Solid State Chemistry
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Lecture – 38
X-ray diffraction, Bragg's law, reciprocal lattice

Now, I will go to the 3rd lecture of week 8 and in this lecture we will put to use our understanding of a miller indices and a distance between lattice planes in order to explain X-ray diffraction ok. So; and so I will introduce X-ray diffraction. So, how you can relate the X-ray diffraction to the miller indices and the distance between planes, and then also look at try to talk a little bit about the reciprocal lattice ok. So, week 8, lecture 3 will be X-ray diffraction Bragg's law and reciprocal lattice.

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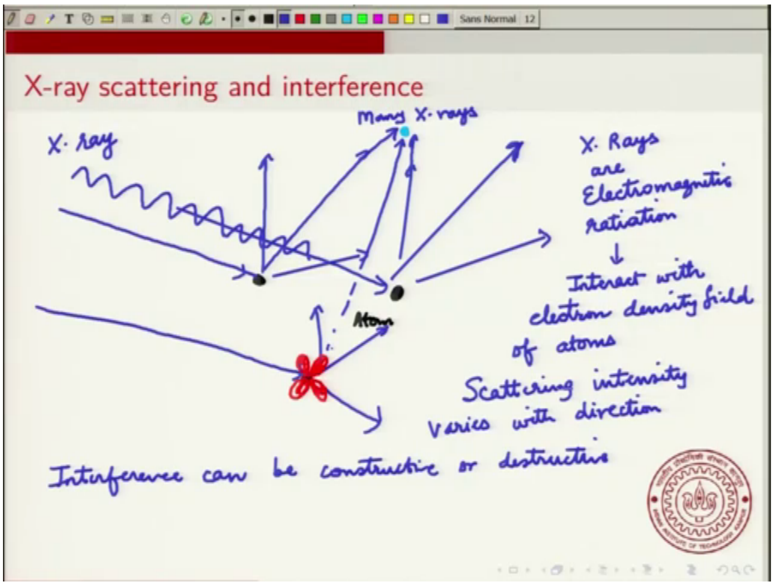

So, let us talk in general about X- ray scattering and interference ok. Now, I will later on describe in detail how X-rays are generated, but for now let me just mention that X-ray is some ray; of some wavelength and this is your X-ray and it is travelling in some direction ok. So, this is my X-ray it is some beam; X-ray is some beam of electromagnetic radiation that is travelling in some direction. And now, what is interesting things happen when it interacts with atoms when it interacts with atoms ok. So, this is an atom, it basically interacts with the electrons in the atom and then it gets scattered in some direction ok.

Now, typically it will get scattered in several directions, but there is a scattering intensity which says that in certain directions so, scattering will be the largest. So, now, if there are several atoms; if there are several atoms then each of them will scatter X-rays ok. So, each of them will scatter X-rays and actually I should emphasize that they are act they are also scattered in other directions ok.

They are not only scattered in one direction they are scattered in several directions and X-rays are electromagnetic radiations that interact with the electron density of atoms. So, I will just emphasize this part that X-rays are electromagnetic radiation and they interact with electron density field of atoms and what we mean by electron density field is really the spatially varying electron density.

So, whatever the structure of these electron density is around an atom, it c is going to interact with that. So, if you have a d orbital it will have some structure, some electron density, some spatially varying electron density and this X-ray is going to interact with that. So, whatever the electron density is around the atom it will interact with that ok. And it gets scattered in all directions ok, but the scattering intensity is typically larger in certain directions than others ok. So, the scattering intensity varies with direction.

Now so, what we see is that, now if you look at; if you look at some faraway point, let us say you look at this point ok. Now, this point is getting X-rays that are scattered by different atoms. So, it is getting an X-ray; let us say it is getting an X- ray scattered by this atom by this atom maybe there is some X-ray that is being scattered by this atom that is also interfering. So, there are lot of X-rays coming due to scattering from different atoms at any point. So, so many X-rays and so the question is there constructive or destructive interference and so there is interference of all these waves and interference can be constructive or destructive ok.

