MAE 212
SPRING 2001
HW 3 SOLUTIONS

1.

$$N_{ATOMS} = \rho V \left(\frac{N_{AV}}{AT.WT.} \right)$$

$$= 2.7 \times 10^{6}\ g\ Al/m^3 \times 12.7 \times 10^{-6}\ m$$

$$\times\ 304 \times 10^{-3}\ m \times 22.8\ m \times \left(\frac{0.6023 \times 10^{24}\ ATOMS}{26.98\ g\ Al} \right)$$

$$= \underline{\underline{5.31 \times 10^{24}\ ATOMS}}$$

2.

$$x\, Cu^{63} + y\, Cu^{65} = Cu^{63.55}$$

$$x + y = 1$$

$$\Rightarrow \underline{\underline{72.5\%\ Cu^{63}\ \text{and}\ 27.5\%\ Cu^{65}}}$$

3.

$$\frac{75g}{MW_{Cu}} = \frac{75g}{63.55\ g/mol} = 1.18\ mol\ Cu$$

$$\frac{25g}{MW_{Ni}} = \frac{25g}{58.71\ g/mol} = 0.43\ mol\ Ni$$

$$\frac{1.18}{1.18 + 0.43} = \underline{\underline{73.5\ mol\ \%\ Cu}}$$

$$\Rightarrow \underline{\underline{26.5\ mol\ \%\ Ni}}$$

4. $Z_1 = +1$ for Na^+, $Z_2 = -1$ for Cl^-

$e = 1.6\ 10^{-19}\ C$, $\varepsilon_0 = 8.85\ 10^{-12}\ C^2/Nm^2$

a_0 = sum of the radii of Na^+ and Cl^- ions

$= 0.095\ nm + 0.181\ nm$

$= 0.276\ nm\ 10^{-9}\ \frac{m}{nm} = 2.76\ 10^{-10}\ m$

Finally,

$$F_{attractive} = -\frac{Z_1 Z_2 e^2}{4\pi \varepsilon_0 a_0^2} = -\frac{(+1)(-1)(1.6\ 10^{-19}\ C)^2}{4\pi\left[8.85\ 10^{-12}\ \frac{C^2}{Nm^2}\right](2.76\ 10^{-10}\ m)^2} \Rightarrow$$

$$\boxed{F_{attractive} = +3.02\ 10^{-9}\ N}$$

The repulsive force will be equal and opposite in sign and thus will be $-3.02\ 10^{-9}\ N$. We will use this value in Problem 4.

5.

From $U_{net} = \frac{Z_1 Z_2 e^2}{4\pi \epsilon_0 a} + \frac{b}{a^n} \Rightarrow$

$$F = \underbrace{-\frac{Z_1 Z_2 e^2}{4\pi \epsilon_0 a^2}}_{\text{attractive}} \underbrace{- \frac{nb}{a^{n+1}}}_{\text{repulsive}}$$

At equilibrium $(a = a_0)$, $F = 0$

$$F = F_{attractive} + F_{repulsive} = 0$$

Using the $F_{repulsive}$ value from the previous Problem $\Rightarrow$

$$-\frac{nb}{a_0^{n+1}} = -3.02\ 10^{-9}\ m \Rightarrow$$

$$-\frac{9b}{(2.76\ 10^{-10} m)^{10}} = -3.02\ 10^{-9}\ Nt \Rightarrow$$

$$\boxed{b = 8.6 \times 10^{-106} \cdot Nt\ m^{10}}$$

$$U_{Na^+Cl^-} = \frac{Z_1 Z_2 e^2}{4\pi \epsilon_0 a_0} + \frac{b}{a_0^n} = \frac{(+1)(-1)(1.6\ 10^{-19}\ C)^2}{4\pi[8.85\ 10^{-12}\ \frac{C^2}{Nm^2}](2.76\ 10^{-10} m)}$$

$$+ \frac{8.6\ 10^{-106}\ Nt\ m^{10}}{(2.76\ 10^{-10}\ m)^9} \Rightarrow$$

$$\boxed{U_{Na^+Cl^-} = -7.42\ 10^{-19}\ J}$$ (recall $1 J = 1\ Nt \cdot m$)

