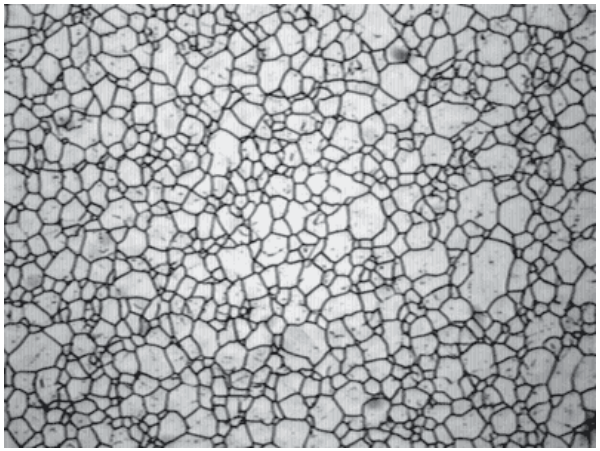
Crystal Structures

Academic Resource Center

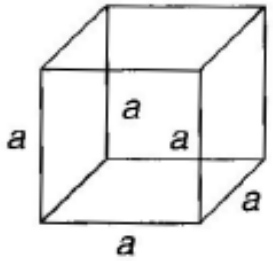
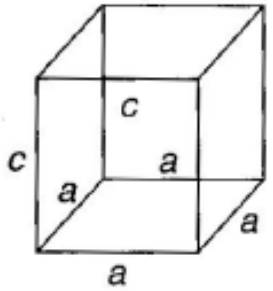
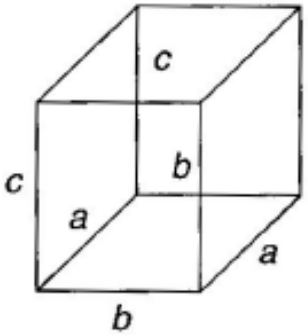
Crystallinity: Repeating or periodic array over large atomic distances. 3-D pattern in which each atom is bonded to its nearest neighbors

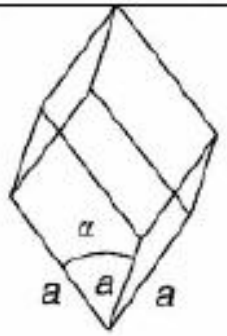
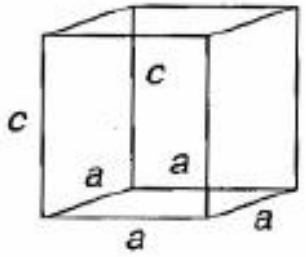
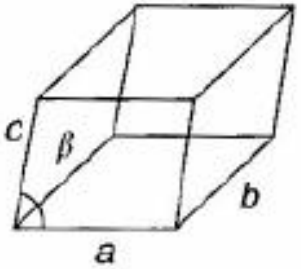
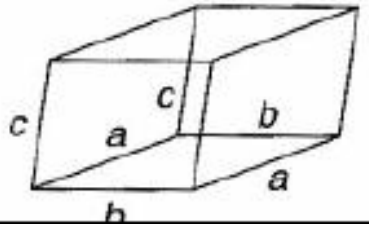
Crystal structure: the manner in which atoms, ions, or molecules are spatially arranged.



Unit cell: small repeating entity of the atomic structure. The basic building block of the crystal structure. It defines the entire crystal structure with the atom positions within.

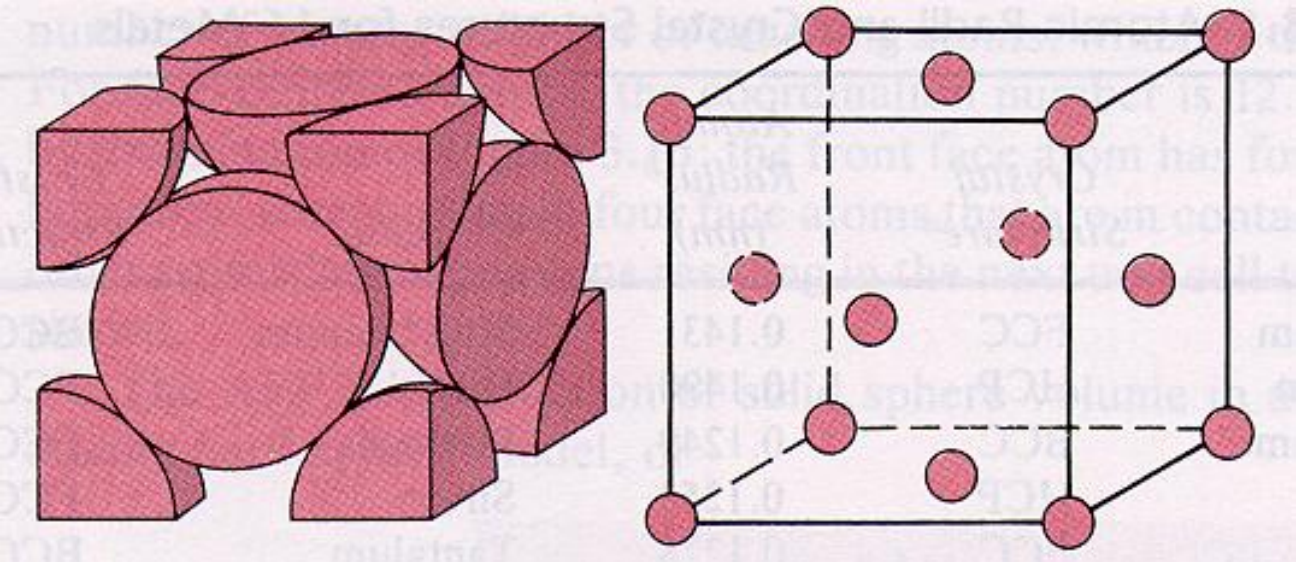
Lattice: 3D array of points coinciding with atom positions (center of spheres)

