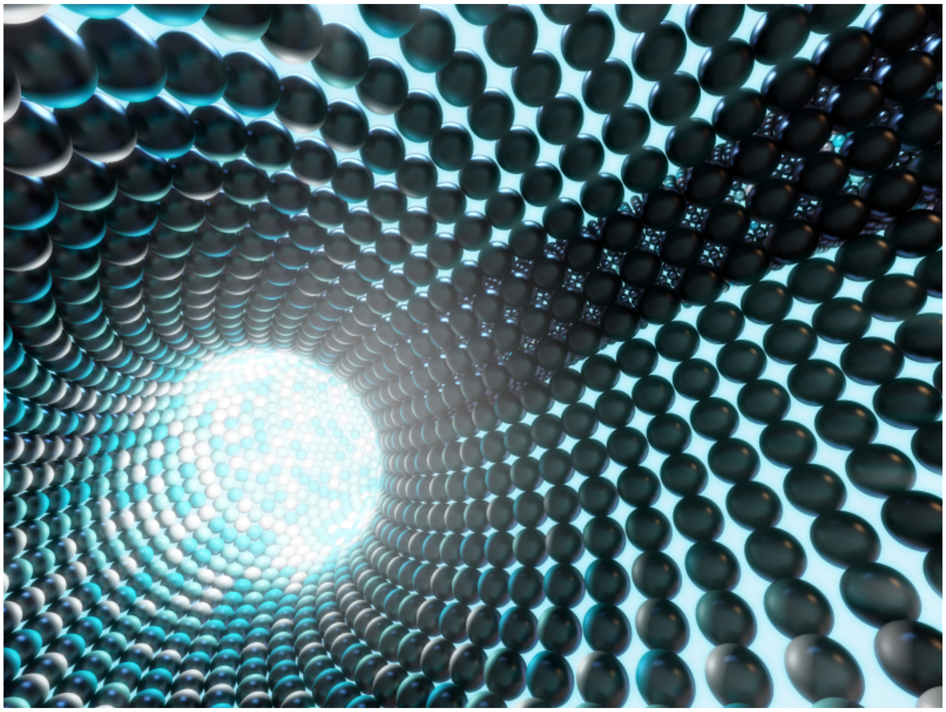
AUB-SPRING 2012- MECH 340- MIDTERM I



STUDENT NAME: **ID:**

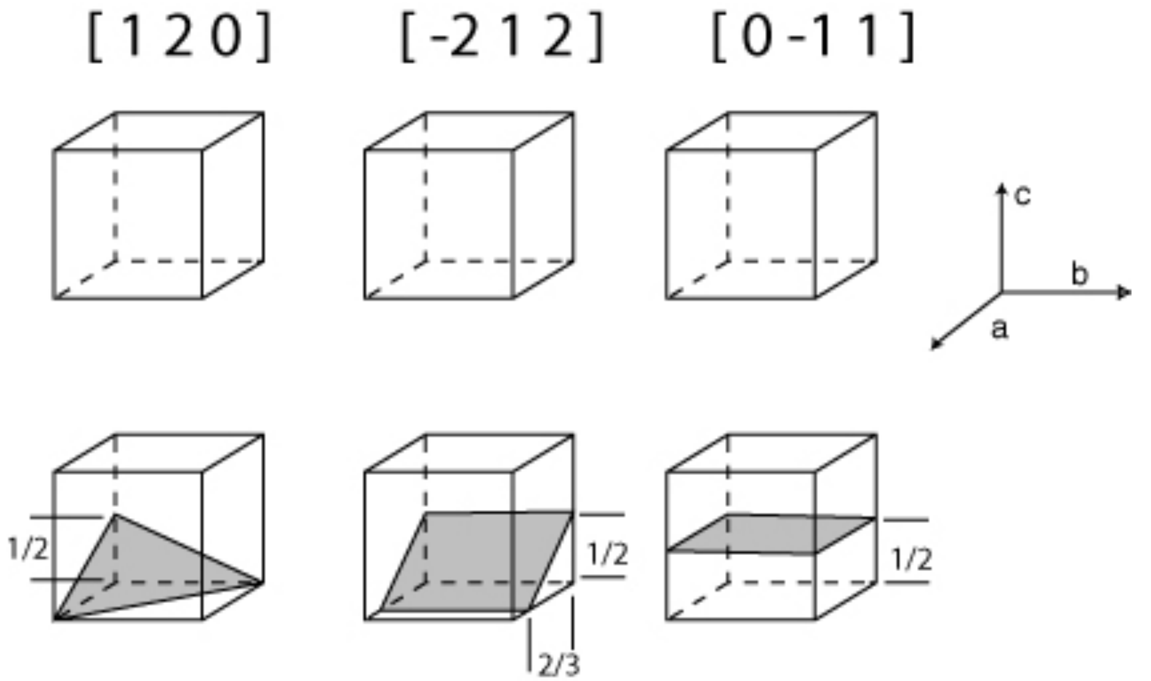
For instructor use only:

