MECH 221 Session # 2 and # 4

MECH 221

Chapter 3: Crystalline Solids

Chapter 4: Imperfections in Solids

2.1 ~~Question 1:~~

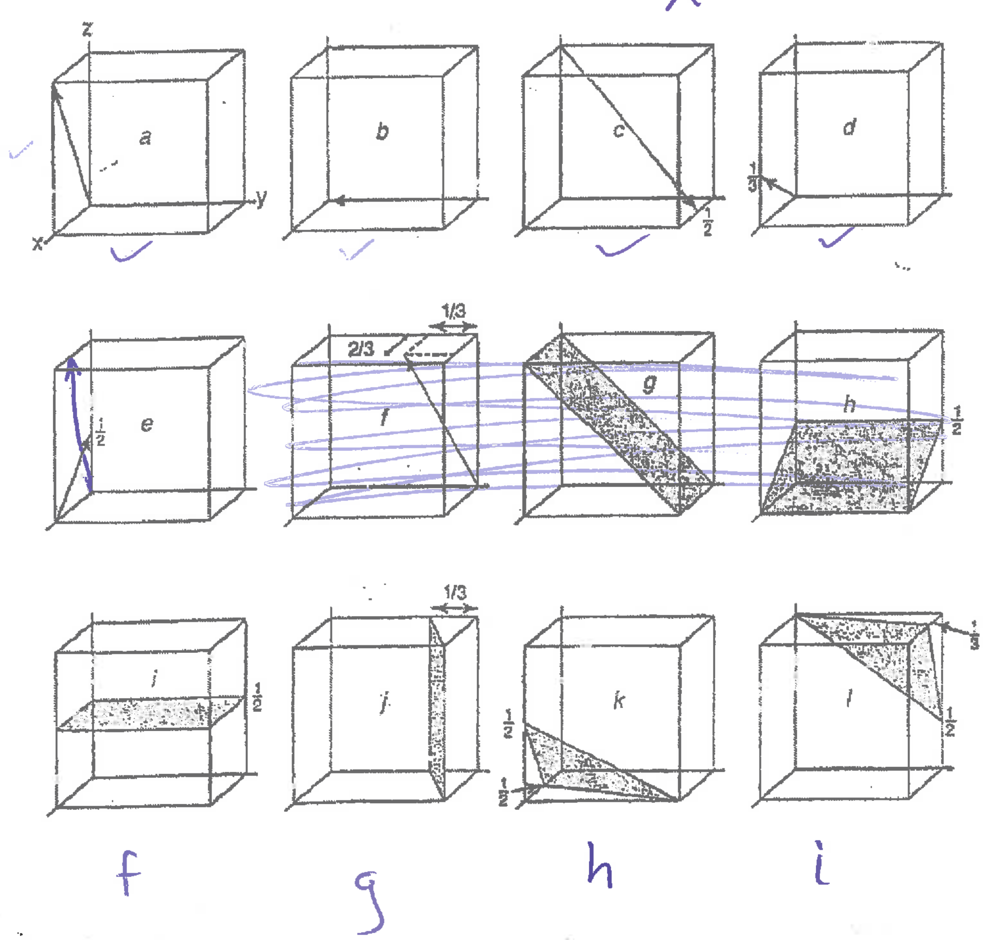
Explain why the properties of polycrystalline materials are most often isotropic.

An individual grain, which is a single crystal, is anisotropic but the random orientations of all grains of a polycrystalline material result in isotropy.

2.2 ~~Question 2:~~

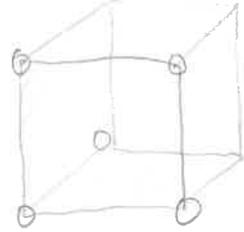
Sketch the following planes and directions within a cubic unit cell:

(a) [101] (b) [0$\bar{1}$0] (c) [12$\bar{2}$] (d) [301] (e) [102] (f) (002) (g) (1$\bar{3}$0) (h) ($\bar{2}$12) (i) (3$\bar{1}\bar{2}$)

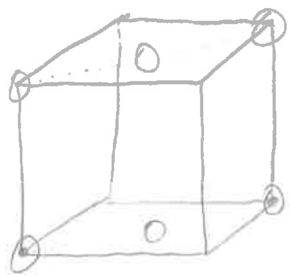


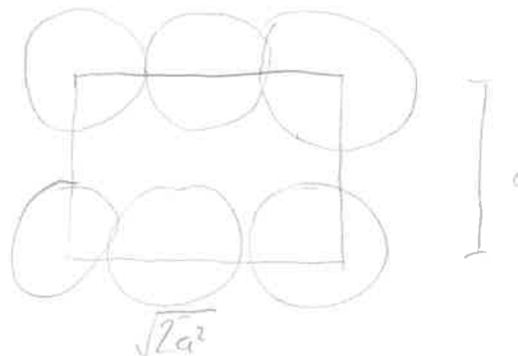
2.3 cont.

