

Stanford University
MatSci 152: Principles of Electronic Materials and Devices
Spring Quarter, 2009-2010
Homework #1



Issued: March 31, 2010

Due: April 7, 2010 (at the start of class)

Suggested reading: Kasap, Chapter 1

Problems:

(Full problems printed online at <http://dionne.stanford.edu> → Classes)

1. Kasap Problem 1.4 (Ionic Bonding in CsCl)
2. Kasap Problem 1.8 (Kinetic Molecular Theory, applied to Ar-ion lasers)
3. Kasap Problem 1.9 (Kinetic Molecular Theory, applied to He-Ne lasers)
4. Kasap Problem 1.12 (Heat Capacity)
5. Kasap Problem 1.20 (Diffusion in Si)
6. Kasap Problem 1.25 (Diamond and Zinc Blende)

1. (Kasap problem 1.4) Ionic bonding and CsCl

The potential energy E per $\text{Cs}^+\text{-Cl}^-$ pair within the CsCl crystal depends on the interionic separation r in the same fashion as in the NaCl crystal,

$$E(r) = -\frac{e^2 M}{4\pi\epsilon_0 r} + \frac{B}{r^m}$$

Energy per ion pair in ionic crystals [1.38]

where for CsCl, $M = 1.763$, $B = 1.192 \times 10^{-104} \text{ J m}^9$ or $7.442 \times 10^{-5} \text{ eV (nm)}^9$ and $m = 9$. Find the equilibrium separation (r_0) of the ions in the crystal and the ionic bonding energy, that is, the ionic cohesive energy; and compare the latter value to the experimental value of 657 kJ mol^{-1} . Given the *ionization energy* of Cs is 3.89 eV and the *electron affinity* of Cl (energy released when an electron is added) is 3.61 eV , calculate the atomic cohesive energy of the CsCl crystal as joules per mole.

2. (Kasap problem 1.8) Kinetic molecular theory

a. In particular Ar-ion laser tube the gas pressure due to Ar atoms is about 0.1 torr at $25 \text{ }^\circ\text{C}$ when the laser is off. What is the concentration of Ar atoms per cm^3 at $25 \text{ }^\circ\text{C}$ in this laser? ($760 \text{ torr} = 1 \text{ atm} = 1.013 \times 10^5 \text{ Pa}$.)

b. In the He-Ne laser tube He and Ne gases are mixed and sealed. The total pressure P in the gas is given by contributions arising from He and Ne atoms

$$P = P_{\text{He}} + P_{\text{Ne}}$$

where P_{He} and P_{Ne} are the *partial pressures* of He and Ne in the gas mixture, that is, pressures due to He and Ne gasses alone,

$$P_{\text{He}} = \frac{N_{\text{He}}}{N_A} \left(\frac{RT}{V} \right)$$

and

$$P_{\text{Ne}} = \frac{N_{\text{Ne}}}{N_A} \left(\frac{RT}{V} \right)$$

In a particular He-Ne laser tube the ratio of He and Ne atoms is $7:1$, and the total pressure is about 1 torr at $22 \text{ }^\circ\text{C}$. Calculate the concentrations of He and Ne atoms in the gas at $22 \text{ }^\circ\text{C}$. What is the pressure at an operating temperature of $130 \text{ }^\circ\text{C}$?

3. (Kasap problem 1.9) Kinetic Molecular Theory

Calculate the effective (rms) speeds of the He and Ne atoms in the He-Ne gas laser tube at room temperature (300 K).

4. (Kasap problem 1.12) Heat capacity

- Calculate the heat capacity per mole and per gram of N_2 gas, neglecting the vibrations of the molecule. How does this compare with the experimental value of $0.743 \text{ J g}^{-1} \text{ K}^{-1}$?
- Calculate the heat capacity per mole and per gram of CO_2 gas, neglecting the vibrations of the molecule. How does this compare with the experimental value of $0.648 \text{ J K}^{-1} \text{ g}^{-1}$? Assume that CO_2 molecule is linear (O-C-O), so that it has two rotational degrees of freedom.
- Based on the Dulong-Petit rule, calculate the heat capacity per mole and per gram of solid silver. How does this compare with the experimental value of $0.235 \text{ J K}^{-1} \text{ g}^{-1}$?
- Based on the Dulong-Petit rule, calculate the heat capacity per mole and per gram of the silicon crystal. How does this compare with the experimental value of $0.71 \text{ J K}^{-1} \text{ g}^{-1}$?

5. (Kasap problem 1.20) Diffusion in Si

The diffusion coefficient of boron (B) atoms in a single crystal of Si has been measured to be $1.5 \times 10^{-18} \text{ m}^2 \text{ s}^{-1}$ at $1000 \text{ }^\circ\text{C}$ and $1.1 \times 10^{-16} \text{ m}^2 \text{ s}^{-1}$ at $1200 \text{ }^\circ\text{C}$.

- What is the activation energy for the diffusion of B, in eV/atom?
- What is the preexponential constant D_0 ?
- What is the rms distance (in micrometers) diffused in 1 hour by the B atom in the Si crystal at $1200 \text{ }^\circ\text{C}$ and $1000 \text{ }^\circ\text{C}$?
- The diffusion coefficient of B in polycrystalline Si has an activation energy of 2.4-2.5 eV/atom and $D_0 = (1.5-6) \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$. What constitutes the diffusion difference between the single crystal sample and the polycrystalline sample?

6. (Kasap problem 1.25) Diamond and zinc blende

Si has the diamond and GaAs has the zinc blende crystal structure. Given the lattice parameters of Si and GaAs, $a = 0.357 \text{ nm}$ and $a = 0.356 \text{ nm}$, respectively, and the atomic masses of Si, Ga, and As as 28.08, 69.73 g/mol, and 74.92, respectively, calculate the density of Si and GaAs. What is the atomic concentration (atoms per unit volume) in each crystal?