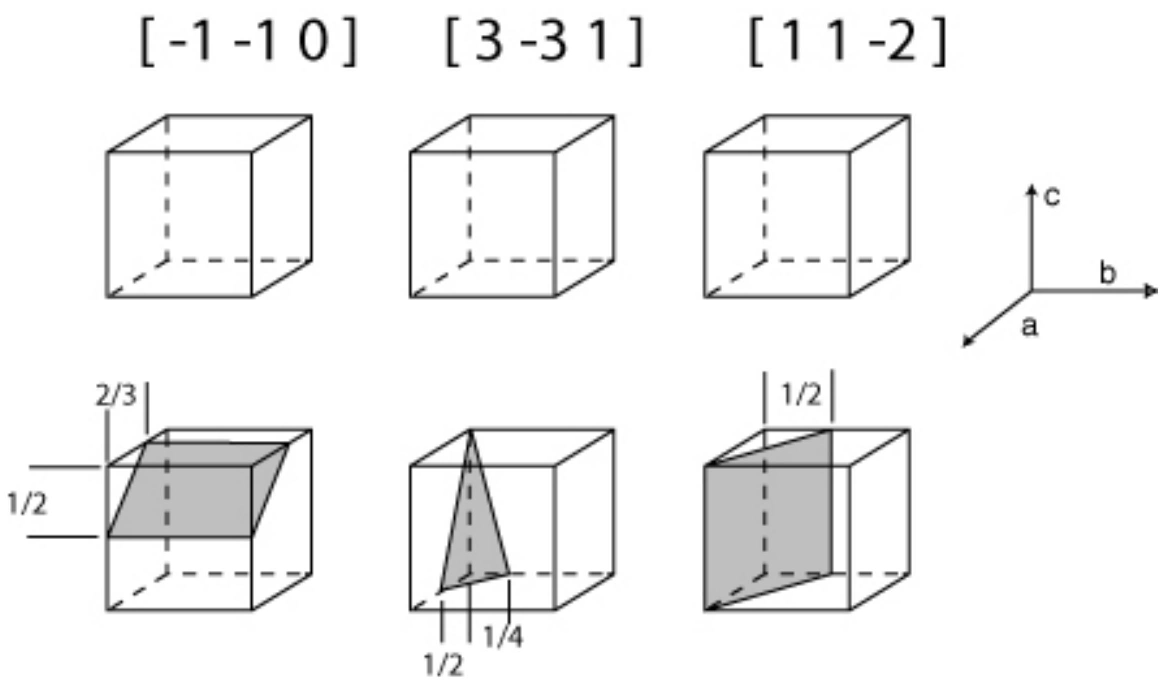
Problem 1:
Problem 2:
Problem 3:

Final Grade:

Part I - Crystalline structures-18 pts Total

a) On the unit cells below, draw the listed DIRECTIONS in the top row, and determine the Miller Indices of the PLANES in the bottom row.

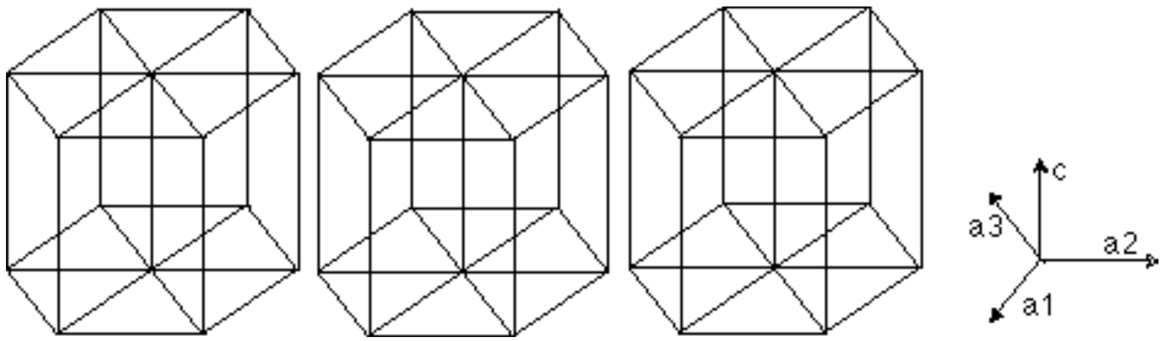


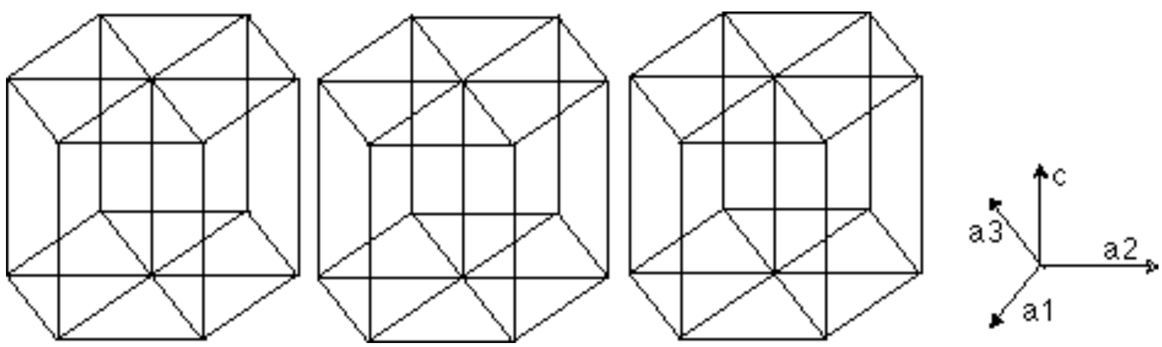


b) Illustrate on the drawings the positions of the planes within the hexagonal unit cells given below:

