PHYS40352 Solid State Physics Examples 2

1. Over a limited range of composition, an alloy of copper (valence 1) with silicon (valence 4) adopts the BCC structure. Assuming that the free-electron Fermi sphere would fit inside the first Brillouin zone, just touching the zone boundaries, show (as in lectures) that the electron density

$$n = \frac{k_F^3}{3\pi^2} \simeq \frac{1}{3\pi^2}\left\{\frac{\sqrt{2}\,\pi}{a}\right\}^3.$$

Hence show that the electron/atom ratio is approximately 1.48. Calculate the proportions (atomic percentages) of copper and silicon in the alloy.

2. For *small* amounts of zinc, a zinc–copper alloy adopts the FCC structure. As the amount of zinc is increased, this structure (so-called α-brass) remains stable until the electron/atom ratio exceeds 1.38. This critical value of the electron/atom ratio agrees well with the value 1.36 at which the free electron Fermi sphere just touches the faces of the Brillouin zone that are closest to $\boldsymbol{k} = \boldsymbol{0}$. Verify the theoretical result 1.36 and calculate the proportions of copper and zinc (valence 2) in this case.

Note: The 8 shortest reciprocal lattice vectors of the FCC lattice are $(1\,1\,1) \times 2\pi/a$ and the vectors related to this by cubic symmetry. The zone faces closest to $\boldsymbol{k} = \boldsymbol{0}$ bisect these 8 reciprocal lattice vectors. The remaining zone faces (such as the one bisecting $(2\,0\,0) \times 2\pi/a$) are further from $\boldsymbol{k} = \boldsymbol{0}$.

3. Show that the volume of the Jones zone of the diamond structure is $16 \times (2\pi/a)^3$. From this, show that the Jones zone contains enough states to accommodate 32 electrons per cubic unit cell; i.e., 4 electrons per atom.

Reminder: The boundaries of the Jones zone bisect $(2\,2\,0) \times 2\pi/a$ and symmetry-related reciprocal lattice vectors. To simplify the calculation of the volume, regard it as a cube of side $4\pi/a$ with pyramids of height $2\pi/a$ and square bases of side $4\pi/a$ attached to each face of the cube. The volume of a pyramid is $\frac{1}{3} \times$ [basal area] $\times$ [height].

4. For a uniform electron gas with Fermi wave vector k_F, show that the radius of an "atomic sphere" containing Z electrons is

$$r_0 = (9\pi Z/4)^{1/3}/k_F.$$

Show that the total electrostatic energy of an atomic sphere containing an ion of charge $+Ze$ at its centre is

$$-\frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\frac{Z^2\alpha}{r_0} \qquad \text{with} \qquad \alpha = \tfrac{9}{5} = 1.8.$$

Method: Work out the energy change in adding a spherical shell of charge with radius r and thickness δr, and integrate to obtain the total energy.

Note that α is very close to the precise value $\alpha = 1.79$ for close-packed structures. The Wigner–Seitz unit cells for close-packed structures are electrically neutral and roughly spherical in shape; they interact weakly with each other, leading to the small deviation from $\alpha = 1.8$.

5. Near the conduction band minima of silicon, the surfaces of constant energy are ellipsoids of revolution with their long axes directed along the k_x, k_y and k_z axes. For example, near a CB minimum lying at $\boldsymbol{k}_0$ on the k_x axis,

$$E(\boldsymbol{k}) = \text{const.} + \frac{\hbar^2}{2}\left[\frac{\Delta {k_x}^2}{m_l} + \frac{\Delta {k_y}^2 + \Delta {k_z}^2}{m_t}\right],$$

where $\Delta\boldsymbol{k} = \boldsymbol{k} - \boldsymbol{k}_0$ is the "distance" from the minimum.

In a cyclotron resonance experiment on silicon, the applied magnetic field is in the x-direction and the frequency of the applied microwave field is 24 GHz. By considering the shapes of the electron orbits on the k_x, k_y and k_z ellipsoids, explain why only *two* electron resonance peaks are observed in the experiment.

Given that the resonances occur at $B = 0.1$ and 0.3 tesla, calculate the transverse and longitudinal effective masses m_t and m_l for electrons in silicon, expressing your results in terms of the free-electron mass m_0. [You can assume that $m_l > m_t$.]

6. Sketch the shape of cyclotron orbits (in $\boldsymbol{k}$-space) for electrons at the Fermi energy in

(a) the monovalent metal potassium, regarding the electrons as free, and

(b) a nearly-free electron divalent metal with the simple cubic structure.

In both cases, take the magnetic field to be in the positive z direction. Note that in case (b) there are *at least* three distinct orbits you can draw.

Given that the number density of electrons in potassium is $1.4 \times 10^{28}\,\mathrm{m}^{-3}$, calculate the radius of closed cyclotron orbits in $\boldsymbol{r}$-space when the magnetic field strength is 0.2 tesla.