ME 254: Materials Engineering

Chapter 3: The Structure of Crystalline Solids

1st Semester 1435-1436 (Fall 2014)

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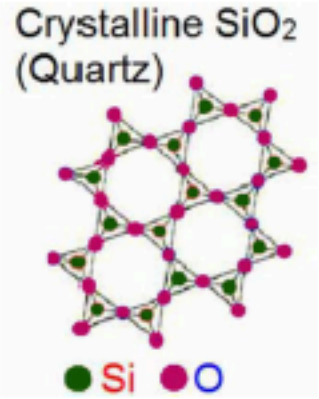
- Crystalline vs. non-crystalline materials
- Crystal structure, crystal system, lattice, unit cell, lattice parameters
- SC, BCC, FCC, HCP
  - Close packed direction
  - Coordination # (Z)
  - # of atoms/unit cell
  - APF
  - Stacking sequence
- Theoretical Density
- Single crystal vs. polycrystalline materials
- Point coordinates
- **Crystal direction**
- **Crystal planes**
- Linear density, $LD_{[xxx]}$
- Planar density, $PD_{(xxx)}$

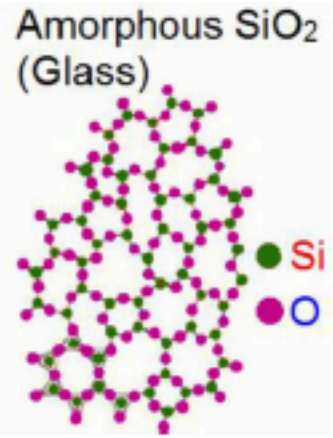
Atomic arrangement



Solid

Crystalline

Amorphous

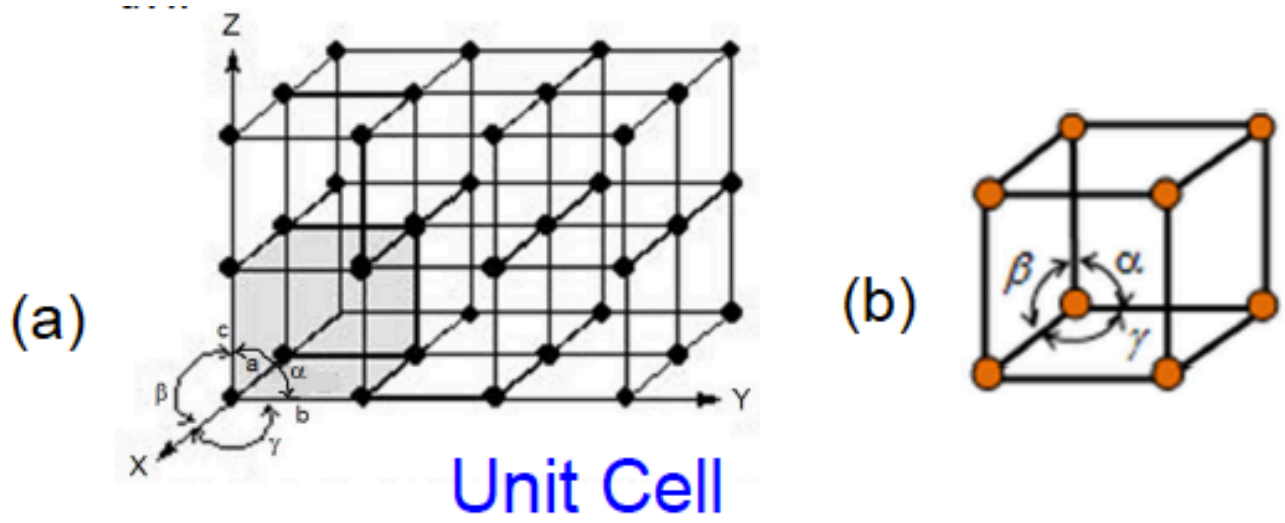


Crystalline – periodic arrangement of atoms: definite repetitive pattern

Non-crystalline or Amorphous – random arrangement of atoms.

Crystal structure

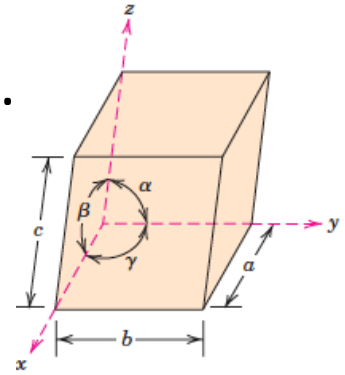
Crystal structure: spatial arrangement of atoms



Lattice: 3D array of points *(lattice points) with infinite repetition.*

Unit cell: The basic structural unit of the lattice structure.

Crystal system: defined based on the geometry of a unit cell (lattice parameters: a, b, c, α, β, γ)

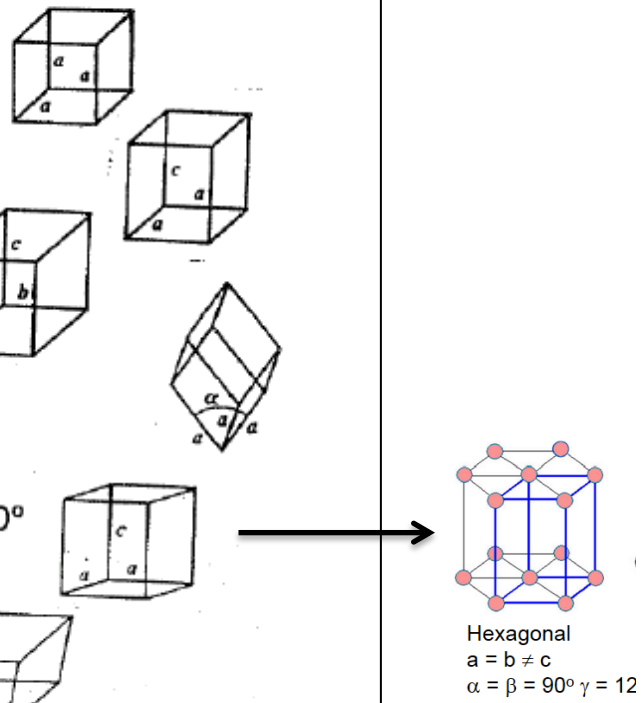


Crystal structure

- **7** Crystal systems ← 7 unique "shapes" of unit cells

Shape of unite cell → **7** Crystal Systems

Cubic	$a=b=c,\ \alpha=\beta=\gamma=90^o$
Tetragonal	$a=b\neq c,\ \alpha=\beta=\gamma=90^o$
Orthorhombic (or Rhombic)	$a\neq b\neq c,\ \alpha=\beta=\gamma=90^o$
Rhombohedral (or Trigonal)	$a=b=c,\ \alpha=\beta=\gamma\neq 90^o$
Hexagonal	$a=b\neq c,\ \alpha=\beta=90^o,\ \gamma=120^o$
Monoclinic	$a\neq b\neq c,\ \alpha=\gamma=90^o\neq\beta$
Triclinic	$a\neq b\neq c,\ \alpha\neq\beta\neq\gamma\neq 90^o$



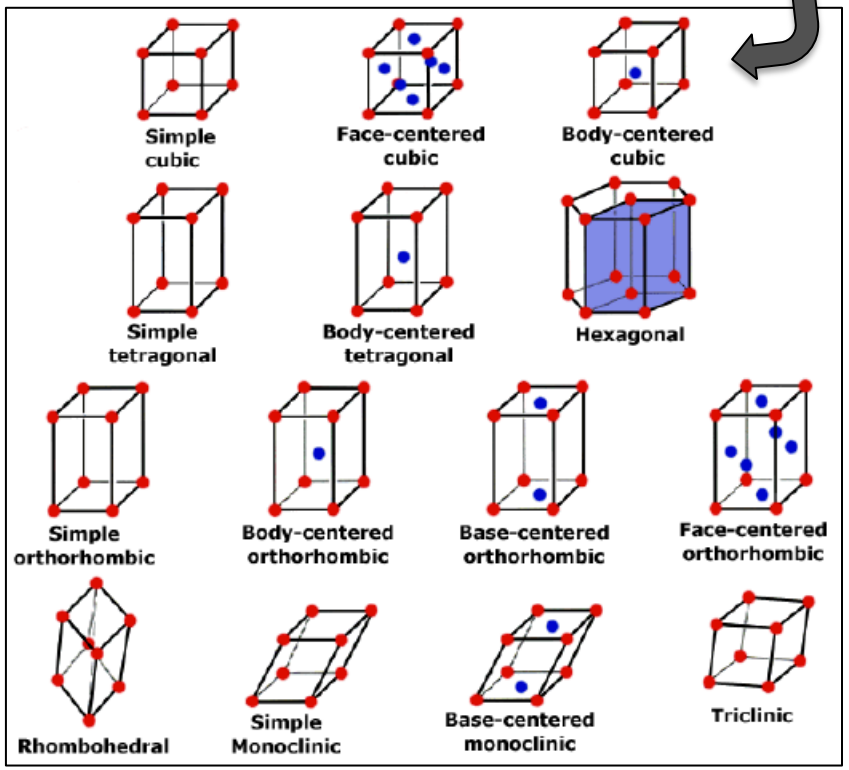
Hexagonal
a = b ≠ c
α = β = 90° γ = 12

Crystal structure

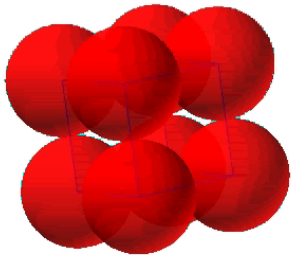
- **7** Crystal systems ← 7 unique "shapes" of unit cells
- **14** Bravais lattices ← 14 unique "arrangements" of lattice points in unit cells

Shape of unite cell → **7** Crystal Systems

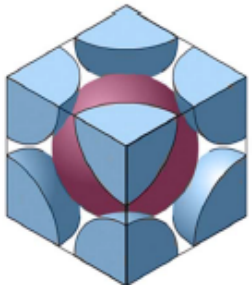
Cubic	$a=b=c,\ \alpha=\beta=\gamma=90^\circ$
Tetragonal	$a=b\neq c,\ \alpha=\beta=\gamma=90^\circ$
Orthorhombic (or Rhombic)	$a\neq b\neq c,\ \alpha=\beta=\gamma=90^\circ$
Rhombohedral (or Trigonal)	$a=b=c,\ \alpha=\beta=\gamma\neq 90^\circ$
Hexagonal	$a=b\neq c,\ \alpha=\beta=90^\circ,\ \gamma=120^\circ$
Monoclinic	$a\neq b\neq c,\ \alpha=\gamma=90^\circ\neq\beta$
Triclinic	$a\neq b\neq c,\ \alpha\neq\beta\neq\gamma\neq 90^\circ$

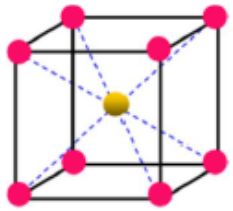


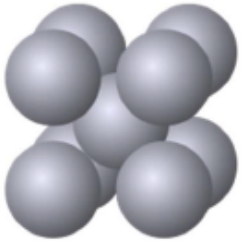
SIMPLE CUBIC STRUCTURE (SC)



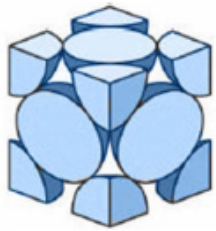
Body Centered Cubic (BCC)

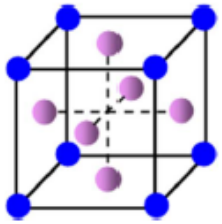


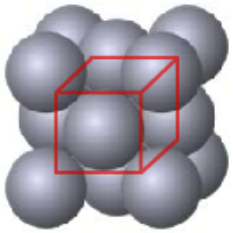




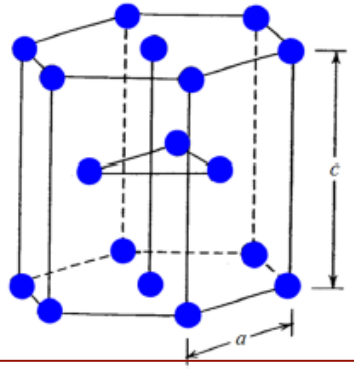
Face Centered Cubic (FCC)