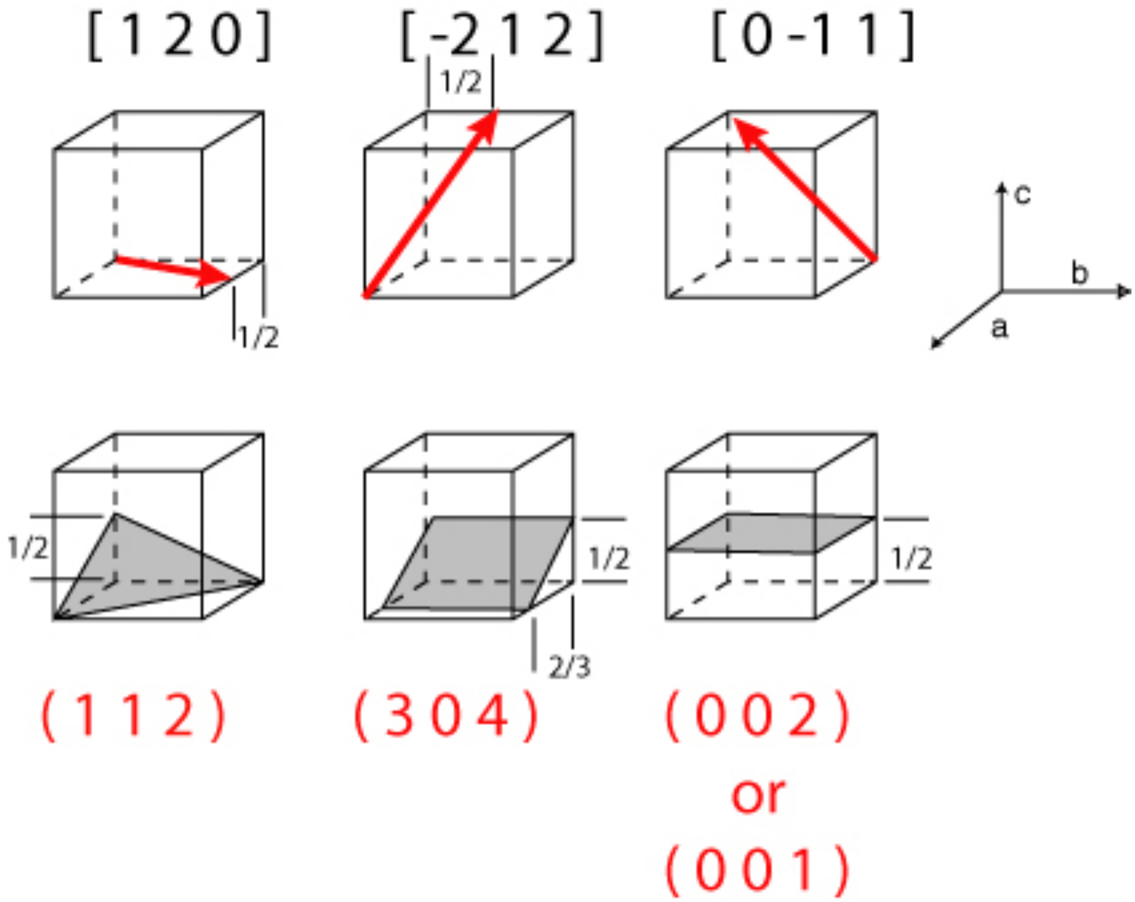
(1 -1 0 0) plane (0 0 0 2) plane (1 0 -1 1) plane

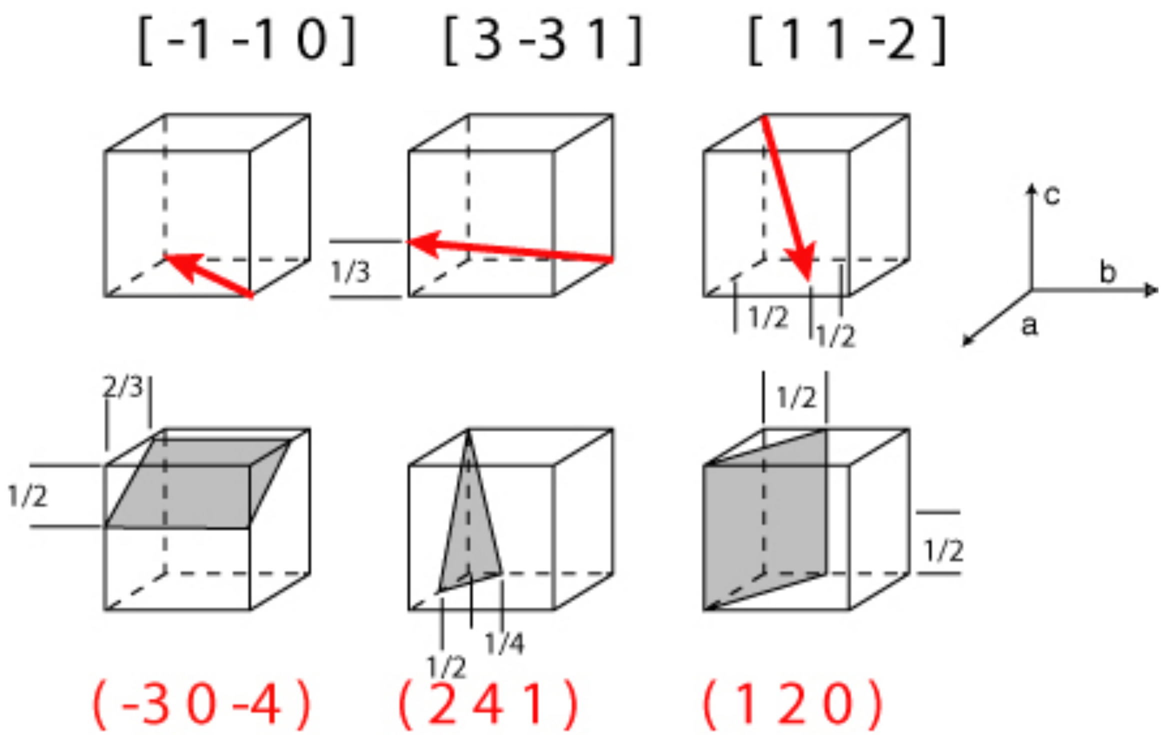
(0 1 -1 0) plane (-1 -1 2 1) plane (2 -1 -1 0) plane