So, basically at every point you will see a different pattern of X-rays ok. So, this is a basic idea of X-ray scattering and interference and now, what we are going to see is how the underlying structure of the, how the underlying. So; obviously, whether it is constructive or destructive depends on depends on how the atoms are spaced with respect to each other ok. It depends on the relative distance and the relative positions of the atoms ok.

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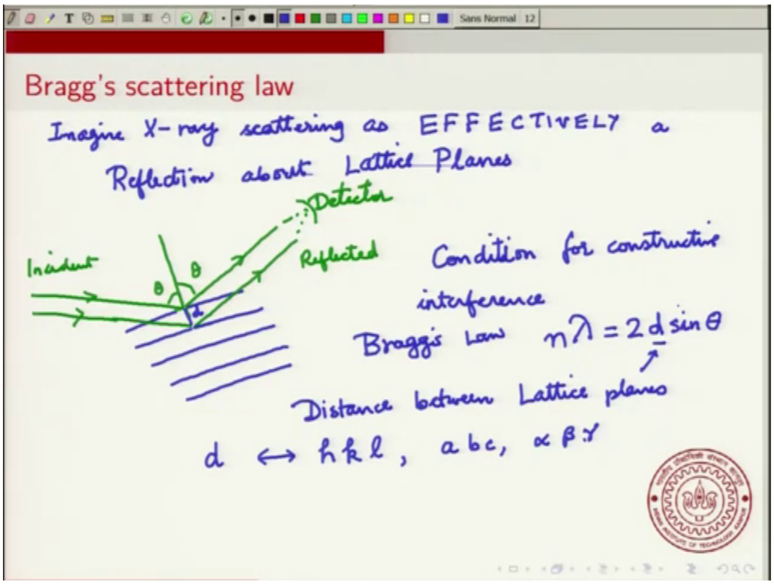

So now let us look at Bragg's scattering law, which is actually a hugely simplified version it is a very simple result and what that says is that, this scattering of X-rays by all atoms can be imagined in the following way. So, what it says is that we can imagine X-ray scattering as effectively a reflection about lattice planes.

So, what the idea is that, you can take this picture of X-ray scattering and think of it as effectively as a reflection about lattice planes ok. Now; obviously, you do not really have reflections I mean, what you have is a fairly; you can see that scattering is fairly complicated process and scattering is of individual atoms not of planes; however, you can look at X-ray scattering ok so, the at least as far as the interference process is concerned, you can look at, you can imagine X-ray scattering effectively as a reflection about lattice planes.

So, what this allows you to do is to look at look at this family of lattice planes. And now, imagine that that if you have an incident; if you have an incident X-ray beam let me use a different colour; if you had an incident X- ray beam ok. Now you can imagine that, this will be reflected of this ok. So therefore, the if this angle is theta then it will be reflected in such a way that this angle is also theta.

And now, these are lattice planes and you can imagine so Bragg's scattering law can be derived using this picture that X–rays; that these are X-rays are actually getting reflected of lattice planes and so, if you take another parallel X-ray beam. So, these two are the incident beams and these other reflected beams and what the idea is that, there is going to be some interference here if you put a detector here ok. Then you have to see whether these two beams interfere constructively or destructively at the detector ok. And the condition for constructive interference is given by Bragg's law, which is given by n lambda equal to 2 d sin theta ok. This is the very well known Bragg's law which I am sure all of you have seen before.

What is important to emphasize is that, you know actually the interaction of X-rays with atoms is much more complicated than simple reflection of planes, but effectively if you do the entire calculation, if you do the entire scattering theory ok, it is actually a fairly complicated quantum mechanical theory. The result that you get is just the same as this simple Bragg's scattering law ok. And I will not be doing this, I will not be trying to derive this, but what is interesting is that this quantity d that appears is the distance between lattice planes.

