

Name \_\_\_\_\_

Student Number \_\_\_\_\_

**Exercise N°1** 2 pts

Give the Miller indices of all the crystallographic directions and planes indicated

(A)

$$\begin{array}{r} -1, 0, 1 \\ -0, 1, 1 \\ \hline 1 \quad -1 \quad 0 \\ h' \quad k' \quad l' \end{array}$$

$$h = \frac{1}{3}(2h' - k')$$

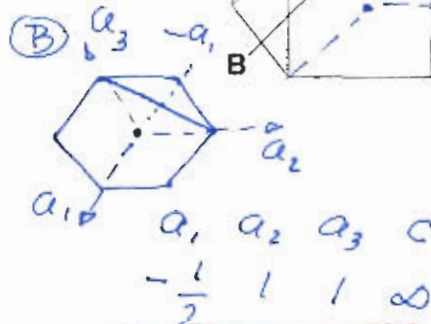
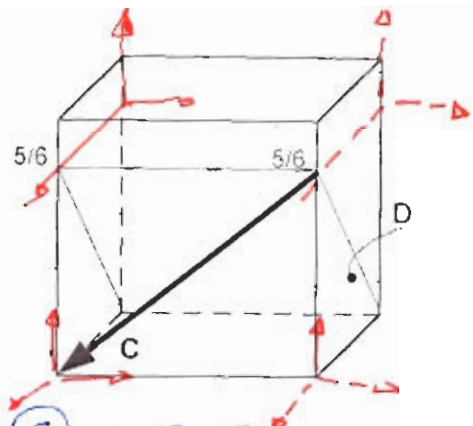
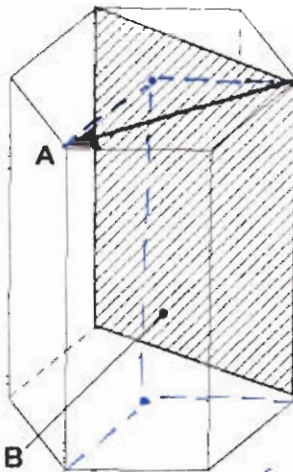
$$h = \frac{1}{3}(2 + 1) = 1$$

$$k = \frac{1}{3}(-2 - 1) = -1$$

$$i = -\frac{1}{3}(1 - 1) = 0$$

$$l = 0$$

$$\boxed{(1 \bar{1} 0)}$$



$$\boxed{(\bar{2} 1 1 0)}$$

(C)

$$\begin{array}{r} 1, 0, 0 \\ 1, 1, \frac{5}{6} \\ \hline 0, -1, -\frac{5}{6} \\ \boxed{[0 \bar{6} \bar{5}]} \end{array}$$

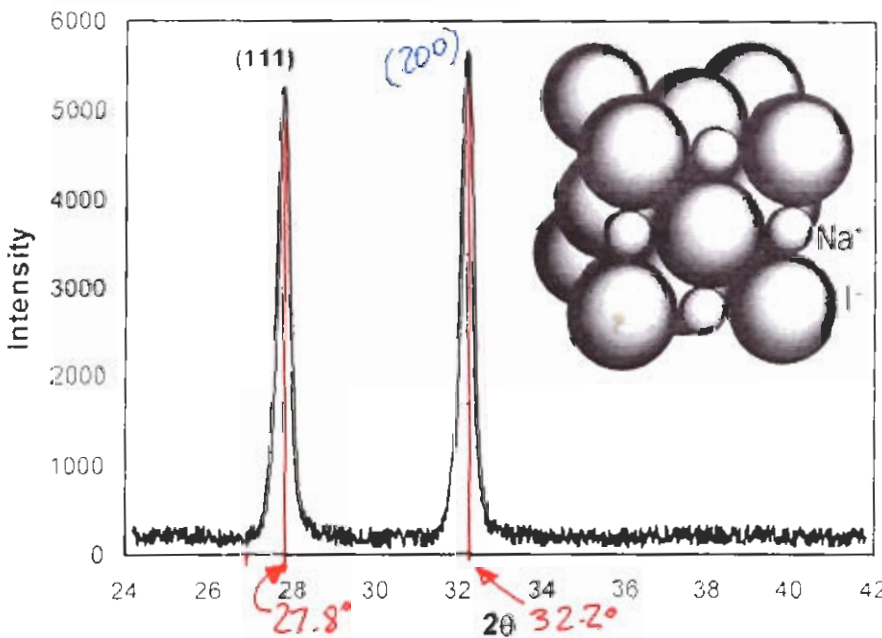
(D) four possible positions of origin  $\Rightarrow$  2 results.

$$\begin{array}{r} x \quad y \quad z \\ -1, \infty, \frac{5}{6} \Rightarrow -1, 0, \frac{6}{5} \\ \Rightarrow \boxed{(\bar{5} 0 6)} \end{array}$$

$$\begin{array}{r} x \quad y \quad z \\ 1, \infty, -\frac{5}{6} \Rightarrow 1, 0, -\frac{6}{5} \Rightarrow \boxed{(5 0 \bar{6})} \end{array}$$

**Exercise N°2** 8 pts

Sodium iodide (NaI) is being used in scintillation counters developed recently for electron microscopy. The following is a partial x-diffraction spectrum obtained from NaI using a cobalt target ( $\text{Co-K}\alpha = 0.178897 \text{ nm}$ )



$Z_{\text{Na}} = 11$   
 $Z_{\text{I}} = 53$   
 $A_{\text{Na}} = 22.990$   
 $A_{\text{I}} = 126.905$   
 $N_A = 6.022 \cdot 10^{23} \frac{\text{atoms}}{\text{mole}}$   
 $R_{\text{Na}^+} = 0.098 \text{ nm}$

- What type of structure does NaI have? (e.g. zinc blende, perovskite, etc.)
- What is the coordination number of  $\text{Na}^+$ ? What type of site do those cations occupy?
- Indicate what is the plane that caused the second peak in the x-ray spectrum.
- Using both sets of  $hkl$  (Miller indices) calculate the measured lattice parameter of NaI.
- Calculate the density at room temperature of NaI in  $\text{g/cm}^3$ .
- What type of point defect can you expect to find in this solid? Explain.
- Explain how a "diffraction cone" is formed (3 sentences with a sketch).