for (100)



for (110)

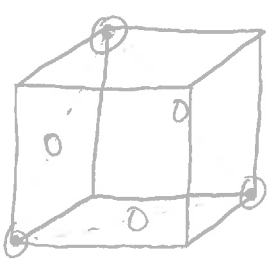


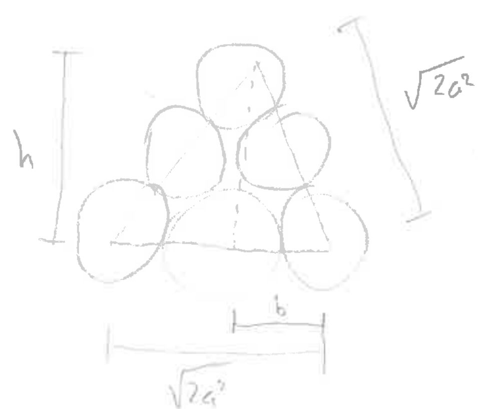


$$\text{planar density} = \frac{2}{a\sqrt{2a^2}} = 1.143 * 10^{19} \frac{\text{atoms}}{m^2}$$

$$PF = \frac{2(\pi R^2)}{(2\sqrt{2}R)\sqrt{2((2\sqrt{2}R)^2)}} = 0.934\ ?$$

for (111)





$$b = \frac{\sqrt{2a^2}}{2} = 2.48668 * 10^{-10}$$

$$h = \sqrt{2a^2 - \frac{2a^2}{4}} = \sqrt{\frac{3}{2}a^2} = 4.307 * 10^{-10}$$

$$\text{planar dens.} = \frac{3\frac{1}{6} + 3\frac{1}{2}}{\frac{1}{2}bh} = \frac{2}{\frac{1}{2}(2.486 * 10^{-10})(4.307 * 10^{-10})}$$

$$= 3.73 * 10^{19} \frac{\text{atoms}}{m^2}$$

$$PF = \frac{2(2\pi R^2)}{\quad}$$

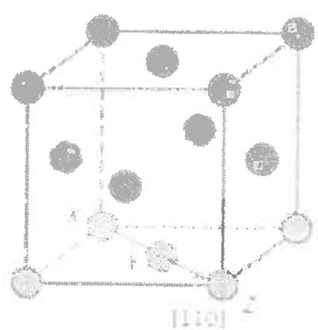
2.3 ~~Question 3:~~

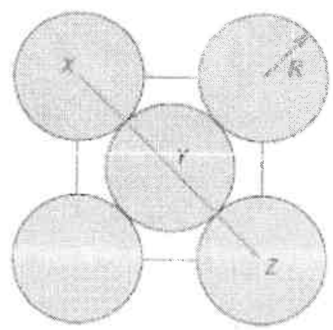
Determine the planar density and packing fraction for FCC nickel in the (100) (110) and (111) planes. Which if any of these planes is closed packed?

Hint: Packing fraction is the fraction of the plane actually covered by atoms. The lattice parameter of Ni is 3.5167 A.

A: Angstrom

$1 A = 10^{-10} m$





For

$$\text{planar density} = \frac{2}{(3.5167*10^{-10})^2} = 1.617*10^{19}\ \frac{\text{atoms}}{m^2}$$

$$\text{packing factor} = \frac{2\pi R^2}{(2\sqrt{2}R)^2} = 0.7854$$

4.1 ~~Question 4:~~

Calculate the number of vacancies per cubic metre in iron at 850°C. The energy for vacancy formation is 1.08 eV/atom. Furthermore, the density and atomic weight for Fe are 7.65 g/cm3 and 55.85 g/mol, respectively.