System	Lattice constants and angles	Unit cell geometry
Cubic	$a = b = c, \alpha = \beta = \gamma = 90°$	
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90°$	
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90°$	

System	Axial lengths and angles	Unit cell geometry
Rhombohedral	$a = b = c$, $\alpha = \beta = \gamma \neq 90°$	
Hexagonal	$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$	
Monoclinic	$a \neq b \neq c$, $\alpha = \gamma = 90°$, $\neq \beta$	
Triclinic	$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90°$	

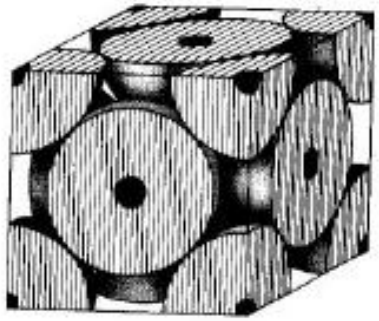
Metallic Crystal Structures

FCC (face centered cubic): Atoms are arranged at the corners and center of each cube face of the cell.



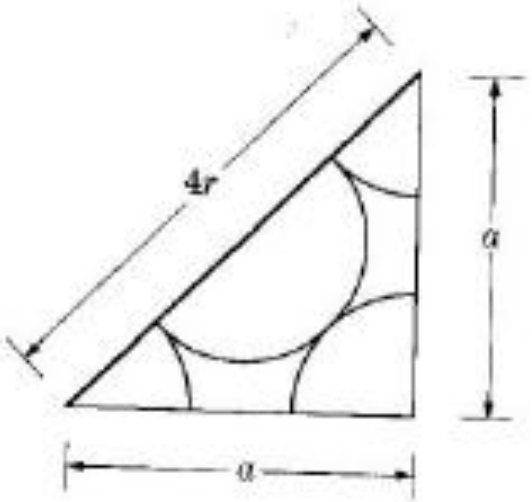
FCC continued

Close packed Plane: On each face of the cube



Atoms are assumed to touch along face diagonals.

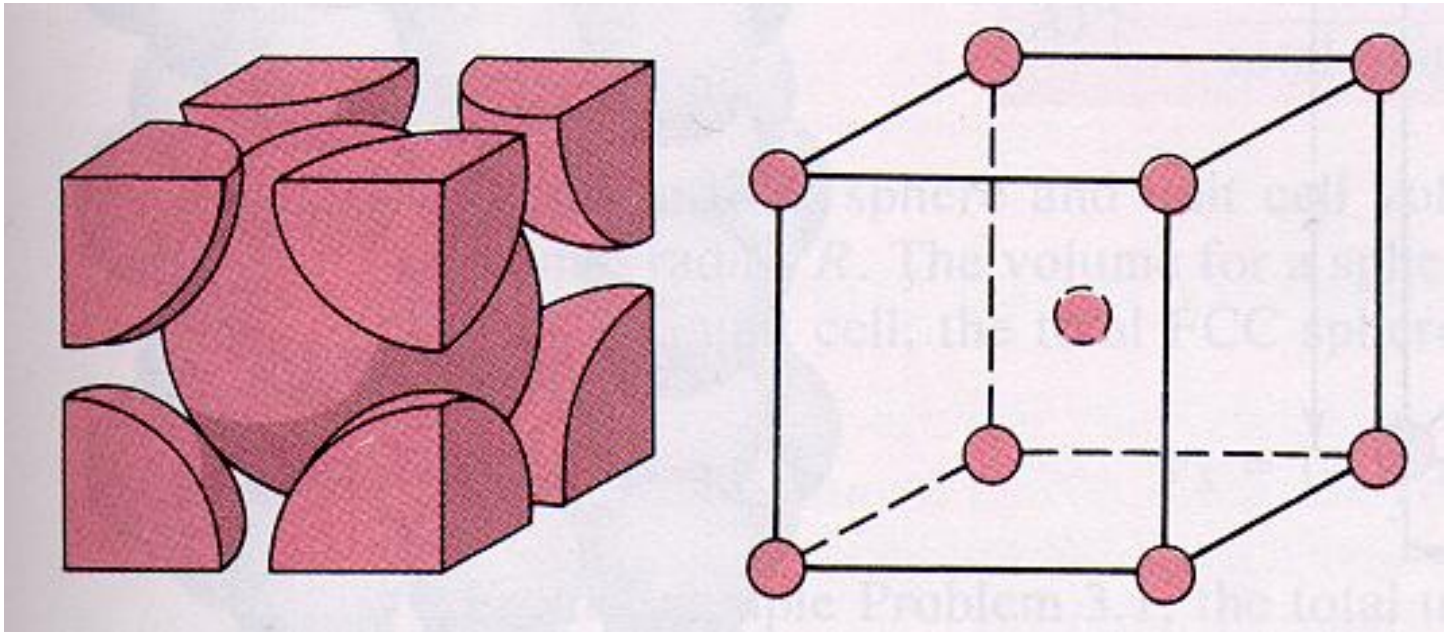
4 atoms in one unit cell.



