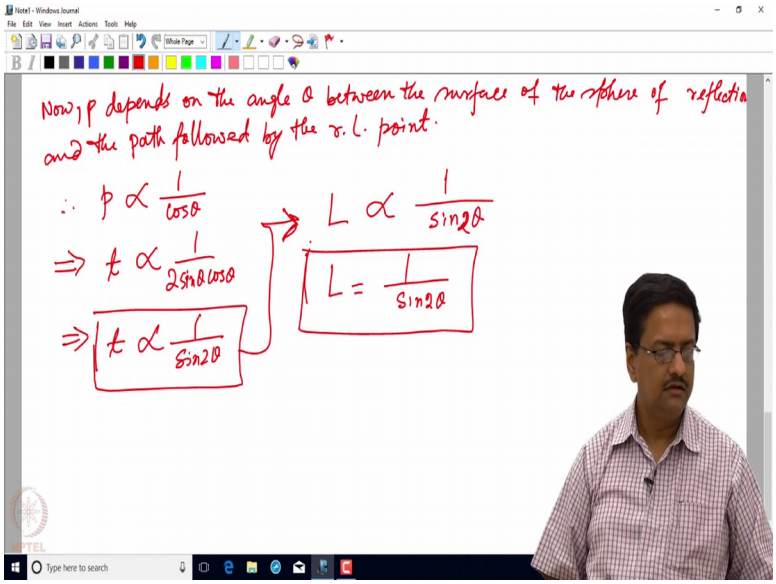

Now, this p depends on the angle theta between the surface of the sphere of reflection, and the path followed by the reciprocal lattice point. Therefore, it is easy to show that p is proportional to 1 by cos theta, which implies that t is proportional to 1 by 2 sin theta cos theta that means, t is proportional to 1 by sin 2 theta, so which means this t is the time taken for a reciprocal lattice point to pass through a given Ewald sphere.

And the Lorentz term is what these represented by this time t. So, eventually this t can be replaced by L. And we can write L is proportional to 1 by sin 2 theta. For all practical purposes this L is written as 1 by sin 2 theta. And this correction term is applied to the data that is collected. So, this is how the Lorentz correction is applied to all the reflections, by this to all the reciprocal lattice points that are responsible for corresponding X-ray diffraction in different directions.

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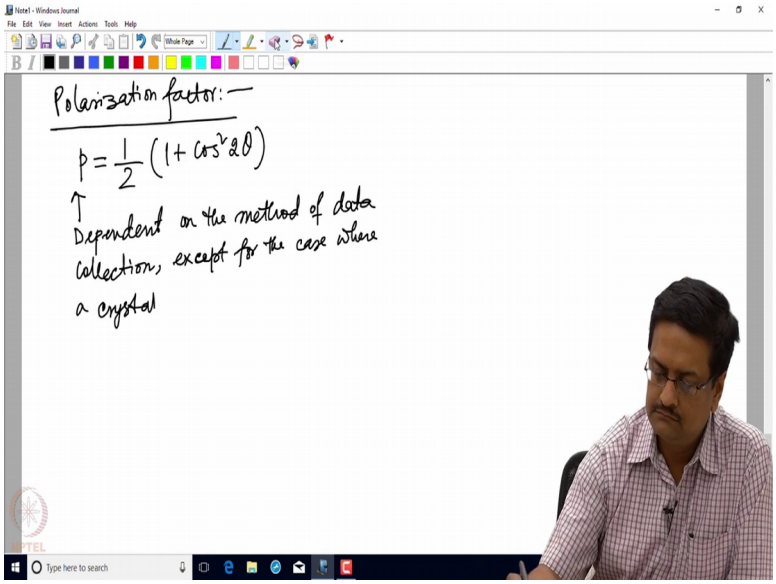

Now, let us try to understand the polarization term. The polarization factor p is written as 1 by 2 1 plus cos square 2 theta. This p is dependent on the method of data collection, except for the case where a crystal.

