Ch. 2 Atomic Structure and Bonding

Net, Attractive, Repulsive **Energies** between two ions:

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n};\ n \sim 8$$

$$A = \frac{1}{4\pi\varepsilon_o}(q_1)(q_2)\ ;\quad q = \text{magnitude of net charge}$$

Force between two ions

$$F_N = F_A + F_R = +\frac{A}{r^2} - \frac{B}{r^{n+1}}$$

$$\%\ \text{ionic character} = \left\{1 - e^{-(1/4)(X_1 - X_2)^2}\right\} \times 100\%$$

X = electronegativity

Chapt 3 Structure of Crystalline Solids

	Lattice Parameter	APF
FCC:	$a = 2\sqrt{2}R$	0.74
BCC:	$a = \frac{4}{\sqrt{3}}R$	0.68
HCP	$a = 2R;\ c = 1.633a$	0.74

$$APF = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{nV_{sph}}{V_{cell}}$$

Density: $$\rho = \frac{nA}{V_{cell}N_A}$$

$$LD = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$

$$PD = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$

Points: coordinates in terms of fractional distances of lattice parameters

Naming Direction Vectors

1. Move tail to origin
2. Write point where direction leaves unit cell
3. Multiply by LCD to get integers
4. Enclose in square brackets [*h k l*]

Naming Planes

1. Move plane off origin
2. Write intercepts of plane with *x*-, *y*-, and *z*-axes
3. Flip intercepts
4. Multiply by LCD to get integers
5. Enclose in parenthesis (*h k l*)

Families of directions: same orientation and LD; < >
Families of planes: same orientation, and packing density; { }

Crystal Systems (systems that have only right-angles):
Cubic (3 sides equal)
Tetragonal (2 sides equal)
Orthogonal (no sides equal)

Stacking: FCC: ABCABCABC…; HCP: ABABABAB…

Chapt 12 Structure of Ceramics

Determined by ratio of ionic radii r_c/r_a; electric charge.

Ch 4. Imperfections

Vacancies. Solid Solutions: substitutional, interstitial
Dislocations. Grain Boundaries, Interphase Bnds, Free Surfaces.
Voids, Inclusions, other Phases.

Number of vacancies:	$N_v = N\exp\left(\frac{-Q_v}{kT}\right)$
Number of atomic sites per unit volume:	$N = \frac{(N_A)\rho}{A}$
Composition, wt% of Element 1	$C_1 = \frac{m_1}{m_1 + m_2} \times 100\ \text{wt\%}$
Composition, at%	$C_1' = \frac{n_1}{n_1 + n_2} \times 100\ \text{at\%}$
Conversion wt% to at%	$C_1' = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100\ \text{at\%}$
Conversion at% to wt%	$C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \times 100\ \text{wt\%}$
Concentration: ρ[g/cm^3] C''[kg/m^3]	$C_1'' = \frac{C_1}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} \times 10^3$
Average Density, two-element solid-solution:	$\rho_{\text{ave}} = \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}}$

Grain Size

ASTM Method: $N = 2^{n-1} = 2^{G-1}$

N = # of grains per in.^{2} at 100×, $n = G$ = grain-size number

Intersection Method (on photomicrograph magnified M times)

- draw ~7+ lines of same length L in random directions; the lines should be as long as possible.
- determine average number of grains per line: g; OR the average number grain boundaries intersected per line: p.
- divide line length by average number of grains per line (or intersections per line) to give the grain size as seen in picture: $l = L/g$ (or $d_i = L/p$)
- divide by mag. M to give the ***grain diameter***: $D = l/M$, or the *mean intercept length:* $\bar{\ell} = d_i/M$

Alternate: Take the total length of the lines L_T (e.g., L_T=7L) divide by the total grains R covered by the lines, or the number G.B. intersections, and divide again by the magnification M:

$$D = \frac{L_T}{RM} \qquad \bar{\ell} = \frac{L_T}{PM}$$

Chapt 5 Diffusion

Diffusion Flux	$J = \frac{M}{At}$
Fick's First Law: C = concentration [kg/m^3]	$J = -D\frac{\Delta C}{\Delta x}$
Diffusion Coefficient [m^2/s]	$D = D_o\exp\left(\frac{-Q_d}{RT}\right)$