So, we see immediately that, this distance between lattice planes that we calculated in the last lecture is something that appears in Bragg's scattering law ok. Now, what is this distance between lattice planes; ? so, we know how to relate d is related to kl, abc, alpha beta gamma. So, if you if you know abc, alpha beta gamma and h k l you can calculate the distance between lattice planes ok. So, this is the basic idea of X-ray diffraction, that you have an incident beam, you have a reflected beam and you can calculate; you can calculate the condition for constructive interference.

And it is only when there is constructive interference you will see a maximum at the detector and in that case you will have this Bragg's condition ok. We will discuss this in more detail as we go on, but I just wanted to introduce the Bragg's scattering law ok.

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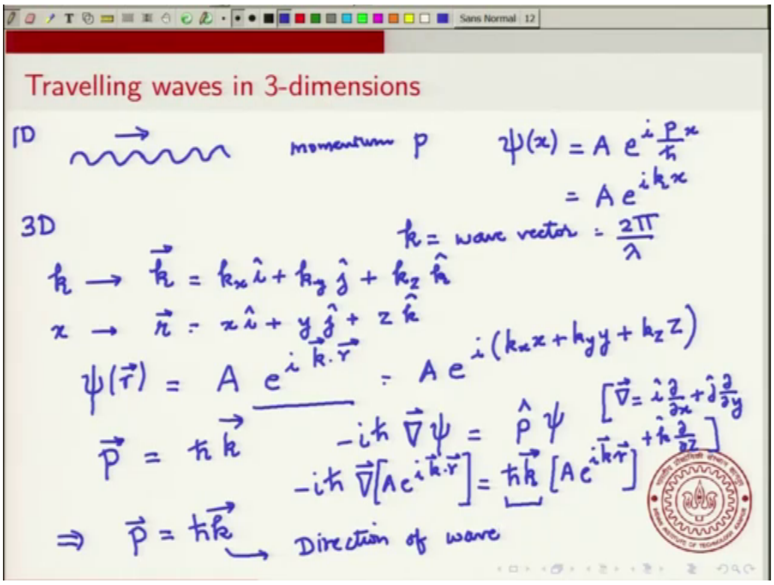

Now, a slightly different way to look at X-ray diffraction is to do the following ok. If you have a travelling wave; if you have a traveling wave in one dimension, this is travelling in this direction.

So, it is a wave that keeps moving with time ok. Now so, this wave has a momentum; it has a momentum of k and if it has a momentum P, then you can write its wave function; so, the wave function for a travelling wave in one dimension so this is 1D ok. So, psi of x you can write as I will just put A constant and I can write e to the i P by h cross x. This is a wave that is travelling with momentum of P in the x direction ok. So, this is a travelling wave in one dimension.

Now, if you had in 3D, before I go to 3D this quantity P by h cross is written as its written as wave vector i k x. So, k equal to wave vector this is again related to the de Broglie hypothesis that you know, chorus wave has a momentum P and P by h cross will be what is called a wave vector. Wave vector is basically you can think of it as 2 pi by lambda, lambda is a wavelength ok. Now, what happens in 3D? In 3D you have k, goes to k vector this is k x i plus k y j plus k z k.

So now k becomes a vector and now instead of x you have r which is x i plus yj plus zk ok so, instead of x you have r and now your wave function psi is a function of r ok. So, that this is a travelling wave in 3 dimensions and this is given by some constant times e to the i k dot r. So, it is a k dot r that is that is same as A e to the i times k x x plus k y y plus k z z ok.

So, this is the travelling wave in three dimensions and this is an equation of a travelling wave in three dimensions and this is, I have not explicitly put time ok, but you know that, you can calculate the momentum the momentum will be equal to h cross k you can work it out ok. Momentum you can work it out by using minus i h cross dou psi dou psi by or gradient of psi cross k k bit. So, minus i h cross gradient of psi ok so if psi has this form minus i h cross gradient of psi. Now, this is equal to the operator; quantum mechanical operator for the momentum operator on psi ok.

And this will be you can show by if you put this particular form of the wave function, you can show that minus i h cross now gradient, gradient if for those who are not familiar with gradient, I will just put the expression for the gradient operator. Gradient is equal to i times dou by dou x plus j times dou by dou y plus k times dou by dou z ok.