Boltzmann's constant: $k = 1.38*10^{-25}$ J/atom*K = $8.62*10^{-5}$ eV/atom*K

$$N_v = Ne^{-\frac{Q_v}{KT}}$$

$$850°C = 1123 K$$

$$Q_v = 1.08\ eV/atom$$

$$N = \frac{N_A \rho}{A} = \frac{(6.023*10^{23})(7.65)}{55.85} = 8.25*10^{22}\ \frac{atom}{cm^3}$$

$$N_v = 8.25*10^{22}\, e^{\frac{-1.08}{(8.62*10^{-5})(1123)}} = 1.178*10^{18}\ \frac{vac.}{cm^3} = 1.178*10^{24}\ \frac{vac.}{m^3}$$

4.2 ~~Question 5:~~

In the table below, atomic radius, crystal structure, electronegativity, and the most common valence are tabulated, for several elements; for those that are nonmetals, only atomic radii are indicated. Which of these elements would you expect to form the following with copper:
(a) A substitutional solid solution having complete solubility?
(b) A substitutional solid solution of incomplete solubility?
(c) An interstitial solid solution?

Element	*Atomic Radius (nm)*	*Crystal Structure*	*Electro-negativity*	*Valence*
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Pt	0.1387	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

For complete substitutional solubility, the variation in atomic radii must be ± 15%, must have the same crystal structure and the electronegativities must be similar and volences should be similar.

a) Ni, Pd and Pt because they meet all criteria

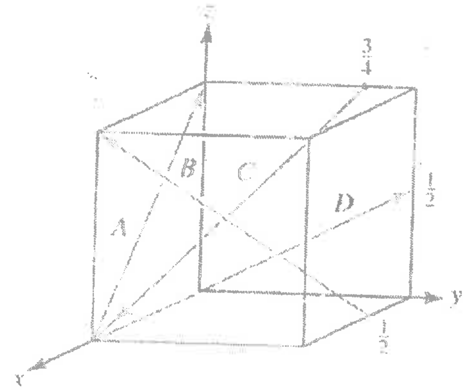
b) Ag, Al, Co, Cr, Fe and Zn are missing one or more of the criteria

c) C, H and O because they are significantly smaller.

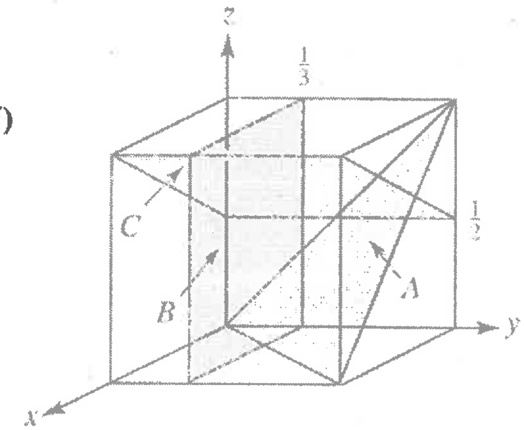
2.4 ~~Question 6:~~

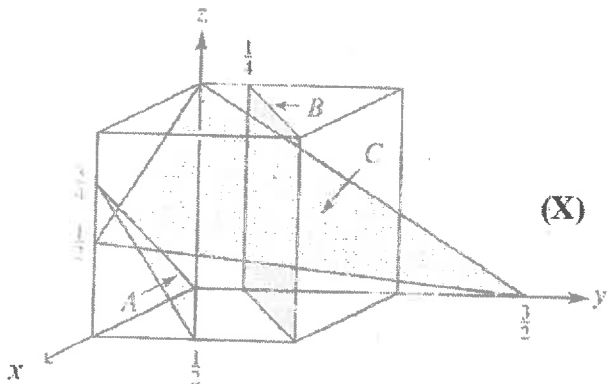
Determine the indices for the directions and planes shown in Figures V, W and X.

(V)



(W)





(X)

V A: $[\bar{1}\,0\,1]$ B: $[1\,\bar{2}\,2]$ C: $[4\,\bar{3}\,\bar{4}]$ D: $[0\,2\,1]$

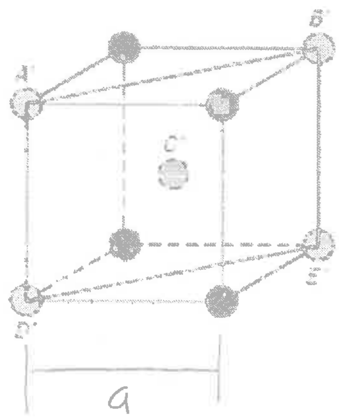
W A: $[1\,\bar{1}\,1]$ B: $[0\,3\,0]$ C: $[1\,0\,\bar{2}]$

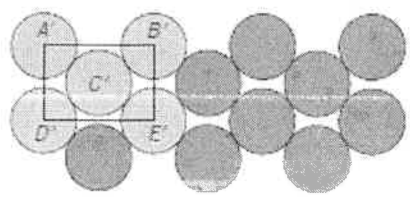
X A: $[\bar{3}\,6\,4]$ B: $[3\,\bar{4}\,0]$ C: $[3\,4\,6]$

2.5 ~~Question 7~~

Derive the atomic packing factor for both BCC and FCC crystal structures.

