# Electrons in crystals Final written test academic year 2008/2009 January 26, 2009

(Time: 3 hours)

Exercise 1: Drude and Sommerfeld model of free electron gas

Copper has a mass density  $\rho = 8.95 \text{ g/cm}^{-3}$ , and electrical resistivity  $1.56 \cdot 10^{-8} \text{ ohm} \cdot \text{m}$  at room temperature. Assuming that the effective mass of electron in Cu  $m^* = m_0$ ,  $(m_0 \text{ is the free electron mass})$  calculate:

- 1. The concentration of the conduction electrons and the mean relaxation time  $\tau$
- 2. The Fermi energy  $E_F$  and the Fermi velocity  $v_F$
- 3. The mean free path  $\ell_F$  at the Fermi level  $l_F$

#### **Exercise 2**: Bravais lattices with basis and structure factors

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

|   | В |   | С |   | А |   | В |   | С |   |
|---|---|---|---|---|---|---|---|---|---|---|
| С |   | A |   | В |   | С |   | A |   | В |
|   | В |   | С |   | A |   | В |   | С |   |
| С |   | A |   | В |   | С |   | A |   | В |
|   | В |   | С |   | A |   | В |   | С |   |

- 1. Describe and sketch the primitive cell, write the formula unit  $(A_n B_m C_\ell \text{ with } m, n, \ell = ...?)$ , a possible choice of the primitive translation vectors  $\{\mathbf{a}_i\}$  and the basis vectors  $\{\mathbf{d}_i\}$ .
- 2. Write the primitive translation vectors of the reciprocal lattice  $\{\mathbf{b}_i\}$ .
- 3. Assuming that the atomic form factors are  $f_A$ ,  $f_B$  and  $f_C$ , calculate the geometrical structure factor  $S(\mathbf{K})$  on the reciprocal lattice vectors, and specify the conditions that need to be satisfied to have interference maxima in case of  $f_A = f_B = f_C$ .

#### Exercise 3: Electrons in 2d: Fermi surfaces, weak potential

- 1. Consider a two-dimensional metal with rectangular Bravais lattice with basis vectors  $\mathbf{a_1} = (a,0)$  and  $\mathbf{a_2} = (0,b)$ , with a=2Å and b=2a. Give the basis vectors  $\mathbf{b_1}$  and  $\mathbf{b_2}$  of the reciprocal lattice (using  $cm^{-1}$ ) and sketch the first Brillouin zone.
- 2. Consider free electrons, give the general expression of the Fermi "sphere" (or better, "circle", in 2d) as a function of the electron density; then, calculate explicitly the numerical value of its radius in the present case, considering one electron per unit cell.
- 3. Draw such free-electron Fermi "sphere" in the same  $(k_x, k_y)$  plot of the first Brillouin zone, showing and specifying whether it is totally within the first Brillouin zone or not. If not, make a sketch concerning *where* and *how* it would be modified by the presence of a weak periodic potential, and a sketch of a possible second band within the first Brillouin zone.

### Exercise 4: Tight-binding model

Consider s-type electrons in a 1D lattice with lattice spacing a. Use a tight binding model with first and second neighbor hopping and no overlap. With reference to the definition  $\gamma(\mathbf{R})$  in the texbook, consider:  $\gamma(\mathbf{R}_{NN})=t$  where  $\mathbf{R}_{NN}$  is between two nearest beighbors,  $\gamma(\mathbf{R}_{NNN})=t'$  where  $\mathbf{R}_{NNN}$  is between two next- nearest beighbors, otherwise  $\gamma(\mathbf{R})=0$ .

1. Show that the explicit expression for the energy band (using  $E_s - \beta \equiv E_0$  (see again the textbook for the definition of  $\beta$ ) is:

$$E(k) = E_0 - 2[t \cos(ka) + t' \cos(2ka)]$$

- 2. Consider t' = -t and make a plot in the first Brillouin zone, identifying and writing the maxima and minima points.
- 3. Calculate the effective mass in those points.

## 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.
- When required, numerical evaluations should be given exactly with 3 significant figures, if not otherwise indicated.