The University of Western Ontario   Name:_____
Department of Physics and Astronomy   Student #:_____

P2800 Fall 2008

Questions (Total - 20 points):

1.   Of the noble gases Ne, Ar, Kr and Xe, which should be the most chemically reactive and why? (0.5 point)

Xenon should be most reactive since its outermost electrons ($5s^2 6p^6$) are further away from the nucleus than the other noble gases, and thus easier to remove.

2.   Write the electron configuration of the following 5 elements and their ions (1.5 point):

F	$1s^2 2s^2 2p^5$	F^{-1}	$1s^2 2s^2 2p^6$
Ti	[Ar] $4s^2\ 3d^2$	Ti^{+2}	[Ar] $3d^2$
		Ti^{+4}	[Ar]
Y	[Kr] $5s^2\ 4d^1$	Y^{+3}	[Kr]
Ag	[Kr] $5s^1\ 4d^{10}$	Ag^{+1}	[Kr] $4d^{10}$
As	[Ar] $4s^2\ 3d^{10}\ 4p^3$	As^{+3}	[Ar] $4s^2\ 3d^{10}$
		As^{-3}	[Ar] $4s^2\ 3d^{10}\ 4p^6$ or [Kr]
		As^{+5}	[Ar] $3d^{10}$

3.   (a) The melting point of the metal potassium is 63.5°C, while that of titanium is 1660°C. What explanation can be given for this great difference in melting temperatures?

The significantly higher melting point of titanium, as compared to potassium, is in part attributed to the hybridized covalent bonding between the $3d$ and $4s$ orbitals of titanium.

(b) Explain the trend of the melting temperatures in the series: HF, HCl, HBr and HI in terms of difference in the bonding in these compounds. (1.5 point)

Melting temperature changes as a function of the polarizability; it is higher for the larger molecules higher, their intermolecular interactions are stronger

The polarizability ⇑ and the van der Waals attraction ⇑ from Cl to I , abrupt change between HCl and HF ⇒ formation of hydrogen bonding
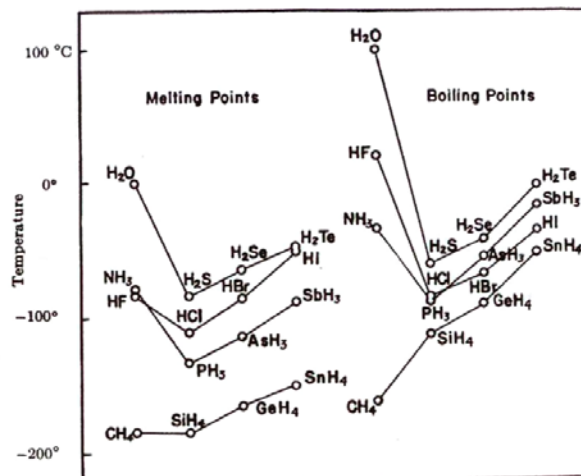

Fig. 6-6 The melting and boiling points of isoelectronic sequences of hydrides. (After Pauling.)

4.   A direction vector passes through a unit cube from point A to point B. What are its direction Miller indices? (1.5 point).

      (a)   A: x = 0.75; y = 0; z = 0.25;   B: x=0.5; y = 1; z = 0

      (b)   A: x = 1; y = 1; z = 0;   B: x=0.25; y = 0; z = 1

      (c)   A: x = 1; y = 0; z = 1;   B: x=0; y = 1; z = 1

(a) $[\bar{1}4\bar{1}]$ (b) $[\bar{3}4\bar{4}]$ (c) $[\bar{1}10]$

5.   What are the Miller indices of the cubic crystallographic planes shown in Figure 1? (1 point)
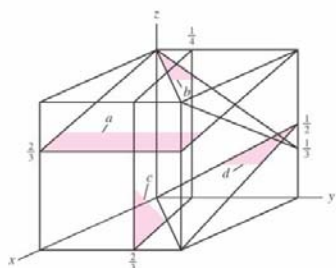

Figure 1.