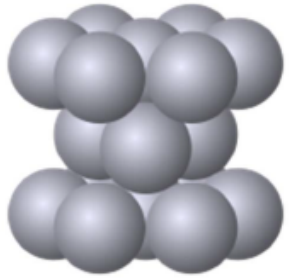






Hexagonal Close Packed (HCP)





	Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF
Simple cubic (SC)				
Body Centered Cubic (BCC)				
Face Centered Cubic (FCC)				
Hexagonal Close Packed (HCP)				

Close packed direction:

Coordination # (Z): no. of nearest neighbor to a particular atom in the crystal

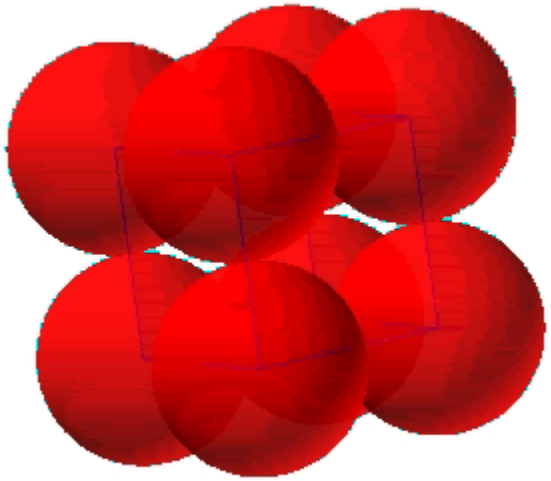
# of atoms/unit cell:

Atomic Packing Factor =

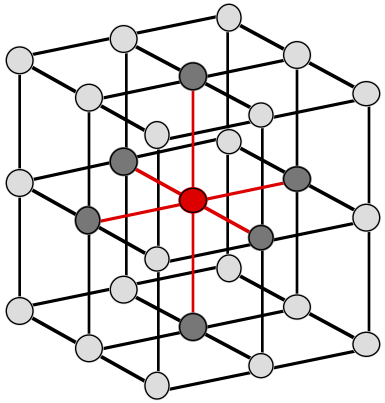
$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

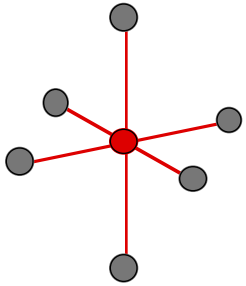
SIMPLE CUBIC STRUCTURE (SC)

- **Rare due to poor packing (only Po has this structure)**
- **Close-packed directions are cube edges.**



- **Coordination # = 6**
  (# nearest neighbors)





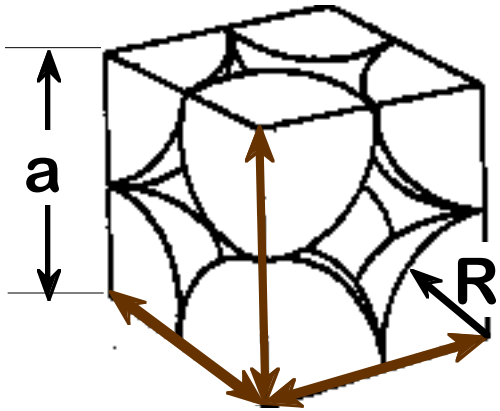
No. of atoms/ unit cell: 8*1/8 = 1

ATOMIC PACKING FACTOR

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

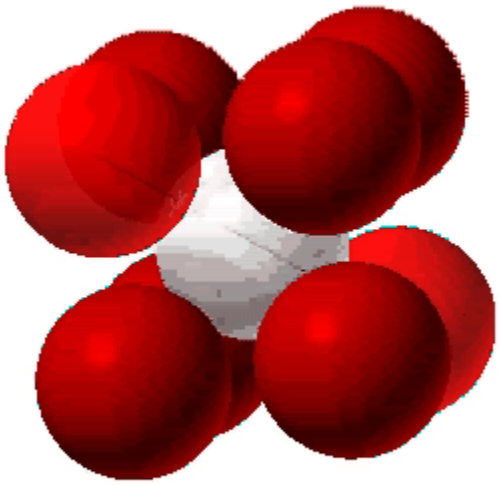
contains 8 x 1/8 =

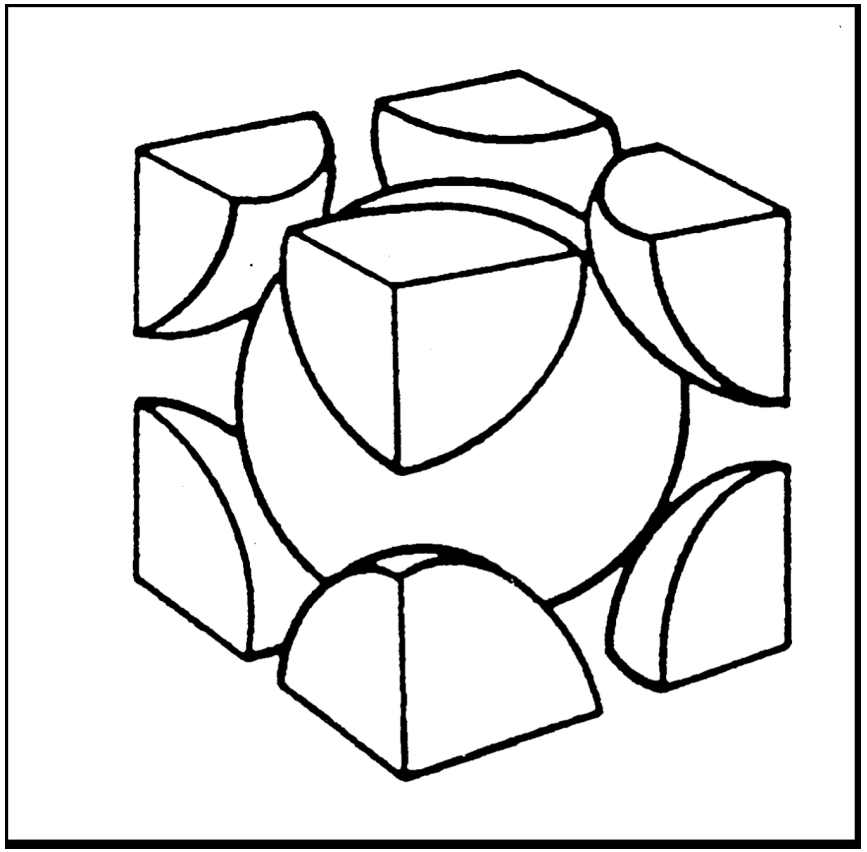
1 atom/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

	Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF
Simple cubic	Cube edge	6	1	0.52
Body Centered Cubic (BCC)				
Face Centered Cubic (FCC)				
Hexagonal Close Packed				

BODY CENTERED CUBIC STRUCTURE (BCC)





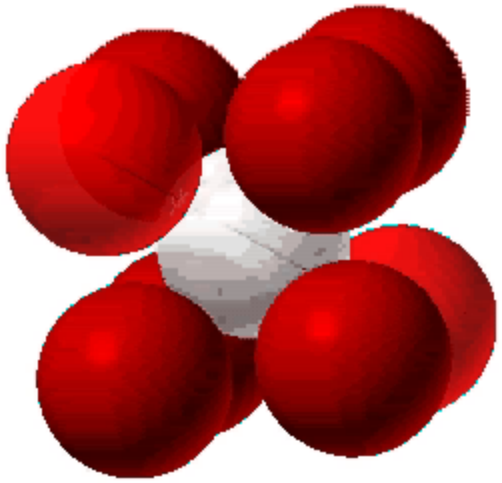
Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF

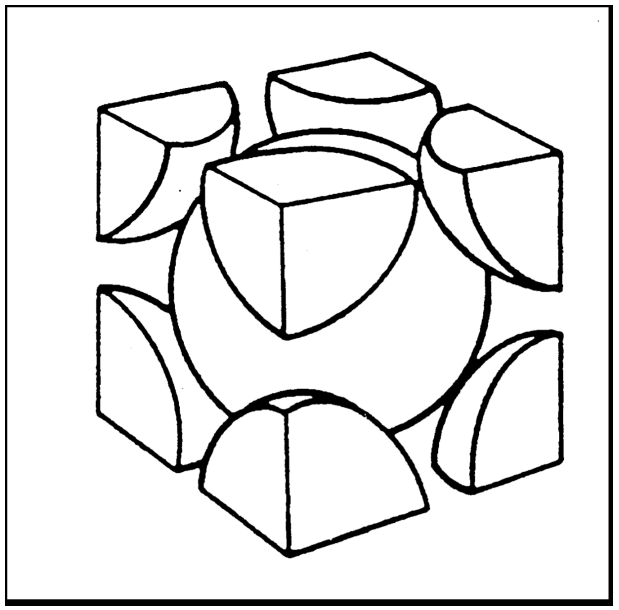
BODY CENTERED CUBIC STRUCTURE (BCC)

- **Close packed directions are cube diagonals.**

  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

- **Coordination # = 8**

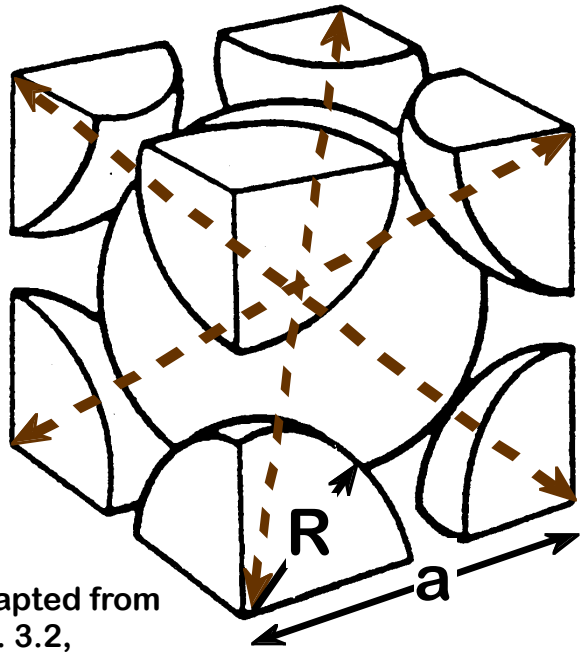




No. of atoms/ unit cell: 8*1/8 + 1 = 2

ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from Fig. 3.2, *Callister 6e.*

Close-packed directions:

length = 4R

$= \sqrt{3}\, a$

Unit cell contains:

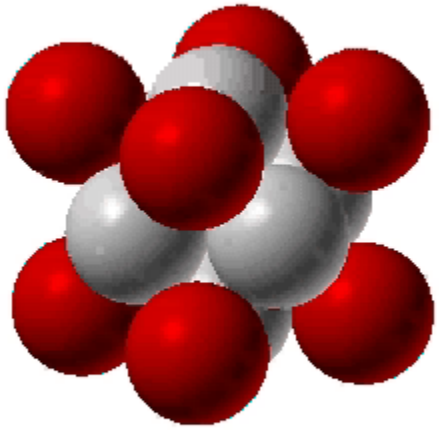
1 + 8 x 1/8

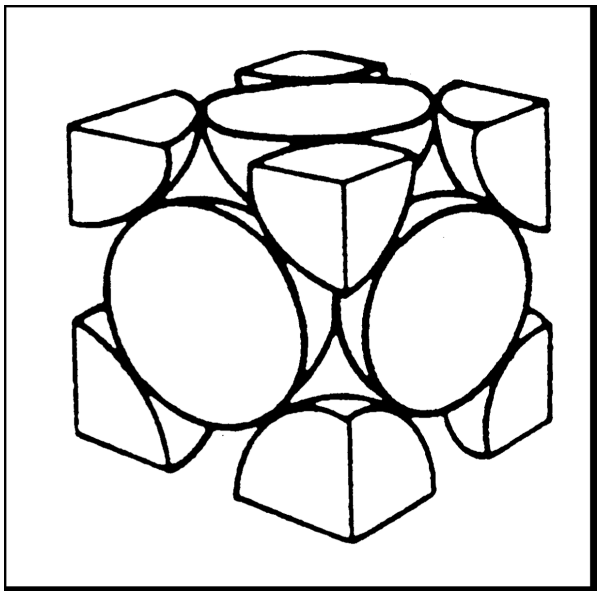
= 2 atoms/unit cell

$$APF = \frac{\left(\frac{\text{atoms}}{\text{unit cell}}\right)\left(\frac{\text{volume}}{\text{atom}}\right)}{\frac{\text{volume}}{\text{unit cell}}} = \frac{2\left(\frac{4}{3}\pi\left(\sqrt{3}a/4\right)^3\right)}{a^3}$$

	Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF
Simple cubic	Cube edge	6	1	0.52
Body Centered Cubic (BCC)	Cube Diagonal	8	2	0.68
Face Centered Cubic (FCC)				
Hexagonal Close Packed				

FACE CENTERED CUBIC STRUCTURE (FCC)





Close packed direction

Coordination # (Z)

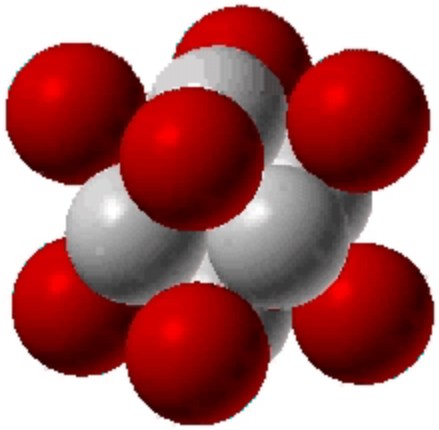
# of atoms/ unit cell

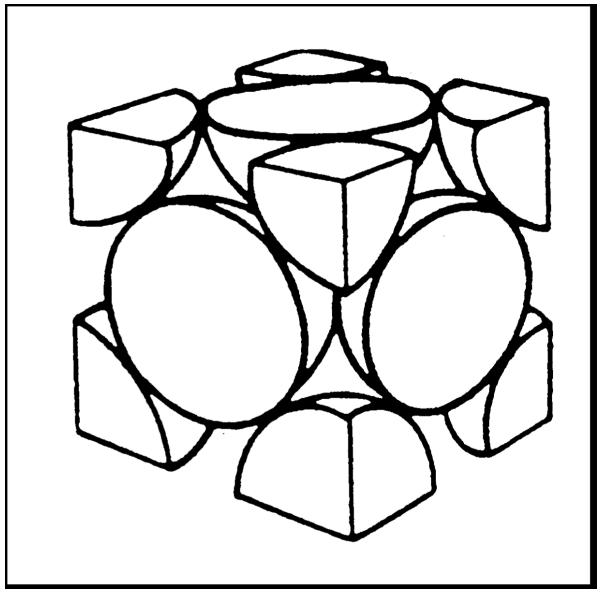
APF

FACE CENTERED CUBIC STRUCTURE (FCC)

- **Close packed directions are face diagonals.**
  - **--Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.**

- **Coordination # = 12**

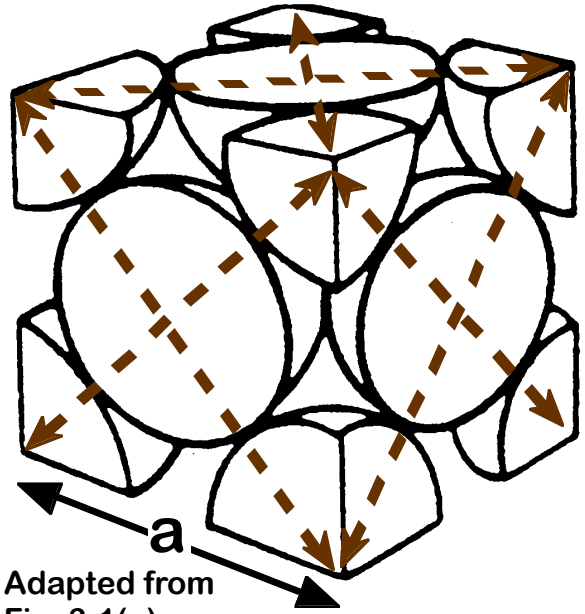




No. of atoms/ unit cell: 8*1/8 + 6 * 1/2 = 4

ATOMIC PACKING FACTOR: FCC

- APF for a body-centered cubic structure = 0.74



Adapted from Fig. 3.1(a), *Callister 6e.*

Close-packed directions:

length = 4R

$= \sqrt{2}\,a$

Unit cell contains:

6 x 1/2 + 8 x 1/8

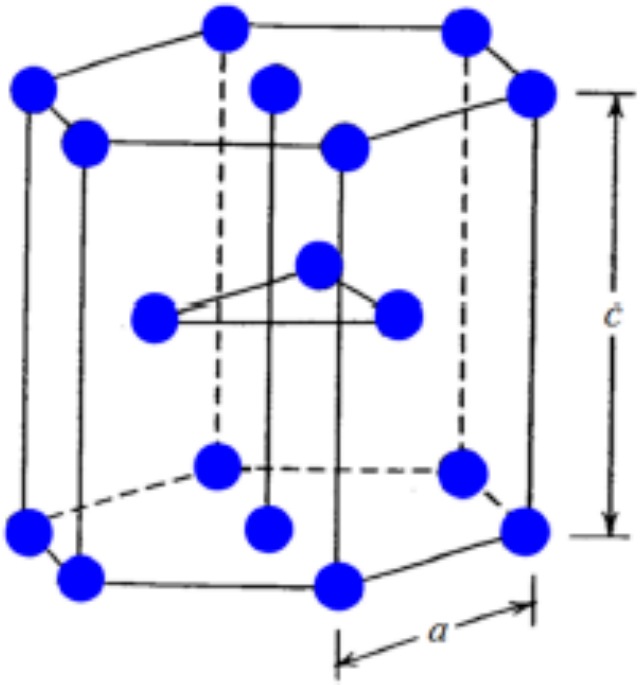
= 4 atoms/unit cell

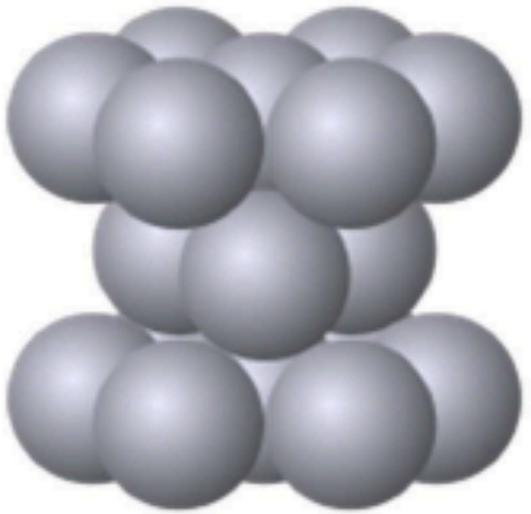
$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{4 \cdot \frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}$$

	Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF
Simple cubic	Cube edge	6	1	0.52
Body Centered Cubic (BCC)	Cube diagonal	8	2	0.68
Face Centered Cubic (FCC)	Face Diagonal	12	4	0.74
Hexagonal Close Packed	Edge	12	6	0.74

Hexagonal Close Packed Crystal (HCP)

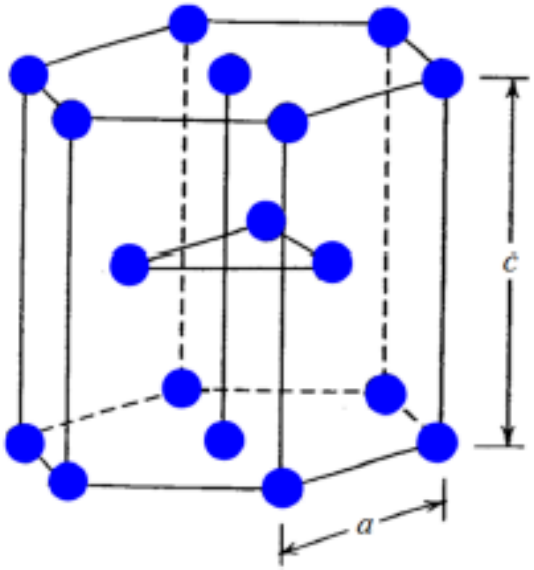
c/ a
=1.633
(ideal)

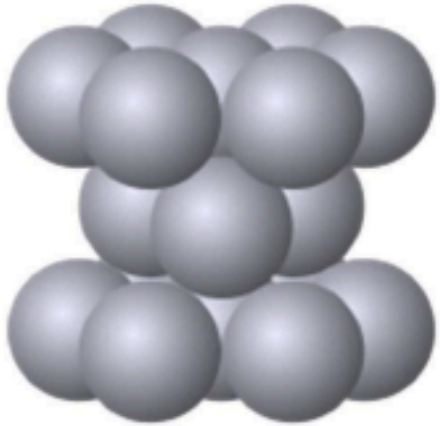




Close packed direction	Coordination # (Z)	# of atoms/ unit cell	APF

Coordination number





In Hexagonal lattice Z = 12. The center atom of the top face is in touch with six corner atoms, three atoms of the mid layer and other three atoms of the mid layer of the unit cell above it.

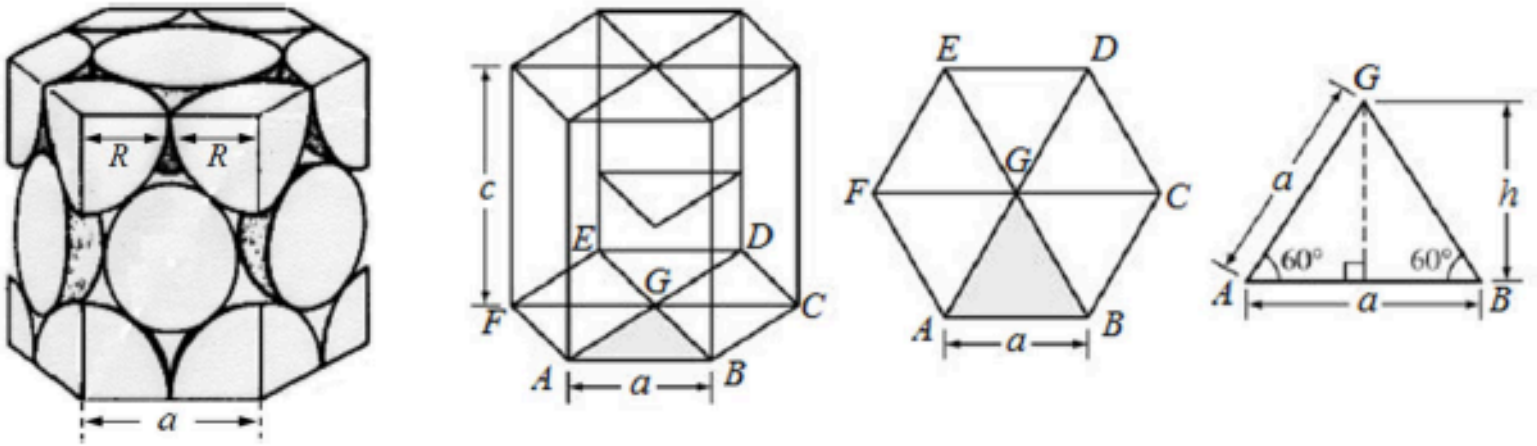
Atomic packing factor

Hexagonal lattice

In the Hexagonal unit cell, number of atoms = 12 corner atoms x 1/6 (shared by six unit cells) + Two face atoms x 1/2 + 3 interior = 6.

$$2R = a$$

Unit cell volume = (6 x ½ x a x h) x c = (3 x a x a sin60°) x c = $3a^2$ c sin60°



APF for HCP = 0.74 (similar to FCC)

