

CHEM 3420: Physical Chemistry II — Spring 2009

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Lecture 34: Diffraction and Bragg's Law

References

1. Levine, *Physical Chemistry*, Chapter 23
2. Solid state handout
3. Slides distributed in class

Key Concepts

- We can probe various structure types and states of order using diffraction of x-rays, neutrons, and/or electrons.
- Diffraction is a cooperative scattering phenomena that occurs when the incident radiation wavelength is on the order of the spacing between objects (in this case atoms).
- The periodic arrangement of atoms in a crystal leads to diffraction which can be quantified a complex analysis of scattering physics. However, this analysis becomes cumbersome in 3D, so the simpler and elegant Bragg's Law is usually employed:

$$\lambda = 2d_{hkl} \sin \theta_{hkl}$$

where d_{hkl} is the spacing between planes with indices hkl and θ_{hkl} is the angle at which one should observe diffracted radiation from plane (hkl) .

- For a cubic crystal, $[hkl] \perp (hkl)$ so we can write the following relationship between the inter-planar spacing and the lattice constant, a :

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Combining this with Bragg's Law:

$$\frac{\lambda^2}{4a^2} = \frac{\sin^2 \theta}{h^2 + k^2 + l^2}$$

- By using these relations we can see that in a diffraction pattern, cubic crystals would have a single peak of intensity at one angle due to diffraction from $\{100\}$ since $d_{100} = d_{010} = d_{001} = a$. Tetragonal would have two peaks one from $(100)/(010)$ and the other from (001) ($d_{100} = d_{010} = a$ and $d_{001} = c$).