(a) use (1, 0, 1) as origin; intercepts: x=-1, y = ∞, z= -1/3 ⇒reciprocals: -1, 0, -3 ⇒ $(\bar{1}0\bar{3})$

(b) use (0, 1, 1) as origin; intercepts: x=1, y = -1, z= -2/3 ⇒reciprocals: 1, -1, -3/2 ⇒ $(2\bar{2}\bar{3})$

(c) use (0, 0, 0) as origin; intercepts: x=-3/5, y = 1/4, z= ∞⇒reciprocals: 1, -12/5, 0⇒ $(\bar{5}12\,0)$

(d) use (0, 1, 0) as origin; intercepts: x=1, y = -1, z= 1/2⇒reciprocals: 1, -1, 2 ⇒ $(1\bar{1}2)$

6.   Determine the Miller-Bravais direction indices of the 6 vectors (a-f) originating at the center of the lower plane and ending at the endpoints of the upper basal plane as indicated in Figure 2. (1.5 point)
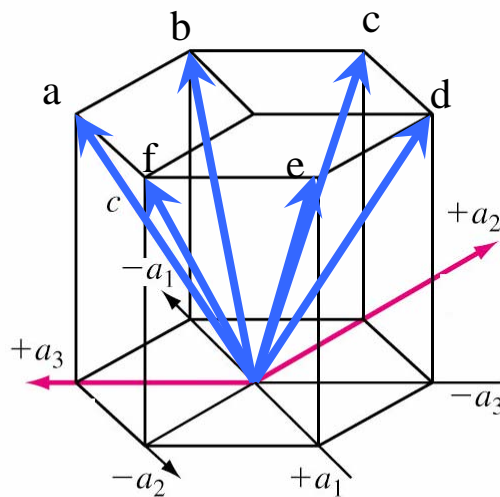
a) $[\bar{1}\,\bar{1}21]$

b) $[\bar{2}111]$

c) $[\bar{1}2\bar{1}1]$

d) $[11\bar{2}1]$

e) $[2\bar{1}\,\bar{1}1]$

f) $[1\bar{2}11]$

Figure 2.

7.   Determine the Miller-Bravais indices of the hexagonal crystal planes *a, b, c* in Figure 3. (1.5 point)

a) Intercepts: $a_1=\infty$, $a_2=1$, $a_3=-1$, $c=\infty$
reciprocals: 0, 1, -1, 0 $(01\bar{1}0)$

b) New origin, intercepts: $a_1=1$, $a_2=-1$, $a_3=\infty$, $c=1$
reciprocals: 1, -1, 0, 1 $(1\bar{1}01)$

c) Intercepts: $a_1=1$, $a_2=-1$, $a_3=\infty$, $c=1$
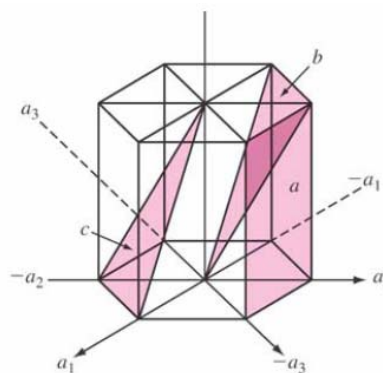reciprocals: 1, -1, 0 , 1 $(1\bar{1}01)$

Figure 3

8.   The lattice constant for *bcc* tantalum at 20°C is 0.33026 nm and its density is 16.6 g/cm³. Calculate a value for its atomic mass. (1 point).