Theoretical Density

ρ= n M / Vc

M=mass of an atom

= Atomic weight (A)/ N_A

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

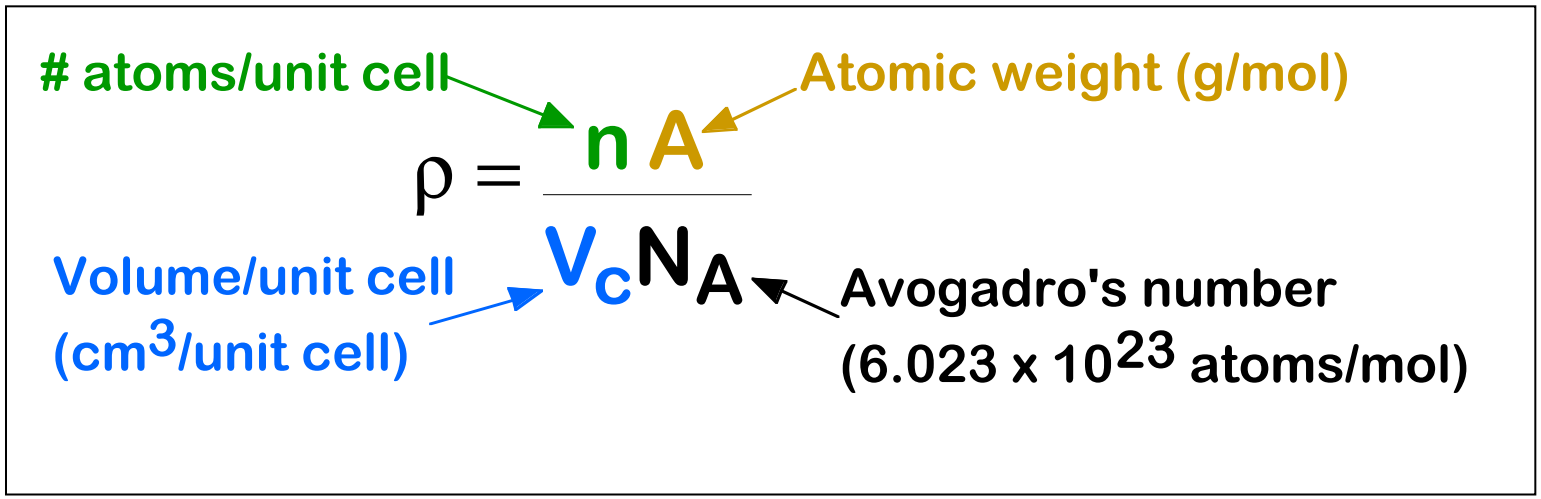
n = number of atoms associated with each unit cell

A = atomic weight

V_C = volume of the unit cell

N_A = Avogadro's number (6.023×10^{23} atoms/mol)

THEORETICAL DENSITY



Example: Copper

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7}cm)

  $V_C = a^3$; For FCC, $a = 4R/\sqrt{2}$; $V_C = 4.75 \times 10^{-23} cm^3$

Result: theoretical $\rho_{Cu} = 8.89$ g/cm^3
Compare to actual: $\rho_{Cu} = 8.94$ g/cm^3

Examples

Ex. 1: Theoretical density calculation from crystal structure.

Theoretical density, $\rho = \dfrac{nA}{V_C N_A}$

n = number of atoms in the unit cell

A = atomic weight

V_C = volume of unit cell

N_A = Avogadro's number (6.023×10^{23} atoms/mol)

Calculate the theoretical density of Al.

Al is FCC, lattice parameter, a = 4.05 Å, n = 4.

Atomic weight of Al is 26.98 g/mol

$$\rho = \frac{4 \times 26.98}{(4.05 \times 10^{-8})^3 \times 6.023 \times 10^{23}} = 2.697\, g/cc$$

Characteristics of Selected Elements at 20C

Element	Symbol	At. Weight (amu)	Density (g/cm^3)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	------	------	------
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	------
Bromine	Br	79.90	------	------	------
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	------	------	------
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	------	------	------
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	------	------	------
Hydrogen	H	1.008	------	------	------

- Crystalline vs. non-crystalline materials
- Crystal structure, crystal system, lattice, unit cell, lattice parameters
- SC, BCC, FCC, HCP
  - Close packed direction
  - Coordination # (Z)
  - # of atoms/unit cell
  - APF
  - Stacking sequence
- Theoretical Density
- Single crystal vs. polycrystalline materials
- Point coordinates
- **Crystal direction**
- **Crystal planes**
- Linear density, $LD_{[xxx]}$
- Planar density, $PD_{(xxx)}$

- Point coordinates
- Crystal direction
- Crystal planes

❑ Point coordinates

Position of any point in a unit cell is given as a fraction of length a (x-axis), fraction of length b (y-axis), and fraction of length c (z-axis)

- Pick an origin
- Put the three axes (x, y, z) along a, b, & c

Example: Find the position of

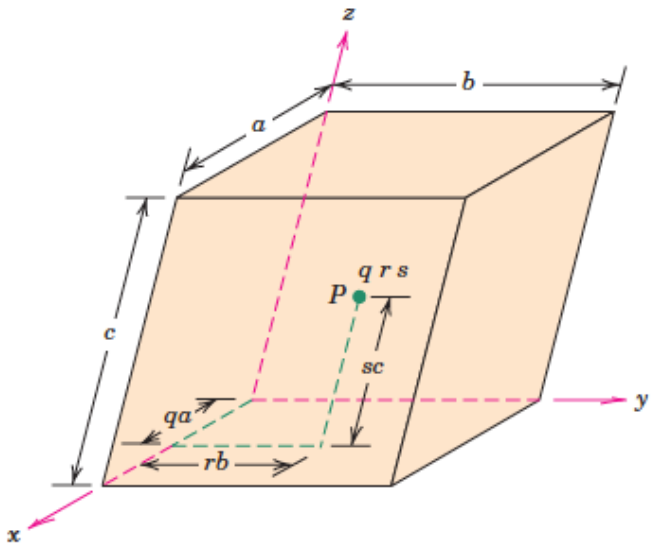
q r s

=>

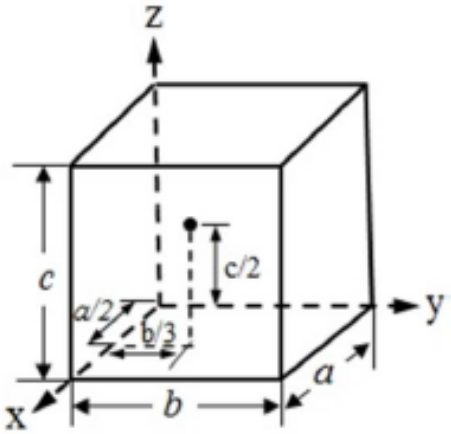
Distance along x-axis = qa

Distance along y-axis = rb

Distance along z-axis = sc

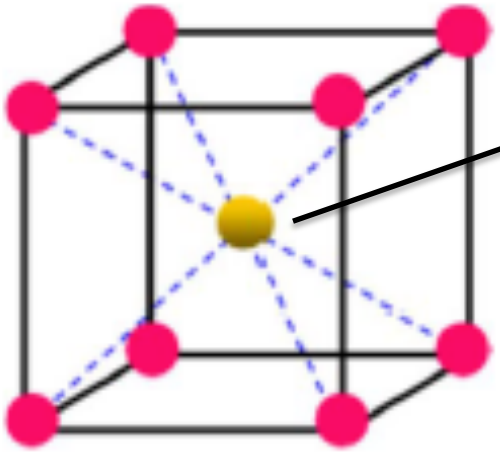


$$\frac{1}{2}\,\frac{1}{3}\,\frac{1}{2}$$

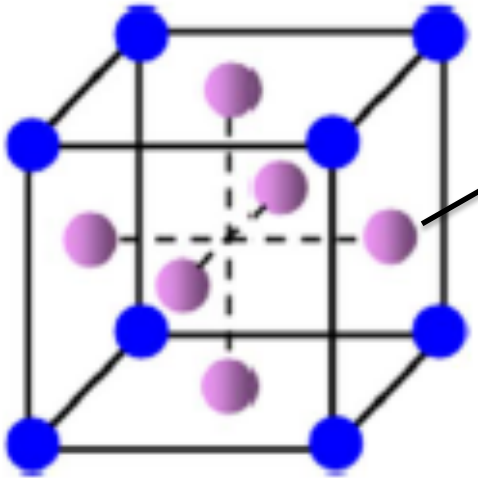


❑ Cont'd: Point coordinates

Example:



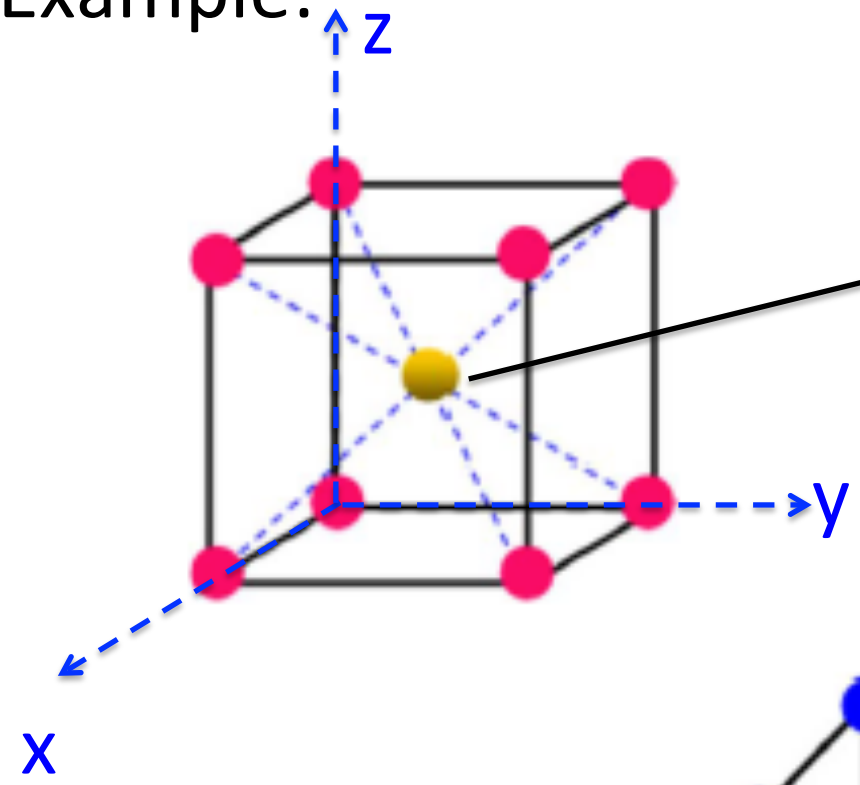
q r s = ??



q r s = ??