Ch. 6 Mechanical Properties of Metals

Stress in Axial Bar:	$\sigma = \frac{F}{A_o}$
Strain:	$\varepsilon = \frac{l - l_o}{l_o} = \frac{\Delta l}{l_o}$
Hooke's Law:	$\sigma = E\varepsilon$
Young's Modulus:	E
Proportional Limit:	$\sigma_p = P$
Yield Strength (0.2% offset):	σ_y
Tensile Strength:	*TS* (*UTS*)
Resilience/Modulus of R.	$U_R = \frac{1\sigma_y^2}{2E}$
Toughness:	Area under σ–ε curve

Poisson's Ratio:

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\varepsilon_y}{\varepsilon_z} = -\frac{\varepsilon_T}{\varepsilon_{direct}} = -\frac{transverse\ strain}{direct\ strain}$$

Failure Strain (Ductility):

$$\%EL = \varepsilon_f = \left(\frac{l_f - l_o}{l_o}\right) \times 100\%; \quad l_f = \text{final length}$$

Reduction of Area (Ductility):

$$\%RA = \left(\frac{A_o - A_f}{A_o}\right) \times 100\%; \quad A_f = \text{area at failure (neck)}$$

Working Stress (Allowable Stress) σ_w; **Factor of Safety**:

$$\sigma_w = \frac{\sigma_y}{N} = \frac{\sigma_y}{FS} \quad \ldots\ldots FS = \frac{\sigma_y}{\sigma_w}$$

Ch. 7 Dislocations and Strengthening Mechanisms

Slip System: Slip Plane and Slip Direction

Shear Stress τ causes dislocations to move.

Hall-Petch Equation:

$$\sigma_y = \sigma_o + \frac{k}{d^{1/2}}$$

Percent Cold Work:

$$\%CW = \left(\frac{A_o - A_d}{A_o}\right) \times 100\%;$$

A_d = cross-sec. area at deformed length

Grain Growth:

$$d^n - d_o^n = Kt$$

Constants

Avogadro's Number

N_A = 6.022 ×10^{23} atoms/mole, *or*:

N_A = 6.022 ×10^{23} molecules/mole

Boltzman's Constant:

k = 8.62 ×10^{-5} eV/atom-K

= 1.38 ×10^{-23} J/atom-K

Gas Constant:

R = 8.31 J/mol-K

Chapt 8 Failure

Fracture (Brittle Fracture/Fast Fracture)

Half Crack Length: a (center crack $2a$, edge crack a)

Stress Intensity Factor:

$$K_I = Y\sigma\sqrt{\pi a}$$

Y = geometric factor: Center crack: 1.0

Edge crack: 1.12

Critical Stress Intensity Factor or **Fracture Toughness**

K_{Ic} - material property

Critical Stress (to cause fracture at crack size a)

$$\sigma_c = \frac{K_{Ic}}{Y\sqrt{\pi a}}$$

Critical Crack Size (to cause fracture at applied stress σ)

$$a_c = \frac{1}{\pi}\left(\frac{K_{Ic}}{Y\sigma}\right)^2$$

Maximum Crack Size to ensure yielding and not fracture

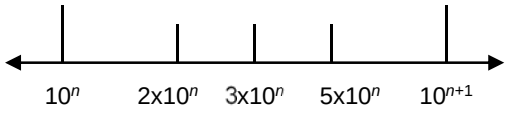
$$a_c = \frac{1}{\pi}\left(\frac{K_{Ic}}{Y\sigma_y}\right)^2$$

Fatigue

Mean Stress	$\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$
Stress Amplitude	$\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$
R-ratio	$R = \frac{\sigma_{min}}{\sigma_{max}}$

Guide to Reading a Log-Scale:

A decade is roughly divided as shown:



Creep

Minimum Temperature for Creep ~0.4T_m

Creep Rate

$$\dot{\varepsilon}_s = K_1\sigma^n$$

$$\dot{\varepsilon}_s = K_2\sigma^n \exp\left(\frac{-Q_c}{RT}\right)$$

Chapt 9 Phase Diagram

PHASE DIAGRAMS. Knowing system composition C_o, and Temperature T, you can find:

1. Phases present
2. Composition of each phase (end of tie-line)
3. Weight fraction (mass fraction) W, of each phase.

Draw microstructure of system when cooled from liquid.

Composition C_1, of Element 1 (Elem1) in system, wt%[Elem1]	$C_1 = \frac{m_1}{m_1 + m_2} \times 100$ wt%[Elem1]
Mass Fraction (Weight Fraction) of Phase α in α-β region (α on left)	Lever Rule $W_\alpha = \frac{C_\beta - C_o}{C_\beta - C_\alpha}$
Mass Fraction (Weight Fraction) of Phase β in α-β region (α on left)	Lever Rule $W_\beta = \frac{C_o - C_\alpha}{C_\beta - C_\alpha}$

Eutectic: $L \rightarrow \alpha + \beta$

Eutectoid: $\gamma \rightarrow \alpha + \beta$

Hypoeutectic: System with composition below eutectic composition C_E.