Density   16.6 g/cm³   Volume   1 cm³
Mass/unit cell X   Volume $(0.33026nm)^3=(0.33026 \times 10^{-9}m)^3$
X = 16.6 g/cm³ (10^6 cm³/m³) $(0.33026 \times 10^{-9}m)^3$=5.98×10⁻²² g/unit cell

$$\text{Atomic mass} = \frac{5.98 \times 10^{-22} g / \text{unit cell}(6.023 \times 10^{23} atoms / mol)}{2 atoms / \text{unit cell}} = 180.09 g / mol$$

9.   Aluminum is diffused into a thick slice of silicon with <u>no previous aluminum</u> in it at a temperature of 1100°C for 6 h. What is the depth below the surface (in cm) at which the concentration is 10^{16} atoms/cm³ if the surface concentration is 10^{18} atoms/cm³? $D = 2 \times 10^{-12}$ cm²/s for aluminum diffusing in silicon at 1100°C. Use the value of the error function from the table below for a solution (2 point).

Given: $C_s = 10^{18}$ atoms/cm³ $C_x = 10^{16}$ atoms/cm³ $C_o = 0.0$

$t = 6.0$ h $= 2.16 \times 10^4$ s $D_{1100°C} = 2.0 \times 10^{-12}$ cm²/s

$$\frac{C_s - C_x}{C_s - C_o} = \frac{10^{18} - 10^{16}}{10^{18} - 0} = erf\left[\frac{x}{2\sqrt{(2.0 \times 10^{-12} \text{ cm}^2/s)(2.16 \times 10^4 \text{ s})}}\right]$$

$$0.99 = erf\left(\frac{x}{4.157 \times 10^{-4}}\right) = erf\,z$$

Interpolating from Table 5.3,

erf z	z
0.9891	1.8
0.9900	x
0.9928	1.9

$$\frac{0.9900 - 0.9891}{0.9928 - 0.9891} = \frac{x_1 - 1.8}{1.9 - 1.8} \quad x_1 = 1.824$$

Substituting,

$$z = 1.824 = \frac{x}{4.157 \times 10^{-4}}$$

$$x = 7.58 \times 10^{-4} \text{ cm}$$

10.   What $\underline{5}$ factors affect the diffusion rate in solid metal crystals? (0.5 point).

1. Type of diffusion mechanism;
2. Temperature of diffusion;
3. Concentration of the diffusion species (
4. Type of crystal structure;
5. Type of crystal imperfections present.

11.   Based on the data in the table below, is it easier for carbon atoms to diffuse in the *bcc* iron or in *fcc* iron? What is the physical reason for this? (Hint: think about the size of interstitial sites for *fcc* and *bcc* structures)(1.5 points)

Table 5.2 Diffusivities at 500°C and 1000°C for selected solute-solvent diffusion systems

Solute	Solvent (host structure)	Diffusivity (m^2/s) 500°C (930°F)	1000°C (1830°F)
1. Carbon	FCC iron	(5×10^{-15})*	3×10^{-11}
2. Carbon	BCC iron	10^{-12}	(2×10^{-9})
3. Iron	FCC iron	(2×10^{-23})	2×10^{-16}
4. Iron	BCC iron	10^{-20}	(3×10^{-14})

Diffusion is easier in *bcc* iron (diffusivity is higher, see table above)

Consider *bcc* iron lattice, the atomic radius of the Fe is R, and the interstitials are at the
A: (½, 0, 0), (0, ½, 0), (0, 0, ½), and B: (½, ½, 0), positions
$4R = \sqrt{3}a$ $R = (\sqrt{3}a)/4$ or $a = (4R)/\sqrt{3}$
A interstitials: radius of interstitial is r_A
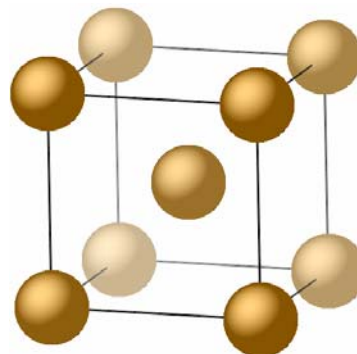$2R + 2r_A = a = (4R)/\sqrt{3}$
$2r_A = R(4/\sqrt{3} - 2)$
$r_A = R((2/\sqrt{3}) - 1) = 0.154 R$