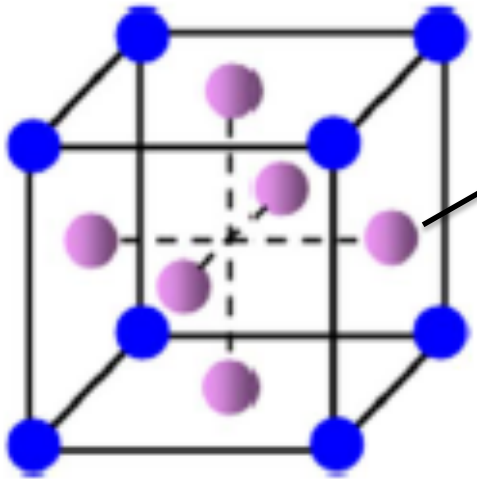
❑ Cont'd: Point coordinates

Example:



q r s = ½ ½ ½

q r s = ½ 1 ½



❑ Crystallographic direction

To specify a direction:

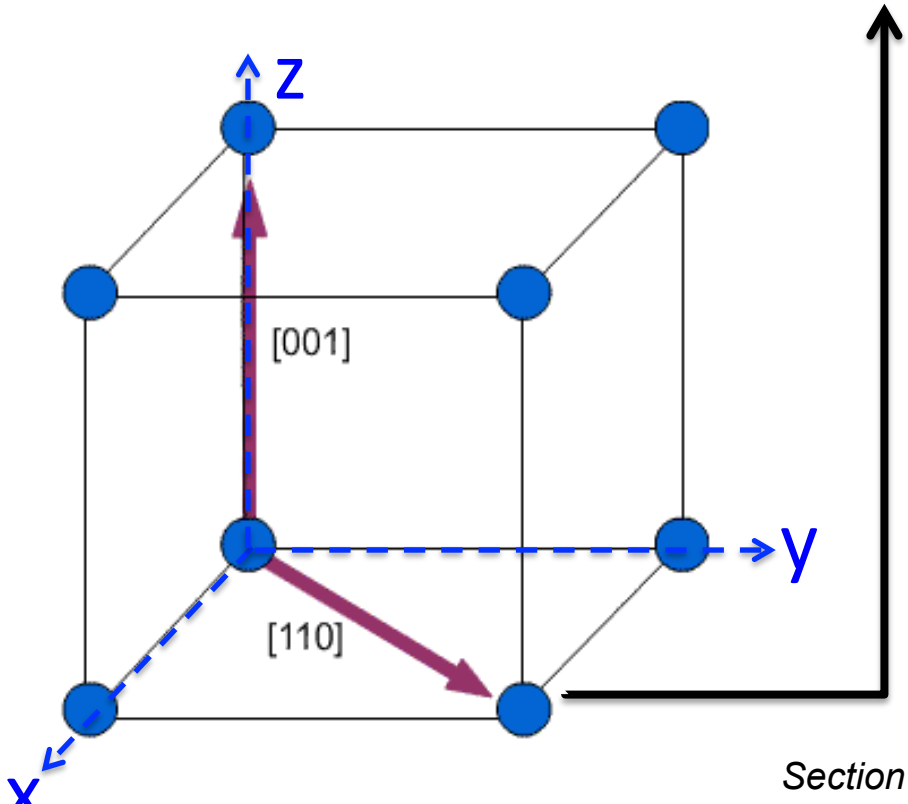
Position the vector such that it passes through the origin

1. Find the coordinates of the two ends of the line (head & tail)
2. Subtract the coordinates of the two ends (head-tail)
3. Convert fractions, if any, into integers (multiply by a common factor) and reduce to lowest terms
4. Enclose in square brackets [u v w]

Coordinates of Head:	1	1	0
Coordinates of Tail:	0	0	0
Subtract:	1	1	0

No fractions

=> [u v w] = [1 1 0]



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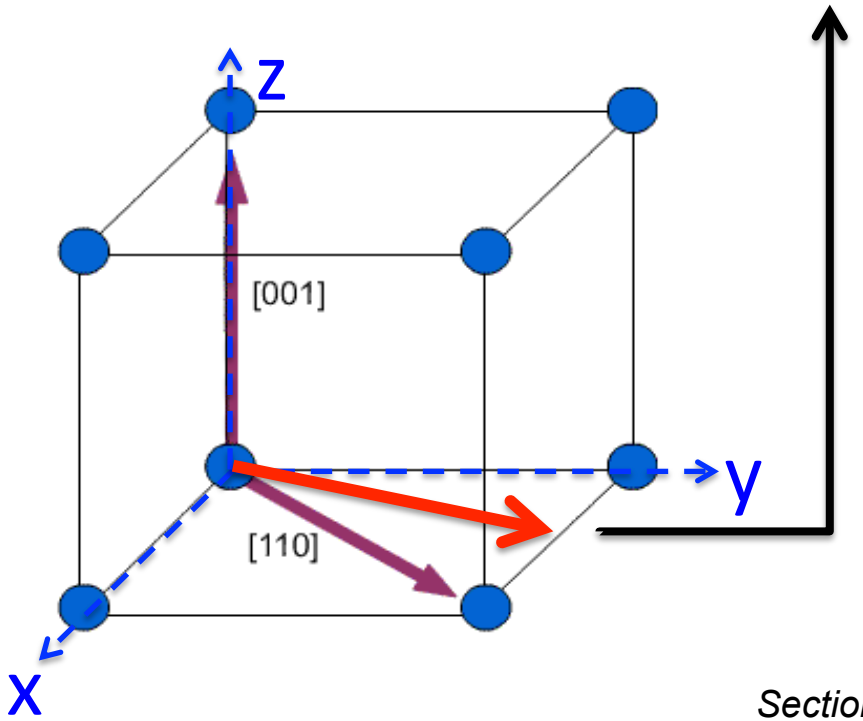
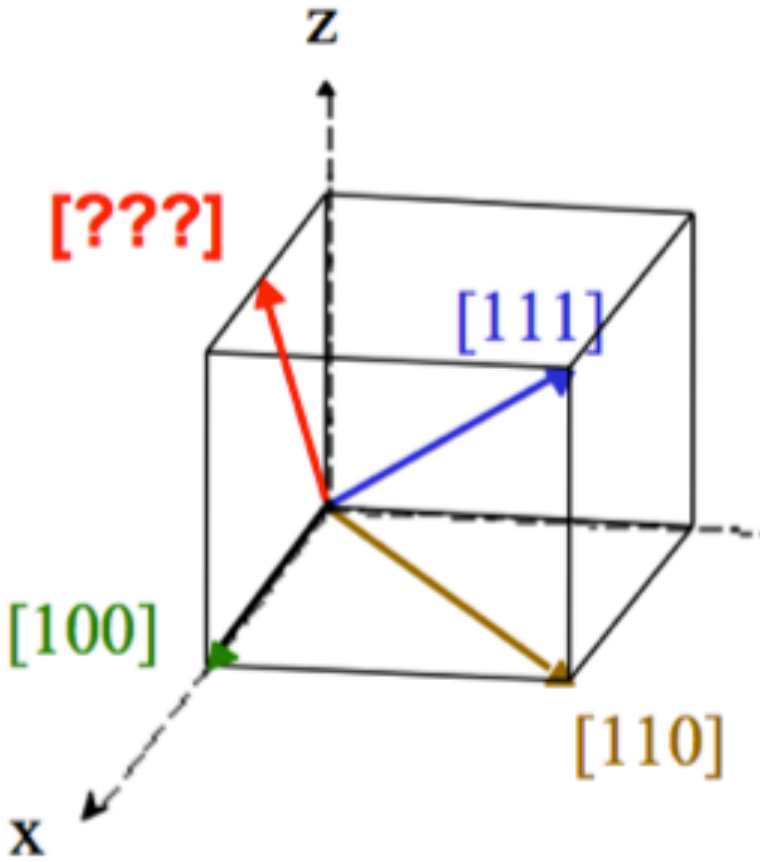
2. Subtract the coordinates of the two ends (head-tail)
3. Convert fractions, if any, into integers (multiply by a common factor) and reduce to lowest terms
4. Enclose in square brackets [u v w]

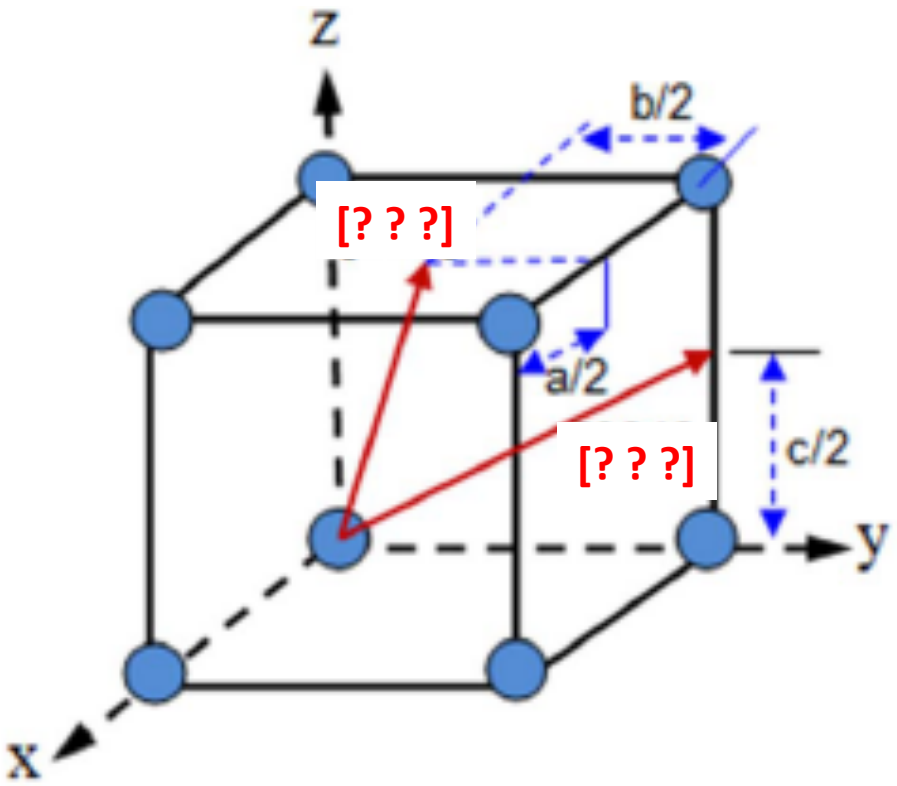
Coordinates of Head:	½	1	0
Coordinates of Tail:	0	0	0
Subtract:	½	1	0
Convert to integers:	1	2	0

=> [u v w] = [1 2 0]



❑ Cont'd: Crystallographic direction

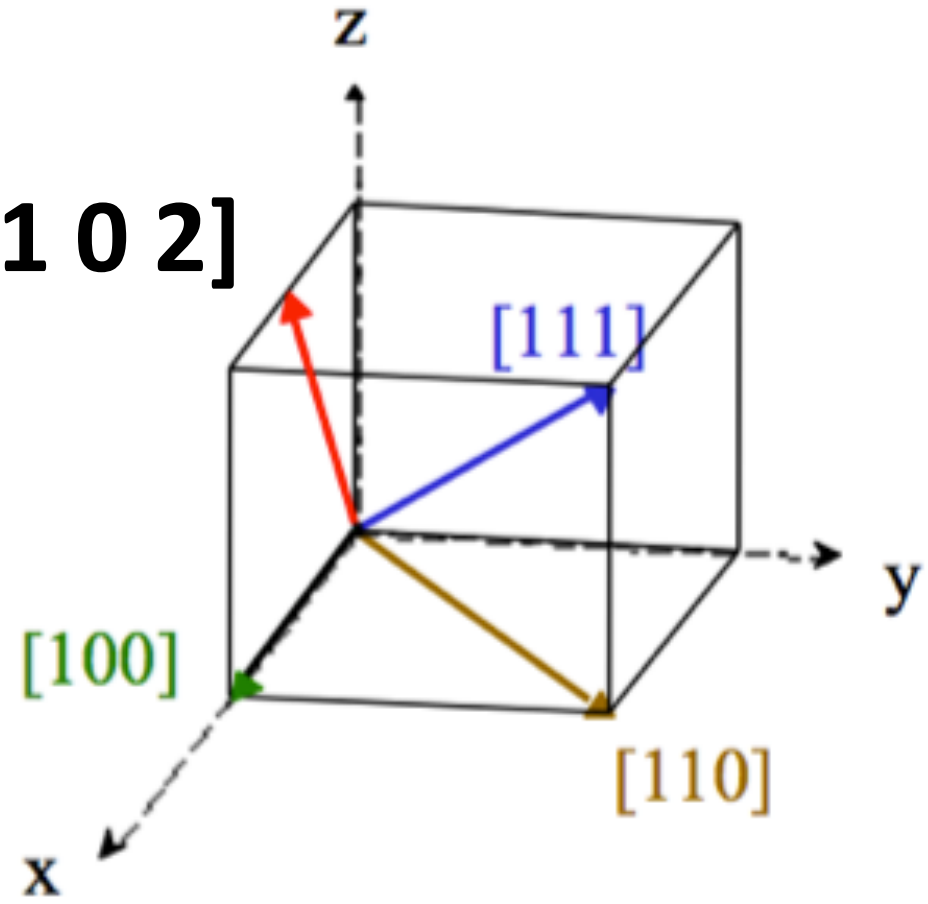


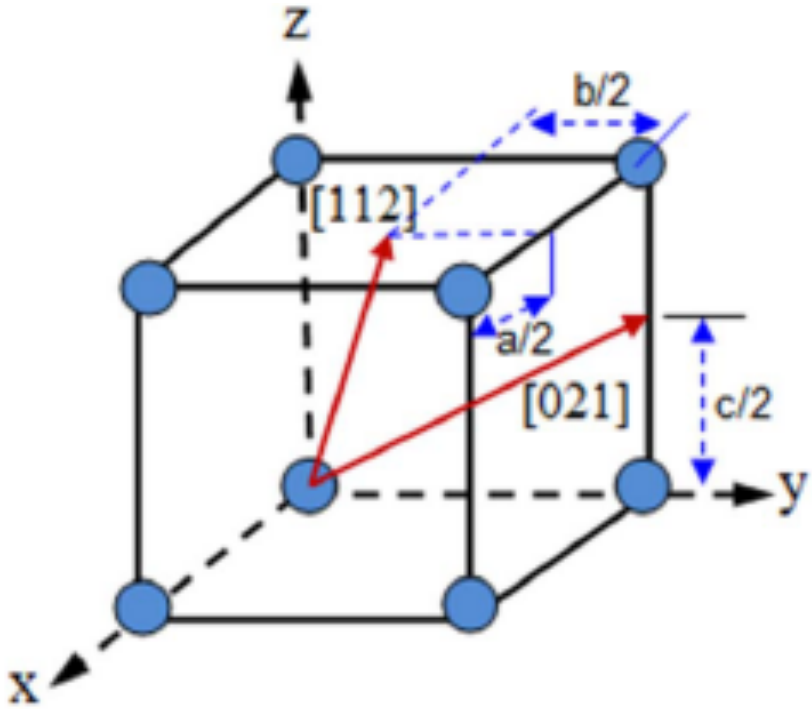


– What is ???

