

CHEM 3420: Physical Chemistry II — Spring 2009

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Lecture 35: Systematic absences

References

1. Levine, *Physical Chemistry*, Chapter 23
2. Solid state handout

Key Concepts

- Primitive cells will show all reflections due to only one lattice point per unit cell. However, multiple cells (ex: BCC, FCC) will have systematic absences due to the extra lattice points in the unit cell.
- The systematic absences are quantified through the structure factor, F_{hkl} defined as follows:

$$F_{hkl} = \sum_{cell} f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

where f_n is the atomic scattering factor of atom n and (u_n, v_n, w_n) are the coordinates of each atom in the unit cell. For example, a BCC structure might have one atom at 0,0,0 and another at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

- The atomic scattering factor, f_n quantifies the “effectiveness” of an atoms x-ray scattering. It is a function of the chemical identity of an atom (primarily the number of electrons) and the scattering angle θ . At diffraction angles of $\theta = 0$ the number of electrons equals f_n , but the atomic scattering factor decreases as θ gets larger.
- The intensity of a diffracted beam is proportional to F^2 .
- Calculation of the structure factor for specific crystal structure leads some common systematic absences:

Primitive Cubic	BCC	FCC
All reflections allowed	$h + k + l = \text{even}, F \neq 0$ $h + k + l = \text{odd}, F = 0$	h, k, l all even or all odd, $F \neq 0$ h, k, l mixed even and odd, $F = 0$