FYSM300 FINAL EXAM 29.11.2013

Each problem gives 6 points. Time limit 4h.

1. Explain shortly
a) crystal structure
b) van der Waals interaction
c) What is the meaning of enthalpy ΔH and entropy ΔS in the energetics of lattice defects? (Gibbs free energy can be written as $\Delta G = \Delta H + T\Delta S$.)
d) sp^3-hybrid
e) chemical potential μ
f) depletion layer

2. BCC-lattice can be described by primitive vectors $\mathbf{a_1} = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$, $\mathbf{a_2} = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$ and $\mathbf{a_3} = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$, where a is a lattice parameter.
a) Determine the coordination number and the nearest neighbour distance for the lattice.
b) Determine, draw and identify the reciprocal space lattice and the corresponding reciprocal space lattice parameter.
c) Calculate packing fraction $\eta = \frac{V_{\text{sphere}}}{V_{\text{unit cell}}}$ for the whole 3-dimensional lattice and also for the (111) 2-dimensional surface of the same lattice, $\eta = \frac{A_{\text{disk}}}{A_{\text{unit cell}}}$. A_{disk} describes the area of the disks and V_{sphere} the volume of the spheres in the unit cell.
d) Sketch the first two Brillouin zones for a simple square lattice in 2-dimensions.

3. Define the equation of motion for a periodic 1D monoatomic chain with atom mass m. Assume only the nearest neighbour harmonic interactions described by a spring constant K. Solve the dispersion relation from the equation motion and sketch the solution in the first Brillouin zone. Based on the solution you got, how is the velocity of sound (group velocity) behaving at the first Brillioun zone and how the spring constant affects the velocity?

4. Explain the temperature dependence of electrical conductivity in:
a) metals (3 p)
b) intrinsic and extrinsic semiconductors (3 p)

5. a) Show that the tight-binding (LCAO) wavefunction

$$\Phi_{ki} = N^{-1/2} \sum_n e^{i\vec{k}.\vec{R}_n} \phi_i(\vec{r} - \vec{R}_n) \tag{1}$$

satisfies Bloch's theorem, and that the normalization constant is $N^{-1/2}$, where N is the number of atoms in the crystal.(3 p)
b) Obtain expressions for the three sp^2-hybrids resulting from the combination of an s-orbital with a p$_x$ and a p$_y$ orbital. Show that hybrids lie in the $x - y$ plane, with a subtended angle of 120°. (3 p)

$$\exp(ix) = \cos(x) + i\sin(x) \qquad a + ar + ar^2 + ar^3 + ... = \frac{a}{1-r}$$