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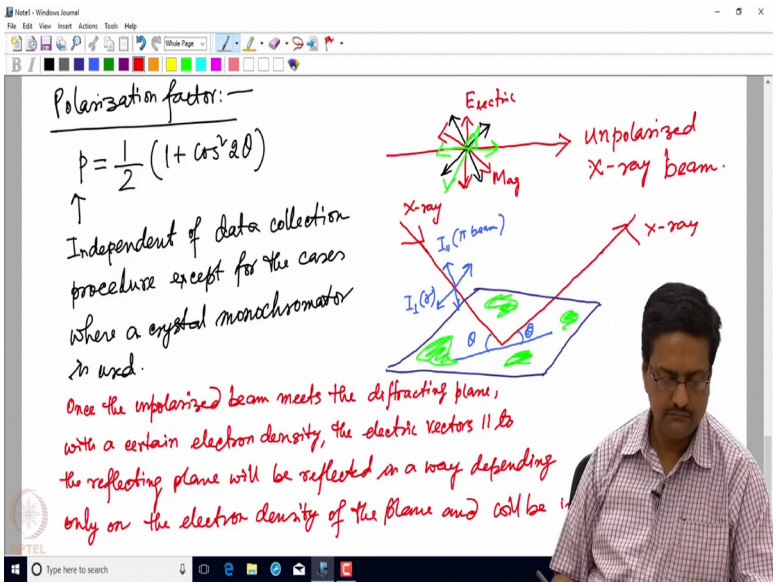

This polarization factor p is independent of data collection procedure except for the cases, where a crystal monochromator is used. This polarization factor p arises from the nature of incident beam, the polarization of the incident beam. A general incident beam, which is used for X-ray diffraction measurement is unpolarized in a sense that it will it is

electric vector and the magnetic vector are perpendicular to each other. And they are in all possible directions.

So, if the electric and magnetic vectors are perpendicular like this, it may be possible that electric vector and the corresponding perpendicular magnetic vector is like that. And if it is like this, the other one goes from this side to that side and so on. So, this these electric and magnetic vectors are all in all possible directions, and it is unpolarized. But then when this unpolarized X-ray beam is made to interact with a plane in crystal, the unpolarized beam falls and gets reflected from a plane in a crystal.

So, in this is case if this is the angle of incidence and this is the angle of diffraction, the unpolarized beam the vectors can be classified as two ways. One beam, which is parallel to the plane of diffraction is written as I parallel or identified as a pi beam. And the 2nd beam the one which is perpendicular to I parallel is written as I perpendicular or the sigma beam. So, the one which is parallel to the plane of reflection, it interacts with the plane in a different way compared to the beam, which is I perpendicular that is the vector of electric and magnetic field.

So, due to all random orientation of these I parallel, and I perpendicular for the incident beam, the incident beam the sum of I parallel is same as I sum of I perpendicular in terms of intensity for the electric vector. But, then when it interacts with the plane, which has different electron density associated somewhere here and there, the way the I parallel interacts is different in a way that I perpendicular interacts.

So, what we observed is the following, once the unpolarized beam meets the diffracting plane with a certain electron density, the electric vectors parallel to the reflecting plane will be reflected in a way depending only on the electron density of the plane and will be independent of theta that is the angle of incidence.