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

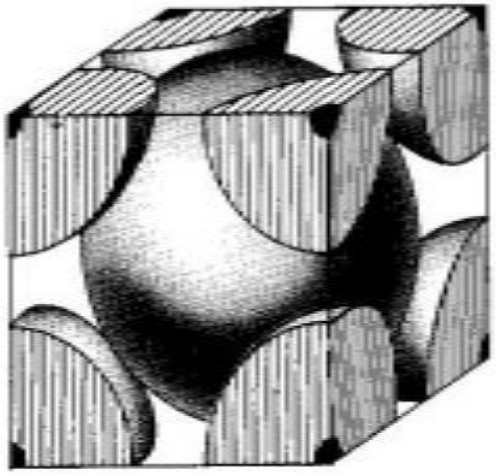
BCC: Body Centered Cubic

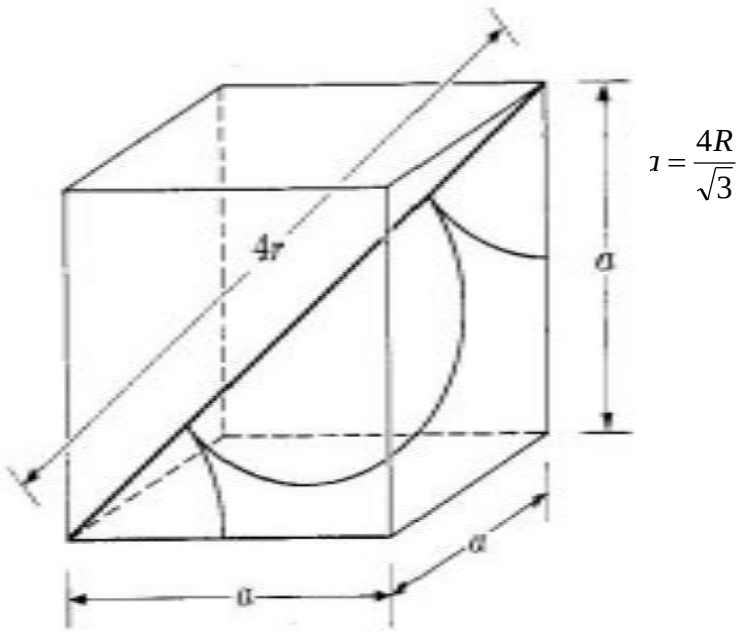
- Atoms are arranged at the corners of the cube with another atom at the cube center.



BCC continued

- Close Packed Plane cuts the unit cube in half diagonally
- 2 atoms in one unit cell

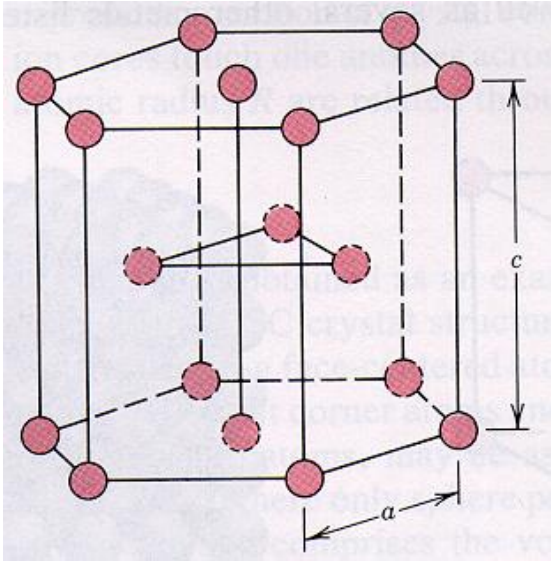




$$1 = \frac{4R}{\sqrt{3}}$$

Hexagonal Close Packed (HCP)