❑ Cont'd: Crystallographic direction

[1 0 2]



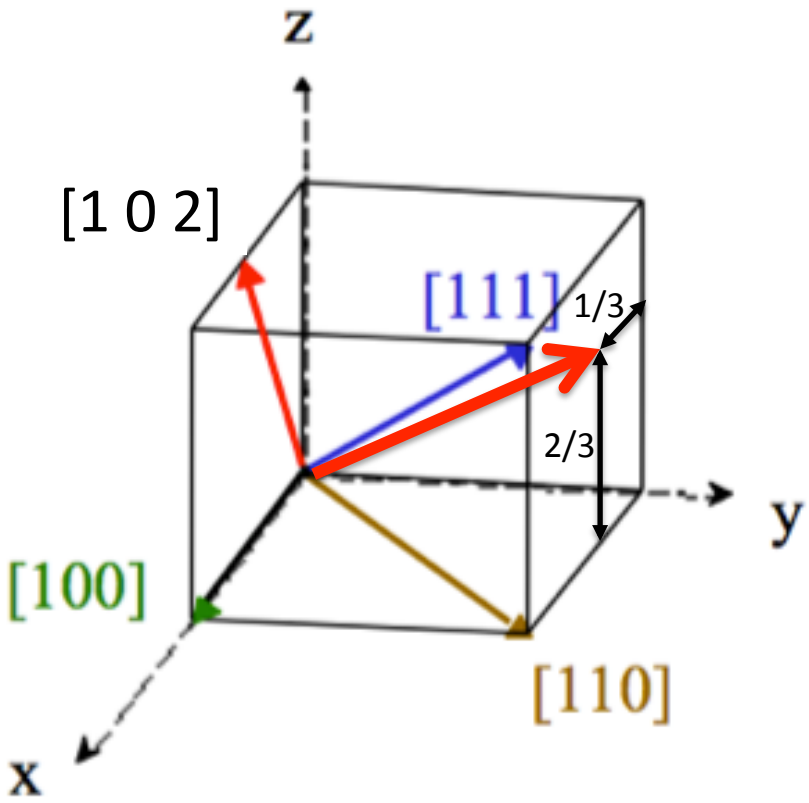


❑ Cont'd: Crystallographic direction

Draw [1 3 2]

[1 3 2]
=>
Multiply by (1/largest term)
1/3 * [1 3 2]:

1/3 1 2/3

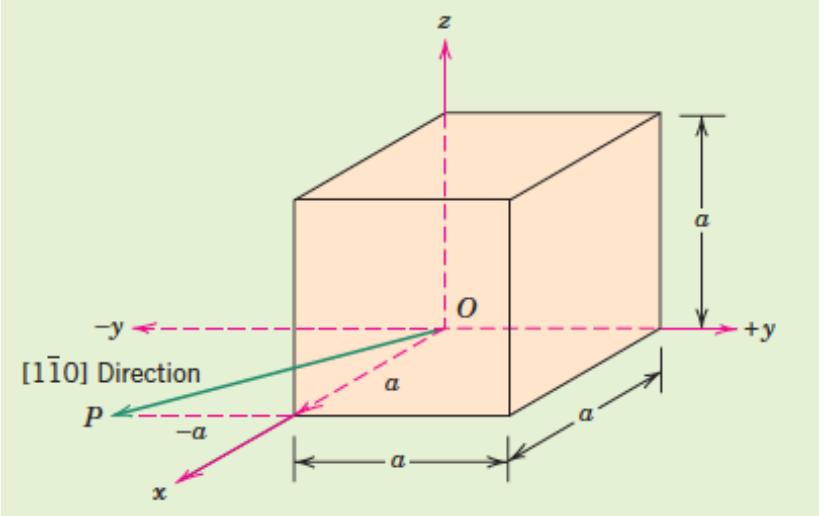


❑ Cont'd: Crystallographic direction

Negative values are expressed with a bar over the number

Example: -2 is expressed $\bar{2}$

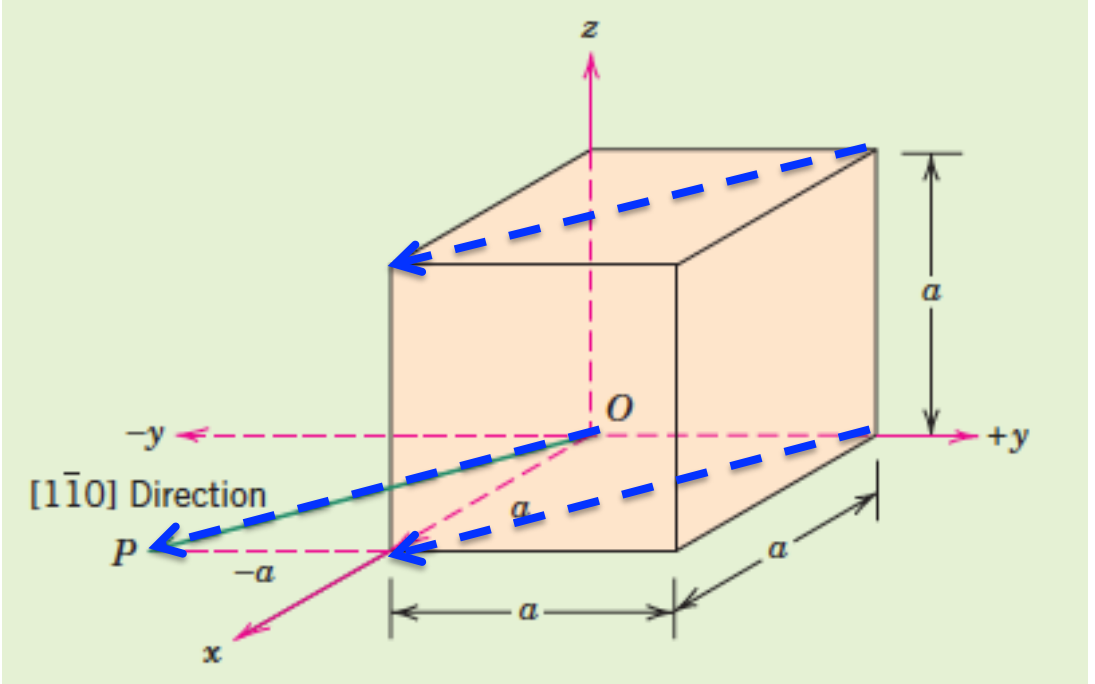
Draw a $[1\bar{1}0]$ direction



❑ Crystallographic direction

Notes:

- ❑ Parallel vectors have the same indices
- ❑ A direction and its multiple are identical
  e.g. [1 0 0] & [2 0 0],
  [½ ½ ½] & [1 1 1]



- ❑ Family of directions <u v w>:
  The spacing of atoms along each direction is the same

For cubic system: directions with same indices are equivalent without regard to order or signs: <100> : [100] [100], [010] [010], [001] [001]

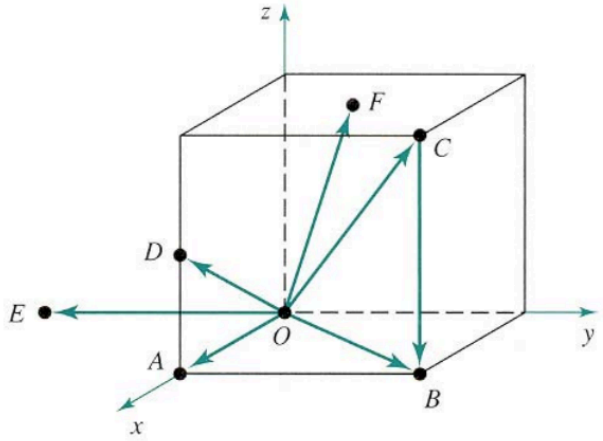
❑ Cont'd: Crystallographic direction

Construction of specified crystallographic direction

Sketch the following directions: [111], [121], $[\bar{1}10]$

Or

Determination of the directional indices



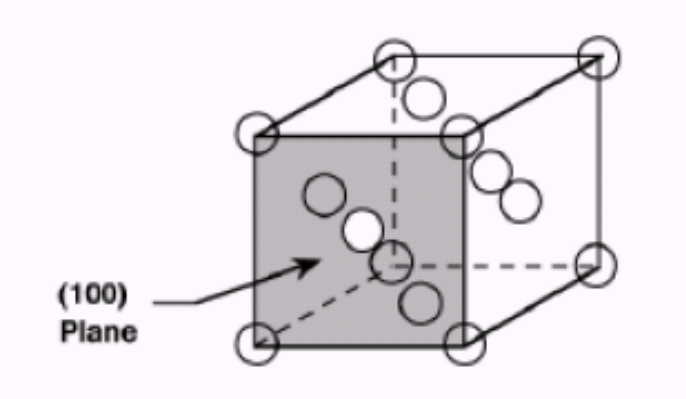
- ✓ **Point coordinates**
- ✓ **Crystal direction**
- ❑ **Crystal planes**

❑ Crystallographic Planes:

Planes are described by notations, called **Miller indices (h k l)**

To find the Miller Indices of a plane, follow these steps:

- Determine the intercepts of the plane along the crystal axes
- Take the reciprocals
- Clear fractions
- Reduce to lowest terms and enclose in brackets ()



