

CHEM 3420: Physical Chemistry II — Spring 2009

April 10, 2009

Lecture 31: 2-D and 3-D lattices

### References

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

### Key Concepts

- A lattice is defined as an array of points with translational symmetry. In three dimensions, this consists of 3 non-colinear translation of arbitrary length. These translations will reproduce the entire structure.
- Each lattice point is not necessarily one atom. Multiple atoms can be associated with each lattice point.
- We defined a primitive unit cell as the simplest unit that will reproduce the entire structure using the defined translations. A primitive unit cell only contains one lattice point per cell.
- In certain situations it may be advantageous to define a multiple cell that contains more than one lattice point per cell. For example, in two dimensions a centered rectangular cell has two lattice points per cell.
- In three dimensions there are 14 Bravais lattice types, some are primitive while others are multiple cells. (See figure in the Lecture Slides)
- In order to generate real structures, additional symmetry elements are combined with the different Bravais lattice types to produce the 230 space groups. The additional elements include 1,2,3,4, and 6-fold rotation, reflection, and inversion.
- The length of the sides of a unit cell are called lattice constants or lattice parameters. For a cubic structure, there is only a single lattice constant,  $a$  (since  $a = b = c$ ). For a tetragonal unit cell,  $a = b \neq c$  and for orthorhombic  $a \neq b \neq c$ .
- 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  $\sqrt{2}a$ .