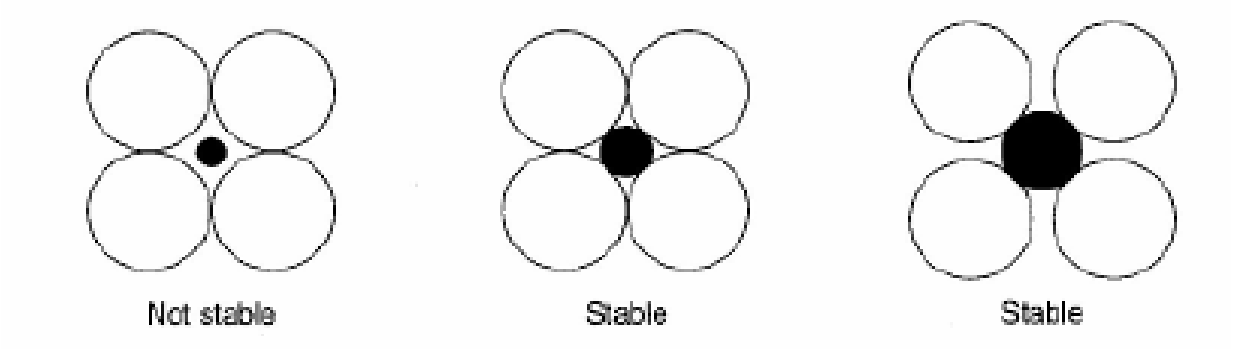
- Cell of an HCP lattice is visualized as a top and bottom plane of 7 atoms, forming a regular hexagon around a central atom. In between these planes is a half-hexagon of 3 atoms.
- There are two lattice parameters in HCP, *a* and *c*, representing the basal and height parameters respectively.



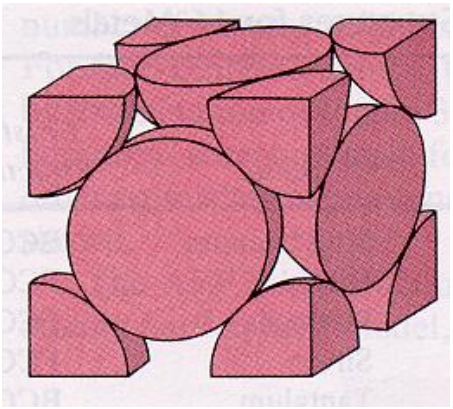
Volume $\frac{3\sqrt{3}\ a^2 c}{2}$

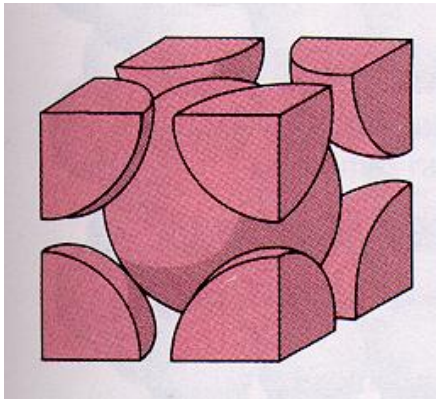
6 atoms per unit cell

Coordination number – the number of nearest neighbor atoms or ions surrounding an atom or ion.