6.

$$U = -\frac{A}{r^2} + \frac{B}{r^{10}}, \quad r_0 = 0.4\,nm, \quad U_0 = -5\,eV$$

FIND A & B FROM DATA FOR r AND U

@ EQUILIBRIUM, AND NOTING THAT AT EQUILIBRIUM

$$\frac{dU}{dr} = F = 0$$

$$U_0 = -\frac{A}{r_0^2} + \frac{B}{r_0^{10}}$$

$$\frac{dU}{dr} = \frac{2A}{r^3} - \frac{10B}{r^{11}}$$

$$\therefore \quad 0 = \frac{2A}{r_0^3} - \frac{10B}{r_0^{11}}$$

$$B = \frac{-U_0}{4} r_0^{10}$$

$$A = -\frac{5U_0}{4} r_0^2$$

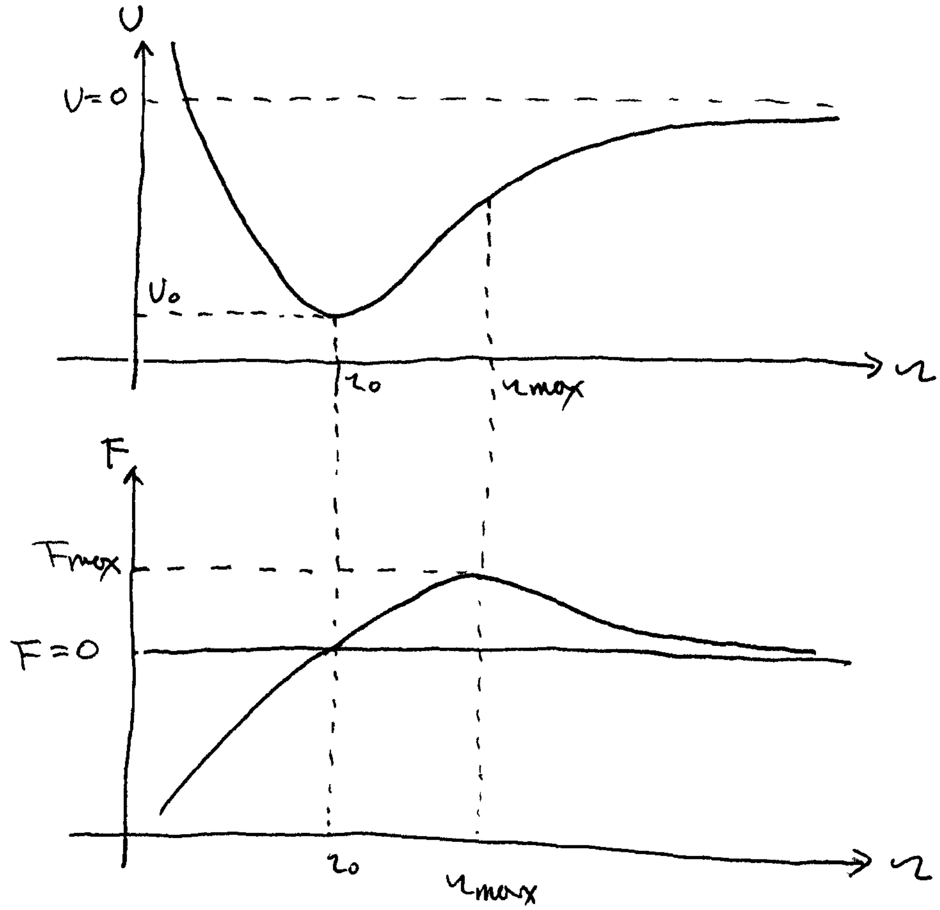
SUBSTITUTING NUMBERS

$$A = 1.59 \times 10^{-19}\ J \cdot nm^2$$

$$B = 2.10 \times 10^{-23}\ J \cdot nm^{10}$$

THE CRITICAL VALUE FOR r_{max} & F_{max} ARE OBTAINED FROM THE FORCE/DISTANCE CURVE: AT $r = r_{max}$, $\frac{dF}{dr} = 0$ AND $F = F_{max}$. BUT $\frac{dU}{dr} = F$, SO AT $r = r_{max}$,

