Solid State Physics: Problem Set #1

Cohesion in Solids and Crystal Structure

Due: Friday Jan. 17 by 5pm

Reading assignment: for Monday, 1.1-1.4 (cohesion in solids)
for Wednesday, 2.1-2.2 (crystal lattices)
for Friday, 2.4 (the reciprocal lattice)

Additional reading: Chapter 1 from Kittel

Problem assignment:

Chapter 2 Problems: *1 Hard sphere crystals - packing density and geometry
5 Tetragonal lattices - why no end or face-centered form?

A1. The density of iron at 20ºC is 7.874 g/cm^3. Look up the crystal structure formed by iron at this temperature and calculate both the volume and side length of the cubic unit cell and the nearest neighbor separation for this crystal.

A2. The potential energy of a pair of atoms in a certain ionic crystal is of the form $U(R)=B/R^9-A/R$, when their separation is R. Given that the equilibrium separation is R_o=0.280 nm and the dissociation energy is 5.00 eV, determine the constants A and B. Use Maple to plot $U(R)/|U(R_o)|$ vs. R/R_o. [Answer: B=6.6x10^{-6} eV·nm^9, A=1.58 eV·nm]

A3. Use the Lennard-Jones potential, $U_{ij} = 4\varepsilon\left[\frac{\sigma^{12}}{R_{ij}^{12}} - \frac{\sigma^{6}}{R_{ij}^{6}}\right]$ where ε and σ are constants, to calculate the ratio of the cohesive energies of neon in the bcc and fcc structures. The required lattice sums are

bcc: $\sum_j R_{ij}^{-12} = 9.114\,R^{-12}$ $\sum_j R_{ij}^{-6} = 12.253\,R^{-6}$

fcc: $\sum_j R_{ij}^{-12} = 12.132\,R^{-12}$ $\sum_j R_{ij}^{-6} = 14.454\,R^{-6}$

where R is the nearest neighbor distance for the given lattice. Note that you must compute the equilibrium separation R_o for each lattice. [Answer: 0.957]

*To be presented in class on Friday ... one part per person.