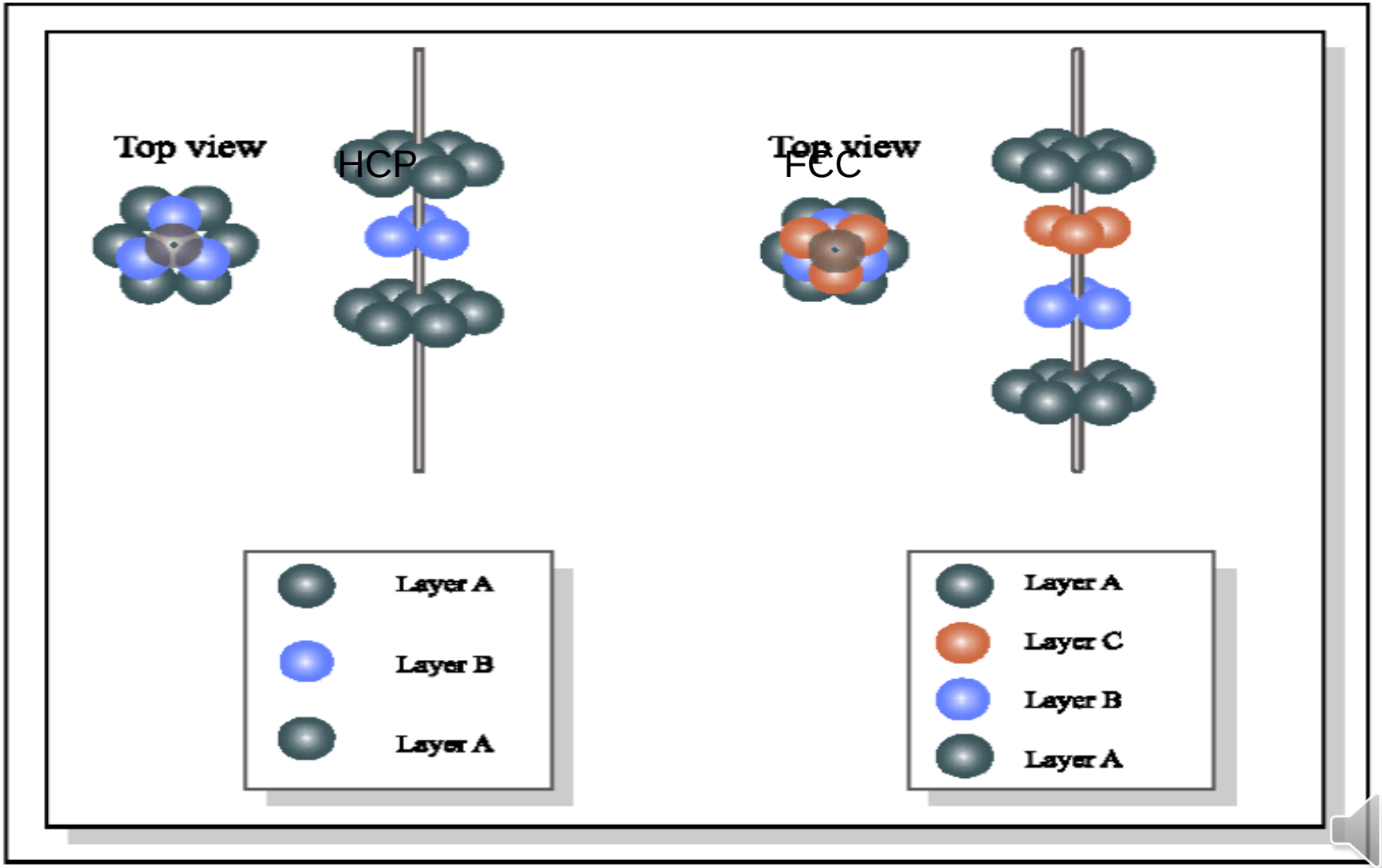


For FCC and HCP systems, the coordination number is 12. For BCC it's 8.



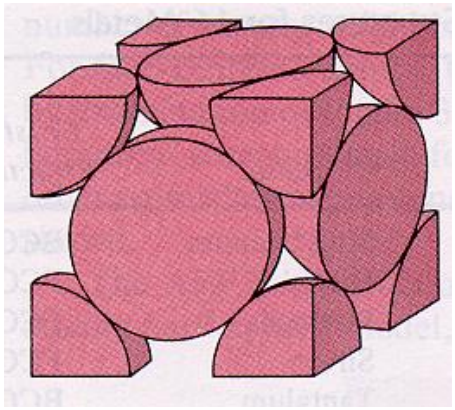


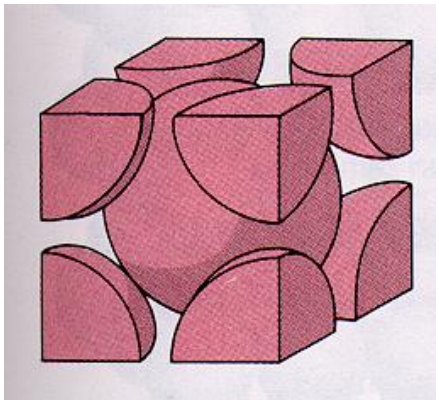
Close Packed Structures



Atomic Packing Factor

- The ratio of atomic sphere volume to unit cell volume, assuming a hard sphere model.
- FCC = HCP = 74% (26% void space in unit cell)
- BCC = 68%





Problem 1

- If the atomic radius for Pb= 0.175nm, find the volume of the unit cell.
- Solution: Pb is fcc, hence $a = 2R\sqrt{2}$

R = 0.175nm

a = 0.495 nm

Volume for cubic = a^3 = 1.21e-28 m^3

Problem 2

Magnesium is hcp with c/a =1.624, density = 1.74g/cm^3. Find the atomic radius of magnesium.

Solution: density = n*MW / (Vc*NA)

For hcp n = 6

Vc = $\frac{3\sqrt{3}\ a^2 c}{2}$ = 2.6*(1.624)a^3 = 4.22a^3

c = 1.624a

NA = 6.02*10^23 atoms/mol

MW magnesium = 24.3 g/mol

Problem 2 continued

4.22a^3 = (6*24.3g/mol)/(1.74g/cm^3*6.02e23atom/mol)

