MatSci 193/203 – Atomic Arrangements in Solids

Autumn 2012

Instructor: Prof. Evan Reed
Durand 133
evanreed@stanford.edu

Time/room: MWF 10:00-10:50am, Cummings 2
M 2:15-5:00pm, 260-113

Note: The Monday afternoon session is for group problem-solving with real-time help from the CA. Attendance is optional but *strongly encouraged.*

Texts: This course will draw from multiple sources, including:

1. "Crystallography and Crystal Defects," Kelly and Knowles. (Available electronically through Stanford Libraries.)
2. "The Basics of Crystallography and Diffraction," C. Hammond (3rd edition, 2010).
3. "Structure of Materials," M. de Graef and M. E. McHenry, (2007).

You may find that Ref. 1 is sufficient for your needs, but you may also find that Ref. 2 and or Ref. 3 are useful for some portions of the class.

Tentative syllabus:

1. Structures and bonding in materials:
    a. Metallic structures
        i. FCC
        ii. BCC
        iii. HCP
        iv. Interstitial sites
        v. Ordered alloys and superlattices
    b. Semiconductors
        i. Diamond cubic
        ii. Zinc blende
        iii. Wurtzite
        iv. Amorphous structures
    c. Carbon structures and monolayer materials
    d. Ionic structures
        i. CsCl
        ii. NaCl
        iii. ZnS
        iv. NiAs
        v. CaF_2

        vi. $CaTiO_3$
        vii. SiO_2
        viii. Ice
        ix. Ionic radius ratio
    e. Energy models
        i. Lennard-Jones and structure prediction
        ii. Ionic models
        iii. Density functional theory
    f. Themodynamics of crystals
        i. High pressure; Enthalpy
        ii. Lattice vibrations; Helmholtz energy
2. Crystal symmetry
    a. Unit cells and lattice
    b. Miller and Miller-Bravais indices
    c. Weiss zone law
    d. Reciprocal lattice
    e. 2D and 3D point groups
    f. 2D space groups
3. Macroscopic consequences of symmetry
    a. Tensor transformations
    b. Optical, piezoelectric, and transport properties