Learning Objectives

- Explain X-rays.
- Interpret the symbols used in the Bragg equation.

Like light, X-rays are electromagnetic radiation with very short wavelengths. Thus, X-ray photons have high energy, and they penetrate opaque material, but are absorbed by materials containing heavy elements.

---

**X-ray Diffraction**

When light passes through a series of equal-spaced pinholes, it gives rise to a pattern due to wave interference, and such a phenomenon is known as diffraction. X-rays have wavelengths comparable to the interatomic distances of crystals, and the interference patterns are developed by crystals when a beam of X-rays passes a crystal or a sample of crystal powder. The phenomena are known as **diffraction of X-rays by crystals**. More theory is given in Introduction to X-ray Diffraction.

X-ray diffraction, discovered by von Laue in 1912, is a well established technique for material analysis. This link is the home page of Lambda Research, which provide various services using X-ray diffractions. For example:

- Residual Stress Measurement
- Qualitative Phase Analysis
- Quantitative Phase Analysis
- Precise Lattice Parameter Determination

In 1913, the father and son team of W.H. Bragg and W.L. Bragg gave the equation for the interpretation of X-ray diffraction, and this is known as the Bragg equation.

$$2d \sin \theta = n \lambda$$

where $d$ is the distance between crystallographic planes, $\theta$ is half the angle of diffraction, $n$ is an integer, and $\lambda$ is the wavelength of the X-ray. A set of planes gives several diffraction beams; each is known as the $n$th order.

Example 1

The X-ray wavelength from a copper X-ray is 154.2 pm. If the inter-planar distance from $\text{NaCl}$ is 286 pm, what is the angle $\theta$?

**Solution**

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

$$\sin \theta = \frac{154}{2 \times 282}$$

$$\theta = 0.273$$
Example 2

An X-ray of unknown wavelength is used. If the inter-planar distance from $\text{NaCl}$ is 286 pm, and the angle $\theta$ is found to be 7.23°, what is $\lambda$?

Solution

\[
\begin{align*}
\lambda &= 2 \times d \times \sin(\theta) \\
&= 2 \times 282 \times \sin(7.23^\circ) \\
&= 71 \text{ pm}
\end{align*}
\]

Example 3

The X-ray of wavelength 71 pm is used. If the inter-planar distance from $\text{KI}$ is 353 pm, what is the angle $\theta$ for the second order diffracted beam?

Solution

The calculation is shown below:

\[
\begin{align*}
\sin \theta &= \frac{\lambda}{2d} \\
&= \frac{71}{2 \times 353} \\
&= 0.100 \\
\theta &= 5.8^\circ
\end{align*}
\]

These examples illustrate some example of the applications of X-ray diffraction for the study of solids.

Questions

1. Hint: 30 degrees

2. If the wavelength is 150 pm and the interplanar distance $d$ is 300 pm, what is the angle $\theta$ in the Bragg equation, for $n = 2$?

   Hint: 30 degrees

3. Hint: $\text{NaCl}$

Discussion -

The larger the interplanar distance $d$, the smaller the angle.
Contributors and Attributions

- Chung (Peter) Chieh (Professor Emeritus, Chemistry @ University of Waterloo)