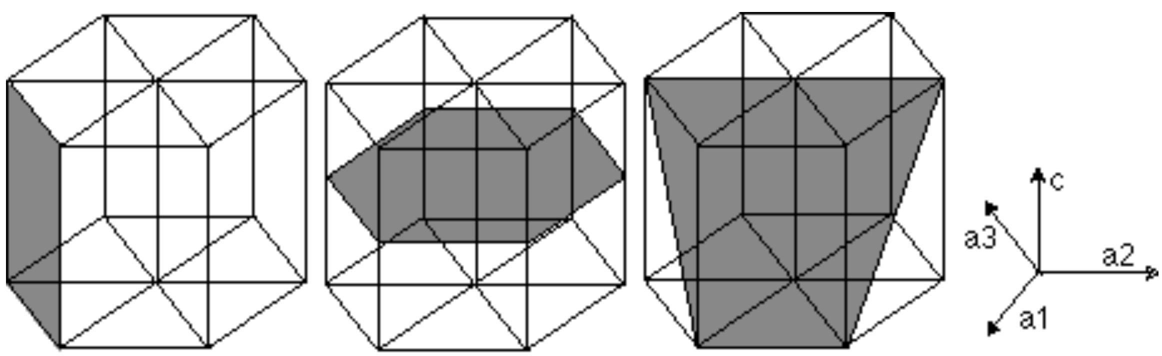


Solution:

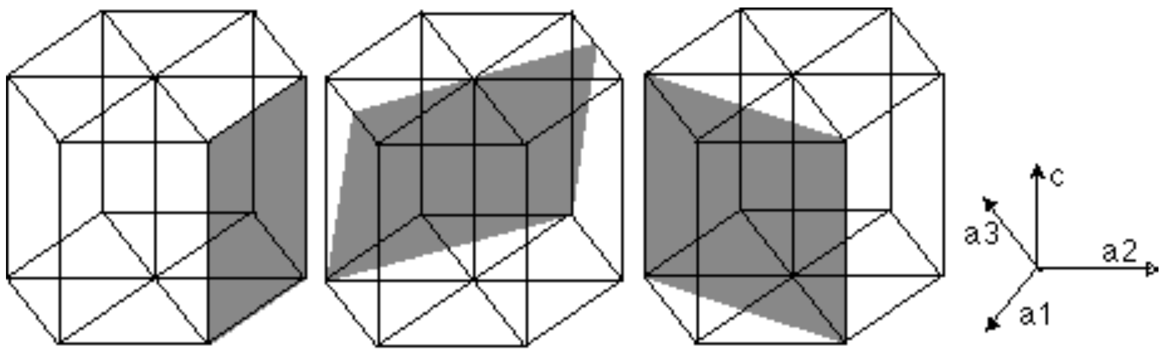




(1 -1 0 0) plane (0 0 0 2) plane (1 0 -1 1) plane



(0 1 -1 0) plane (-1 -1 2 1) plane (2 -1 -1 0) plane



Part II- Miscellaneous Problems-15 pts/qst

1-Select Type I or Type II

2-Do 5 of the 6 problems. Each problem is equally weighted. Some extra information is given at the end of the problem.

3-Solving the 6th question will give you a bonus of 5 pts

TYPE I	TYPE II
1) Compute the number of atoms/m^3 in pure Al. Density of Al = 2.71 g/cm^3 A(Al) = 26.98 Z(Al) = 13 Crystal Structure = FCC	1) An Fe-C alloy initially containing 0.15wt%C is heated in an carbon-rich environment in a furnace at 1400 K. The carbon atmosphere reacts at the surface of the alloy so that the surface carbon content is 0.45wt%C. Given that the D for carbon in iron at 1400 K is 6.9 X 10^-11 m^2/s, at what position will the carbon concentration be 0.35wt%C in 10 hours?
2) Show that the minimum ionic radius ratio for a coordination number of 6 is 0.414. (HINT: some ionic solid crystal structures are included on the last page.)	2) We have a 100kg ingot "master" alloy of composition Nb-10at%Hf. We add 50kg of Nb to this master alloy. What is the overall composition IN WEIGHT PERCENT of the new 150kg ingot? A(Nb) = 92.91 g/mole A(Hf) = 178.49 g/mole
3) An Fe-C alloy initially containing 0.35wt%C is heated in an oxygen-rich environment in a furnace at 1400 K. The	3) The diffusion coefficients for iron in nickel are: D = 9.4 X 10^-16 m^2/s at T = 1273 K, and D = 2.4 X 10^-14 m^2/s at

oxygen atmosphere reacts with the carbon at the surface of the alloy so that the surface carbon content is essentially ZERO, causing the carbon to diffuse out of the alloy (decarburization). Given that the D for carbon in iron at 1400 K is 6.9 X 10^-11 m^2/s, at what position will the carbon concentration be 0.15wt%C in 10 hours?	1473 K. Find the values of Do and Qd, and the temperature at which the diffusion coefficient is D = 5.0 X 10^-15 m^2/s.
4) We have a 100kg ingot "master" alloy of composition Nb-10at%Hf. How many kg of Nb would we need to add to this master alloy to make the overall composition Nb-5at%Hf? ANb = 92.91 g/mole AHf = 178.49 g/mole	4) A hypothetical ceramic material of composition XY is found to have a density of 10.45 g/cm^3 and a unit cell of cubic symmetry with a cell edge of a = 0.43 nm. The atomic weights of the components are A(X) = 86.6 g/mole and A(Y) = 40.3 g/mole. Given this information, which of the following crystal structures are possible for this ceramic? Rock salt, cesium chloride, or zinc blende. (There may be more than one answer…)
5) A hypothetical ceramic material of composition XY is found to have a density of 2.65 g/cm^3 and a unit cell of cubic symmetry with a cell edge of a = 0.43 nm. The atomic weights of the components are A(X) = 86.6 g/mole and A(Y) = 40.3 g/mole. Given this	5) Show that the minimum ionic radius ratio for a coordination number of 8 is 0.732. (HINT: some ionic solid crystal structures are included on the last page.)