$$\frac{d^2U}{dr^2} = 0 \quad \text{AND} \quad \frac{dU}{dr} = F_{max}$$



$$\frac{d^2U}{dr^2} = -\frac{6A}{r^4} + \frac{110B}{r^{12}} \Rightarrow \frac{15U_0}{2}\frac{r_0^2}{r_{max}^4} - \frac{55U_0 r_0^{10}}{2\, r_{max}^{12}} = 0$$

$$\Rightarrow 15 r_0^2 r_{max}^8 = 55 r_0^{10}$$

$$\Rightarrow r_{max} = 1.176 r_0 = \underline{\underline{0.471\text{ nm}}}$$

$$F_{max} = \frac{2A}{r_{max}^3} - \frac{10B}{r_{max}^{11}} = -\frac{5U_0}{2}\frac{r_0^2}{r_{max}^3} + \frac{5U_0}{2}\frac{r_0^{10}}{r_{max}^{11}}$$

$$= \frac{5}{2}\left(\frac{1}{1.176^{10}} - \frac{1}{1.176^2}\right)\frac{U_0}{1.176 r_0}$$

$$= \underline{\underline{2.23 \times 10^{-9}\text{ N}}}$$

7\. TO FIND THE INTERCEPTS TAKE THE RECIPROCALS OF THE PLANE INDICES

	(X)	(Y)	(Z)
PLANE :	3	$\bar{1}$	1
RECIPROCALS :	$\frac{1}{3}$	-1	1

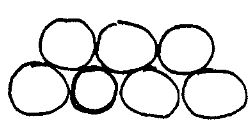
SO THE INTERCEPTS ARE $(\frac{1}{3},0,0)$, $(0,-1,0)$, $(0,0,1)$

8\. THE DIRECTION INDICATED GOES THROUGH (0,0,0) AND (1,0,1). THE VECTOR IN THAT DIRECTION IS (1.0.1) $\Rightarrow$ MILLER INDICES OF THAT DIRECTION ARE [101]. A COLLECTIVE DESCRIPTION FOR THE FACE DIAGONALS IS $\langle 110 \rangle$.

9\. SAME METHOD AS ABOVE. TAKE THE TWO POINTS JOINED BY A VECTOR, DETERMINE THAT VECTOR AND OBTAIN INTEGERS BY USING THE APPROPRIATE MULTIPLIER.

$u_1 : [011]$ $\quad u_2 : [1\bar{1}0]$

$u_3 : [\bar{1}01]$ $\quad u_4 : [01\bar{1}]$

 $\longrightarrow [110]$

IN EACH OF THOSE 4 DIRECTIONS, WE HAVE AN ATOM AT THE ORIGIN AND AT THE END OF THE VECTOR, AS WELL AS ONE HALFWAY, FOR A FCC CRYSTAL. NOTE THAT ALL THESE VECTORS ARE FACE DIAGONALS.

10. THE $\{110\}$ FAMILY OF PLANES ARE THE PLANES CONTAINING THE FACE DIAGONAL, PARALLEL TO ONE AXIS:

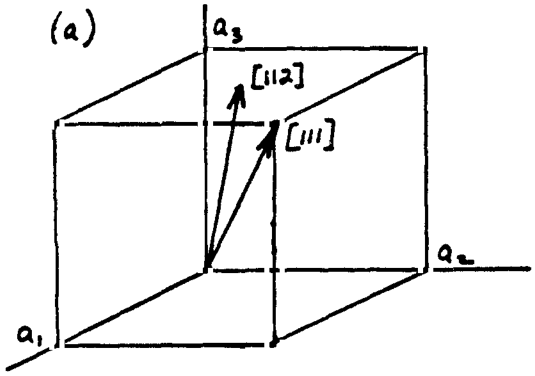
$$\left.\begin{array}{l}(110)\ (011)\ (101)\ (1\bar{1}0)\ (01\bar{1})\ (\bar{1}01) \\ \text{or}\ (\bar{1}\bar{1}0)\ (0\bar{1}\bar{1})\ (\bar{1}0\bar{1})\ (\bar{1}10)\ (0\bar{1}1)\ (10\bar{1})\end{array}\right\}\ \text{SAME PLANES}$$

11.

