Condensed Matter Physics I
Final written test
academic year 2011/2012
June 20, 2012

(*Time: 3 hours*)

NOTE: Give all the steps necessary to understand in detail the solution procedure. Answers with the final result only or with insufficient details will not be considered valid.

Exercise 1: *Copper*

Copper has a mass density $\rho = 8.95$ g/cm^3, and electrical resistivity $1.55\times10^{-}8$ ohm-m at room temperature. Assuming valid the Sommerfeld model, calculate:

1. The concentration of the conduction electrons
2. The mean relaxation time τ
3. The Fermi energy E_F, the Fermi velocity v_F and wave vector k_F.
4. The mean free path ℓ_F at the Fermi level.
5. Using the free-electron model you obtained in (c) the Fermi wave vector k_F. Consider now the effects of the periodicity of the crystalline structure. Knowing that Cu crystallizes in a fcc lattice, indicate whether the Fermi sphere is contained or not within the first Brillouin zone.
6. Suppose that some atoms in Cu crystal are replaced by Zn atoms. Taking into account that Zn is bivalent, while Cu is monovalent, calculate the atomic ratio of Zn to Cu in ZnCu alloy (brass) at which the Fermi surface touches the first Brillouin zone faces. (Use again the free-electron model to estimate the electron concentration.)

Exercise 2: *Crystalline structures*

Consider the 2D lattice in the figure, constituted by 3 different atomic species A, B and C, occupying sites of a triangular lattice.

Which of the following constitute a correct set of primitive lattice vectors? (i) $a_1 = u\hat{x}, a_2 = v\hat{y}$.
(ii) $a_1 = 2u\hat{x}, a_2 = v\hat{y}$.
(iii) $a_1 = u\hat{x}, a_2 = 2v\hat{y}$.
(iv) $a_1 = u\hat{x}, a_2 = u\hat{x} + v\hat{y}$.

How many atoms of each kind are there per primitive cell?

Find the primitive reciprocal lattice vectors, and sketch the Brillouin zone, showing the primitive reciprocal lattice vectors on your sketch.

Exercise 3: *Tight binding*

For a simple cubic structure (lattice parameter a) the energy expression in the tight-binding approximation is

$$\epsilon(\mathbf{k}) = \epsilon_0 - \alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$$

where α and γ are overlap integrals typical of the TB approximation.

1. Expand the energy $\epsilon(\mathbf{k})$ near the bottom of the band (i.e., near the Γ point, $\mathbf{k}$=0) where $ka \ll 1$ to the second order in k (k=$|\mathbf{k}|$). You may define for simplicity $\epsilon_\Gamma = \epsilon_0 - \alpha - 6\gamma$ and $m_e^* = \hbar^2 \left(\frac{\delta^2 \epsilon}{\delta k^2}\right)^{-1}$ (effective mass of the electron) and use ϵ_Γ and m_e^* in the expression of the energy.
2. Expand $\epsilon(\mathbf{k})$ near the zone boundary at the W point ($k_x = k_y = k_z = \pi/a$) in terms of $\delta k = |\delta \mathbf{k}|$, $\delta k \ll 1$, where $k_i = \pi/a - \delta k_i$, $i = x, y, z$. Also in this case give the result using ϵ_Γ and m_e^*.
3. Sketch $\epsilon(\mathbf{k})$ along the symmetry line ΓW in the above tight-binding approximation and for free electrons, considering for the latters: $\epsilon_{free}(\mathbf{k}) = \epsilon_\Gamma + E_0(k)$ and $E_0(k) = \hbar^2 k^2/(2m_e)$. Let $\gamma = (1/6)$ eV and $m_e^* = 1.1 m_e$.