a= 320 pm

For hcp a = 2R

R (atomic radius) magnesium = 160 pm

Crystallographic Points, Directions and Planes

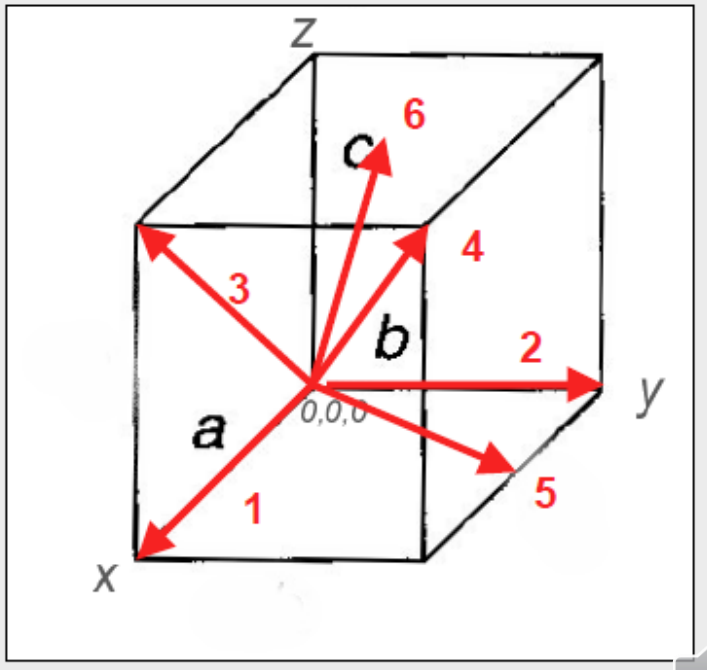
- Directions

Based on intersection with the cell boundaries

Indicated with square brackets [*h, k, l*]

- **Direction 1** — **1, 0, 0 = [100]**
- **Direction 2** — **0,1,0 = [010]**
- **Direction 3** — **1, 0, 1 = [101]**
- **Direction 4** — **1, 1, 1 = [111]**
- **Direction 5** — **½, 1, 0 = [120]**
- **Direction 6** — **½, ½, 1 = [112]**

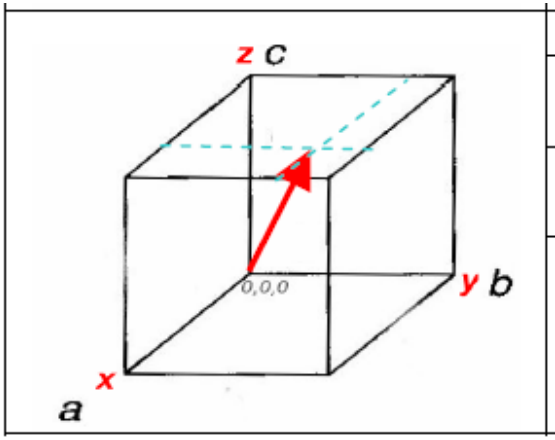
-- Parallel directions have the same value
Lowest Integer Value [111] = [222]



Directions Continued

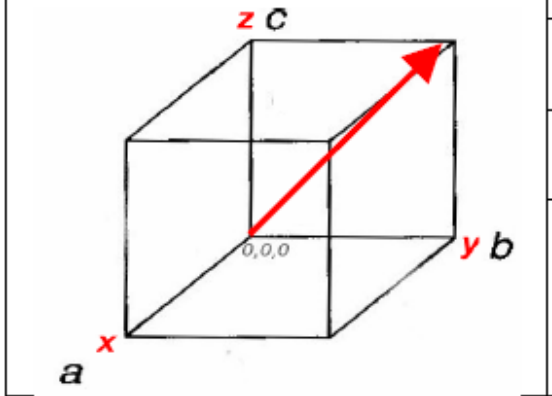
-- No Fractions, Convert to Integers [½ ½ 1] = [112]

-- Negative Direction has a top bar on the hkl value $[1\bar{1}1]$

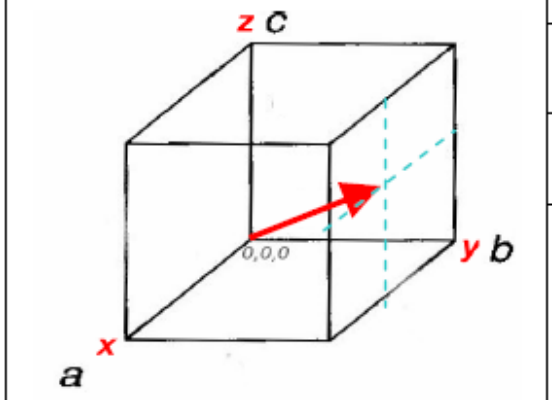


	x (a)	y (b)	z (c)
Point Coordinates	¾	¾	1
Clear Fractions	3	3	4
Crystal Direction	[334]		

Directions Continued



	x (a)	y (b)	z (c)
Point Coordinates	0	1	1
Clear Fractions	0	1	1
Crystal Direction	[011]		