B interstitials: radius of interstitial is r_B
$2R + 2r_B = \sqrt{2} a = (4\sqrt{2} R)/\sqrt{3}$
$r_B = R(2\sqrt{2}/\sqrt{3}) - 1 = 0.63 R$

Consider *fcc* Fe lattice, the atomic radius of the iron is R, and the largest interstitials occur at the
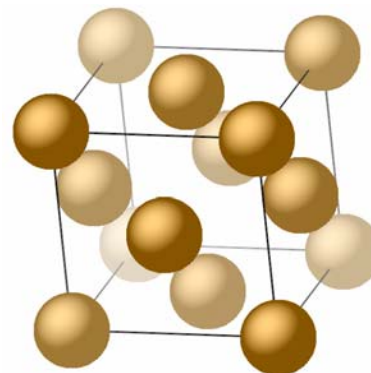(½, 0, 0), (0, ½, 0), (0, 0, ½), *etc.* type positions
$4R = \sqrt{2}a$ $R = (\sqrt{2}a)/4$
Interstitials: radius of interstitial is r
$2R + 2r = a = (4R)/\sqrt{2}$
$r = R(\sqrt{2} - 1) = 0.414 R$

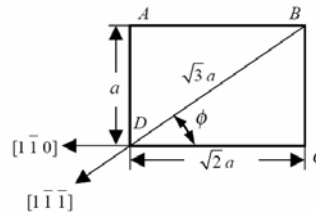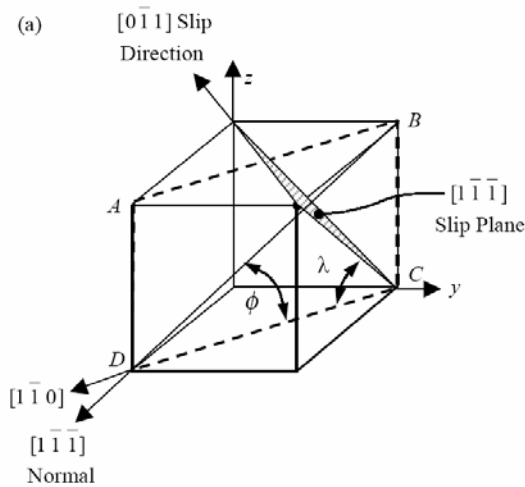*bcc*: $r_B = 0.63 R$ $> fcc$ $r = 0.414 R$

12.   Determine the tensile stress that must be applied to the $[1\bar{1}0]$ axis of a high-purity copper single crystal to cause a slip on the $(1\bar{1}\bar{1})[0\bar{1}\bar{1}]$ system. The resolved shear stress for the crystal is 0.85 MPa. (1.5 points)

$$\tau_r = \sigma\cos\phi\cos\lambda; \quad \sigma = \frac{\tau_r}{\cos\phi\cos\lambda}$$

The angle λ between $[1\bar{1}0]$ stress application and $[0\bar{1}\bar{1}]$ slip direction is

$\lambda = 60°$ $\cos\phi = \sqrt{2}/\sqrt{3} = 0.8165, \phi = 35.3°$

$$\sigma = \frac{0.85 MPa}{\cos 60° \cos 35.3°} = 2.08 MPa$$

13.   Twenty-cm-long rod ($l_0 = 0.22$m) with a diameter of 0.250 cm is loaded (vertically) with a 5000 N weight. If the diameter decreases to 0.210 cm, and assuming that $A_o l_o = A_i l_i$, determine
(a) the engineering stress and strain at this load and
(b) the true stress and strain at this load. (1 point)

Area at start $A_0 = \dfrac{\pi d_0^2}{4} = \dfrac{\pi}{4}(0.25\text{ cm})^2 = 0.04909\text{ cm}^2 = 4.909\times10^{-6}\text{ m}^2$