information, which of the following crystal structures are possible for this ceramic? Rock salt, cesium chloride, or zinc blende.	
6) The diffusion coefficients for silver in copper are: D = 5.5 X 10^-16 m^2/s at T = 650 degree C, and D = 1.3 X 10^-13 m^2/s at 900 degrees C. Find the values of Do and Qd, and calculate the diffusion coefficient for a temperature of T = 875 degrees C.	6) Compute the number of atoms/m^3 in pure K. Density of K = 0.862 g/cm^3 A(K) = 39.09 Z(K) = 19 Crystal Structure = BCC

Useful information

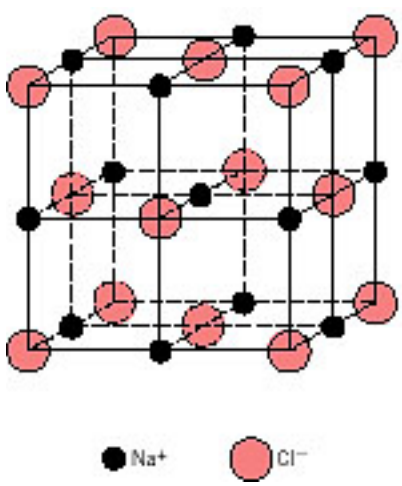


FIGURE 13.2 A unit cell for the rock salt, or sodium chloride (NaCl), crystal structure.

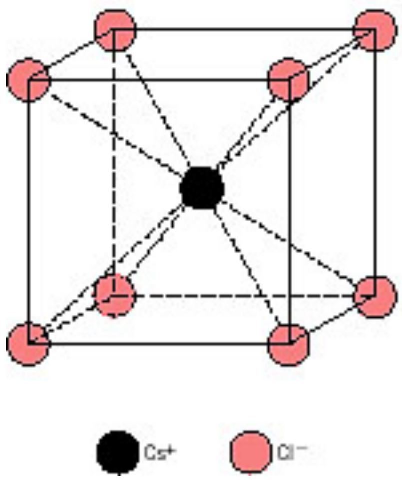


FIGURE 13.3 A unit cell for the cesium chloride (CsCl) crystal structure.

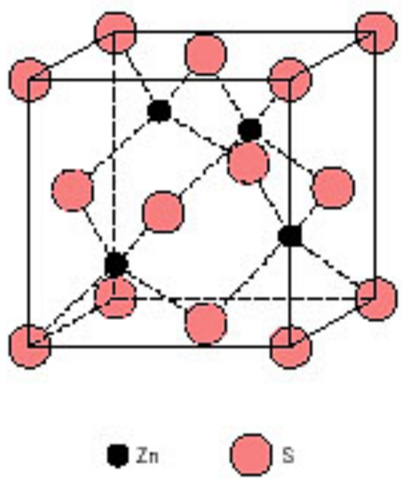


FIGURE 13.4 A unit cell for the zinc blende (ZnS) crystal structure.

Table 5.1 Tabulation of Error Function Values

z	$erf(z)$	z	$erf(z)$	z	$erf(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

SOLUTIONS

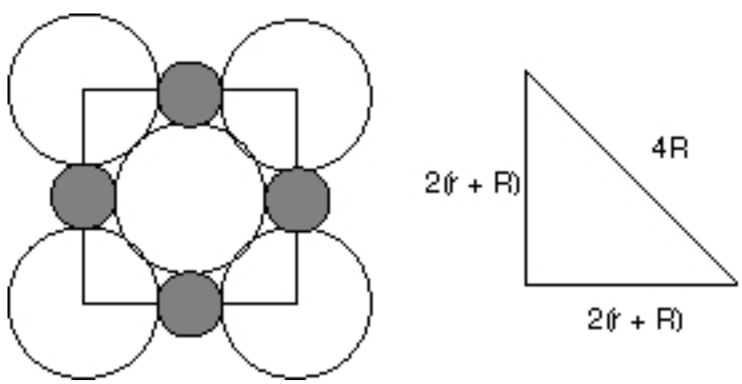
TYPE I

1)

$$\frac{\#\text{atoms}}{m^3} = \frac{\rho\left[g/m^3\right]}{A_{Al}\left[g/\text{mole}\right]} N_o\left[\text{atoms}/\text{mole}\right] = \frac{2.71\times10^6\left[g/m^3\right]}{26.98\left[g/\text{mole}\right]}\left(6.02\times10^{23}\left[\text{atoms}/\text{mole}\right]\right)$$

$$\frac{\#\text{atoms}}{m^3} = 6.05\times10^{28}\left[\text{atoms}/m^3\right].$$

2) The crystal structure we should use is the NaCl structure. Look at the geometry of the (001) plane: The smallest atom size is found when the three large atoms touch each other along the face diagonal, and the small and large atoms touch along the unit cell edge. This gives us the right triangle shown below:



Solving for the atomic ratio, we get:

$$4R^2 = 2(r+R)^2 = 2R^2\left(\frac{r}{R}+1\right)^2$$

$$2 = \left(\frac{r}{R}+1\right)^2 \Rightarrow \sqrt{2}-1 = \frac{r}{R}$$

$$\frac{r}{R} = 0.414$$

3) We can apply the "standard" solution to Ficks Second Law from class: a semi-infinite bar with an

infinite source at x=0.