Bonus (2pts.): Calculate the position ( $2\theta$ ) of the next peak you should expect to appear to the right.

a) Rock salt (as in NaCl)

b)  $\boxed{\text{CN} = 6} \Rightarrow$  octahedral sites

c) This is an FCC type formed with  $\text{I}^-$  anions. Therefore the next peak should be (200)

$$d_{111} = \frac{a}{\sqrt{1+1+1}} = \frac{a}{\sqrt{3}} \quad ; \quad d_{200} = \frac{a'}{\sqrt{4+0+0}} = \frac{a'}{2}$$

$$\lambda = 2d_{111} \sin \theta_{111} \Rightarrow d_{111} = \frac{\lambda}{2 \sin \theta_{111}} = \frac{0.178897 \text{ nm}}{2 \sin \left(\frac{27.8^\circ}{2}\right)} = 0.3723 \text{ nm}$$

$$d_{200} = \frac{0.178897}{2 \sin \left(\frac{32.2^\circ}{2}\right)} = 0.3225 \text{ nm}$$

Notice that both values of  $a$  are very close  $\Rightarrow$  proving that the planes are correctly labeled

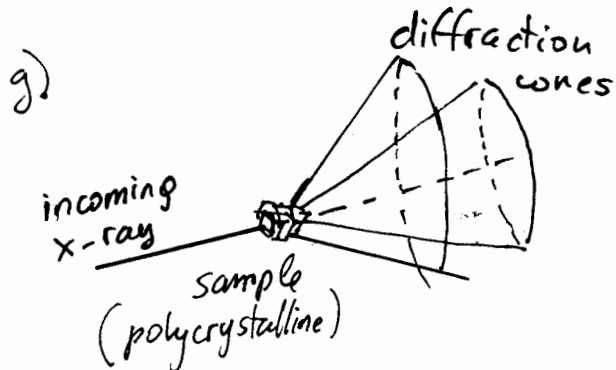
$$a = \sqrt{3} \cdot 0.3723 \text{ nm} = 0.6448$$

$$a' = 2 \cdot 0.3225 \text{ nm} = 0.6451 \text{ nm}$$

$$\text{average } \boxed{a = 0.6450 \text{ nm}}$$

$$e) \rho = \frac{4 \cdot 22.990 + 4 \cdot 126.905}{6.022 \cdot 10^{23} (0.6450)^3} \times 10^{21} \frac{\text{g}}{\text{cm}^3} = \boxed{3.71 \frac{\text{g}}{\text{cm}^3} = \rho_{\text{NaI}}}$$

f) This is an ionic solid  $\Rightarrow$  Schottky and Frenkel defects are expected.

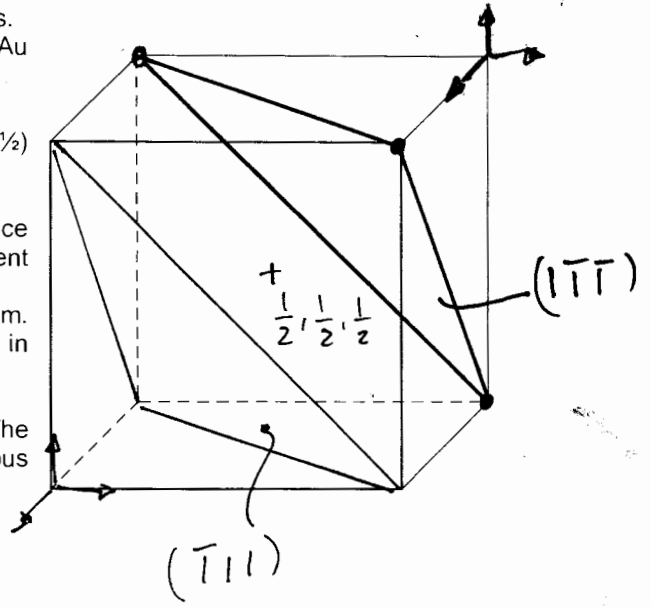


Each cone is produced by the x-ray diffraction on each plane (e.g. (011), (111), etc) for each piece of powder in a polycrystalline sample

**Exercise N°3** 7 pts.

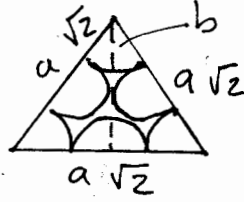
Assume that the unit cell on the right belongs to a gold ( $Z_{Au}=79$ ;  $A_{Au}=196.9665$ ) crystal, which is FCC.

- Please draw the  $(\bar{1}11)$  and  $(1\bar{1}\bar{1})$  planes.
- Does any of those two planes cross the center point  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  of the unit cell? Explain.
- Calculate the planar density of both planes.
- If they are parallel to each other, calculate the distance between these two planes (not between equivalent planes!!!).
- The hydrogen atom has an atomic radius of  $r_H=0.078\text{nm}$ . Calculate whether hydrogen can be an interstitial impurity in gold, assuming that  $a_{Au}=0.4078\text{ nm}$ .
- Calculate the APF of gold.
- Mercury is next to gold ( $Z_{Hg}=80$ ) in the Periodic Table. The melting point of Au is  $1,064^\circ\text{C}$ . Please explain this enormous difference in melting points between both metals.



b) No they do not cross the center point

c) Both are compact planes and have the same  $P_p$



$$b = \sqrt{\left(a\frac{\sqrt{2}}{2}\right)^2 - \left(\frac{a\sqrt{2}}{2}\right)^2}$$

$$b = a \sqrt{\frac{2}{2} - \frac{1}{2}} = a \sqrt{\frac{1}{2}}$$

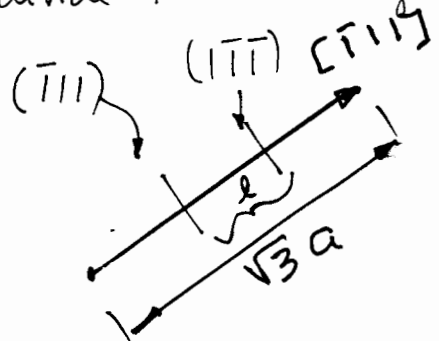
$$\text{Area} = \frac{a^2 \sqrt{2}}{2} \cdot \frac{\sqrt{3}}{2} = \frac{\sqrt{6}}{2} a^2 = \frac{\sqrt{3}}{2} a^2$$

$$\# \text{ atoms} = 3 \cdot \frac{1}{6} + 3 \cdot \frac{1}{2} = \frac{1}{2} + \frac{3}{2} = 2 \text{ atoms}$$

$$P_p = \frac{2 \text{ atoms}}{\sqrt{3} a^2}$$

d) The compact planes  $(\bar{1}11)$  and  $(1\bar{1}\bar{1})$  divide the cube diagonal in three equal segments - therefore the distance between both planes is

$$l = \frac{\sqrt{3}}{3} a$$



$$e) a = 2R + 2r = \frac{2\sqrt{2}}{4} a + 2r$$

$$\therefore r = \frac{a}{2} \left(1 - \frac{\sqrt{2}}{2}\right) = 0.0597 \text{ nm} < 0.0778 \text{ nm}$$

Apparently the hydrogen atom doesn't fit in the octahedral site.