Hypereutectic: System with composition above eutectic composition C_E.

Chapt 17 Corrosion

Corrosion: Chemical Attack

Oxidation: metal electrode loses electrons … goes into solution; can bond with oxygen (oxidize). The ***anode***.

Reduction: metal ion gains electrons to become solid. The ***cathode***.

Standard EMF Series

EMF Series rates metals from most chemically inert (most cathodic) to most active (most anodic) by measuring the voltage difference between a metal anode in 1 molar solution of its own ion with respect to (w.r.t.) platinum anode in 1 molar solution of H+ (standard hydrogen electrode). The electrodes are electrically connected to each other, and the solutions are separated by a membrane that only lets electric charge pass through.

The more positive V^o (w.r.t. platinum electrode), the less likely that metal is to corrode. The less positive V^o, the more likely to corrode.

Eletrochemical Cell

Connecting two metals in an electrochemical cell (electrode of metal in its own solution, connected electrically to another electrode metal in its own solution), gives a voltage difference:

$$\Delta V^o = V_2^o - V_1^o$$

If $\Delta V^o > 0$, Metal 1 corrodes; if $\Delta V^o < 0$, Metal 2 corrodes.

The metal that corrodes (loses material is the anode. The metal that does not corroded is the cathode.

Galvanic Series

Galvanic Series rates metals resistance to corrosion in seawater. The higher on the series, the more resistant to corrosion.

Corrosion: eight types

Remember your two favorite types of corrosion and be able to describe them.

Corrosion Prevention

How do you prevent/impede corrosion?

Chapt 18 Electrical Properties

Material properties:

Resistivity: ρ [Ω•m]

Conductivity: $\sigma = \rho^{-1}$ [Ω•m]$^{-1}$

Ohm's Law	$V = IR$
Resistance of wire Length l, cross-sect. A	$R = \frac{\rho l}{A}$

Semi-Conductors

Based on Column-IV elements (Si, Ge). Doped to increased conductivity.

Conductors of electricity *electrons* (–) and *holes* (+)

n-type: dope with an element with more valence elections (negative charge carrier)

p-type: dope with an element with less valence elections (positive charge carrier)

Updated: 12/07/2015

USEFUL INFORMATION

Constants

Avogadro's Number

$N_A = 6.022 \times 10^{23}$ molecules/mole

Boltzman's Constant:

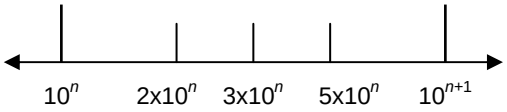
$k = 8.62 \times 10^{-5}$ eV/atom-K

$= 1.38 \times 10^{-23}$ J/atom-K

Ideal Gas Constant:

$R = 8.31$ J/mol-K

Guide to Reading a Log-Scale:
A decade is roughly divided as shown:



The Three Moe s of Fracture

Moe I **Moe II** **Moe III**

The Standard emf Series

Further down the chart, electrodes become increasingly active.

Electrode Reaction	Standard Potential V^0(V)
$Au^{3+} + 3e^- \rightarrow Au$	+1.420
$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$	+1.229
$Pt^{2+} + 2e^- \rightarrow Pt$	+1.20
$Ag^+ + e^- \rightarrow Ag$	+0.800
$Fe^{3+} + 3e^- \rightarrow Fe$	+0.771
$O_2 + 2H_2O + 4e^- \rightarrow 4(OH^-)$	+0.401
$Cu^{2+} + 2e^- \rightarrow Cu$	+0.340
$2H^+ + 2e^- \rightarrow H_2$	+0.000
$Pb^{2+} + 2e^- \rightarrow Pb$	–0.126
$Sn^{2+} + 2e^- \rightarrow Sn$	–0.136
$Ni^{2+} + 2e^- \rightarrow Ni$	–0.250
$Co^{2+} + 2e^- \rightarrow Co$	–0.277
$Cd^{2+} + 2e^- \rightarrow Cd$	–0.403
$Fe^{2+} + 2e^- \rightarrow Fe$	–0.440
$Cr^{3+} + 3e^- \rightarrow Cr$	–0.744
$Zn^{2+} + 2e^- \rightarrow Zn$	–0.763
$Al^{3+} + 3e^- \rightarrow Al$	–1.662
$Mg^{2+} + 2e^- \rightarrow Mg$	–2.363
$Na^+ + e^- \rightarrow Na$	–2.714
$K^+ + e^- \rightarrow K$	–2.924