$$C_x = 0.15\ ;\ C_o = 0.35\ ;\ C_s = 0.0\ ;$$

$$\frac{C_x - C_o}{C_s - C_o} = \frac{0.15-0.35}{0.0-0.35} = 0.571 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.429 \Rightarrow \frac{x}{2\sqrt{Dt}} = 0.401$$

$$x = (0.401)\left(2\sqrt{Dt}\right) = (0.401)\left(2\sqrt{\left(6.9\times10^{-11}\,m^2/s\right)(10\,hr)(3600s/hr)}\right)$$

$$x = 1.26\times10^{-3}m = 1.26mm.$$

4) Four steps to take here:

(1) Convert master alloy composition to wt% :

$$wt\%Hf = \frac{(at\%Hf)(A_{Hf})}{(at\%Hf)(A_{Hf}) + (at\%Nb)(A_{Nb})}$$

$$wt\%Hf = \frac{(10)(178.49g/mole)}{(10)(178.49g/mole) + (90)(92.91g/mole)}$$

$$wt\%Hf = 0.176 = 17.6\%$$

(2) Convert target composition to wt% :

$$wt\%Hf = \frac{(5)(178.49g/mole)}{(5)(178.49g/mole) + (95)(92.91g/mole)}$$

$$wt\%Hf = 0.092 = 9.2\%Hf \Rightarrow 90.8wt\%Nb$$

(3) How much mass of Nb, Hf do we have in the master alloy?

$$M_{Hf} = (100kg)17.6\% = 17.6kgHf$$

$$M_{Nb} = 100kg - 17.6kg = 82.4kg.$$

(4) Find how much new Nb to get target wt% composition :

$$wt\%Nb = 0.908 = \frac{82.4kg + Xkg}{100kg + Xkg}$$

$$90.8kg - 82.4kg = (1-0.908)X \Rightarrow X = 91.3kgNb.$$

5) We know a couple of things about these ceramic crystal structures. Since the composition of the ceramic is an equal mixture (by atomic fraction) of X and Y, the crystal unit cell will have the same number of X atoms as Y atoms. We also know the relation for calculating the density of a crystalline

solid. We can use these together to find out how many atoms per unit cell the ceramic compound has.

$$\rho = \frac{\text{weight of atoms/u.c.}}{\text{volume/u.c.}}$$

$$\text{Volume} = \left(0.43\times10^{-7}\,\text{cm}\right)^3 = 7.9\times10^{-23}\,\text{cm}^3.$$

$$\text{Weight} = \frac{(\#\,\text{atoms / u.c.})\left(A_x + A_y\right)}{2N_o} = \frac{(\#\,\text{atoms / u.c.})(86.6\,\text{g / mole} + 40.3\,\text{g / mole})}{2\left(6.02\times10^{23}\,\text{atoms / mole}\right)}$$

$$\text{Weight} = (\#\,\text{atoms / u.c.})\left(1.05\times10^{-22}\,\text{g / atom}\right)$$

So that :

$$\rho = \frac{(\#\,\text{atoms / u.c.})\left(1.05\times10^{-22}\,\text{g / atom}\right)}{7.9\times10^{-23}\,\text{cm}^3} = 2.65\,\text{g / cm}^3 \Rightarrow (\#\,\text{atoms / u.c.}) = 1.99 \approx 2.$$

Compare with the crystal structures:

Rock Salt has (8 corners/8)+(6 faces/2)+(12edges/4)+(1body) = 8 atoms/u.c.

CsCl has (8 corners/8)+(1body) = 2 atoms/u.c.

Zinc Blende has (8 corners/8)+(6 faces/2)+(4 inside the body) = 8 atoms/u.c.

Thus, there is one possible answer: **CsCl structure.**

6) Just like the homework problem; two equations and two unknowns to find Do and Qd, then plug and chug to find D:

$$D_{650} = D_o \exp\left(-\frac{Q_d}{RT_{650}}\right); \quad D_{900} = D_o \exp\left(-\frac{Q_d}{RT_{900}}\right)$$

$$\frac{D_{650}}{D_{900}} = \exp\left(-\frac{Q_d}{R}\left[\frac{1}{T_{650}} - \frac{1}{T_{900}}\right]\right) \Rightarrow Q_d = \frac{-R\ln\left(\frac{D_{650}}{D_{900}}\right)}{\left[\frac{1}{T_{650}} - \frac{1}{T_{900}}\right]}$$

$$Q_d = \frac{-(8.314\,\mathrm{J/mole-K})\ln\left(\frac{5.5\times10^{-16}\,\mathrm{m^2/s}}{1.3\times10^{-13}\,\mathrm{m^2/s}}\right)}{\left[\frac{1}{923\mathrm{K}} - \frac{1}{1173\mathrm{K}}\right]} = 197\ \mathrm{kJ/mole}.$$

$$D_{650} = D_o \exp\left(-\frac{Q_d}{RT_{650}}\right) \Rightarrow D_o = \frac{D_{650}}{\exp\left(-\frac{Q_d}{RT_{650}}\right)} = \frac{\left(5.5\times10^{-16}\,\mathrm{m^2/s}\right)}{\exp\left(-\frac{197{,}000\,\mathrm{J/mole}}{(8.314\,\mathrm{J/mole-K})(923\mathrm{K})}\right)}$$

$$D_o = 7.75\times10^{-5}\ \mathrm{m^2/s}.$$

$$D_{875} = D_o \exp\left(-\frac{Q_d}{RT_{875}}\right) = \left(7.75\times10^{-5}\ \mathrm{m^2/s}\right)\exp\left(-\frac{197{,}000\,\mathrm{J/mole}}{(8.314\,\mathrm{J/mole-K})(1148\mathrm{K})}\right)$$

$$D_{875} = 8.42\times10^{-14}\ \mathrm{m^2/s}.$$

SOLUTIONS

TYPE II
1) We can apply the "standard" solution to Ficks Second Law from class: a semi-infinite bar with an infinite source at x=0.