Area under load $A_i = \dfrac{\pi d_i^2}{4} = \dfrac{\pi}{4}(0.21\text{ cm})^2 = 0.03464\text{ cm}^2 = 3.464\times10^{-6}\text{ m}^2$

Assuming $A_0 l_0 = A_i l_i$ or $l_i / l_0 = A_0 / A_i$,

A   Engineering stress $= \dfrac{F}{A_0} = \dfrac{5000\text{ N}}{4.909\times10^{-6}\text{ m}^2} = 1019\times10^6\text{ Pa} = 1019\text{ MPa}$

B   Engineering strain $= \varepsilon = \dfrac{l_i - l_0}{l_0} = \dfrac{A_0}{A_i} - 1 = \dfrac{4.909\times10^{-6}\text{ m}^2}{3.464\times10^{-6}\text{ m}^2} - 1 = 1.417 - 1 = 0.417$

True stress $= \sigma_T = \dfrac{F}{A_i} = \dfrac{5000\text{ N}}{3.464\times10^{-6}\text{ m}^2} = 1443\times10^6\text{ Pa} = 1443\text{ MPa}$

True strain $= \varepsilon_T = \ln\dfrac{l_i}{l_0} = \ln\dfrac{A_0}{A_i} = \ln\left[\dfrac{0.04909\text{ cm}^2}{0.03462\text{ cm}^2}\right] = \ln(1.418) = 0.349$

14.   Discuss the advantages and disadvantages of using electron microscopes in comparison with X-ray diffraction for determining the structure of a crystal. (1.5 point).

The main advantage of electron microscopes is that they produce a direct image of the crystal, whereas X-ray methods produce a diffraction pattern from which the crystal structure must be calculated. Having a direct image means that it is easy to identify defects in the crystal structure.

The main disadvantage of an electron microscope is that only very thin samples can be measured, whereas X-ray methods can be used with bulk samples In addition, X-ray methods allow quantitative measurements of the atomic spacing to be made with great accuracy (up to hundredths of Å). Such information cannot be obtained from an electron microscopy.

15.   An *fcc* metal crystal is illuminated with X-rays of wavelength of 0.09nm. The crystal is rotated and the angles at which Bragg reflections occur are measured. Which set of crystal planes will give the smallest angle for first-order reflection (n = 1)? If the angle (Θ) is 18.9° determine the spacing between these crystal planes. At what angle will first-order reflection be obtained from the (200) and (220) crystal planes? (1.5 point).

For *fcc* crystals first diffraction peaks are for the {111}, {200}, {220}, … planes $\Rightarrow$

$\Rightarrow$ {111}

$$n \times \lambda = 2d \sin \Theta \qquad \sin \Theta = \frac{n \times \lambda}{2d} = \frac{\lambda}{2d}$$

The smallest angle $\Rightarrow$ the smallest $\sin \Theta \Rightarrow$ for the largest interplanar separation d

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \Rightarrow \text{the smallest observable } \sqrt{h^2 + k^2 + l^2}$$

$$\Theta = 18.9^o, \quad \sin \Theta = 0.32392, \quad d = \frac{0.09nm}{2 \times 0.32392} = 0.13892nm$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}, \quad a = d\sqrt{h^2 + k^2 + l^2} = 0.13892\sqrt{1^2 + 1^2 + 1^2} = 0.13892\sqrt{3} = 0.24061nm$$

$$d_{200} = \frac{0.24061nm}{\sqrt{2^2 + 0^2 + 0^2}} = \frac{0.24061}{\sqrt{4}} = 0.1203nm \,; \Theta_{200} = 22.0^o$$

$$d_{220} = \frac{0.24061nm}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{0.24061}{\sqrt{8}} = 0.08507nm;; \Theta_{220} = 31.9^o$$