f) It's FCC: we don't need to calculate it  
We know it: 0.74

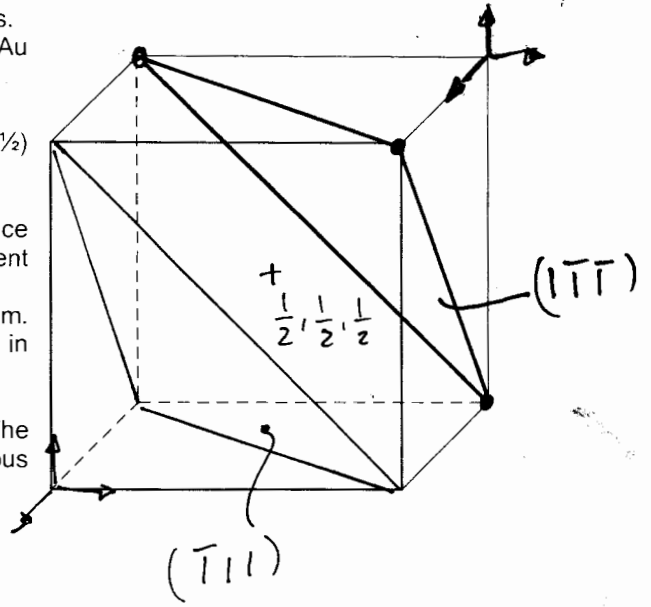
g) Au has a covalent bond added to the metallic one. This combined nature of the bond creates a much more stable crystal, i.e. higher melting point

If you need more space continue your work on the back of the paper

**Exercise N°3** 7 pts.

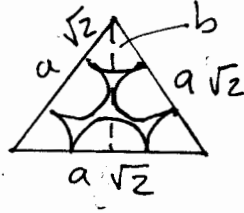
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b) No they do not cross the center point

c) Both are compact planes and have the same  $\rho_p$



Area =  $\frac{b}{2} \cdot a\sqrt{2}$

$$b = \sqrt{\left(a\frac{\sqrt{2}}{2}\right)^2 - \left(\frac{a\sqrt{2}}{2}\right)^2}$$

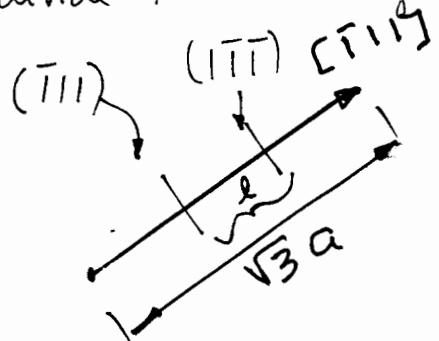
$$b = a \sqrt{\frac{2}{2} - \frac{1}{2}} = a \sqrt{\frac{3}{2}}$$

$$\text{Area} = \frac{a^2 \sqrt{2}}{2} \cdot \sqrt{\frac{3}{2}} = \frac{\sqrt{6}}{2} a^2 = \frac{\sqrt{3}}{2} a^2$$

$$\# \text{ atoms} = 3 \cdot \frac{1}{6} + 3 \cdot \frac{1}{2} = \frac{1}{2} + \frac{3}{2} = 2 \text{ atoms}$$

$$\rho_p = \frac{2 \text{ atoms}}{\sqrt{3} a^2}$$

d) The compact planes  $(\bar{1}11)$  and  $(1\bar{1}\bar{1})$  divide the cube diagonal in three equal segments - therefore the distance between both planes is



$$l = \frac{\sqrt{3}}{3} a$$

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g) Au has a covalent bond added to the metallic one. This combined nature of the bond creates a much more stable crystal, i.e. higher melting point

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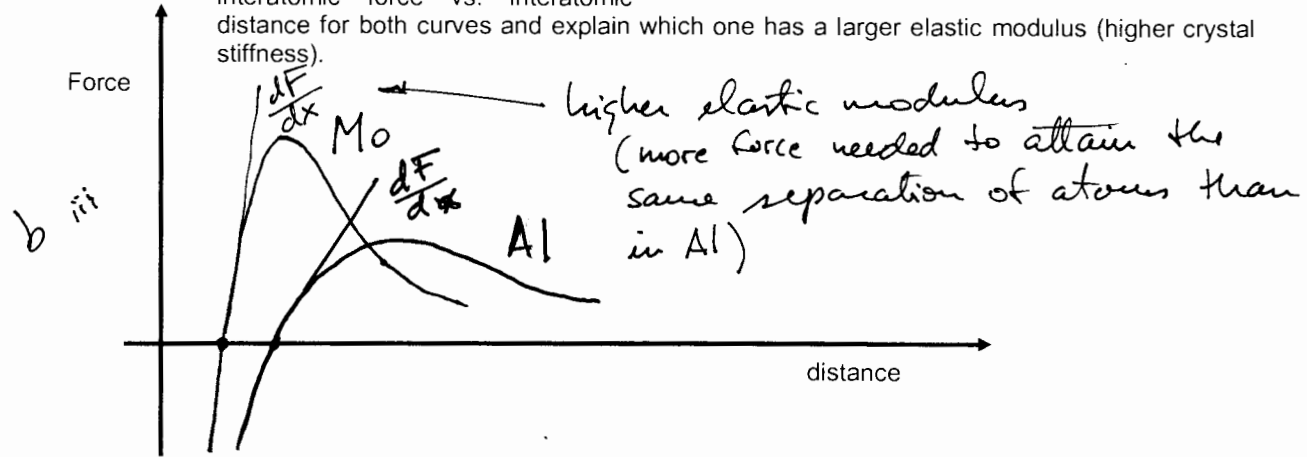
Exercise N°4 8 pts.

The following questions may or may not be related to each other:

- a) What is called *thermoionic emission*? (two sentences).
- b) Consider aluminum (melting point M.P.= 660°C) and molybdenum (M.P. 2,600°C). Respond to the following:

23	24	25	26	27	28	29	30	31
V	Cr	Mn						
	42							
	Mo							
	74							

- i. Which one has a vacancy activation energy of 460 kJ/mol and which one, 165 kJ/mol? Justify your answer.
- ii. Most likely which one has a higher expansion coefficient?
- iii. On the axes below sketch the interatomic force vs. interatomic distance for both curves and explain which one has a larger elastic modulus (higher crystal stiffness).



- c) Explain the delocalization of electrons in metallic bonds and how that affects the electrical properties of metals (three sentences). What is different in ionic conductors?
- d) The molecular weight (MW) distribution of a polymer sample was found to be: 30% with MW = 5,400 g/mol, 40% with MW = 50,000 g/mol, 30% with MW = 100,000 g/mol. Calculate the molecular weight of the polymer.
- e) Describe the formation of sulfur crosslinks in the vulcanization of natural rubber (4 sentences).
- f) Provide at least three unit cells of plutonium.
- g) Uranium dioxide (UO<sub>2</sub>) is highly toxic and has a fluorite type unit cell. How many internal tetrahedral sites are occupied in that cell? Who occupies them: O<sup>2-</sup> or U<sup>4+</sup>? Explain.

Bonus (2 pts.): Based on the reading assignment on metallic glasses, please respond:

- i. Provide two medical applications of Vitreloy and the main reasons for its use.
- ii. Explain the following criterion in the formation (manufacturing) of metallic glasses: "Atomic radius mismatch between elements,  $\Delta r / r$ , should be greater than 12% to have a higher packing density" (think of the slide shown in class).