$C_x = 0.35$; $C_o = 0.15$; $C_s = 0.45$; $\frac{C_x - C_o}{C_s - C_o} = \frac{0.35-0.15}{0.45-0.15} = 0.6667 = 1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$ $\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.3333 \Rightarrow \frac{x}{2\sqrt{Dt}} = 0.305$ $x = (0.305)(2\sqrt{Dt}) = (0.305)\left(2\sqrt{\left(6.9\times10^{-11}\,m^2/s\right)(10hr)(3600s/hr)}\right)$ $x = 9.6\times10^{-4}\,m = 0.96mm = 960\mu m.$
2) Three steps to take here: (1) Convert master alloy composition to wt% : $wt\%Hf = \frac{(at\%Hf)(A_{Hf})}{(at\%Hf)(A_{Hf}) + (at\%Nb)(A_{Nb})}$ $wt\%Hf = \frac{(10)(178.49g/mole)}{(10)(178.49g/mole) + (90)(92.91g/mole)}$ $wt\%Hf = 0.176 = 17.6\%$ (2) How much mass of Nb, Hf do we have in the master alloy? $M_{Hf} = (100kg)17.6\% = 17.6kgHf$ $M_{Nb} = 100kg - 17.6\,kg = 82.4kg.$ (3) Add new Nb and find wt% compositions : $wt\%Hf = \frac{17.6kg}{150kg} = 11.7wt\%Hf.$
3) Just like the homework problem; two equations and two unknowns to find Do and Qd, then plug and chug to find T:

$$D_{1273} = D_o \exp\left(-\frac{Q_d}{RT_{1273}}\right); \quad D_{1473} = D_o \exp\left(-\frac{Q_d}{RT_{1473}}\right)$$

$$\frac{D_{1273}}{D_{1473}} = \exp\left(-\frac{Q_d}{R}\left[\frac{1}{1273K} - \frac{1}{1473K}\right]\right) \Rightarrow Q_d = \frac{-R\ln\left(\frac{D_{1273}}{D_{1473}}\right)}{\left[\frac{1}{1273K} - \frac{1}{1473K}\right]}$$

$$Q_d = \frac{-(8.314 J/mole-K)\ln\left(\frac{9.4\times10^{-16} m^2/s}{2.4\times10^{-14} m^2/s}\right)}{\left[\frac{1}{1273K} - \frac{1}{1473K}\right]} = 253\ kJ/mole.$$

$$D_{1273} = D_o \exp\left(-\frac{Q_d}{RT_{1273}}\right) \Rightarrow D_o = \frac{D_{1273}}{\exp\left(-\frac{Q_d}{RT_{1273}}\right)} = \frac{\left(9.4\times10^{-16} m^2/s\right)}{\exp\left(-\frac{253{,}000 J/mole}{(8.314 J/mole-K)(1273K)}\right)}$$

$$D_o = 2.26\times10^{-5}\ m^2/s.$$

$$D = D_o \exp\left(-\frac{Q_d}{RT}\right) \Rightarrow T = -\frac{Q_d}{R\ln\left(\frac{D}{D_o}\right)} = -\frac{(253{,}000 J/mole)}{(8.314 J/mole-K)\ln\left(\frac{5.0\times10^{-15}\ m^2/s}{2.26\times10^{-5}\ m^2/s}\right)}$$

$$T = 1369K.$$

4) We know a couple of things about these ceramic crystal structures. Since the composition of the ceramic is an equal mixture (by atomic fraction) of X and Y, the crystal unit cell will have the same number of X atoms as Y atoms. We also know the relation for calculating the density of a crystalline solid. We can use these together to find out how many atoms per unit cell the ceramic compound has.

$$\rho = \frac{\text{weight of atoms/u.c.}}{\text{volume/u.c.}}$$

$$\text{Volume} = \left(0.43\times10^{-7}\,\text{cm}\right)^3 = 7.9\times10^{-23}\,\text{cm}^3.$$

$$\text{Weight} = \frac{(\#\,\text{atoms / u.c.})\left(A_x + A_y\right)}{2N_o} = \frac{(\#\,\text{atoms / u.c.})(86.6\,\text{g / mole} + 40.3\,\text{g / mole})}{2\left(6.02\times10^{23}\,\text{atoms / mole}\right)}$$

$$\text{Weight} = (\#\,\text{atoms / u.c.})\left(1.05\times10^{-22}\,\text{g / atom}\right)$$

So that :

$$\rho = \frac{(\#\,\text{atoms / u.c.})\left(1.05\times10^{-22}\,\text{g / atom}\right)}{7.9\times10^{-23}\,\text{cm}^3} = 10.45\,\text{g / cm}^3 \Rightarrow (\#\,\text{atoms / u.c.}) = 7.86 \approx 8.$$

Compare with the crystal structures:

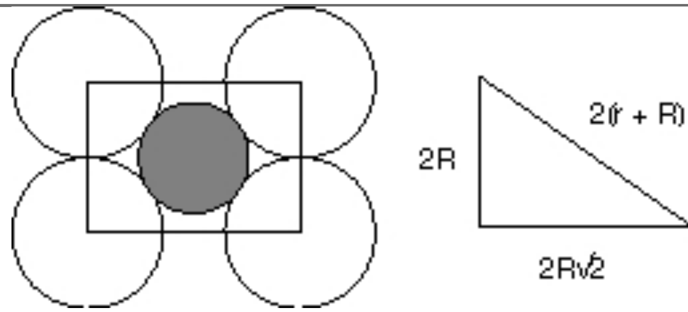
Rock Salt has (8 corners/8)+(6 faces/2)+(12edges/4)+(1body) = 8 atoms/u.c.

