CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 41: X-Ray Diffraction: Bragg's Law

So, in this lecture we are going to start discussion on diffraction of X-rays from crystals. In the last lecture we looked at diffraction in which the grating that was used was a DVD and we had used a green laser as our source with a specific wavelength to show diffraction.

Now, in crystals it is a similar thing. Now, we have a three-dimensional grating in which each atom in a crystal is a scattering center. Now, but here we cannot use something that we use for the DVD like the green laser, because the wavelength of the green laser, or for that matter any visible light, is much more than the spacing between atoms.

For example, if I look at the following cubic crystals and we look at the lattice parameter a. Now let us take copper. Its lattice is FCC and the lattice parameter is 0.362 nanometers, or in another unit it could be written as 3.62 angstroms. Now, generally we will prefer to use the nanometer unit rather than the angstrom unit.

Diamond again is an FCC lattice and its lattice parameter is $0.357\ nm$. Consider silicon, again FCC, its lattice parameter is $0.343\ nm$. Consider iron, which is a body-centered cubic crystal, we have $0.294\ nm$. Finally, if I look at molybdenum, which is BCC, the lattice parameter is $0.315\ nm$.

So, in each case the lattice parameter, and therefore the spacing between atoms, is much smaller than the wavelength of green laser. Now, for diffraction to occur, the beam that is being used has to be of a similar order of magnitude. The wavelength of that beam should be of similar order of magnitude as the spacing between atoms, and that is why we use X-rays.

Now, typically the wavelength of X-rays λ varies between $0.1\,nm$, or one can write 1 angstrom, to about $1\,nm$, that is about 10 angstroms. So, you can very clearly see that X-rays are going to have the right wavelength to be able to get diffraction from a crystal.

Now, just before we start talking about X-ray diffraction, let me say a little bit about production of X-rays. How are X-rays produced? Well, essentially we bombard a target metal. So, this is a metal target. We bombard this metal target with high-energy electrons, and that results in the production of X-rays.

Now, what is the mechanism behind it? Well, first of all, when the electrons hit the metal target, there will be a rapid deceleration of the electrons and their energy will get converted into various radiations, and a big chunk of that radiation would be in the X-ray wavelength range. So, rapid deceleration produces X-rays.

For instance, if this metal target was molybdenum, and if I look at what kind of spectrum I will get when I target electrons onto the molybdenum target, we might get something like this. On the horizontal axis we have wavelength in angstroms, say 1 angstrom, 2 angstroms, 3 angstroms, and on the vertical axis we have the intensity of X-rays that are produced. At an accelerating voltage of $20\,kV$, we might get a spectrum like this.

Now, if I increase the accelerating potential to $25\,kV$, then we get some interesting effects. When the potential is increased from $20\,kV$ to $25\,kV$, we start getting what is called characteristic radiation, and these characteristic radiations have very specific wavelengths which are signatures of the target metal that we are using.

Now, what is this characteristic radiation? Let us look at it. Let us say this is the nucleus of an atom, then we have the K shell, the L shell, and the M shell. Now, suppose an incoming electron collides with an electron in the K shell and ejects it out. This takes the atom into a higher energy state, and it can recover back by an electron jumping from the L shell to the K shell. As a result, radiation is emitted which is characteristic radiation.

It could also happen that an electron from the M shell jumps into the vacant site in the K shell, and that will also result in characteristic radiation. So, an electron jumping from the M shell to the K shell produces what is called K_β radiation, and jumping from the L shell to the K shell produces what is called K_α radiation.

If I go back to the spectrum, this is K_β and this one is K_α. Normally, we use the K_α characteristic radiation when we want to do experiments with monochromatic X-rays, which means X-rays of a specific wavelength.

So, how do we get a specific wavelength? We use filters. Filters are used to filter out what is called white radiation. So, white radiation is filtered out and only the characteristic radiation is left. This can be used for conducting X-ray diffraction experiments. There are also techniques in which we need the white radiation, and then we will use it as is, but I will not get into the theory of filters in this course since it is beyond the scope of this course.

So, we will assume that either we have white radiation or we have characteristic radiation, and we can work with these to do X-ray diffraction experiments.

Now, we will get into the theory of X-ray diffraction starting with scattering of X-rays from atoms. Now, I have a crystal where atoms are at specific locations, and when an incoming X-ray beam hits the crystal, the X-ray photons hit individual atoms, and as a result each atom scatters X-rays in all directions, in a kind of spherical manner.

So, each atom scatters X-rays in different directions. The intensity may vary depending on the direction, but all atoms scatter X-rays in this manner. So, we can say that atoms scatter X-rays in all directions in three-dimensional space.

Now, using these ideas, let us come to the famous Bragg equation, also referred to as Bragg's law. Imagine we have atomic planes and an incident beam of X-rays. The beam gets scattered by atoms on one plane, and similarly atoms on the next plane also scatter X-rays.

We consider two rays, ray 1 and ray 2, scattered from two successive atomic planes, and we consider a detector at point Q. We choose a direction such that the scattered beam makes an angle θ with the atomic planes, which is equal to the angle of incidence. This looks like reflection, but it is not reflection. It is a scattering process.

