**X-ray diffraction (XRD)**

**Slide 1:** X-ray diffraction methods are the most effective methods for determining the crystal structure of materials. In this short lecture I will first explain the basic fundamentals of XRD, then show some applications of this method, before finishing it off with elaborating more about a specific example of a XRD-lab. The specific example is the XRD-lab in Oslo which is a place I have personally visited.

**Slide 2:** Within XRD, you have two different methods: spectroscopic and photographic. The first one is widely used, while the second is not. So we will only focus on the first one!

With regards to the theory of XRD, it is important to mention that the biggest aspect of this is something called Braggs law. X-rays are electromagnetic waves at the size of about 0.1nm, meaning much smaller than visible light. An important part of Braggs law is the theory of interference. You need constructive interference, which basically is two waves adding to each other, for a diffracted beam to leave the crystal plane with the same scattering angle as incident angle. In the figure two beams are deflected by the plane. These two beams won’t be in phase (meaning constructive) unless Braggs law is fulfilled.

In the actual law, d represents the atomic spacing; meaning the distance between atoms in the crystal lattice. n = an integer or “order of reflection”, ʎ is the incident wavelength and theta is the angle of incidence.

**Slide 3:** If we have constructive interference detected, and a known wavelength and angle of incidence we could find the atomic spacing. This also gives us the opportunity to find the crystal structure of the material. We have the Miller indices h, k, l and the lattice parameter a (which is the constant distance between components of the lattice).

**Slide 4:** I will now go further into the applications of the method XRD. First of all I worked on a project that decided whether a component was heusler-material or half-heusler material. A heusler material has ferromagnetic properties despite neither of the materials involved being magnetic. Ferromagnetism = magnetism to metals like iron. You basically follow the formula XYZ or X2YZ where X = electropositive transition metal like Ti, Y = transition metal like Co and Z = main group elements like Sn. The functionality is basically like this: you shoot x-rays at a powder-form of the sample and measure it by a detector. When shooting in the incident x-rays you have to make sure that all the planes are covered. From this you get a distance, a. After this you compare with known values. 6.06 Å gives a half-heusler with properties similar to a semiconductor and 6.36 Å gives a heusler gives a conductor-material.

**Slide 5:** An another application is the use of XRD in pharmaceutical industry. X-ray diffraction can be used to characterize the composition of the pharmaceutical. There is a certain process that all companies have to go through that involves XRD. First step is to isolate the active drug, then use XRD on power-form of drug to look at the crystal structure. Then you send that into a commission and secure a patent before manufacturing the drug.

**Slide 6:** This last part is about my trip to the XRD-lab in Oslo. It is affiliated with the University in Oslo and is according to the employees there the foremost XRD-lab in all of Norway. The lab has one crystal XRD instrument (the APEX) and several powder XRD instruments. Picture 1is of the APEX. With the APEX you have an instrument that does not involve destroying the material into powder-shape. It can give the unit cell dimension, bond-bond length and gives the crystal structure through a process called crystal refinement.

The other XRD instruments are high temperature powder diffraction instruments like D500, transmission powder XRD like DIFF1 (both pictured). Other instruments are: DIFF2 for surface diffraction, DIFF3 and the Huber which uses high and low temperature transmission powder.

Any question?