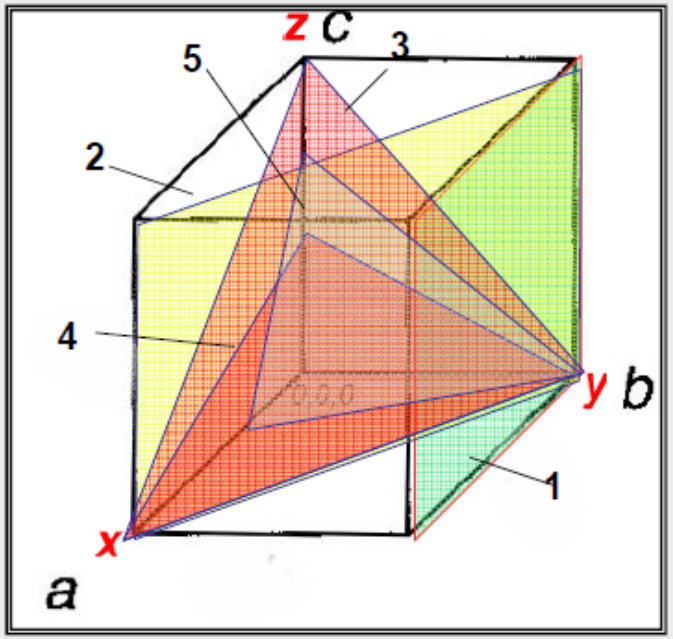


	x (a)	y (b)	z (c)
Point Coordinates	½	1	½
Clear Fractions	1	2	1
Crystal Direction	[121]		

Crystal Planes

Miller Indices-- Based on reciprocal of the intersection of the plane with the cell axes, indicated with parenthesis (*h, k, l*)

- Plane 1 $1/\infty$, 1/1, $1/\infty$ = (010)
- Plane 2 1/1 , 1/1, $1/\infty$ = (110)
- Plane 3 1/1, 1/1, 1/1 = (111)
- Plane 4 1/1 , 1/1, 1/(½) = (112)
- Plane 5 1/(½) , 1/1, 1/(¾) = (634)



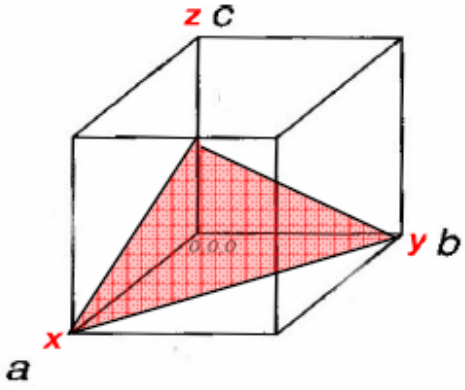
-- Parallel planes have the same value (111) = (222)

-- No Fractions, convert to integers (½ ½ 1) = (112)

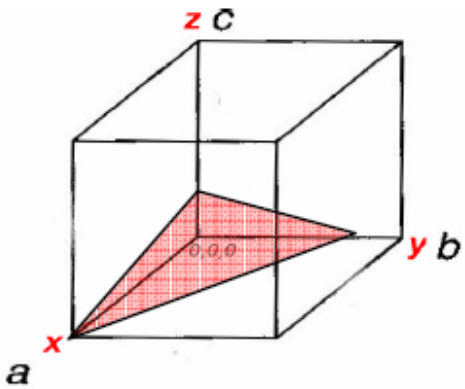
-- Negative Direction has a top bar on the hkl value $(11\bar{1})$

Wiliam H. Miller, 1801-1880, Professor of Mineralogy, Cambridge

Indexing Planes

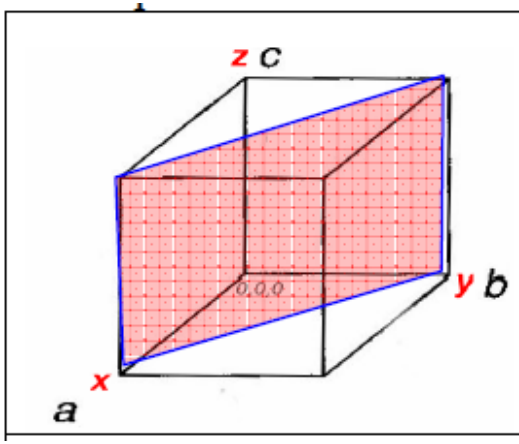


	x (a)	y (b)	z (c)
Intercept on axes	1	1	½
Reciprocal	1	1	2
Integer Clear	1	1	2
Miller Indices	(112)		



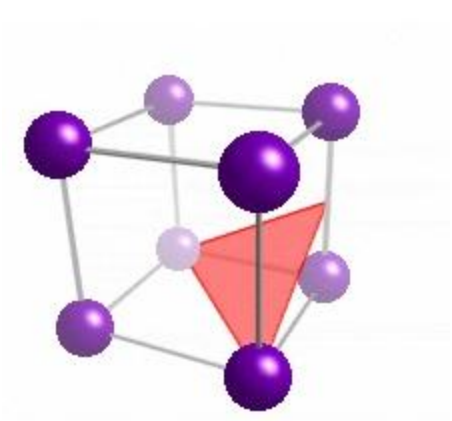
	x (a)	y (b)	z (c)
Intercept on axes	1	¾	¼
Reciprocal	1	4/3	4
Integer Clear	3	4	12
Miller Indices	(3 4 12)		

