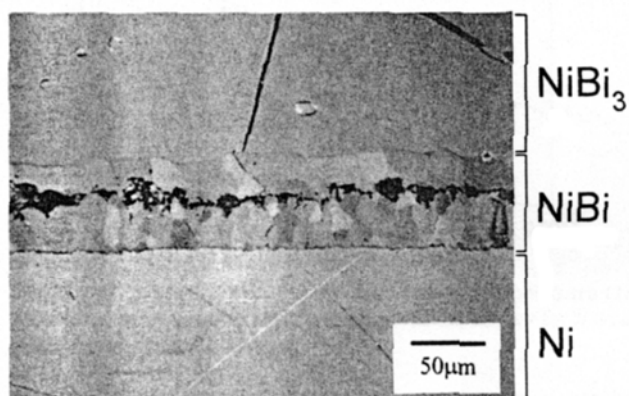


<b>HW 1</b>	<b>Inorganic Materials Chemistry</b>	<b>Name:</b>	
<b>Points:</b>	<b>C7780</b>	<b>Date:</b>	
Max. 100 points	<b>Fall 2013</b>	<b>A</b>	

- (8 pts)** A unit cell has in general shape of a) cube b) tetrahedron c) parallelepiped
- (12 pts)** In the crystalline  $\text{Cu}_2\text{O}$ , oxygen atoms possess coordination number 4. What is the coordination number of Cu? Show how you arrive to the answer.
- (30 pts)** A solid state reaction between Ni and  $\text{NiBi}_3$  discs leads to the product shown below. Consider three cases:
  - only Ni diffuses through the interfaces
  - only Bi diffuses through the interfaces
  - both Ni and Bi diffuse through the interfaces at the same rate
Calculate for each case the Kirkendall ratio, compare your results with Figure 5, and suggest which mechanism is the most plausible.



**Figure 5.** A cross sectional picture (polarized) showing the reaction product  $\text{NiBi}$  for the reaction between  $\text{NiBi}_3$  and  $\text{Ni}$  at  $370\text{ }^\circ\text{C}$  for 600 h. From top to bottom, the three layers are  $\text{NiBi}_3$ ,  $\text{NiBi}$ , and  $\text{Ni}$ , respectively. The crack within  $\text{NiBi}$  delineates the original interface between  $\text{Ni}$  and  $\text{NiBi}_3$  before the reaction.

4. (15 pts) A (111) diffraction in the powder X-ray diffractogram appears at 41 degree  $2\theta$  when Cu  $K\alpha$  radiation was used ( $\lambda = 1.54059 \text{ \AA}$ ).

a) What is the value of the interplanar distance  $d_{hkl}$  ?

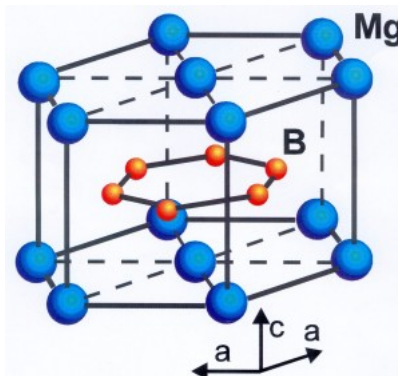
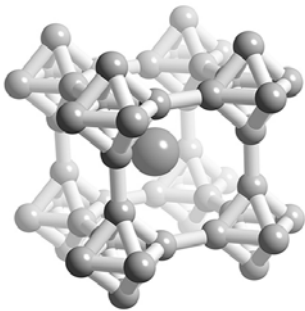
b) What would be the value of the diffraction angle when Mo  $K\alpha$  radiation is used instead ( $\lambda = 0.70932 \text{ \AA}$ ).

c) The relationship between  $d_{hkl}$  and cubic lattice parameter  $a$  is:

$$\frac{1}{d^2_{hkl}} = \frac{h^2 + k^2 + l^2}{a^2}$$

Calculate the cubic cell size.

5. (15 pts) Give stoichiometric formulas for these structures. Large atoms = A, small atoms = B



6. (20 pts) Specific surface area of  $\alpha\text{-Fe}_2\text{O}_3$  was measured by nitrogen adsorption at 77 K and its value is  $120 \text{ m}^2 \text{ g}^{-1}$ . Density of this oxide is  $5.277 \text{ g cm}^{-3}$ . Calculate the particle size assuming a spherical particle shape.