So, that is a gradient operator, it is a three dimensional version of the derivative operator ok. So, if you take this gradient and operate it on this particular on psi of r ok. So, if I take a gradient of A e to the i k dot r you can show it, again it is fairly elementary, but I will not do it in detail you can show that this is exactly equal to h cross k vector times A e to the i k dot r ok. So, what that implies? This implies that the momentum the eigenvalue of momentum is equal to h cross k ok.

So, you see that this constant that is multiplying the wave function is nothing, but the eigenvalue and that is equal to the momentum. So, the momentum eigenvalue is equal to h cross k for a travelling wave in three dimensions and this is again seen in elementary books in co in quantum mechanics ok. So, the point is that this sort of expression e to the i dot r represents a travelling wave in three dimensions, it is a wave that is travelling along the direction of k because it has momentum of h cross k it is travelling along.

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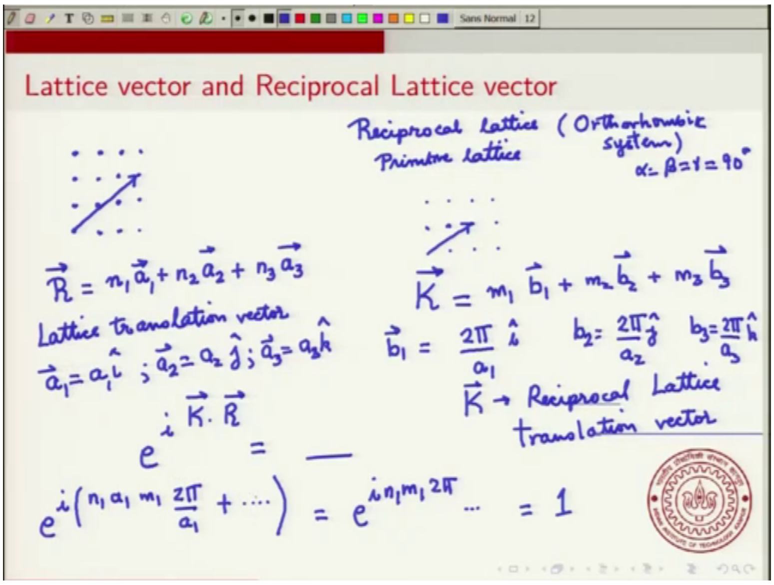

So, k gives the direction of wave and now this will actually be fairly useful to analyze the Bragg's scattering. Now, before we do; I do that I just want to introduce a concept of a reciprocal lattice vector ok. Now, to do this we will start with the following way. So, if we have a lattice then let me start with a key ok. And we take some arbitrary vector R from one lattice point to another

We can write this as; let me write it as n 1 a plus n 2 b ok. So, you can you can write it in this form ok. So, this is called a lattice translation vector. Now, we define a reciprocal lattice.; so, we define something called a reciprocal lattice and for now let me consider that we consider orthorhombic system. Again for simplicity we will just consider the orthorhombic system and so in other words alpha equal to beta equal to gamma equal to 90 degrees.

So now imagine a lattice, and let me also consider a primitive lattice ok; for now I will consider a primitive lattice. So, initially I will start with orthorhombic system and a primitive lattice. And now, you imagine a lattice which is given by translation vectors so, I will just; I think I want to change my notation a little bit instead of calling it abc, I will call it a 1 a 2 and a 3 ok.

So, I am just changing the notation into a from abc into a 1 a 2 a 3 and this is I am just calling my lattice translation vectors as a 1 a 2 and a 3 instead of abc, because I want to use the b for the reciprocal lattice. So, the reciprocal lattice is given a general translation vector in this reciprocal lattice is given by m 1 into m 3 into b 3 where b 1 in this particular case equal to 2 pi by a 1; a 1 is a magnitude of a 1, into i hat b 2 is equal to 2 pi by a 2 into j hat and b 3 equal to 2 pi by a 3 into k hat.