The Galvanic Series

	Platinum
	Gold
	Graphite
↑	Titanium
	Silver
Increasingly Inert	Stainless Steel (passive)
	Nickel (Passive)
	Copper-Nickel alloys
	Bronzes (Cu-Sn)
	Copper
	Brasses (Cu-Zn)
	Nickel (active)
	Tin
	Lead
	Stainless Steel (active)
	Cast Iron
Increasingly Active	Iron and Steel
	Aluminum Alloys
↓	Cadmium
	Commercially pure Aluminum
	Zinc
	Magnesium Alloys

Periodic Table of the Elements

1A												3A	4A	5A	6A	7A	8A
1 **H** 1.00794 Hydrogen	2A																2 **He** 4.002602 Helium
3 **Li** 6.941 Lithium	4 **Be** 9.012182 Beryllium											5 **B** 10.811 Boron	6 **C** 12.0107 Carbon	7 **N** 14.0067 Nitrogen	8 **O** 15.9994 Oxygen	9 **F** 18.9984032 Fluorine	10 **Ne** 20.1797 Neon
11 **Na** 22.989769 Sodium	12 **Mg** 24.3050 Magnesium	3B	4B	5B	6B	7B	8B			1B	2B	13 **Al** 26.9815386 Aluminum	14 **Si** 28.0855 Silicon	15 **P** 30.973762 Phosphorus	16 **S** 32.065 Sulfur	17 **Cl** 35.453 Chlorine	18 **Ar** 39.948 Argon
19 **K** 39.0983 Potassium	20 **Ca** 40.078 Calcium	21 **Sc** 44.955912 Scandium	22 **Ti** 47.867 Titanium	23 **V** 50.9415 Vanadium	24 **Cr** 51.9961 Chromium	25 **Mn** 54.938045 Manganese	26 **Fe** 55.845 Iron	27 **Co** 58.933195 Cobalt	28 **Ni** 58.6934 Nickel	29 **Cu** 63.546 Copper	30 **Zn** 65.38 Zinc	31 **Ga** 69.723 Gallium	32 **Ge** 72.64 Germanium	33 **As** 74.92160 Arsenic	34 **Se** 78.96 Selenium	35 **Br** 79.904 Bromine	36 **Kr** 83.798 Krypton
37 **Rb** 85.4678 Rubidium	38 **Sr** 87.62 Strontium	39 **Y** 88.90585 Yttrium	40 **Zr** 91.224 Zirconium	41 **Nb** 92.90638 Niobium	42 **Mo** 95.96 Molybdenum	43 **Tc** [98] Technetium	44 **Ru** 101.07 Ruthenium	45 **Rh** 102.90550 Rhodium	46 **Pd** 106.42 Palladium	47 **Ag** 107.8682 Silver	48 **Cd** 112.411 Cadmium	49 **In** 114.818 Indium	50 **Sn** 118.710 Tin	51 **Sb** 121.760 Antimony	52 **Te** 127.60 Tellurium	53 **I** 126.90447 Iodine	54 **Xe** 131.293 Xenon
55 **Cs** 132.9054519 Cesium	56 **Ba** 137.327 Barium	57-71 Lanthanides	72 **Hf** 178.49 Hafnium	73 **Ta** 180.94788 Tantalum	74 **W** 183.84 Tungsten	75 **Re** 186.207 Rhenium	76 **Os** 190.23 Osmium	77 **Ir** 192.217 Iridium	78 **Pt** 195.084 Platinum	79 **Au** 196.966569 Gold	80 **Hg** 200.59 Mercury	81 **Tl** 204.3833 Thallium	82 **Pb** 207.2 Lead	83 **Bi** 208.98040 Bismuth	84 **Po** [209] Polonium	85 **At** [210] Astatine	86 **Rn** [222] Radon
87 **Fr** [223] Francium	88 **Ra** [226] Radium	89-103 Actinides	104 **Rf** [267] Rutherfordium	105 **Db** [268] Dubnium	106 **Sg** [271] Seaborgium	107 **Bh** [272] Bohrium	108 **Hs** [270] Hassium	109 **Mt** [276] Meitnerium	110 **Ds** [281] Darmstadtium	111 **Rg** [280] Roentgenium	112 **Cn** [285] Copernicium	113 **Uut** [284] Ununtrium	114 **Uuq** [289] Ununquadium	115 **Uup** [288] Ununpentium	116 **Uuh** [293] Ununhexium	117 **Uus** [294] Ununseptium	118 **Uuo** [294] Ununoctium

