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Lecture – 34 Scattering of X-rays from crystals Part-I

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Diffraction of waves by Crystals
-> Direct imaging of an atomic lattice.
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In our earlier lecture, we had seen we had discussed about crystals, and how to describe crystals of a solid which is a periodic arrangement of atoms inside the solid. And we had covered what are the tools required to understand this crystal, namely making a Bravais lattice which is a collection of geometrical points which are corresponding to the crystal. There is no unique choice, but there is a way to make the Bravais lattice. And you can make a Bravais lattice plus bases which are the atoms you will put at each point on the Bravais lattice. And then we describe the primitive lattice, cell and what are the different types of crystal symmetries which are present, and what are the important types of crystals which are present and different materials fall within these different crystal systems which can be described by these different crystal systems.

We came across the concept of a unit cell plus a number of lattice points per unit cell; it can be different from the primitive cell. So, these are the concepts and tools. The toolbox was given to you to actually study and analyze crystal structures. However, how does one know also that there are crystals inside I mean there is a periodic arrangement of atoms inside the solid, how does one even experimentally come to know about that, and that is going to be the topic of our lectures in the subsequent section of lectures is how does one actually analyze the crystal structure when there are beams which are diffracting through the crystal, and how does the periodic arrangement of atoms effect those beams which are passing through the crystal.

So, this brings us to the topic of diffraction of waves by crystals. These waves can be electromagnetic waves, these can be waves corresponding to quantum particles like neutron, you can send a beam of neutrons on a crystal which has a periodic arrangement of atoms. And how would this beam of neutrons emerged, it could be a collimated beam of electrons, and the waves which are associated with that collimated beam of electrons, how they diffract through the crystal, these are the topics that we will sort of buildup upon and try to understand that in the context of this present lecture. And this will help us to get information of the atomic lattice which is present inside the crystal and so, how does one directly emerged atomic lattice, it is basically through the diffraction of waves through the crystal.

And this topic actually started off in 1895 by the discovery of William Rontegen who discovered X-rays. So, basically he had a tube, and there is from one end of the tube there are electrons which are generated which are accelerated and they hit another target which could be tungsten. When the electron beam which is accelerated between the anode and cathode strikes the target, it causes excitation in the electrons in a shell electrons of the atoms in the target which then de excite and produce characteristic X-rays. And from here begins to generate X-rays.

So, this was a very important discovery this generation of X-rays which happened in 1895. And ultimately in 1913 Bragg was able to explain an interesting observation of how X-rays behave when they reflect of a crystal at particular angle. So, you have X-rays which are reflecting of a crystal surface and the reflected intensity of that X-ray has got some particular behaviour depending on the angle of incidence. At some angle of incidences is it was found that you have a lot of reflection ok, whereas at other angles you do not have a reflection and that was related to the crystal structure of the lattice which was explained by Bragg in 1913. So, in 1895 X-rays was discovered which was then apply to study X-ray crystals and there was an important discovery by 1913 which

reveal the atomic nature of the crystals and that there is a periodic arrangement of atoms inside the crystal..

Now, how does one actually understand this phenomena of electromagnetic waves which are interacting with the lattice or with the periodic arrangement of atoms inside the crystal?

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To understand that let us again look at something which you already know from optics and that is the phenomena of diffraction of light by gratings. So, what is a grating, this is like a material in which you have made periodic slits which are periodically spaced, and there is an incoming plane wave which is incident this is the plane wave of light, this is the plane wave front of light which is incident on the diffraction grating. So, this is your diffraction grating. And what will you observe on the screen. So, on the screen which is here this is your screen. So, this is your grating; this is your wave front; and this is your screen. What will you observe on the screen, you will observe maximas which are spaced out.

So, at this point, you will get a central maxima, you will get the first order maxima. On this side, you will also get a first order maxima on this side. This is also a first order maxima. So, when the incoming wave front falls on the diffraction grating, the light gets scattered. And the light from which is getting scattered from different slits actually interfere and give rise to these maximas. You get maximas which are present, this is the central maxima; and there are first order maxima and higher order maximas as you go along.

So, the phenomena of diffraction leads to this periodic brightening of light which you get. And this is the phenomenon of diffraction. It occurs because of the periodic spacing of these slits or grating in your path of incoming light. And if the wavelength of light is of the order of the spacing of the slits, then you observe this sort of a diffraction pattern which is coming basically because of the interference of the scattered light. And depending on the path difference you will get this sort of maximas and minimas.

What is important to note out here is that you will observe this only if the wavelength of light is of the order of these spacing of these slits, the spacing of these splits which are periodically spaced if the wavelength of the light is of the order of spacing of the slits, then you will get this sort of a diffraction pattern. For visible light, your wavelengths could be few thousands of angstroms ok, as a result the spacings between the split slits can be pretty large of this order.