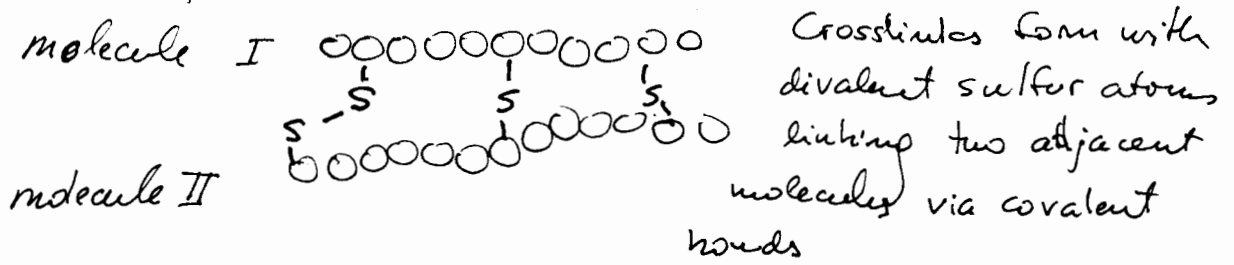
a) Electrons <sup>have enough energy to</sup> leave the metal at high temperatures, favored by a high electrical field.

b) Al has a  $Q_D = 165 \text{ kJ/mol}$  since it's easier to create vacancies in this crystal due to the low melting point (less stable bond) - therefore it will expand more when created -

c) Valence electrons leave the host atoms and form a "cloud" of delocalized electrons. They have high mobility and <sup>their velocities</sup> can be "oriented" by applied electrical field very easily.

d)  $MW = 0.3 \times 5,400 + 0.4 \times 50,000 + 0.3 \times 100,000$   
 $MW = 51,620 \text{ g/mol}$

e)



f) Pu has 6 unit cells:

- 2 are monoclinic
- orthorhombic
- FCC
- tetragonal
- BCC

g) It has a fluorite structure ( $\text{CaF}_2$ ) type. Tetrahedral sites for  $\text{U}^{+4}$

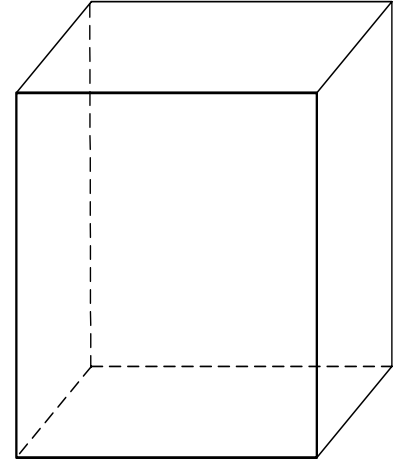
INGE 4001 – 2<sup>nd</sup> Semester - 2005 – 2006 – Sections 066 & 076  
 Instructor: O. M. Suárez – Grad student: Hermes Calderón  
 Mid-Term Exam #1, Thursday February 9, Stéfani S-113  
 Maximum time: 1½ hours - Maximum Grade: 20 pts (without bonus).

Name: \_\_\_\_\_

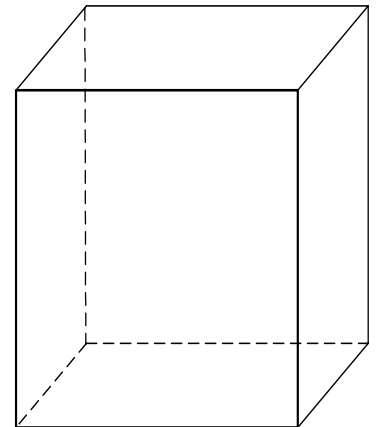
Student Number: \_\_\_\_\_

**Exercise N°1** 6 pts.

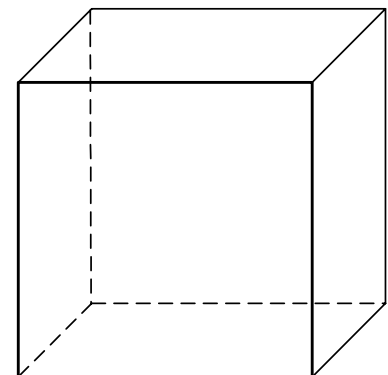
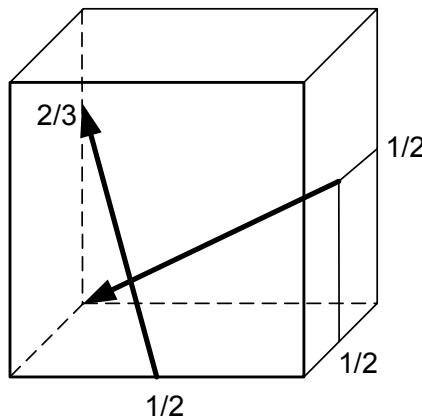
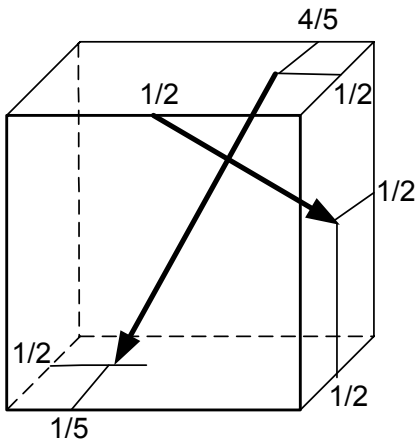
a) The empty unit cell on the right is base-centered orthorhombic. Draw the  $[\bar{1}\bar{1}0]$  direction. Then calculate the linear density of this direction. Is this the direction with maximum linear density in a base-centered orthorhombic unit cell? Name and draw two more directions with identical linear densities.



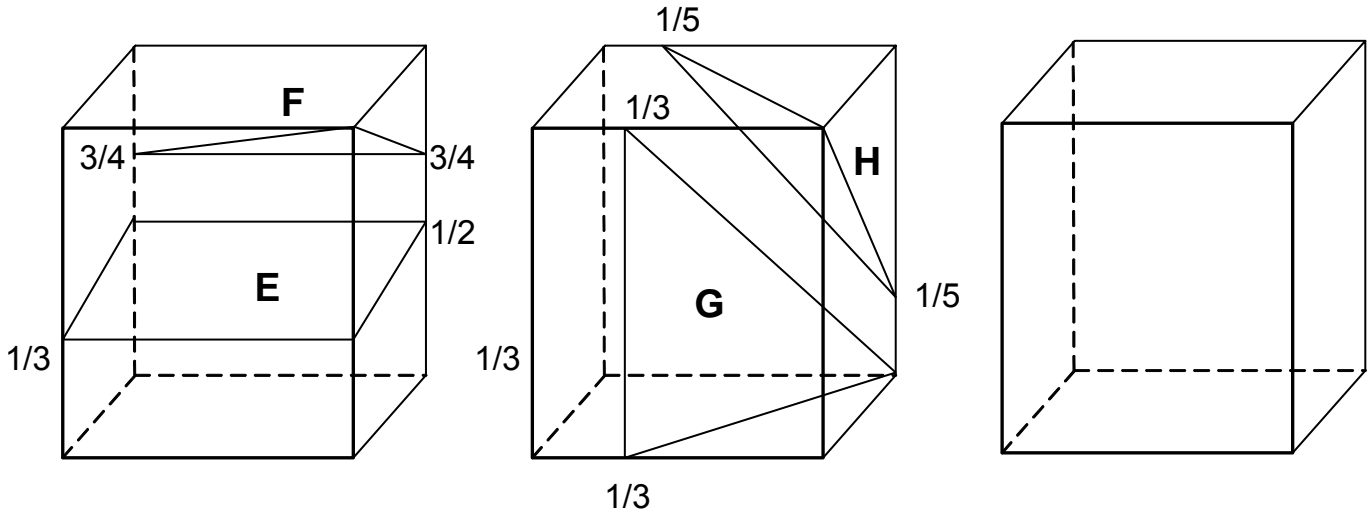
b) The empty unit cell on the right is simple tetragonal. Draw the  $(\bar{1}\bar{1}\bar{1})$  plane. What is the coordination number of the central interstice? What is the coordination number of each atom?



c) Give the Miller indices all crystallographic directions planes shown in the next pictures. On the empty cubes draw the  $[\bar{1}20]$  direction and the  $(4\bar{2}1)$  plane.