Lanthanides	57 **La** 138.90547 Lanthanum	58 **Ce** 140.116 Cerium	59 **Pr** 140.90765 Praseodymium	60 **Nd** 144.242 Neodymium	61 **Pm** [145] Promethium	62 **Sm** 150.36 Samarium	63 **Eu** 151.964 Europium	64 **Gd** 157.25 Gadolinium	65 **Tb** 158.92535 Terbium	66 **Dy** 162.500 Dysprosium	67 **Ho** 164.93032 Holmium	68 **Er** 167.259 Erbium	69 **Tm** 168.93421 Thulium	70 **Yb** 173.054 Ytterbium	71 **Lu** 174.9668 Lutetium
Actinides	89 **Ac** [227] Actinium	90 **Th** 232.03806 Thorium	91 **Pa** 231.03588 Protactinium	92 **U** 238.02891 Uranium	93 **Np** [237] Neptunium	94 **Pu** [244] Plutonium	95 **Am** [243] Americium	96 **Cm** [247] Curium	97 **Bk** [247] Berkelium	98 **Cf** [251] Californium	99 **Es** [252] Einsteinium	100 **Fm** [257] Fermium	101 **Md** [258] Mendelevium	102 **No** [259] Nobelium	103 **Lr** [262] Lawrencium

Electronegativity

Periodic Table of the Elements

Electronegativity

http://chemistry.about.com

About Chemistry

1A												3A	4A	5A	6A	7A	8A
1 H 2.20	2A																2 He no data
3 Li 0.98	4 Be 1.57											5 B 2.04	6 C 2.55	7 N 3.04	8 O 3.44	9 F 3.98	10 Ne no data
11 Na 0.93	12 Mg 1.31	3B	4B	5B	6B	7B	8B			1B	2B	13 Al 1.61	14 Si 1.90	15 P 2.19	16 S 2.58	17 Cl 3.16	18 Ar no data
19 K 0.82	20 Ca 1.00	21 Sc 1.36	22 Ti 1.54	23 V 1.63	24 Cr 1.66	25 Mn 1.55	26 Fe 1.83	27 Co 1.88	28 Ni 1.91	29 Cu 1.90	30 Zn 1.65	31 Ga 1.81	32 Ge 2.01	33 As 2.18	34 Se 2.55	35 Br 2.96	36 Kr 3.00
37 Rb 0.82	38 Sr 0.95	39 Y 1.22	40 Zr 1.33	41 Nb 1.6	42 Mo 2.16	43 Tc 1.9	44 Ru 2.2	45 Rh 2.28	46 Pd 2.20	47 Ag 1.93	48 Cd 1.69	49 In 1.78	50 Sn 1.96	51 Sb 2.05	52 Te 2.1	53 I 2.66	54 Xe 2.6
55 Cs 0.79	56 Ba 0.89	57-71 Lanthanides	72 Hf 1.3	73 Ta 1.5	74 W 2.36	75 Re 1.9	76 Os 2.2	77 Ir 2.20	78 Pt 2.28	79 Au 2.54	80 Hg 2.00	81 Tl 1.62	82 Pb 2.33	83 Bi 2.02	84 Po 2.0	85 At 2.2	86 Rn no data
87 Fr 0.7	88 Ra 0.89	89-103 Actinides															

*** Elements > 104 exist only for very short half-lifes and the data is unknown.***

Lanthanides	57 La 1.10	58 Ce 1.12	59 Pr 1.13	60 Nd 1.14	61 Pm 1.13	62 Sm 1.17	63 Eu 1.2	64 Gd 1.2	65 Tb 1.2	66 Dy 1.22	67 Ho 1.23	68 Er 1.24	69 Tm 1.25	70 Yb 1.1	71 Lu 1.27
Actinides	89 Ac 1.1	90 Th 1.3	91 Pa 1.5	92 U 1.38	93 Np 1.36	94 Pu 1.28	95 Am 1.3	96 Cm 1.3	97 Bk 1.3	98 Cf 1.3	99 Es 1.3	100 Fm 1.3	101 Md 1.3	102 No 1.3	103 Lr no data