

MS/EST 143, Problem Set #2

assigned 04/03/11

due 04/08/11

1. Calculate the equilibrium concentration (#/#) and equilibrium number (#/volume) of vacancies in copper at 1000 °C. The activation enthalpy for vacancy formation is 0.9 eV/atom and the density at 1000 °C is 8.4 g/cm³. State any assumptions.
2. Write formally correct defect information reactions and the corresponding mass action equilibrium constants for the following. Refer to tabulated ionic radii for guidance (*e.g.* provided in Chiang, Table 1.2). If you think more than one incorporation mechanism is possible, briefly discuss why and show the different possibilities.
 - i. Solid solution of CaCl₂ in NaCl
 - ii. Solid solution of CaO in ZrO₂
 - iii. Solid solution of SrTiO₃ in BaTiO₃
 - iv. Solid solution of Y₂O₃ in BaTiO₃
 - v. Solid solution of Nb₂O₅ in BaTiO₃
 - vi. Solid solution of Al₂O₃ in BaTiO₃
3. LiF has a Schottky formation energy of 2.6 eV and a bandgap of 12 eV. At 500 °C estimate the relative concentrations of ionic and electronic defects, and determine which are dominant on an absolute concentration basis.
4. Construct the Brouwer diagram for a pure binary oxide MO of the rocksalt structure for which, at the temperature of interest, $K_i \gg K_s$. (That is, the bandgap is small relative to the Schottky energy).