

## Assignment 1

### Problem 1

A typical paper clip weighs 0.59g and consists of iron (Fe). Calculate (a) the number of unit cells and (b) the number of iron atoms in the paper clip.

Data: structure : BCC; lattice parameter: 2.866 Angstroms; Atomic Mass: 55.847g.mol<sup>-1</sup>

### Problem 2

$\alpha$ -Mn has a cubic structure with a lattice parameter of 0.8931nm and a density of 7.47g.cm<sup>-3</sup>.  $\beta$ -Mn has a different cubic structure with a lattice parameter of 0.6326nm and a density of 7.26g.cm<sup>-3</sup>. Determine the percentage volume change that would occur if  $\alpha$ -Mn transforms to  $\beta$ -Mn

Data: Atomic Mass of Manganese: 54.938g.mol<sup>-1</sup>; Manganese Atomic Radius: 0.112nm

### Problem 3

Would you expect NiO to have the cesium chloride, sodium chloride or zinc blende type of structure? Based on your answer determine (a) the lattice parameter, (b) the density and (c) the packing factor.

Data: Ionic Radii Ni<sup>2+</sup> = 0.69Angstroms, O<sup>2-</sup> = 1.32Angstroms

### Problem 4

The density of a sample of FCC Palladium is 11.98g.cm<sup>-3</sup> and its lattice parameter is 3.8902 Angstroms. Calculate (a) the fraction of lattice points that contain vacancies and (b) the total number of vacancies in a cubic centimeter of palladium.

Data: Atomic Mass of Palladium: 106.4g.mol<sup>-1</sup>

### Problem 5

Homogeneous solid nucleation in liquid metals is thought to occur at undercoolings of 0.2 the melting point of the metal.

- a) Calculate the temperature and number of degrees of undercooling at which iron should nucleate homogeneously.
- b) Calculate the size of the critical radius.
- c) Calculate the number of atoms in the nucleus having the critical radius.
- d) Suppose that an iron nucleus is formed homogeneously with an undercooling of only 25°C. How many atoms would have to spontaneously group together in order for this to occur? The fusion temperature of pure iron is 1538°C.

Data: The lattice parameter of BCC iron is 2.91Angstroms, Heat of Fusion = 1737J.cm<sup>-3</sup>; Solid Liquid Interfacial Energy = 204x10<sup>-7</sup>J.cm<sup>-2</sup>

### Problem 6

Devices such as transistors are made by doping semiconductors with different dopants that generate regions that have p- or n- type semiconductors. The diffusion takes place at a temperature of 1100°C.

Assume the source provides a surface concentration of  $10^{20}$  atoms.cm<sup>-3</sup> and the diffusion time is 1 hour. Assume that the silicon wafer contains no phosphorus or boron to begin with.

- (a) calculate the depth at which the concentration of phosphorus will be  $10^{18}$  atoms.cm<sup>-3</sup>.
- (b) calculate the depth at which the concentration of boron will be  $10^{18}$  atoms.cm<sup>-3</sup>.
- (c) Which one of the two dopants diffuses faster and what type of semiconductor we expect to obtain in each case.

Data:

Diffusion Constant or Pre-exponential of P in Si ( $D_0$ ) =  $4.70\text{cm}^2.\text{s}^{-1}$ ;

Activation energy for Diffusion of P in Si (Q) = 3.68eV/atom;

Diffusion Constant or Pre-exponential of B in Si ( $D_0$ ) =  $1.0\text{cm}^2.\text{s}^{-1}$ ;

Activation energy for Diffusion of B in Si (Q) = 3.50eV/atom;

$R = 8.31415 \text{ J. K}^{-1}.\text{mol}^{-1}$

$\text{eV} = 1.602 \times 10^{-19} \text{ J}$

$\text{mol} = 6.023 \times 10^{23} \text{ atoms}$

Hint: Need to find the value of D (Diffusion Coefficient)