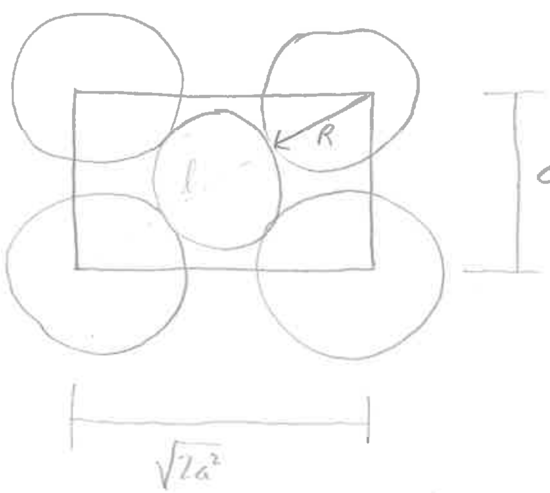
BCC





$$\ell = \sqrt{a^2 + \left(\sqrt{2a^2}\right)^2} = \sqrt{3}\,a$$

BCC

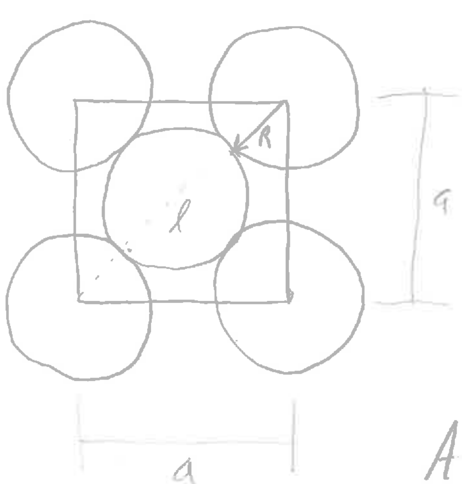


$$\ell = 4R$$

$$\sqrt{3}\,a = 4R \qquad a = \frac{4R}{\sqrt{3}}$$

$$APF = \frac{V_s}{V_c} = \frac{2\,\frac{4}{3}\pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} = 0.68$$

FCC



$$\ell = \sqrt{2a^2} = 4R$$

$$2a^2 = 16R^2$$

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

$$APF = \frac{V_s}{V_c} = \frac{4\,\frac{4}{3}\pi R^3}{\left(2\sqrt{2}R\right)^3} = 0.74$$

2.6 ~~Question 8~~

The atomic weight, density, and atomic radius for three hypothetical alloys are listed in the following table. For each, determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination.

Alloy	Atomic Weight (g/mol)	Density (g/cm^3)	Atomic Radius (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

$$\rho = \frac{nA}{V_C N_A}$$

Trial and error. Assumptions necessary

For A, assume simple cubic $\rightarrow n = 1$ atom per unit cell and $a = 2R$

$$\rho = \frac{1(77.4)}{(2(1.25*10^{-8}))^3 \, 6.023*10^{23}} = 8.22 \text{ g/cm}^3 \therefore \text{assumption correct}$$

For B, assume FCC $\rightarrow n = 4$ and $a = 2\sqrt{2}R$

$$\rho = \frac{4(107.6)}{(2\sqrt{2}(1.33*10^{-8}))^3 \, 6.023*10^{23}} = 13.42 \text{ g/cm}^3 \therefore \text{assumption correct}$$

For C, assume simple cubic $\rightarrow n = 1$ $a = 2R$

$$\rho = \frac{1(127.3)}{(2(1.42*10^{-8}))^3 \, 6.023*10^{23}} = 9.23 \text{ g/cm}^3 \therefore \text{assumption correct}$$

2.7 **Question 9**

Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used.

$$n\lambda = 2d_{hkl}\sin\theta \qquad d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

from table 3.1 (Callister) $R = 0.1387$ nm

$a = 2\sqrt{2}R$

$$d_{hkl} = \frac{2\sqrt{2}(0.1387)}{\sqrt{1^2+1^2+3^2}} = 0.1183 \text{ nm}$$

first order → $n = 1$

$$\theta = \sin^{-1}\frac{n\lambda}{2d_{hkl}} = \sin^{-1}\frac{0.1542}{2(0.1183)} = 40.7°$$

$$2\theta = 81.4°$$

4.3 ~~Question 10~~

Determine the approximate density of a high leaded brass that has a composition of 64.5 wt% Cu, 33.5 wt% Zn, and 2 wt% Pb.