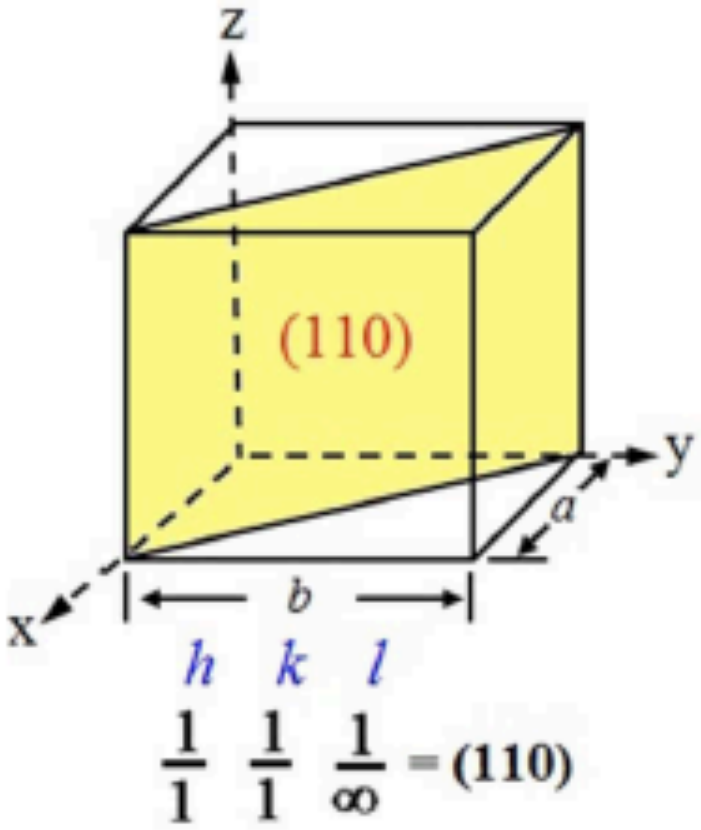
Intercept: 1 ∞ ∞

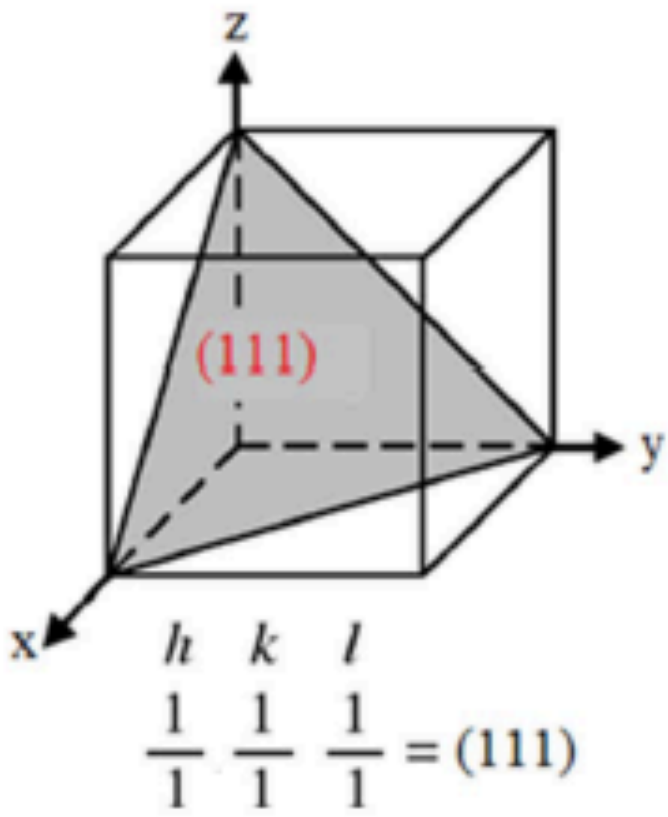
Reciprocal: 1 0 0

Plane: (100)

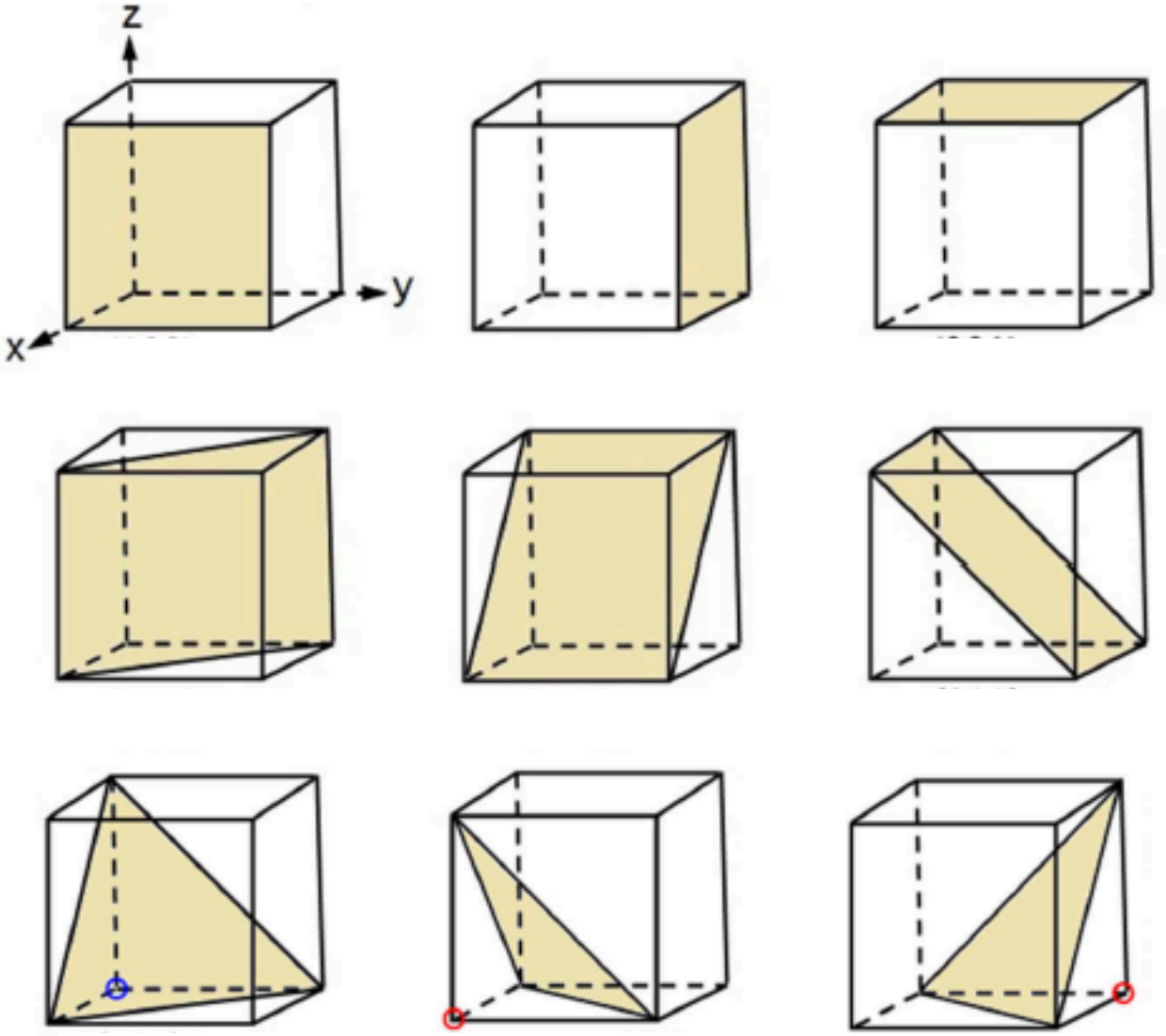
❑ Crystallographic Planes:

Planes are described by notations, called **Miller indices (h k l)**



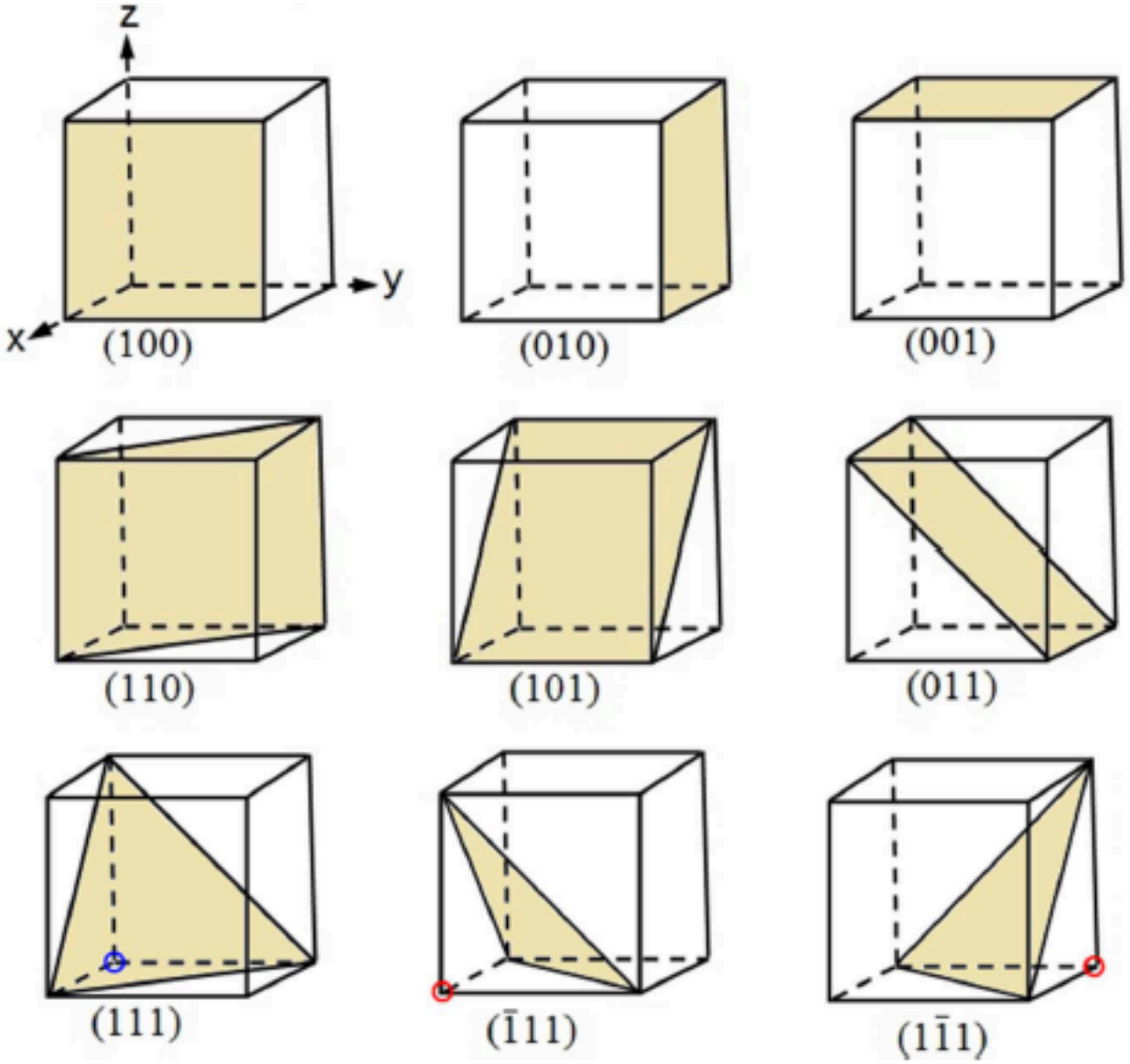


❑ Cont'd: Crystallographic Planes



•If the plane passes through the origin, then the origin point has to be shifted by one lattice parameter to another corner.