*If you need more space continue your work on the back of the paper*



### Exercise N°2 5 pts

Tin ( $Z=50$ ,  $A=118.711$ ) has been used as a solder alloy component for many years. At about  $13^\circ\text{C}$ , gray tin ( $\alpha\text{-Sn}$ ) undergoes a phase transformation to white tin ( $\beta\text{-Sn}$ ).

$\alpha\text{-Sn}$  has a diamond cubic structure (like C and Si) with lattice parameter:  $a = 0.649 \text{ nm}$ .  $\beta\text{-Sn}$  has a body-centered tetragonal structure (BCT) with lattice constants  $a = 0.583 \text{ nm}$  and  $c = 0.318 \text{ nm}$ .

- To which important group in the periodic table does tin belong? Give two more examples of elements in the same group
- Sketch the hybridization of  $\alpha\text{-Sn}$  using the orbital boxes.
- Calculate the theoretical density of the two phases in  $\text{g/cm}^3$ .
- Calculate the % volume change upon cooling, i.e. when Sn goes from  $\beta$  to  $\alpha$ . Does it expand or contract?
- What is the coordination number of any Sn atom in  $\alpha\text{-Sn}$ ?

**Bonus (2pts.):** Calculate the APF of  $\beta\text{-Sn}$ , knowing that  $r_{\text{Sn}}=0.145\text{nm}$

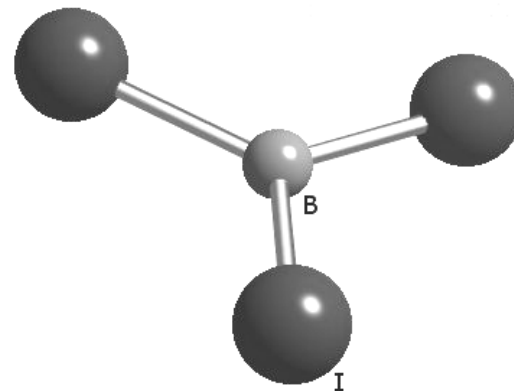
*If you need more space continue your work on the back of the paper*



**Exercise N°3** 5 pts

Boron tri-iodide  $\text{BI}_3$  is a compound used in neutron detectors. The basic molecule is shown in perspective (angles between bonds are  $120^\circ\text{C}$ ). Boron atomic number is  $Z=5$  and iodine,  $Z=53$ . Boron electronegativity is 2.04 and iodine, 2.66. Respond to the following requests:

- Write the electronic configuration of both elements in their ground state.
- What type of bond does  $\text{BI}_3$  have? Why? Do you think this compound may have a mixed bond? If yes, what is the other bond type? Is it large or small? Why?
- Is the boron atom hybridized? Explain using Hund's rule.
- Is this a polar molecule? Why or why not?



**Exercise N°4** 4 pts.

The following questions may or may not be related to each other:

- a) Demonstrate that in an *ideal* HCP structure  $c = 2 \cdot \sqrt{\frac{2}{3}} \cdot a$ .
- b) Using your knowledge of vacancies explain why *volume density* is also called *theoretical density* (three sentences).
- c) Explain the delocalization of electrons in metallic bonds and how that affects the electrical properties of metals (three sentences). What is different in ionic conductors?
- d) Demonstrate that the planar density of (0002) plane in an *HCP* unit cell is the same as the planar density of  $(\bar{1}\bar{1}\bar{1})$  plane in an FCC cell (assume that the atomic radius is the same in both cases).

Bonus (1 pt.): Describe the formation of sulfur crosslinks in the vulcanization of natural rubber (4 sentences).

INGE 4001 – 2<sup>nd</sup> Semester - 2006 – 2007 – Sections 016 & 036

Instructor: O. M. Suárez – Grad student: Hermés Calderón

Mid-Term Exam #1, Thursday Feb. 15, Stéfani S-113

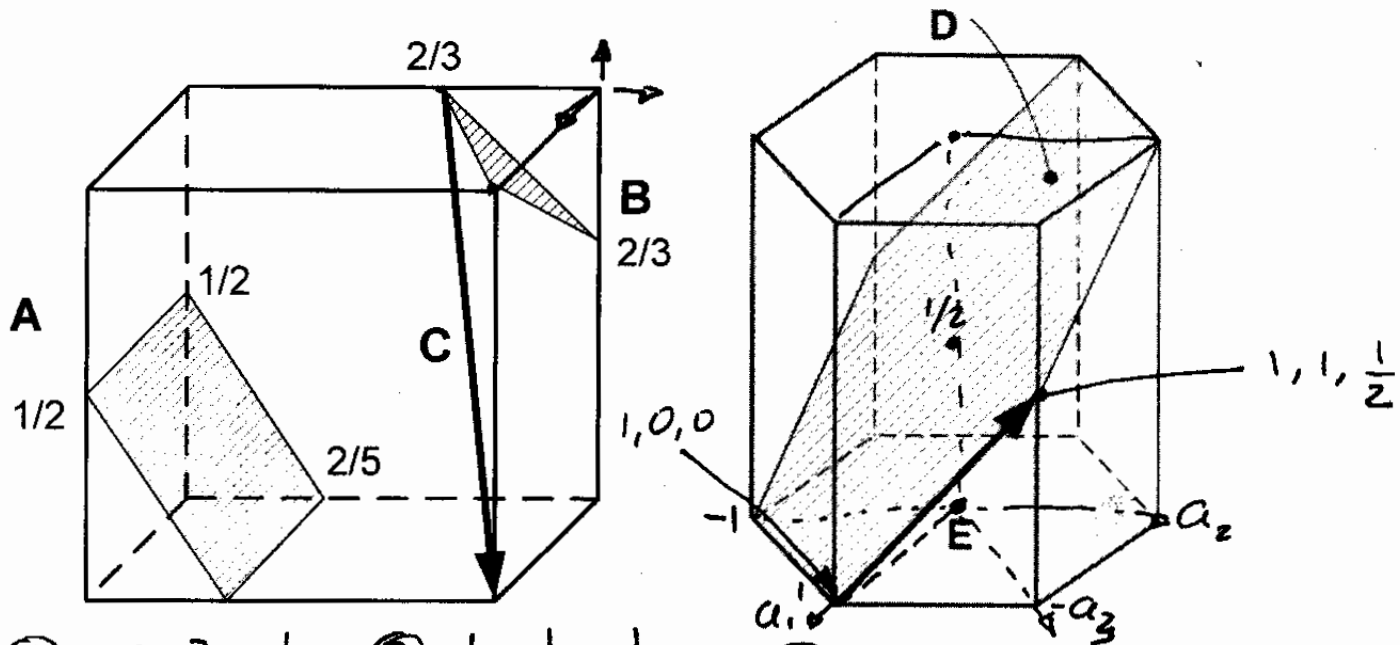
Maximum time: 1½ hours - Maximum Grade: 25 pts.