$$\rho_{ave} = \frac{100}{\frac{C_{Cu}}{\rho_{Cu}} + \frac{C_{Zn}}{\rho_{Zn}} + \frac{C_{Pb}}{\rho_{Pb}}}$$

$\rho_{Cu} = 8.94$ g/cm³

$\rho_{Zn} = 7.13$ g/cm³

$\rho_{Pb} = 11.35$ g/cm³

$$\rho_{ave} = \frac{100}{\frac{64.5}{8.94} + \frac{33.5}{7.13} + \frac{2}{11.35}} = 8.27 \text{ g/cm}^3$$

1.4 **Question 11**

For an FCC single crystal, would you expect the surface energy for a (100) plane to be greater or less than that for a (111) plane? Why?

The surface energy of a single crystal depends on the crystallographic orientation because different planes have different planar densities. The (100) plane would have greater surface energy because its planar density is less than that of the (111) plane therefore leaving more potential atomic bonds unsatisfied.

2.8.// anisotropic

2.9.// Thorium $\rho = 11.72\ g/cm^3$ $A = 232\ \frac{g}{mol}$ FCC $\rightarrow n=4$

$$\rho = \frac{nA}{V_c N_A}$$

$$11.72 = \frac{4(232)}{a^3\ 6.022\times10^{23}} \rightarrow a = 5.085\times10^{-8}\ cm = 0.5085\ nm$$

2.10.// Crystal orientations

2.11.// Rhodium FCC

diffraction angle = 36.12° (3, 1, 1)

$n=1$

$\lambda = 0.0711\ nm$ $R = ?$

$$n\lambda = 2d_{hkl}\sin\Theta \qquad d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$\Theta = \frac{36.12}{2} = 18.06°$$

$$(1)\ 0.0711 = 2\ d_{hkl}\ \sin 18.06$$

$$\rightarrow d_{hkl} = 0.11467$$

$$0.11467 = \frac{a}{\sqrt{3^2+1^2+1^2}}$$

$$\rightarrow a = 0.3803\ nm$$

$$a = 2\sqrt{2}R = 0.3803$$

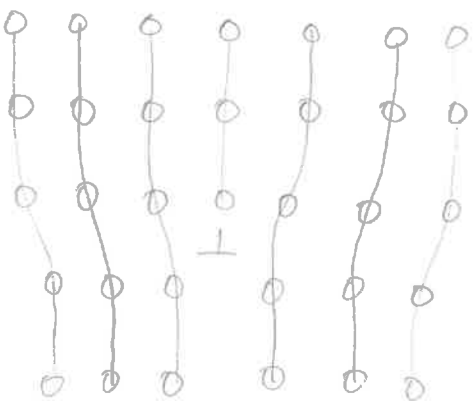
$$\rightarrow R = 0.1344\ nm$$

4.5

~~Question 12~~

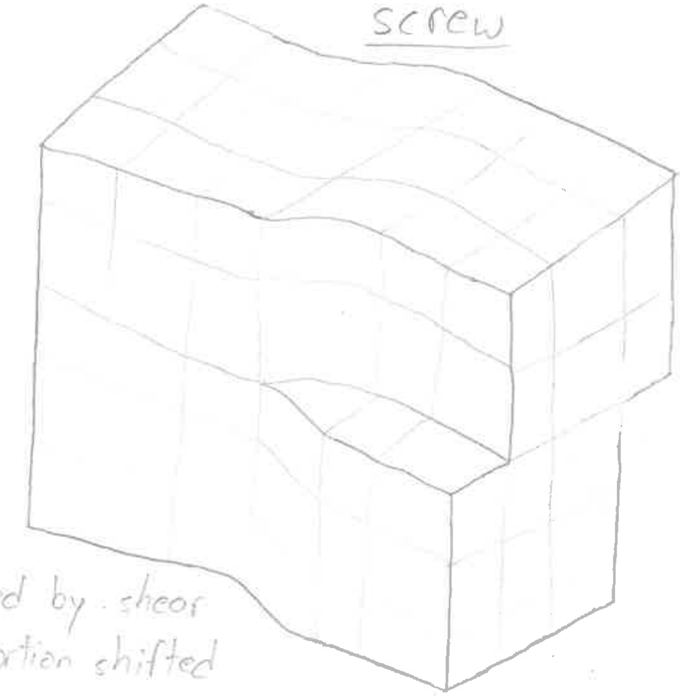
Describe and draw a sketch of an edge dislocation and of a screw dislocation.