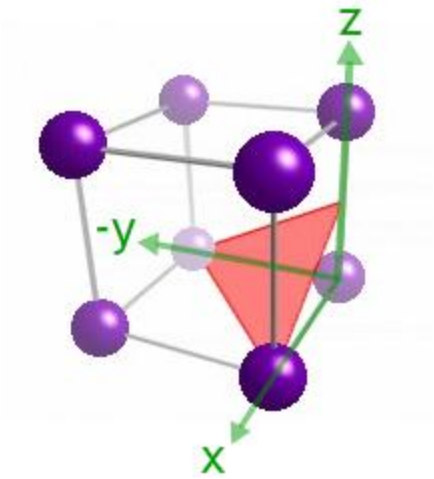
Indexing Planes

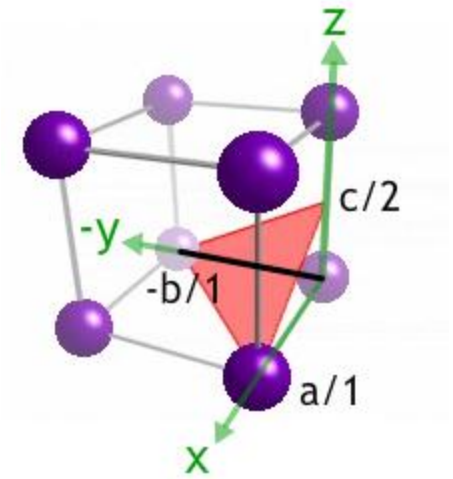


	x (a)	y (b)	z (c)
Intercept on axes	1	1	∞
Reciprocal	1/1	1/1	1/∞ = 0
Integer Clear	1	1	0
Miller Indices	(110)		

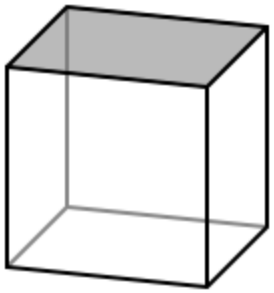
Problem 3: Indexing a negative plane



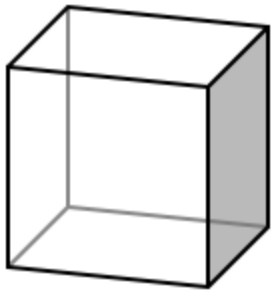




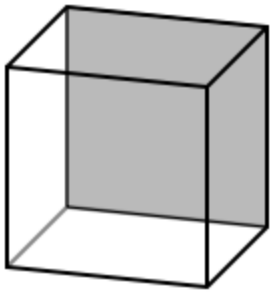
$(1\bar{1}2)$



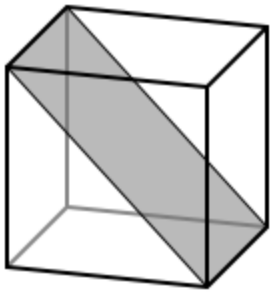
(001)



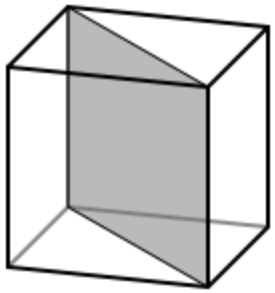
(100)



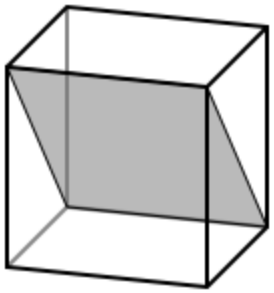
(010)



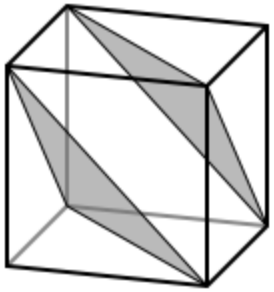
(101)



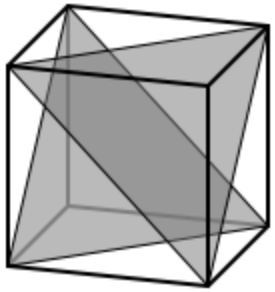
(110)



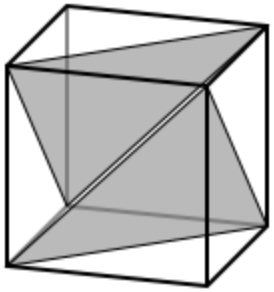
(011)



(111)



$(1\bar{1}1)$



$(\bar{1}11)$

Draw your own lattice planes

- Very useful website:

http://www.doitpoms.ac.uk/tlplib/miller_indices/lattice_draw.php

References

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