Name:

Student Number:

**Exercise N°1** 6 pts.

a) Give the Miller indices of all the crystallographic directions and planes indicated below.



Ⓐ  $\infty, \frac{2}{3}, \frac{1}{2}$   
 $0, \frac{5}{2}, 2$   
 $(0 \ 5 \ 4)$

Ⓑ  $1, -\frac{1}{3}, -\frac{1}{3}$   
 $(1 \ \bar{3} \ \bar{3})$

Ⓒ  $1, 1, 0$   
 $0, \frac{2}{3}, 1$

Ⓓ  $1, -1, \infty, \frac{1}{2}$   
 $(1 \ \bar{1} \ 0 \ 2)$

Ⓔ  $1, 1, \frac{1}{2}$   
 $1, 0, 0$   
 $0, 1, \frac{1}{2}$

$h'k'l' = 0 \ 2 \ 1$

$h = \frac{1}{3}(2h' - k') = \frac{1}{3}(2 \cdot 0 - 2)$   
 $h = -\frac{2}{3}$

$k = \frac{1}{3}(2 \cdot 2 - 0) = \frac{4}{3}$

$i = -\frac{1}{3}(0 + 2) = -\frac{2}{3}$   
 $l' = 1$

$[\frac{1}{3} \ 1 \ \bar{1}]$   
 $[3 \ 1 \ \bar{3}]$

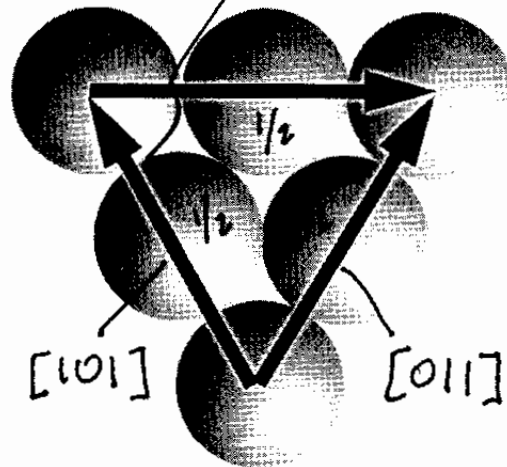
$-\frac{2}{3} \ \frac{4}{3} \ -\frac{2}{3} \ 1$   
 $[\bar{2} \ 4 \ \bar{2} \ 3]$

$[\bar{1} \ 1 \ 0]$

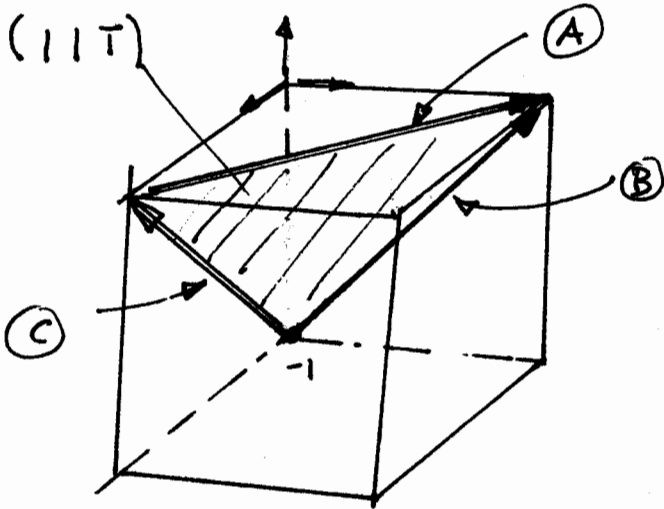
b) The image on the right corresponds to the (111) plane of an FCC unit cell. Using this image:

- Please provide the Miller indices of the three directions indicated.
- Calculate the planar density of the (111) plane as a function of the lattice parameter  $a$ .
- Compute the linear density of all the directions indicated.

**Bonus (1 pt.):** Demonstrate that this plane has the same planar density as the (0001) plane in an HCP crystal (assume that the atoms in both crystals have the same radius:  $R_{HCP} = R_{FCC}$ )



If you need more space continue your work on the back



i) (A) 
$$\begin{array}{r} 0, 1, 1 \\ 1, 0, 1 \\ \hline [1 \ 1 \ 0] \end{array}$$

(B) 
$$\begin{array}{r} 0, 1, 1 \\ 0, 0, 0 \\ \hline [0 \ 1 \ 1] \end{array}$$

(C) 
$$\begin{array}{r} 1, 0, 1 \\ 0, 0, 0 \\ \hline [1 \ 0 \ 1] \end{array}$$

ii) 
$$P_P = \frac{\# \text{ atoms}}{\text{area}}$$

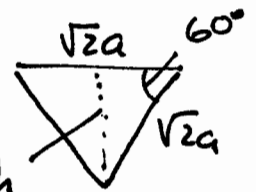
$$\begin{aligned} \# \text{ atoms} &= 3 \times \frac{1}{2} + 3 \times \frac{1}{6} \\ &= \frac{3}{2} + \frac{1}{2} = \frac{4}{2} = 2 \end{aligned}$$

$$P_P = \frac{2}{\frac{a^2 \sqrt{3}}{2}} = \frac{4}{a^2 \sqrt{3}}$$

$$\text{area} = \frac{\sqrt{2} a h}{2}$$

$$\text{area} = \frac{\sqrt{2}}{2} a \cdot \sqrt{2} a \cos 30^\circ$$

$$\text{area} = \frac{a^2 \sqrt{3}}{2}$$



For FCC:

$$\sqrt{2} a = 4R \Rightarrow a = \frac{4R}{\sqrt{2}}$$

$$a^2 = \frac{16}{2} R^2 = 8R^2$$

Bonus:

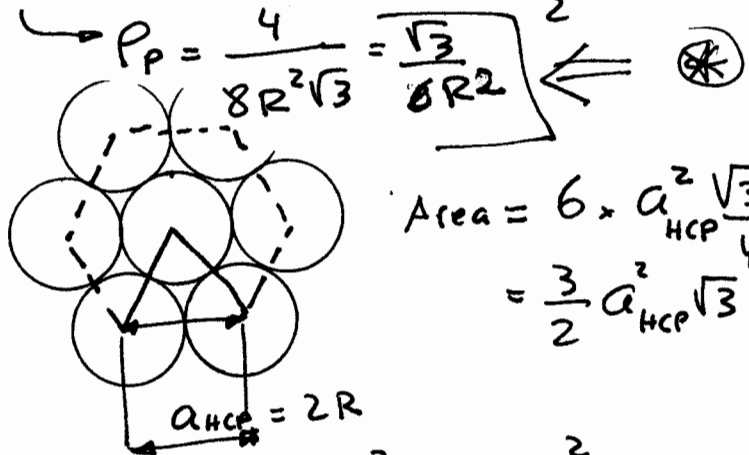
For HCP:

$$a_{\text{HCP}} = 2R$$

$$\# \text{ atoms} = 1 + \frac{1}{3} \times 6 = 3$$

$$P_{\text{HCP}} = \frac{3}{\frac{3}{2} a_{\text{HCP}}^2 \sqrt{3}} = \frac{2}{a_{\text{HCP}}^2 \sqrt{3}}$$

$$P_{\text{HCP}} = \frac{1}{2R^2 \sqrt{3}} = \frac{\sqrt{3}}{6R^2} *$$



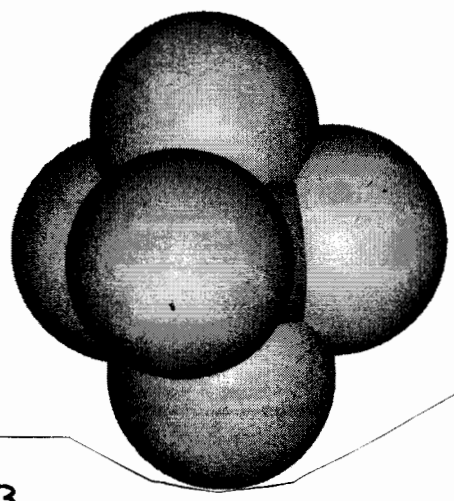
$$\begin{aligned} \text{Area} &= 6 \times \frac{a_{\text{HCP}}^2 \sqrt{3}}{4} \\ &= \frac{3}{2} a_{\text{HCP}}^2 \sqrt{3} \end{aligned}$$

$$a_{\text{HCP}} = 2R \Rightarrow a_{\text{HCP}}^2 = 4R^2$$

same

**Exercise N°3** 5 pts.

Arsenic pentachloride  $AsCl_5$  (molecule shown on the right) is a common environmental hazard in soils that comes from fluorocarbon processing. Arsenic (As) atomic number is  $Z = 33$  with  $A = 74.9216$  while chlorine's  $Z=17$  and  $A = 35.453$ .



- Provide the electronic configuration of both elements in their ground state.
- In which groups of the periodic table are they?
- Why do you think they cannot form ionic bonds?
- Describe the hybridization process of arsenic necessary to combine with chlorine through covalent bonds
- Is this a polar or non-polar molecule? Explain

Bonus (1 pt.): Indicate which type the hybridization is (e.g.  $sp^2$ ,  $sp^3$ ,  $sp^3d$ , etc.).

a) Arsenic  $Z = 33$   $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$  Group VA  
 $2 + 2 + 6 + 2 + 6 + 2 + 10 + 3 = 33$  4s 4p 4d  
 Chlorine  $Z = 17$   $1s^2 2s^2 2p^6 3s^2 3p^5$  Group VII A 3s 3p 3d  
 $2 + 2 + 6 + 2 + 5 = 17$  2s 2p 1s

b) As Group VA (miss 3 electrons to become a noble gas) V VI VII VIII  
 Cl Group VII A (miss 1  $e^-$  to be a noble gas) | As | | Cl | |

c) They are too close (neighboring groups) so there is not enough difference in electronegativities

d) We need Hund's rule:  
 $4s^2 4p^3$  4s 4p Valence 3  
 hybridization 4d Valence 5  
 Bonus: hybrid type  $sp^3d$

e) It's a non polar molecule. Since the charges are symmetrically distributed around the "center" of the molecule

**Exercise N°2** 8 pts.

In medicine thallium (Tl) has limited use because of the narrow margin between toxicity and therapeutic benefits to treat skin diseases. For Tl,  $Z = 81$  and  $A = 204.3833$ . At room temperature thallium is HCP and its lattice constants are:  $a = 0.34566 \text{ nm}$  and  $c = 0.55248 \text{ nm}$ . Respond to the following requests clearly:

- Calculate the APF of this crystal. Does thallium have an ideal HCP unit cell? Explain.
- Calculate the theoretical density in  $\text{g/cm}^3$  of this metal.  $N_A = 6.0221367 \cdot 10^{23}$  atoms/mole
- Consider the interstice (space) located in the position  $0,0,0, \frac{1}{2}$  of thallium unit cell and indicate its coordination number.
- At  $230^\circ\text{C}$ , thallium changes from HCP to BCC ( $a = 0.3882 \text{ nm}$ ). Calculate the percent of volume change of the HCP  $\rightarrow$  BCC phase transformation of thallium. Is it an expansion or a shrinkage (contraction)?

Bonus (1 pt.): Thallium is very close to gold ( $Z=79$ ) in the Periodic Table. While Tl melting point is  $304^\circ\text{C}$ , gold melting point is  $1064.2^\circ\text{C}$ . Explain carefully why you think there is such a large difference in melting points.

a)  $\text{Vol} = \text{Area base} \cdot c$

Area base =  $6 \cdot \Delta$   
 $\frac{h}{a} = \cos 30^\circ = \frac{\sqrt{3}}{2} \therefore h = \frac{\sqrt{3}}{2} a$



$$\Delta = \frac{ah}{2} = \frac{\sqrt{3}}{4} a^2$$

$$\text{Area base} = 6 \frac{\sqrt{3}}{4} a^2 = \frac{3\sqrt{3}}{2} a^2$$

$$\text{Vol} = \frac{3\sqrt{3}}{2} a^2 \cdot c = \frac{3\sqrt{3}}{2} (0.34566)^2 \cdot (0.55248) \text{ nm}^3$$

$$\text{Vol} = 0.1715 \text{ nm}^3$$

$$\text{APF} = \frac{\# \text{ atoms} \cdot \frac{4}{3} \pi R^3}{\text{Vol}}$$

$$R^3 = \left(\frac{a}{2}\right)^3 = \frac{a^3}{8} \quad \# \text{ atoms} = 6$$

$$\text{APF} = \frac{6 \cdot \frac{4}{3} \pi \frac{a^3}{8}}{\text{Vol}} = \frac{\pi a^3}{\text{Vol}} = \frac{\pi (0.34566)^3 \text{ nm}^3}{0.1715 \text{ nm}^3}$$

$$\boxed{\text{APF} = 0.7565}$$

or 75.65%

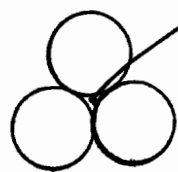
For an ideal HCP  
APF = 74%

b)

$$\rho = \frac{6 \cdot \frac{A}{N_A}}{\text{Vol}} = 6 \times 204.3833 \frac{\text{g}}{\text{mol}} \cdot \frac{1}{6.02 \cdot 10^{23} \frac{\text{atom}}{\text{mol}}} \cdot \frac{10^{21} \text{ nm}^3/\text{cm}^3}{0.1715 \text{ nm}^3}$$

$$\boxed{\rho = 11.87 \frac{\text{g}}{\text{cm}^3}}$$

c)