edge



An extra half plane of atoms

screw

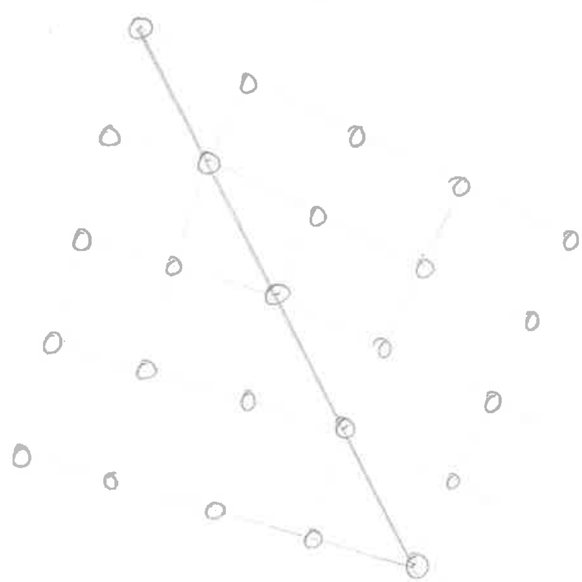


Caused by shear
Upper portion shifted

4.6

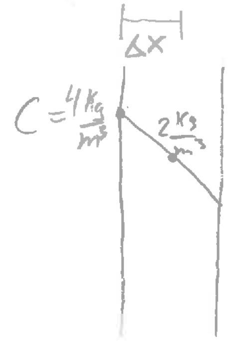
~~Question 13~~

What is a twin boundary? Draw a sketch.



A twin boundary is a grain boundary at which there is a mirror lattice symmetry.

4.7 || $\Delta x = ?$



$D = 6 * 10^{-11}\ \frac{m^2}{s}$ $\qquad$ $J = 1.2 * 10^{-7}\ \frac{kg}{m^2 \cdot s}$

$J = -D \frac{dC}{dx}$ $\qquad$ since linear $\frac{dC}{dx} = \frac{4-2}{\Delta x}$

$1.2 * 10^{-7} = -6 * 10^{-11}\ \frac{4-2}{\Delta x} \longrightarrow \Delta x = 0.001\,m = \underline{1\,mm}$

Concentrations in $\frac{kg}{m^3}$

4.8 ||

$D = 6.9 * 10^{-11}\ \frac{m^2}{s}$

$C_0 = 0.35\ wt\%\ C$

$C_s = 0\ wt\%\ C$

$C_x = 0.15\ wt\%\ C$

$\Delta t = 10h = 36000\,s$

Concentrations in wt%

$$\frac{C_x - C_0}{C_s - C_0} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\frac{0.15 - 0.35}{0 - 0.35} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$erf\left(\frac{x}{2\sqrt{Dt}}\right) = 0.4286$$

interpolation: $\frac{x}{2\sqrt{Dt}} = \frac{0.45 - 0.40}{0.4755 - 0.4284}\left(0.4286 - 0.4284\right) + 0.40 = 0.4002$

$$0.4002 = \frac{x}{2\sqrt{6.9 * 10^{-11}(36000)}} \longrightarrow x = 0.00126\,m = \underline{1.26\,mm}$$

4) B – If the indentations were made too close to each other, errors here could also occur. The area of the second indentation could have possibly been used by the first indentation; therefore, the created indent will be too great and will not be even.

5) The sources of error within this lab would be mostly due to human error. Such as obtaining the proper amount of force. We were told to obtain a force of both 10,000N and 5,000N. To reach exactly 5,000N and 10,000N wasn't the easiest task; therefore, there is some error there as we went over or under the specified force by a bit. The 15 seconds we needed to leave the metal alone for also had to be exact. It is possible that we were a couple of milliseconds off. Lastly, it was difficult to identify a precise measurement using the microscope because the indentation was very small, so with respect to that there could be a miniscule error there. In terms of calculations, the resultant values were rounded to four significant figures. This damages the precision of the final results. In comparison to the ASTM specifications, the Brinell Hardness resultant aluminum values for all three trials were not found within range. This was caused by the excessive amount of load given to the sample.