So, I am just doing this I will explain, why this is useful and just to emphasize again a 1 is equal to a i or a 1 i, a 2 is equal to a 2 j and a 3 is equal to a 3 k ok. So, the a 3 without the vector sign represents the magnitude of a 3, similarly a 2 without the vector sign represents the magnitude of a 2 and a 1 without the vector sign represents the magnitude of a 1.

So, these are the reciprocal lattice lattice vectors ok. So, this is a general translation in the reciprocal lattice and what you can see is that if I take e to the i K dot R. So, if I take e to the i K dot R ok. So, this looks like a travelling wave only thing I have taken K to be a reciprocal lattice translation vector and R to be a lattice translation vector. So, this is a; so, K is a reciprocal lattice translation vector and we will see what happens when you do this.

So, e to the i K dot R ok so, equal to what ok; so, equal to what is this equal to ? So, let us take e to the i K dot R. So, we see that e to the i; now K has m 1, m 1 m 2 m 3 are integers just as n 1 n 2 and n 3 are integers, they can be anything from minus infinity to plus infinity, but they have to be integers ok. So, m 1 into b 1; b 1 is 2 pi by a 1 into i into a and you take K dot R then you have to take m 1 b 1 into n 1 a 1.

And again, using a 1 as a 1 i and substituting this for b 1, what you will get is a following. You will get e to the i so, K dot R will have the first you will have n 1 a 1 m 1 and for b 1 I will put 2 pi by a 1 and you have two other terms I will not bother about it.

So, let us just look at this first term. So, this is e to the i and n 1 into m 1 is a constant a 1 will cancel and so we just have n 1 m 1 into 2 pi and whenever you have an integer n into m is an integer. So, this is just equal to 1, even you have other terms and any e to the i 2 pi into n integer is just 1 ok. So, the product of; so, this term will just give one and similarly the y and z terms will also give one.

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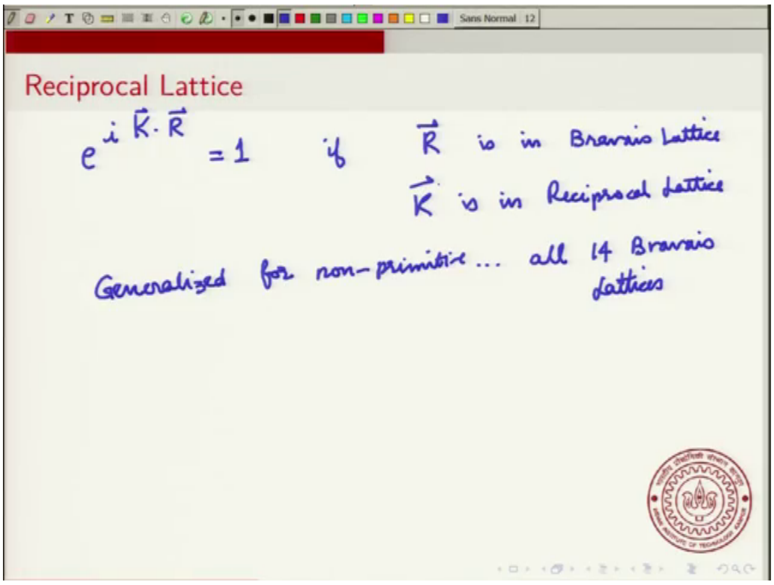

So, that is the property of this reciprocal lattice translation vector that e to the i K dot R equal to 1, 1 if R is in Bravais lattice and K is in reciprocal lattice ok.

Now, I took this for the case ok so, this can be generalized for non primitive basically all 14 Bravais lattices ok. So, just as you have a Bravais lattice. So, for each of the 14 Bravais lattices you have a reciprocal lattice which right now is just another lattice with some different parameters and this actually turns out to be very important in the in both in X-ray diffraction and in the band theory of solids ok.

So, I will conclude this 3rd lecture of week eight here, in the next lecture we look at more details of X-ray diffraction.

Thank you.