We want to find out whether the waves arriving at point Q interfere constructively or destructively. We drop perpendiculars to find the extra distance travelled by ray 2 compared to ray 1. The path difference δ between the two rays is given by the sum of the two segments.

$$\delta = BD + BC$$

If the interplanar spacing is d, then from geometry we can show that each segment is equal to $dsin\theta$. Therefore, the total path difference is

$$\delta = 2dsin\theta$$

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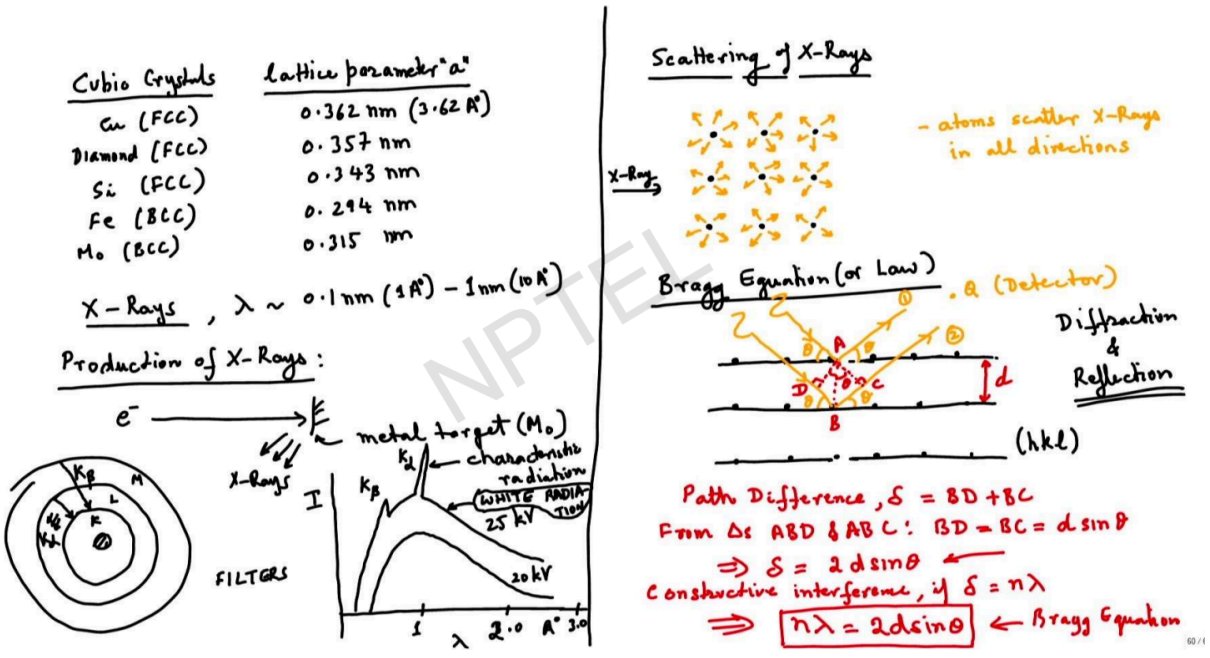

From the previous lecture, we know that constructive interference occurs when the path difference is an integral multiple of the wavelength. Therefore, replacing δ by $n\lambda$, we get

$$n\lambda = 2dsin\theta$$

This is the Bragg equation. Here n is called the order of reflection and can take values $1, 2, 3,$ and so on. When $n = 1$, it is first-order diffraction, when $n = 2$, it is second-order diffraction, and so on.

The terms diffraction and reflection are often used interchangeably because of the geometry, even though physically it is a scattering process and not reflection.

Now, for convenience, we can eliminate n by writing

$$\lambda = 2\frac{d}{n}sin\theta$$

The term $\frac{d}{n}$ corresponds to the interplanar spacing of the (nh, nk, nl) planes if d is the interplanar spacing of the (hkl) planes. This idea was discussed in earlier lectures.

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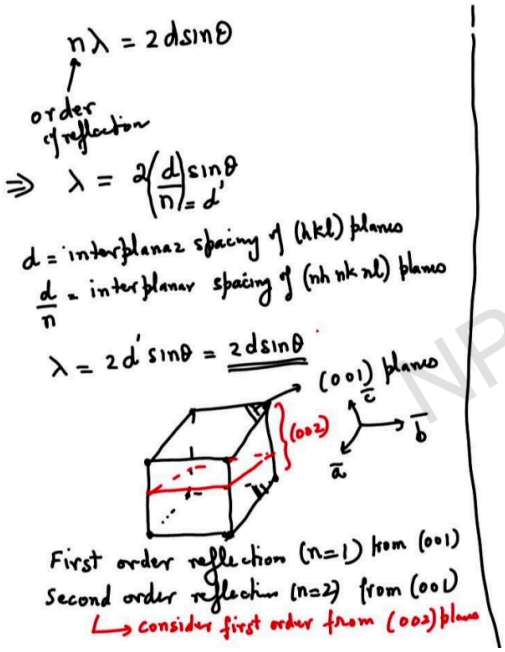

Therefore, we can simply write the Bragg equation as

$$\lambda = 2d'sin\theta = 2dsin\theta$$

and consider everything as first-order diffraction.

For example, if we consider diffraction from (001) planes and look at second-order diffraction, it is equivalent to first-order diffraction from (002) planes. Even though (002) planes may not contain atoms, this is done purely for mathematical convenience.

So, with this I conclude this lecture, and in the next lecture we will look at scattering in more detail and discuss how X-ray intensities depend on atomic distribution and motifs in crystals.