Conclusion

There are a number of different types of hardness tests being used around the world. During the lab, the Brinell Hardness Test was being used. It gives quick results, it is easy to perform, and the results obtained from the test are very accurate. It is also the test used when other tests cannot handle the durability of the metal. By using this test, it was found that the experiment was a success.

4.9||

~~must determine D~~

$$\frac{x^2}{Dt} = \text{const.}$$

$$\frac{x_1^2}{D_1 t_1} = \frac{x_2^2}{D_2 t_2}$$

$$D = D_0 e^{-\frac{Q_d}{RT}}$$

same D_0, R, T and Q_d

$\therefore$ $D_1 = D_2$

$$\frac{x_1^2}{t_1} = \frac{x_2^2}{t_2}$$

$$\frac{0.0025^2}{10(3600)} = \frac{0.005^2}{t_2}$$ ⟶ $t_2 = 144000\,s = 40\,h$

STEEL SAMPLE TRIAL #1

$b = (D^2 - d^2)^{1/2} = ((10)^2-(3)^2)^{1/2} = 9.539392014mm$

$t = (D/2) - (b/2) = 5 - (9.53../2) = 0.230303993mm$

$A = \pi Dt = \pi(10)(0.23..) = 7.235213322mm^2$

$HB = P (kg)/A (mm2) = 1036.9011kg/7.235213322mm^2 = 143.3131345kg/mm^2$

Average Brinell Hardness: HB = (143.3131345+147.286647+148.6865482)/3 =146.4287766mm^2

5/5

Discussion

1) The Brinell Hardness test is most often used to test the metals that have a structure too coarse or a surface that is too rough to be tested using another method. Such as casting and forging. The Brinell test is a simple test that gives results quickly. The information obtained from this test usually associates with ductility, tensile strength, wear resistance, and other physical metallic properties. Hardness tests are most often used to determine the heat treatment of a specific part and to identify whether or not the materials tested have the proper characteristics for its specified use.

2) There are a few other hardness tests used in engineering. Rockwell Hardness Test and Vickers Hardness Test are two of the few. In the Rockwell test, the indenter moves downwards into position onto the chosen surface. A reference position of zero is then determined followed by a specific minor load being applied. Once the minor load is applied, the major load is applied for a specified time. Once the time has passed, one releases the major load and leaves the minor load. The end result is the Rockwell number that identifies the difference in depth from the initial zero position as a result of the major load. The Vickers test uses a 136° pyramidal diamond indenter that forms a square indent. The indenter is applied to the metal by a very precise force. The force is than kept for 10-15 seconds. Once the time has passed, the indenter is removed leaving a square indentation. The size is than determined optically by measuring the two diagonals. Finally to get Vickers Hardness number, you divide the test force by the surface area of the indent.

3) A – If the indentations were made too close to the edge of the metal, an indentation that is unsymmetrical can cause an error in the HB number.

1.10

steady state

$J_1 = 5.4 * 10^{-10}\ Kg/m^2 s \qquad T_1 = 727°C \qquad \frac{dC}{dx} = -350\ \frac{Kg}{m^4}$

$Q_d = 125000\ J/mol \qquad J_2 = ? \qquad T_2 = 1027°C$

$$J_1 = -D_1 \frac{dC}{dx}$$

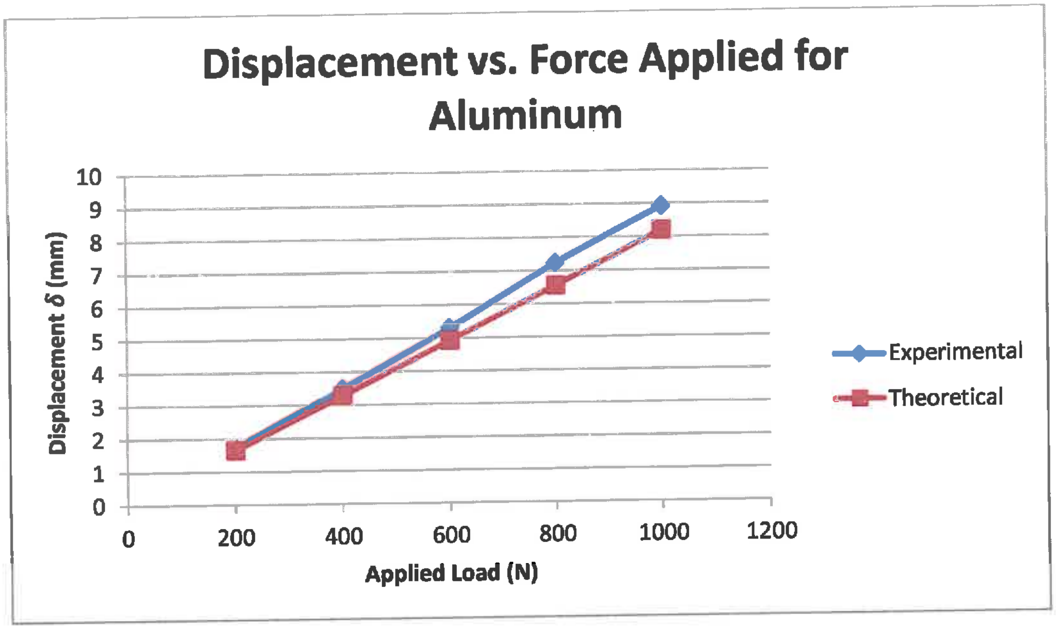
$$5.4*10^{-10} = -D_1(-350) \longrightarrow D_1 = 1.54*10^{-12}\ \frac{m^2}{s}$$