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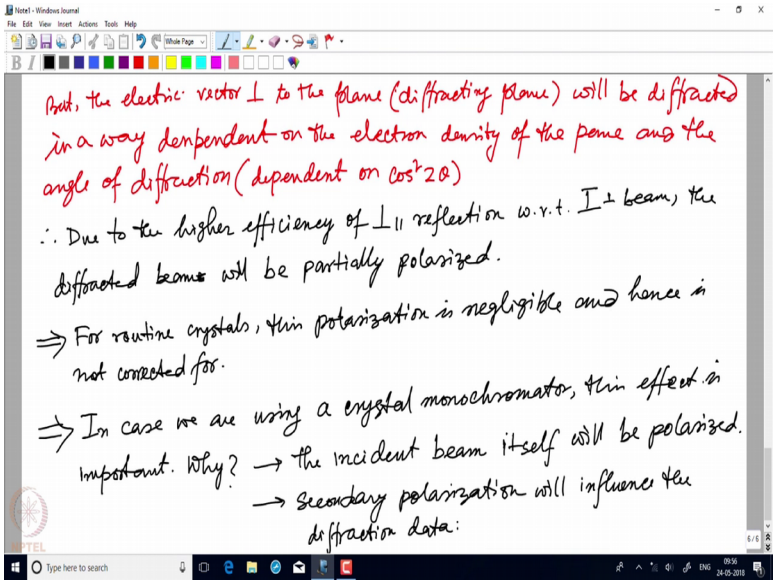

But, the electric vectors perpendicular to the plane that is the diffracting plane will be diffracted in a way dependent on the electron density of the plane of the plane and the angle of diffraction that is will be dependent on sin 2 theta dependent on cos square 2 theta. Therefore, due to the higher efficiency of I parallel reflections with respect to the I perpendicular beam, the diffracted beam will be partially polarized.

So, this partial polarization might cause problem in the X-ray diffracted intensity, and hence there should be a correction term. But, in general for routine crystals for regular in general for routine crystals, this polarization is negligible and hence is not corrected for. But, then if we are using a crystal monochromator, so in case we are using a crystal monochromator, which is like a germanium crystal with it is 1 1 1 plane expose, and we try to generate copper K alpha 1 radiation. So, in case of that kind of experiment where you generate you use a monochromatic X-ray. So, in case of usage of crystal monochromator, this effect is important why, because the incident beam itself will be polarized. And hence secondary polarization will takes place; secondary polarization will influence the diffraction data.

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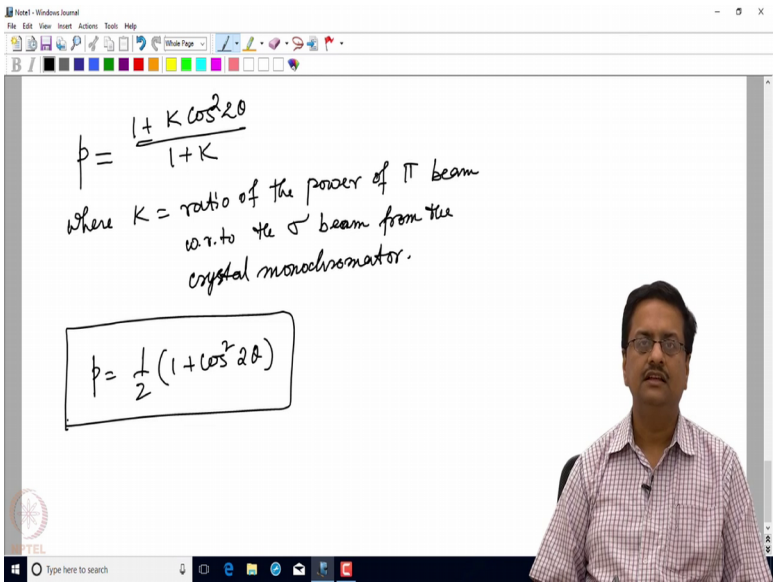

So, that is why in case of diffractometers, where we use a crystal monochromator and appropriate polarization correction is applied, and it is written it is used as 1 plus K cos square 2 theta divided by 1 plus K, where K is the ratio of the power of pi beam with respect to the sigma beam from the crystal monochromator. When crystal monochromator is not used, we write K equal to 1, so it becomes equal to p into equal to half of 1 plus cos square 2 theta.

So, in this lecture, we have discussed about the two important corrections, which are applied are called Lorentz and polarisation terms. And we have tried to express these terms in some mathematical expressions. And these are used during the data reduction process from a routine data that is collected using any type of diffractometer or any type of detector. So, in the next class, we will learn about the scaling and temperature factors that are incorporated in data reduction.