Physics 489 S 04 Lecture 4
Crystal Lattices and Classification (Ashcroft and Mermin, chapter 4)
Also information from chapter 7

1. A Crystal is an ordered state of matter
   Qualitatively different from liquids/gases
   Change from liquid to crystal is a true phase transition
   Paradigm for other ordered states (like magnetism)

2. Crystal = Lattice * Basis (convolution)
   Lattice defines the laws of repetition - set of ideal points
   Basis is the contents of each unit or cell:, real atoms or electron density etc.

   Translational symmetry defines the lattice.
   Point symmetry is the symmetry of the basis - rotation, reflection, inversion
   Crystal symmetry (Space group) combines translation and point symmetries - distinguishes one crystal system from another.
   1-D and 2-D examples

3. Bravais Lattice (1845)
   14 possible ways to make (3D) space translationally invariant.
   Elements of the translation group.
   Infinite array of discrete points in space: crystal appears exactly the same if translated by the vector to any of the points
   (a) 1D: $R = n_1 a_1$
   (b) 2D $R = n_1 a_1 + n_2 a_2$ with a_1, a_2 non-colinear
   (b) 3D: $R = n_1 a_1 + n_2 a_2 + n_3 a_3$ with a_1, a_2, a_3 non-coplanar.

4. Primitive unit cell.
   Volume of space which, when translated by all possible R's, fills space completely with no overlap. Not unique choice.
   In 3D: Cell volume $= a_1 \cdot (a_2 \times a_3)$.
   Wigner-Seitz cell - most compact cell - unique

5. Close-packing of spheres.
   One way (triangular lattice) in 2D
   Infinite number of ways to stack in 3d.
   Simplest are HCP (2 layers AB) and FCC (3 layers ABC).
   FCC is a Bravais lattice
   HCP is not a Bravais lattice, but hexagonal lattice with 2 atom basis.

6. Crystal structures of elements.

SC	Po
FCC	Xe, Kr..., Al, Cu, Ni, Ca, Ag, Au, Pt, Pb.
BCC	Na, K..., Fe, Cr, Cr, Mo, W, Nb
HCP	Be, Cd, Mg, Er, Gd, Ho...
ABAC	La

7. Important lattices with basis
   CsCl, NaCl, Diamond, Zincblende (ZnS) and Graphite.
   Materials of recent interest:
   High Temperature Superconductors, e.g., $YBa_2Cu_3O_7$
   Another superconductor discovered recently, MgB_2

8. Finite number of possible crystal classes
   Example of 2-D Bravais lattices - 5 possible types
   Proof in 2-D that only 60,90,120,180 degree rotations are possible - e.g., 5-fold rotations impossible in a crystal

9. Enumeration of 14 Bravais lattices in 3-D. (See Chapt 7)
   Cubic (3) simple (SC), body-centered (BCC) and face-centered (FCC).
   Tetragonal (2) simple and centered.
   Orthorhombic (4) simple, body-centered, base-centered and face-centered.
   Monoclinic (2) simple and centered.
   Triclinic (1)
   Rhombohedral or trigonal (1)
   Hexagonal (1).