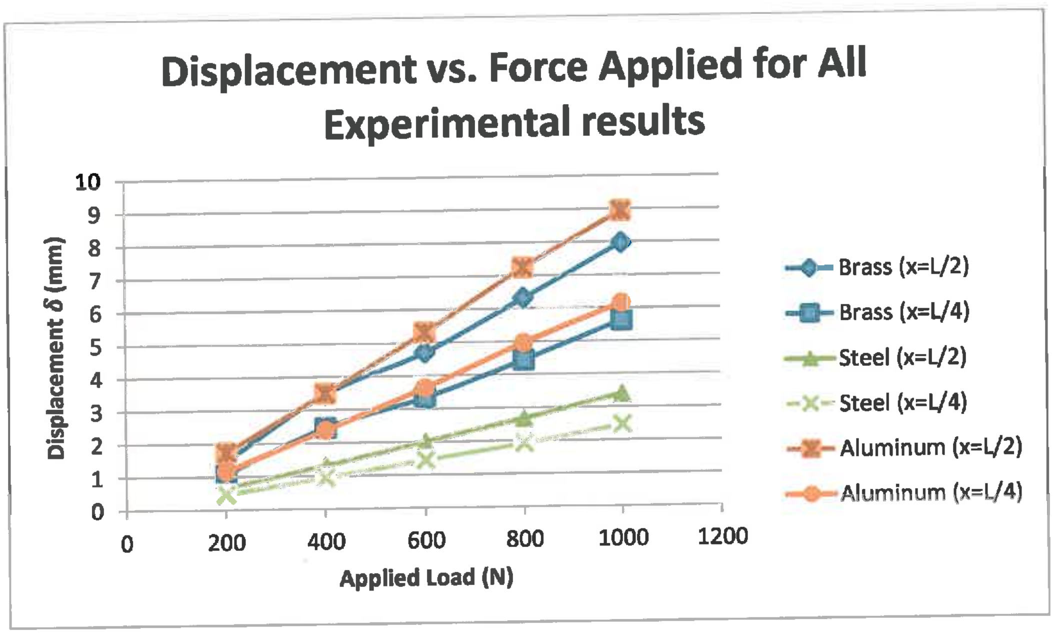
$$D_1 = D_o e^{\frac{-Q_d}{RT_1}}$$

$$1.54*10^{-12} = D_o e^{\frac{-125000}{8.314(1000)}} \longrightarrow D_o = 5.21*10^{-6}\ \frac{m^2}{s}$$

$$D_2 = D_o e^{\frac{-Q_d}{RT_2}} = 5.21*10^{-6} e^{\left(\frac{-125000}{8.314(1300)}\right)} = 4.94*10^{-11}\ \frac{m^2}{s}$$

$$J_2 = -D_2 \frac{dC}{dx} = -4.94*10^{-11}(-350) = \underline{\underline{1.73*10^{-8}\ \frac{Kg}{m^2 s}}}$$


Displacement vs. Force Applied for Aluminum
Displacement δ (mm)
10
9
8
7
6
5
4
3
2
1
0
0
200
400
600
800
1000
1200
Applied Load (N)
Experimental
Theoretical


Displacement vs. Force Applied for All Experimental results
Displacement δ (mm)
10
9
8
7
6
5
4
3
2
1
0
0
200
400
600
800
1000
1200
Applied Load (N)
Brass (x=L/2)
Brass (x=L/4)
Steel (x=L/2)
Steel (x=L/4)
Aluminum (x=L/2)
Aluminum (x=L/4)