

MSEG201 LQ1 formula sheet

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$$\begin{aligned}k &= 1.38 \times 10^{-23} \text{ J/atom} \cdot \text{K} \\k &= 8.62 \times 10^{-5} \text{ eV/atom} \cdot \text{K} \\N_A &= 6.022 \times 10^{23} \text{ atoms/mol}\end{aligned}$$

$$\begin{aligned}R &= 8.314 \text{ J/mol} \cdot \text{K} \\e &= 1.6 \times 10^{-19} \text{ C} \\m_e &= 9.11 \times 10^{-31} \text{ kg}\end{aligned}$$

$$\begin{aligned}m_p &= 1.67 \times 10^{-27} \text{ kg} \\m_n &= 1.67 \times 10^{-27} \text{ kg} \\\lambda_{Cu_{K-\alpha}} &= 1.54 \text{ \AA}\end{aligned}$$

Prefix	Symbol	Factor	Prefix	Symbol	Factor
pico	p	10^{-12}	milli	m	10^{-3}
angstrom	\AA	10^{-10}	centi	c	10^{-2}
nano	n	10^{-9}	deci	d	10^{-1}
micro	μ	10^{-6}			

System	coordination	APF	atoms	r a relationship	close packed	reflection rule	plane ex
FCC	12	0.74	4	$4r = \sqrt{2}a$	face diagonal	h,k,l all even or odd	(111), (200)
BCC	8	0.68	2	$4r = \sqrt{3}a$	body diagonal	$h+k+l = 2n$	(111), (200), (220)
SC	6	0.52	1	$2r = a$	edge	all	all!
HCP	12	0.74	2	$2r = a; c = \sqrt{\frac{8}{3}}a$	base edge		

System	interstitial sites
FCC	octahedral edges; mid diagonals tetrahedral
BCC	octahedral edge centers & face centers; tetrahedral face diamonds

r_{cat}/r_{an}	coordination	structure	example	formula units/cell
< 0.155	2	linear		2
0.155 - 0.225	3	trigonal planar		3
0.225 - 0.414	4	tetrahedral	zincblende	4
0.414 - 0.732	6	octahedral	rock salt; NaCl	4
0.732 - 1.0	8	cubic	CsCl	1
AX_2	8	flourite/antiflourite	CaF_2	4

notation: (hkl) is a plane, [uvw] is a direction, {hkl} is a family of planes

cubics

$$\rho = \frac{n \cdot A}{V \cdot N_A}$$

ceramics

$$\rho = \frac{n(\sum A_c + \sum A_a)}{V \cdot N_A}$$

metals

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

ceramics

$$\frac{N_s}{N} = \exp\left(\frac{-Q_s}{2kT}\right)$$

$$N = \rho \cdot \frac{N_A}{\mu}$$

$$n\lambda = 2d \sin(\theta)$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\ln\left(\frac{N_{v2}}{N_{v1}}\right) = \frac{-Q_v}{k} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$E = E_A + E_R$$

$$E_A = -\frac{A}{r}$$

$$E_R = \frac{B}{r^n}$$

equilateral triangle: $A = \frac{\sqrt{3}}{4}a^2$
 volume of a sphere: $V = \frac{4}{3}\pi r^3$
 area of a circle: $A = \pi r^2$
 volume of a cylinder: $V = \pi r^2 h$

volume of a cone: $V = \frac{1}{3}\pi r^2 h$
 volume of a pyramid: $V = \frac{1}{3}A_b h$
 volume of a tetrahedron:
 $V = \frac{1}{6}\sqrt{2}a^3$

volume of a cube: $V = a^3$
 circle circumference: $C = 2\pi r$
 triangle area: $A = \frac{1}{2}bh$
 pythagorean: $a^2 + b^2 = c^2$

30-60-90: $a, a\sqrt{3}, 2a$
 45-45-90: $a, a, a\sqrt{2}$
 1 radian: 57.3°
 1 degree: $\frac{\pi}{180}$ radians

solid solutions

- $\Delta r < 15\%$ (similar atomic radii)
- as ΔEN decreases, solubility increases
- same structure (i.e. both FCC)
- a metal dissolves better in higher valency host

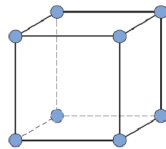
Defects

- vacancies—absence of atom, distorts planes
- dislocations—line defect, edge or screw
- frenkel—cation vacancy + cation interstitial
- shottky—cation and anion vacancy
- edge dislocation—extra half plane of atoms
- bergers vector—direction and magnitude of dislocation
- screw dislocation—spiral planar defect

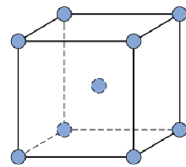
Grains

- grain boundary—interface between grains
- angle boundary—interface between grains with different orientations
- high angle boundaries leads to higher surface energy
- smaller grains have higher surface energy
- anisotropy—directional dependence of properties

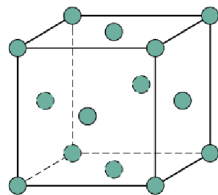
Simple Cubic (SC)



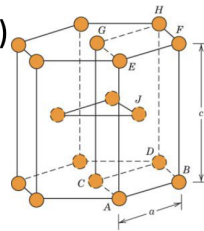
Body-Centered (BCC)



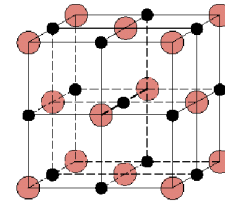
Face-Centered (FCC)



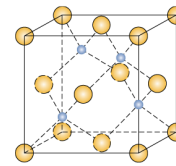
Hexagonal close packed (HCP)



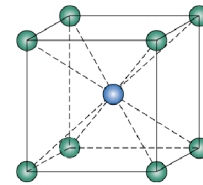
Rock Salt (AX)



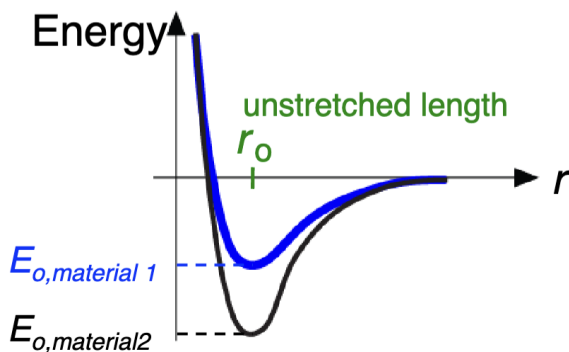
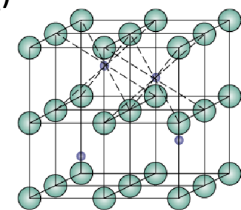
Zincblende (AX)



Cesium Chloride (AX)



Fluorite/Anti-Fluorite (AX₂)



Larger E_0	Larger T_m
Smaller E_0	Larger α

