LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Solid State Physics, F7006T

Examination date: 2016-03-15

The solutions are just suggestions. They may contain several alternative routes.

1. Cu has FCC (a=3.61Å) structure and hence are the primitive basis vectors: $a = \frac{a}{2}(1,1,0)$, $b = \frac{a}{2}(1,0,1)$ and $c = \frac{a}{2}(0,1,1)$. For BZ we have primitive basis vectors: $a^* = \frac{2\pi}{a}(-1,-1,1)$, $b^* = \frac{2\pi}{a}(-1,1,-1)$ and $c^* = \frac{2\pi}{a}(1,-1,-1)$.
   The BZ is a BCC structure $K_{BZ} = \frac{1}{2} \mid a^* \mid = \frac{\pi\sqrt{3}}{a} \approx 1.5073 \cdot 10^{10} m^{-1}$.
   $K_F = (3\pi^2 N)^{1/3} = (\frac{3\pi^2 4}{a^3})^{1/3} \approx 1.36036 \cdot 10^{10} m^{-1}$ and hence $\frac{K_F}{K_{BZ}} = \frac{(12\pi^2)^{1/3}}{\pi\sqrt{3}} \approx 0.90$. The Fermi sphere does not intercept the BZ and one can use the free electron model.

2. (a) Au has FCC structure, the primitive unit cell contains 1 atom and the cubic unit cell contains 4 atoms.
   Mo has BCC structure, the primitive unit cell contains 1 atom and the cubic unit cell contains 2 atoms.
   Si has FCC structure with a basis of two atoms at (0,0,0) and $\frac{a}{4}$(1,1,1), the primitive unit cell contains 2 atoms and the cubic unit cell contains 8 atoms.

   (b) See above

   (c) Nearest neighbour distance r_0 in Si is $\frac{a\sqrt{3}}{4}$, a=5.43Å gives $r_0 \approx 2.35$Å. Next nearest distance is $\frac{a}{\sqrt{2}} \approx 3.84$Å.

3. $C_v = C_v^{el} + C_v^{ph}$. As the temperature in question (300K) is well above the Debye temperature (160K) we can use Dulong-Petits law for the phonons $C_v^{ph} = 3Nk_B$. For the electron contribution $C_v^{el} = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$, $T_F = E_F/k_B$ and $E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$. For Na we have $\rho = 971 kg/m^3$, atomic weight = 22.9898u some calculations gives $T_F = 36599.353$K. Fraction contributed by the electrons: $F = \frac{C_v^{el}}{C_v^{el}+C_v^{ph}} = \frac{1}{1+\frac{6T_E}{\pi^2 T}} \approx 0.0133$.

4. X-rays scatter against the electron distribution around the ions. In KCl the number the number of electrons around the K^+ and Cl^- ion are equal. The X-rays do not see an FCC lattice with a basis of K^+ and Cl^- ions but they see an SC lattice with similar electron distribution on each lattice site. Support motivations with Bragg scattering conditions and form factors.

5. Combining $\sigma = e(n\mu_e + p\mu_h) = 1/\rho$ and $n_i = p_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2}(m_e m_h)^{3/4} e^{-E_g/2k_B T}$ As the mobillity μ only depends algebraically on T the reistance will be dominated by the exponential. Hence we have $R \propto e^{E_g/2k_B T} \rightarrow \ln(R) = constant + E_g/2k_B T$. Plotting $\ln(R)$ versus $1/T$ will produce a straight line and from the slope ($E_g/2k_B = 3917.82157$) we calculate $E_g \approx 0.68eV$.