EP 317.3 MIDTERM TEST (3 WRITTEN PROBLEMS)

Instructor: Yansun Yao
10:00 ~ 11:20 AM, February 24th, 2015

ANSWER ALL QUESTIONS. MARKS PER EACH QUESTION ARE INDICATED.

Physical Constants:

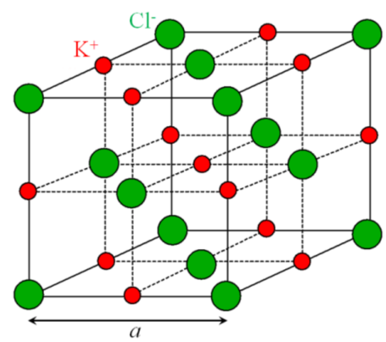
Elementary charge: $e = 1.602 \times 10^{-19}$ C

Avogadro's number: $N_A = 6.022 \times 10^{23}$ mol^{-1}

Wiedemann-Franz-Lorenz coefficent: $C_{WFL} = 2.44 \times 10^{-8}$ W Ω K^{-2}

1. Potassium Chloride (KCl) has an ionic crystal structure (see figure below). When the crystal is in equibrium, the lattice parameter (a) is 0.629 nm.

(a) Find the number of K atoms and the number of Cl atoms per unit cell. (**10%**)



(b) Draw the (100) and (110) planes of the KCl crystal and determine the total number of atoms (add K and Cl together) per cm^2 on the (100) and (110) planes. (**20%**)

(c) The potential energy E per K^+−Cl^- pair as a function of interatomic separation r can be written as the sum of an attractive potential energy (PE) and a repulsive PE,

$$E(r) = -\frac{A}{r} + \frac{B}{r^9}$$

where A and B are constants. When the crystal is in equibrium, $E(r)$ becomes minimum. Find the ratio B/A. (**10%**)

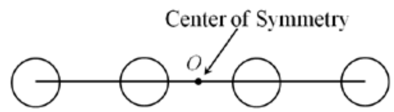
2. Electrical and thermal conductivity. Electron drift mobility in silver has been measured to be 56 cm^2 V^{-1} s^{-1} at 27 °C. The atomic mass and density of Ag are given as 107.87 g mol^{-1} and 10.50 g cm^{-3}, respectively.

(a) Assuming that each Ag atom contributes exactly one conduction electron, calculate the resistivity of Ag at 27 °C. (**10%**)

(b) Compare your calculated resistivity with the measured value of 1.6×10^{-8} Ω m at the same temperature and suggest reasons for the difference. (**10%**)

(c) Calculate the thermal conductivity of silver at 27 °C. If you did not obtain an answer for (a), use $\rho = 2.0 \times 10^{-8}$ Ω m. (**10%**)

3. Linear H_4 molecule. Consider a linear, equal-spacing chain of four hydrogen atoms representing a hypothetical H_4 molecule. Each hydrogen atom has a 1*s* atomic wavefunction. This molecule has a center of symmetry *O* midway between the second and the third atom, *and all molecular wavefunctions must be either symmetric or antisymmetric about O.*



(a) Sketch schematically the atomic wavefunction $\psi_{1s}(r)$ as a function of distance from the nucleus. **(4%)**

(b) Using the linear combination of atomic orbitals (LCAO) method, sketch schematically *all four molecular orbitals*. **(16%)**

(c) Order the energies of the molecular orbitals you just drew and briefly explain your reasoning. **(10%)**