MATERIALS PHYSICS II FALL 2006 HOMEWORK PROBLEMS 2

Return to Michael by Wednesday 27.10.2006 at noon

1. *Periodic potential in one dimension and the Kronig-Penney model, AM problem 8.1. See also Elliott problem 5.11.* (**6 points!**)

2. *A simple model for a monovalent close-packed FCC metal.* Assume that *all* the valence electron density of the metal (1 electron per atom) is uniformly distributed inside close-packed (touching) spheres, centered at fcc lattice sites. Let the radius of the spheres be R.
(a) Show that the electrostatic energy (electron-ion and electron-electron energy) of the electron in one sphere with a positive ion (charge $+e$) at the center, is given by

$$U_{es} = -\frac{9e^2}{40\pi\epsilon_0 R}.$$

(b) Show that the quantum mechanical kinetic energy of (free) electrons inside the sphere is

$$U_{kin} = \frac{3\hbar^2(9\pi/4)^{2/3}}{10mR^2}.$$

(c) The total energy per sphere (atom) in this model is then $U_T = U_{es} + U_{kin}$. Find the equilibrium distance between the nearest-neighbour atoms, R_{eq}, and the optimal total energy (= cohesive energy per atom), $U_T(R_{eq})$. Evaluate R_{eq} and $U_T(R_{eq})$ in Ångstroms and electron volts, respectively, and compare to experimental nearest-neighbour distances and cohesive energies of typical (monovalent) fcc-metals, like Cu, Ag and Au. (Cu: 3.61 Å and 3.49 eV; Ag: 4.09 Å and 2.95 eV ; Au: 4.08 Å and 3.81 eV) (**4 points**)