

HW 2	Inorganic Materials Chemistry	Name:	
Points:	C7780	Date:	
Max. 100 points	Fall 2013	A	

1. (10 pts) In the crystalline Cu_3N , copper atoms possess coordination number 2. What is the coordination number of N?

2. (15 pts) X-ray radiation of a Cu anode ($\lambda = 1.54 \text{ \AA}$) was diffracted under an angle of 14.22° at silicon crystal. Calculate the interplanar distance d in Si for the first order diffraction ($n = 1$).

3. (15 pts) Stishovite is a high-pressure modification of SiO_2 having the rutile structure.

a) What is the coordination number of Si and O?

b) Should it have higher or lower density than quartz?

c) Should it have longer or shorter Si–O bond lengths than quartz?

4. (10 pts) Write balanced chemical equation for a solid state reaction:



5. (20 pts) Cubic spinel ZnFe_2O_4 crystallizes with 8 formula units in the cubic unit cell. The cell parameter $a = 8.42 \text{ \AA}$. Calculate the density in g cm^{-3} of the material.

$N_A = 6.022141 \cdot 10^{23} \text{ mol}^{-1}$, $A_r(\text{Zn}) = 65.41$, $A_r(\text{Fe}) = 55.85$, $A_r(\text{O}) = 15,999$.

6. (30 pts) Gibbs free energy change for nucleation ΔG_N is given by two terms – surface and volume.

$$\Delta G_N = 4\pi r^2 \gamma_{\text{SL}} + 4/3\pi r^3 \Delta G_V$$

γ_{SL} = the solid/liquid interfacial energy

ΔG_V – the free energy change between the ‘monomer’ in solution and unit volume of bulk crystal

$$\Delta G_V = -\frac{RT \ln S}{V_m}$$

S – supersaturation = the quotient (ratio) of the actual concentration and the concentration of the respective species at equilibrium conditions, indicates how far away from equilibrium the system is.

V_m – molar volume of the bulk crystal, r – nucleus radius

a) Explain what is a critical radius of nuclei r_C – draw a graph of ΔG_N versus r .

b) Suggest a way how to control the critical nucleation radius r_C by changing some reaction parameter.