So, what people thought was that all right, you can have this slits which are periodically spaced and they give rise to this diffraction pattern. One can also think of a solid, people are already suspected that the solid has periodic arrangement of atoms even before they saw it; they had actually suspected that crystalline solid can have a periodic arrangement of atoms inside it, and this periodic set of atoms which are present inside a solid.



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So, for a crystalline solid, there is a periodic set of atoms which are present inside the solid. And for a incoming wave front, for a wave front which is incoming, for a plane wave which is incoming and falls on these atoms, each of these atoms will give rise to spherical wave fronts, each of these atoms will start emitting spherical wave fronts. And as a result they will start scattering light from this spherical wave fronts, there will be scattering of light. And just as before in the optical case, if I have a screen then I should observe a diffraction pattern, I should observe a diffraction pattern.

So, just in the optical case if you have light which falls on this diffraction grating you will have a diffraction pattern. For a crystalline solid, you have this periodic arrangement of atoms which are placed inside the crystal. And each of these atoms can act like a source of scattered light, they will generate this spherical wave fronts. The light will get scattered in all directions, and then again they will interfere and you will get a diffraction pattern. So, you should typically observe a diffraction pattern, but what is the requirement to observe such a diffraction pattern, the wavelength of light should be of the order of the spacing between atoms in the crystal. And this spacing between atoms in the crystal is very small ok. It is of the order of 1 to 10 angstroms; it is it is it is within that range ok. And so you need wavelengths which are in that range ok, and these wavelengths are the wavelengths which satisfies this are your X-rays.

So, therefore, discovery of X-rays was very crucial and critical for getting to the point at which you can start detecting the diffraction from an atomic solid, because you need wavelengths which are typically of the lattice constant, if a is the lattice constant of your crystal namely the spacing between lattice points in your crystal, then the wavelength has to be of the order of a only then you will get a diffraction pattern which is coming from this crystal. Ordinary optical light has ordinary visible light, the visible light has wavelengths which of far larger than your lattice constant. So, they will just average over the entire large number of points. So, in a wavelength will average over many such lattice constants and you will not observe anything.

But if you have a wavelength which is coming from an X-ray which is really a small wavelength it is of the order of lambda, then you will observe diffraction pattern. And this was sort of felt and this was suspected that this could happen and so people started exploring how to diffract X-rays from a crystal.

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And so the experiment which was done was that, you have your tube which generates Xrays ok. You have your cathode and you have your anode. This is your cathode. It is generating X-rays. Your electrons are striking you have a high voltage which is applied between this, it accelerates electrons to high velocity, and then they produce X-rays. These are the X-rays which are generated. These X-rays are passed through a collimator, so that you get a collimated parallel beam of X-rays. So, these are the X-rays which are coming. And then from here you get a parallel beam of X-rays which power falls on a crystal.

So, this collimated beam of X-rays falls on the crystal which is made up of periodic spacing of atoms, and then you have a screen placed behind it. This is a screen which is place behind it which will capture the diffraction pattern once the X-rays get diffracted and emerged from this, they will go and strike the screen and generate a diffraction pattern. So, on the screen, you will observe a diffraction pattern. And you will see a distribution of spots, diffraction spots distributed in a particular way around the central maxima.

So, there is a central maxima which is along the direction of the incoming X-rays, and there is first order maximas and higher order maximas which you can see distributed around the central maxima. And this was the diffraction of X-rays by crystals which began the way to explore the crystal structure ok. So, this is called as the lava pattern ok.

However, apart from this and equivalent thing was also seen namely if you take a crystal and you shine a beam of X-rays on it at some angle theta, and you look at the reflected beam of X-rays. So, this is the incident beam of X-rays. And you look at the reflected beam of X-rays, then this reflected beam of X-rays the intensity of the reflected beam is maximum for some specific angles.

And this phenomena, so at some specific angles as you vary the intensity of the incoming X-rays. So, the incoming X-rays falling and then getting reflected, you have a detective which is capturing the intensity of the reflected X-ray as you vary the intensity of the incoming X-ray. And you look at the intensity of the reflected X-ray for some particular angles of incidence; you will find that the intensity of the reflected X-ray becomes maximum.

And this interesting observation as I said was explained by Bragg in 1913 which lead to understanding the crystalline structure of the solid, and the law which he the Bragg's law which he discovered is a very important and a very useful law for understanding the nature of the crystal structure. So, next we go on to the topic of understanding how electromagnetic waves interact with a crystal, and then developing the understanding from there on which we will continue in the next lecture.