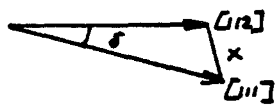
3.28. (a) Sketch, in a cubic unit cell, a [111] and a [112] lattice direction. (b) Use a trigonometric calculation to determine the angle between these two directions. (c) Use Equation 3 3 to determine the angle between these two directions

3.28

(a)



(b)



let $a = a_1 = a_2 = a_3$

$$\overline{[112]} = \sqrt{(\tfrac{1}{2}a)^2 + (\tfrac{1}{2}a)^2 + a^2}$$

$$= \sqrt{1.5a^2} = 1.225\ a$$

$$\overline{[111]} = \sqrt{3}\,a = 1.732a$$

$$x = \frac{\sqrt{2}}{2}a = 0.707a$$

In general,

$$x^2 = (\overline{[111]})^2 + (\overline{[112]})^2 - 2(\overline{[111]})(\overline{[112]})\cos\delta$$

or

$$\cos\delta = -\frac{x^2 - (\overline{[111]})^2 - (\overline{[112]})^2}{2(\overline{[111]})(\overline{[112]})}$$

$$= -\frac{0.5a^2 - 3a^2 - 1.5a^2}{2(\sqrt{3}a)(\sqrt{1.5}a)} = \frac{4}{4.243}$$

$$= 0.9428$$

$$\rightarrow \quad \delta = \underline{\underline{19.5^\circ}}$$

(c)

$$\delta = \arccos \frac{1+1+2}{\sqrt{1+1+1}\sqrt{1+1+4}} =$$

$$= \arccos \frac{4}{\sqrt{3}\sqrt{6}} = \underline{\underline{19.5^\circ}}$$

3.34. What $[hkl]$ direction connects the adjacent face-centered positions $\frac{1}{2}\,\frac{1}{2}\,0$ and $\frac{1}{2}\,0\,\frac{1}{2}$? Illustrate your answer with a sketch.

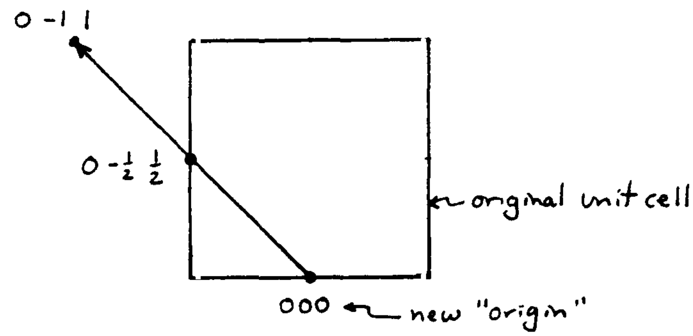
12.

3.34

We can note that, if $\frac{1}{2}\frac{1}{2}0$ becomes the origin 000, then $\frac{1}{2}0\frac{1}{2}$ would become

$$\begin{array}{rccc} & \frac{1}{2} & 0 & \frac{1}{2} \\ - & \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & -\frac{1}{2} & \frac{1}{2} \end{array}$$

Extending the line from the new "origin" through the new $0\,-\frac{1}{2}\,\frac{1}{2}$ position will lead to the position $1\,-1\,0$:



Therefore, it is the $[0\bar{1}1]$ direction.

13.

3.35. A useful rule of thumb for the cubic system is that a given $[hkl]$ direction is the normal to the (hkl) plane. Using this rule and Equation 3.3, determine which members of the $\langle 110 \rangle$ family of directions lie within the (111) plane. (*Hint:* The dot product of two perpendicular vectors is zero.)

3.35

[111] is the plane normal to (111)
and [111] will give a zero dot product with:

$[\bar{1}10]$, $[1\bar{1}0]$, $[\bar{1}01]$, $[10\bar{1}]$, $[01\bar{1}]$, and $[0\bar{1}1]$