$0,0,0, \frac{1}{2}$   
has 3 neighbors  
on the side plus one on  
top and one below  
So: CN = 5

$$d) \frac{\Delta V}{V} \% = \left( \frac{V_{\text{BCC}} - V_{\text{HCP}}}{V_{\text{HCP}}} \right) 100 = \left( \frac{V_{\text{BCC}}}{V_{\text{HCP}}} - 1 \right) 100$$

$$V_{\text{BCC}} = \frac{a_{\text{BCC}}^3}{2} = \frac{(0.3882 \text{ nm})^3}{2} = 0.02925 \text{ nm}^3$$

# atoms  $\rightarrow$  (2)

$$V_{\text{HCP}} = \frac{0.1715 \text{ nm}^3}{6} \text{ (calculated in (a))}$$

# atoms  $\rightarrow$  (6)

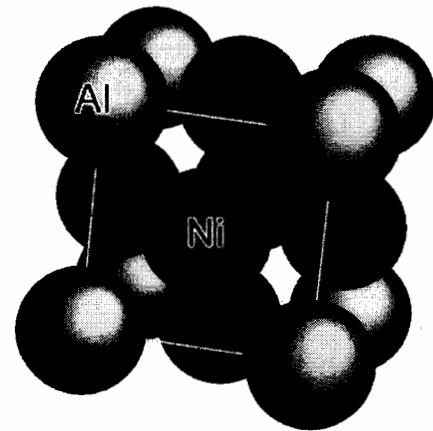
$$V_{\text{HCP}} = 0.02858 \text{ nm}^3$$

$$\frac{\Delta V}{V} \% = \left( \frac{0.02925}{0.02858} - 1 \right) 100 = +2.334\% \text{ Expansion}$$

Bonus: Gold has a covalent component to the metallic nature of the bonding. The bond is stronger and the  $E_{\text{bond}}$  is more negative.

## Exercise N°4 6 pts.

AlNi<sub>3</sub> has been used for its high thermal stability in mechanical parts subject to high heat sources. Its unit cell is shown on the left with aluminum atoms being at the corners of the cube. The x-ray diffraction spectrum shown is a partial one obtained with a Co target (for Co-K $\alpha$ ,  $\lambda = 0.1788965$  nm). This is a cubic intermetallic compound for which you are requested to:



- Compute its lattice parameter in nm.
- Calculate its theoretical density (in g/cm<sup>3</sup>) knowing that for Al, Z=13 and A = 26.9815, and for Ni, Z= 28 and A = 58.71
- We know that in this special cubic compound, the (110) plane should reflect x-rays. Please calculate the position of the (110) plane in the spectrum.
- Justify why we use the term *theoretical density*. How close is this one to the real one? Provide a clear answer in 5 sentences.

**Bonus (2 pts.):** Calculate the chemical composition of this compound in weight percent (Al wt.% and Ni wt.%).

a) Peak (111) @  $51.47^\circ = 2\theta_{111}$

$$\lambda = 2d \sin \theta \quad \therefore \quad d_{111} = \frac{\lambda}{2 \sin \theta_{111}} = \frac{a}{\sqrt{1^2+1^2+1^2}}$$

$$a = \frac{\sqrt{3}}{2} \cdot \frac{0.1788965 \text{ nm}}{\sin\left(\frac{51.47^\circ}{2}\right)}$$

$$a = 0.3568 \text{ nm}$$

b)  $\rho = \frac{n_{\text{Al}} \cdot A_{\text{Al}} + n_{\text{Ni}} \cdot A_{\text{Ni}}}{a^3} \cdot \frac{1}{N_A}$

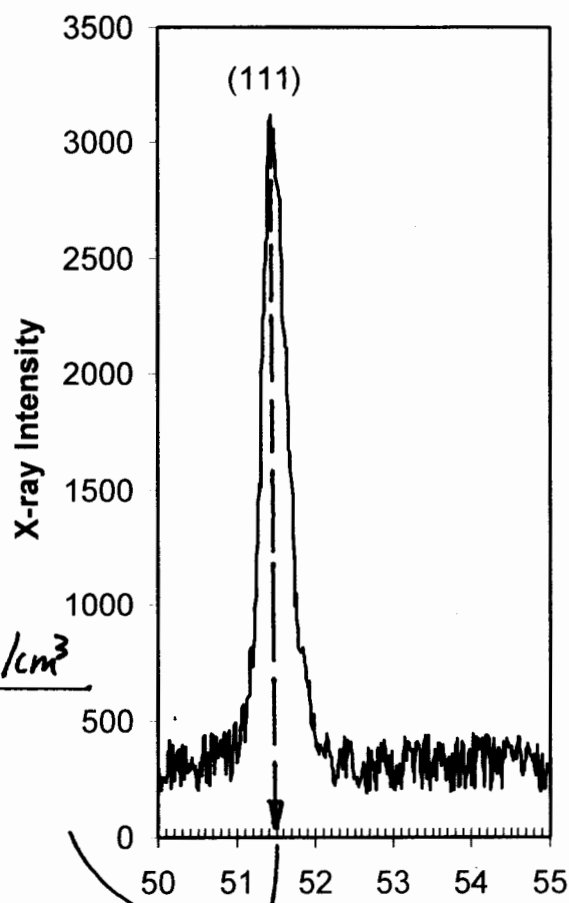
$$n_{\text{Al}} = \frac{1}{8} \times 8 = 1 \quad n_{\text{Ni}} = \frac{1}{2} \times 6 = 3$$

$$\rho = \frac{(26.9815 + 3 \cdot 58.71)}{0.04542 \text{ nm}^3} \cdot \frac{\text{g/mol} \cdot 10^{21} \text{ nm}^3/\text{cm}^3}{6.022 \cdot 10^{23} \text{ at/mol}}$$

$$\rho = 7.42 \text{ g/cm}^3$$

c)  $\sin \theta_{110} = \frac{\lambda}{2d_{110}} = \frac{\lambda}{2} \frac{1}{\frac{a}{\sqrt{1^2+1^2+0^2}}} = \frac{\sqrt{2}}{2} \frac{\lambda}{a}$

$$2\theta_{110} = 2 \cdot \arcsin\left(\frac{\sqrt{2}}{2} \frac{0.1788965}{0.3568}\right) = 42.50^\circ = 2\theta_{110}$$

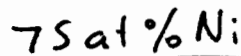


51.47° 2θ



d) "Theoretical" because of the existence of vacancies. The difference between real (measured) density and theoretical density is not much. Only when the solid approaches its melting point the number of vacancies affect the measured density (Al example in class).

Bonus :



$$\text{wt\% Al} = \frac{25 \times 26.9815}{25 \times 26.9815 + 75 \times 58.71} \times 100$$
$$= 13.28 \text{ wt\% Al}$$

$$\text{wt\% Ni} = 100 - 13.28 = 86.72 \text{ wt\% Ni}$$