CsCl has (8 corners/8)+(1body) = 2 atoms/u.c.

Zinc Blende has (8 corners/8)+(6 faces/2)+(4 inside the body) = 8 atoms/u.c.

Thus, there are two possible answers: **Rock Salt and Zinc Blende.**

5) The crystal structure we should use is the CsCl structure. Look at the geometry of the (110) plane: The smallest atom size is found when the two large atoms touch each other along the cube edgel, and the small and large atoms touch along the unit cell diagonal. This gives us the right triangle shown below:



Solving for the atomic ratio, we get:

$$4R^2 + 8R^2 = 4(r+R)^2 = 4R^2\left(\frac{r}{R}+1\right)^2$$

$$3 = \left(\frac{r}{R}+1\right)^2 \Rightarrow \sqrt{3} - 1 = \frac{r}{R}$$

$$\frac{r}{R} = 0.732$$

6)

$$\frac{\#\text{atoms}}{m^3} = \frac{\rho[g/m^3]}{A_K[g/\text{mole}]} N_o[\text{atoms}/\text{mole}] = \frac{0.862\times10^6[g/m^3]}{39.09[g/\text{mole}]}\left(6.02\times10^{23}[\text{atoms}/\text{mole}]\right)$$

$$\frac{\#\text{atoms}}{m^3} = 1.33\times10^{28}[\text{atoms}/m^3]$$

MCQ (7 pts)- 3 pts, 2pts, 2 pts respectively

1-An x-ray diffraction pattern from a FCC crystal has a peak at $2\theta = 45^\circ$ that is indexed to the (111) plane. What is the lattice parameter? The x-ray wavelength = 0.154 nm.

(a) 0.201 nm

(b) 0.348 nm

(c) 0.189 nm

(d) none of the above

2- The grain size of a material can be determined by:

(a) optical microscopy

(b) x-ray diffraction

(c) the density

(d) all of the above

3-Answer is a

A close packed plane in the BCC structure is the:

(a) $(\bar{1}01)$

(b) (001)

(c) $(\bar{1}11)$

(d) none of the above

FORMULA SHEET

$$N_A = 6.02\times10^{23}\ atoms\ /\ mole$$
$$R = 8.314\ J\ /\ mole \bullet K$$
$$k = 8.62\times10^{-5}\ eV\ /\ atom \bullet K$$
$$K = 273 + {}^{\circ}C$$
$$E = \int F dr$$
$$E_N = -\frac{A}{r} + \frac{B}{r^n} = E_{att.} + E_{rep}$$
$$APF = \frac{V_S}{V_C}$$
$$a = 2R\sqrt{2}$$
$$a = 4R\ /\ \sqrt{3}$$
$$N = \frac{\rho N_A}{A}$$
$$\rho = \frac{nA}{V_C N_A}$$
$$LD = \frac{number\ of\ atoms}{length}$$
$$PD = \frac{number\ of\ atoms}{area}$$
$$n\lambda = 2d_{hkl}\sin\theta_{hkl}$$
$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+\ell^2}}$$
$$n_V = \frac{N_V}{N} = \exp\left(\frac{-Q_V}{kT}\right)$$
$$C_1 = \frac{m_1}{m_1+m_2}\times100$$
$$C_1 + C_2 = 100$$
$$n_{m_1} = \frac{m_1'}{A_1}$$
$$C_1' = \frac{n_{m_1}}{n_{m_1}+n_{m_2}}\times100$$
$$C_2' = \frac{n_{m_2}}{n_{m_1}+n_{m_2}}\times100$$
$$C_1' = \frac{C_1A_2}{C_1A_2+C_2A_1}\times100$$
$$C_2' = \frac{C_2A_1}{C_1A_2+C_2A_1}\times100$$
$$C_1 = \frac{C_1'A_1}{C_1'A_1+C_2'A_2}\times100$$
$$C_2 = \frac{C_2'A_2}{C_1'A_1+C_2'A_2}\times100$$
$$C_1'' = \left(\frac{C_1}{\frac{C_1}{\rho_1}+\frac{C_2}{\rho_2}}\right)x10^3$$
$$C_2'' = \left(\frac{C_2}{\frac{C_1}{\rho_1}+\frac{C_2}{\rho_2}}\right)x10^3$$
$$\rho_{ave} = \frac{100}{\frac{C_1}{\rho_1}+\frac{C_2}{\rho_2}}$$
$$\rho_{ave} = \frac{C_1'A_1+C_2'A_2}{\frac{C_1'A_1}{\rho_1}+\frac{C_2'A_2}{\rho_2}}$$
$$A_{ave} = \frac{100}{\frac{C_1}{A_1}+\frac{C_2}{A_2}}$$
$$A_{ave} = \frac{C_1'A_1+C_2'A_2}{100}$$
$$N_1 = \frac{N_A C_1}{\frac{C_1A_1}{\rho_1}+\frac{A_1}{\rho_2}(100-C_1)}$$
$$N = 2^n - 1$$
$$J = -D\frac{dC}{dx}$$
$$D = D_o\exp\left(\frac{-Q_d}{RT}\right)$$
$$\frac{\partial C}{dt} = D\frac{\partial^2 C}{\partial x^2}$$
$$\frac{C_x - C_o}{C_s - C_o} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

Good Luck