

CHEM 3420: Physical Chemistry II — Spring 2009

April 13, 2009

Lecture 32: Describing crystal structures

References

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

Key Concepts

- Body centered cubic (BCC)
 - One lattice point on each corner of a cube, one lattice point in the center of the cube.
 - If we place one at each lattice point, the atoms would touch along a body diagonal of length $\sqrt{3}a$.
- Face centered cubic (FCC)
 - One lattice point on each corner of a cube, one lattice point at the center of each face.
 - There are four lattice points per FCC unit cell.
 - If we place one at each lattice point, the atoms would touch along a face diagonal of length $\sqrt{2}a$.
- We developed a systematic way of talking about crystals and their associated geometry:
 1. Atom locations: points are references as fractions of lattice constants. For example the atom position $\frac{a}{2}, \frac{a}{2}, \frac{a}{2}$ is written: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.
 2. Directions are treated just like vectors:
 - (a) pick an origin
 - (b) end of the vector coordinates treated like atom locations, i.e. written as fractions of cell edges.
 - (c) Specific directions are enclosed in square brackets [] and a family of equivalent directions in angle brackets $\langle \rangle$.

For a hexagonal crystal we need an additional indices for the direction due to the symmetry. We want equivalent directions to have equivalent indices. (See the lecture slides of the mathematical relationship).

3. Planes of atoms: are very important for structure determination and for understanding properties.
 - (a) Find the axial intercepts of the plane (may be negative)
 - (b) Take the reciprocal
 - (c) Clear common factors

A specific plane is enclosed in () while a family of equivalent planes uses { }