❑ Cont'd: Crystallographic Planes



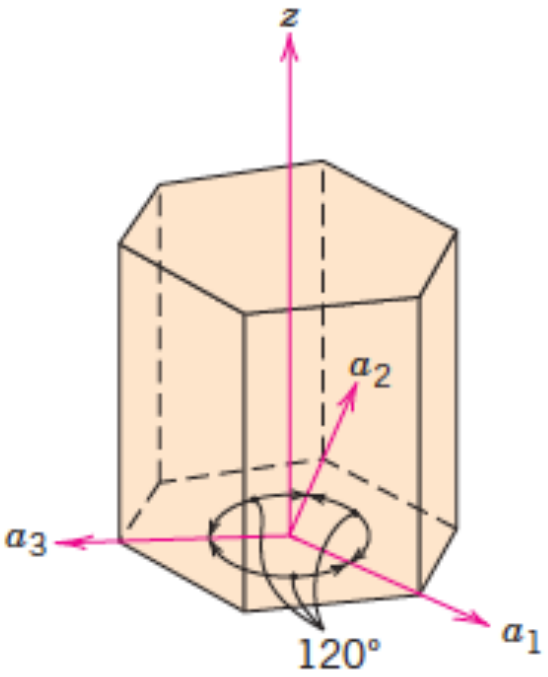
- Crystallographic directions and planes for HCP
- Linear and Planar Densities
- Single crystal vs. polycrystals

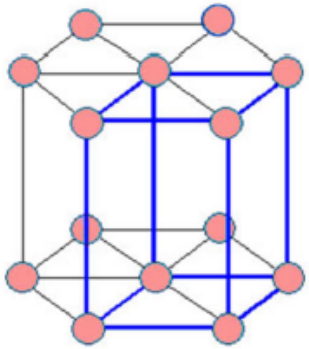
Crystallographic directions and planes for HCP

❑ Cont'd: Crystallographic direction in HCP

Four-index system is commonly used for HCP crystal system

$$[uvtw]$$





Hexagonal
a = b ≠ c
α = β = 90° γ = 12

Conversion between three-index system into four-index system:

$$[u'v'w'] \longrightarrow [uvtw]$$

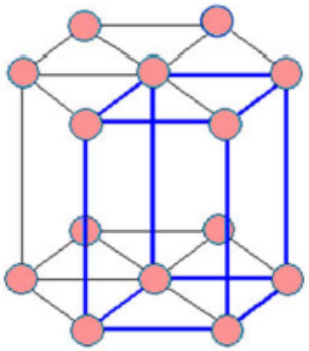
$$u = \frac{1}{3}(2u' - v')$$

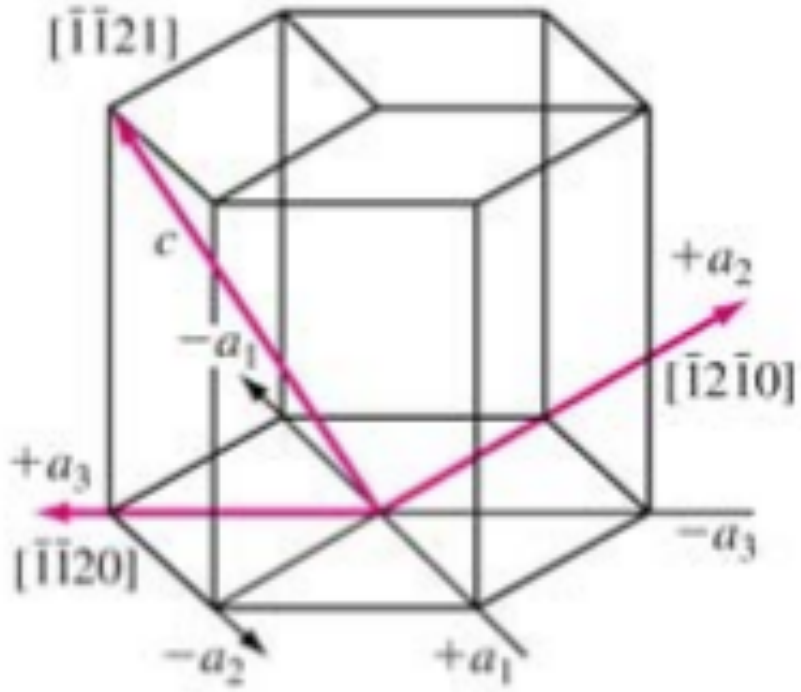
$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

❑ Cont'd: Crystallographic direction in HCP





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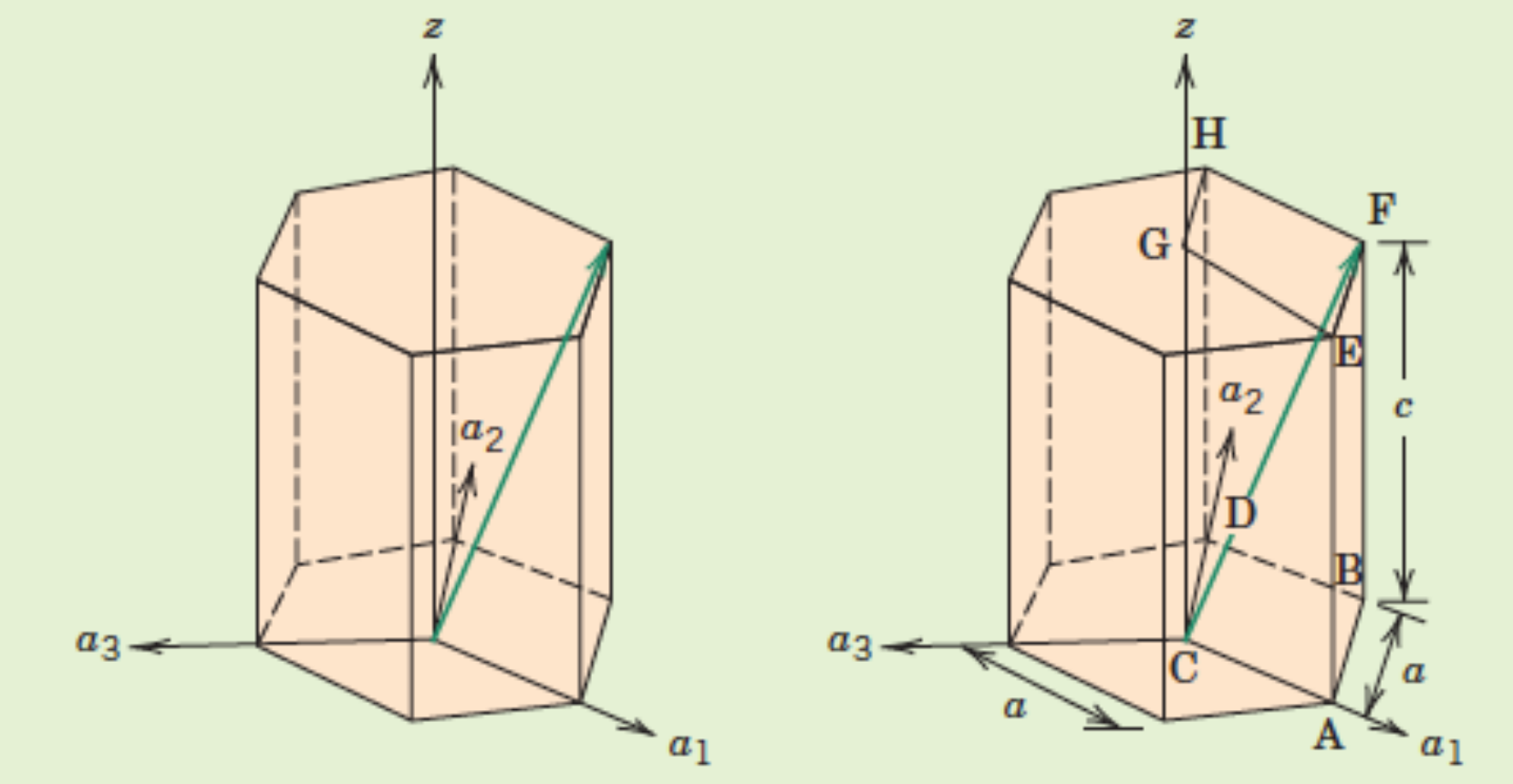
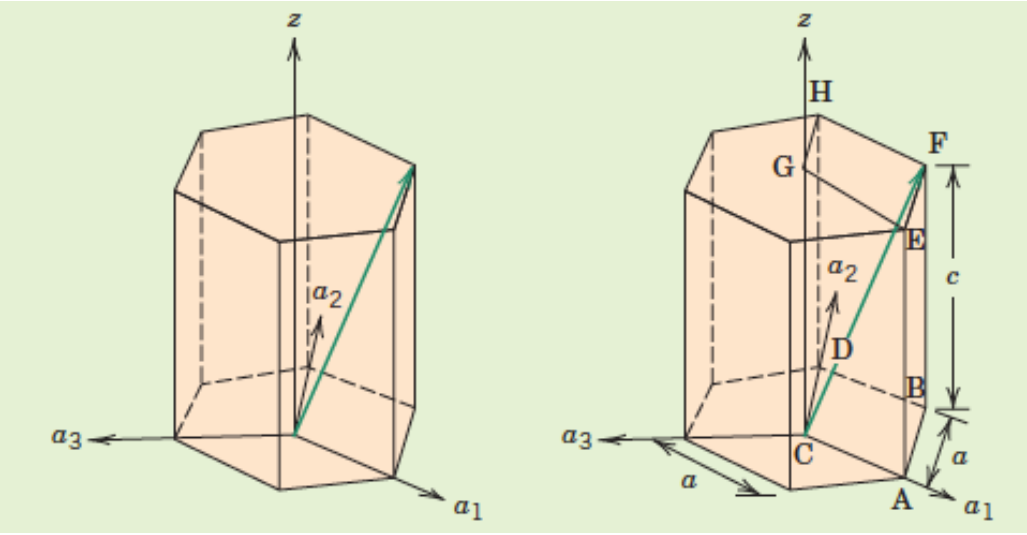
❑ Cont'd: Crystallographic direction in HCP



❑ Cont'd: Crystallographic direction in HCP



$$u' = 1 \qquad v' = 1 \qquad w' = 1$$

Also, from Equations 3.6a, 3.6b, 3.6c, and 3.6d

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

$$t = -(u + v) = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3}$$

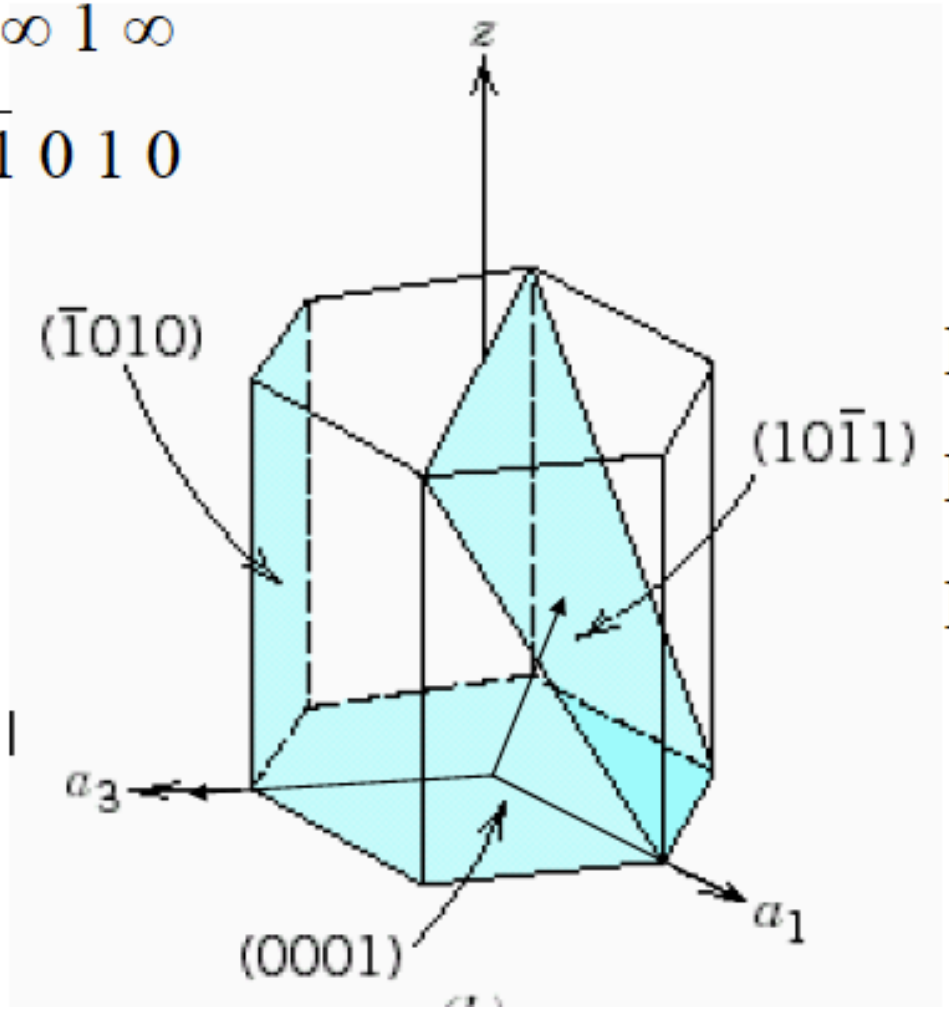
$$w = w' = 1$$

Multiplication of the above indices by 3 reduces them to the lowest set, which yields values for u, v, t, and w of 1, 1, -2 and 3, respectively. Hence, the direction shown in the figure is $[11\bar{2}3]$.

❑ Crystallographic plane in HCP

Intercept: $\bar{1} \infty 1 \infty$

Reciprocal: $\bar{1}$ 0 1 0

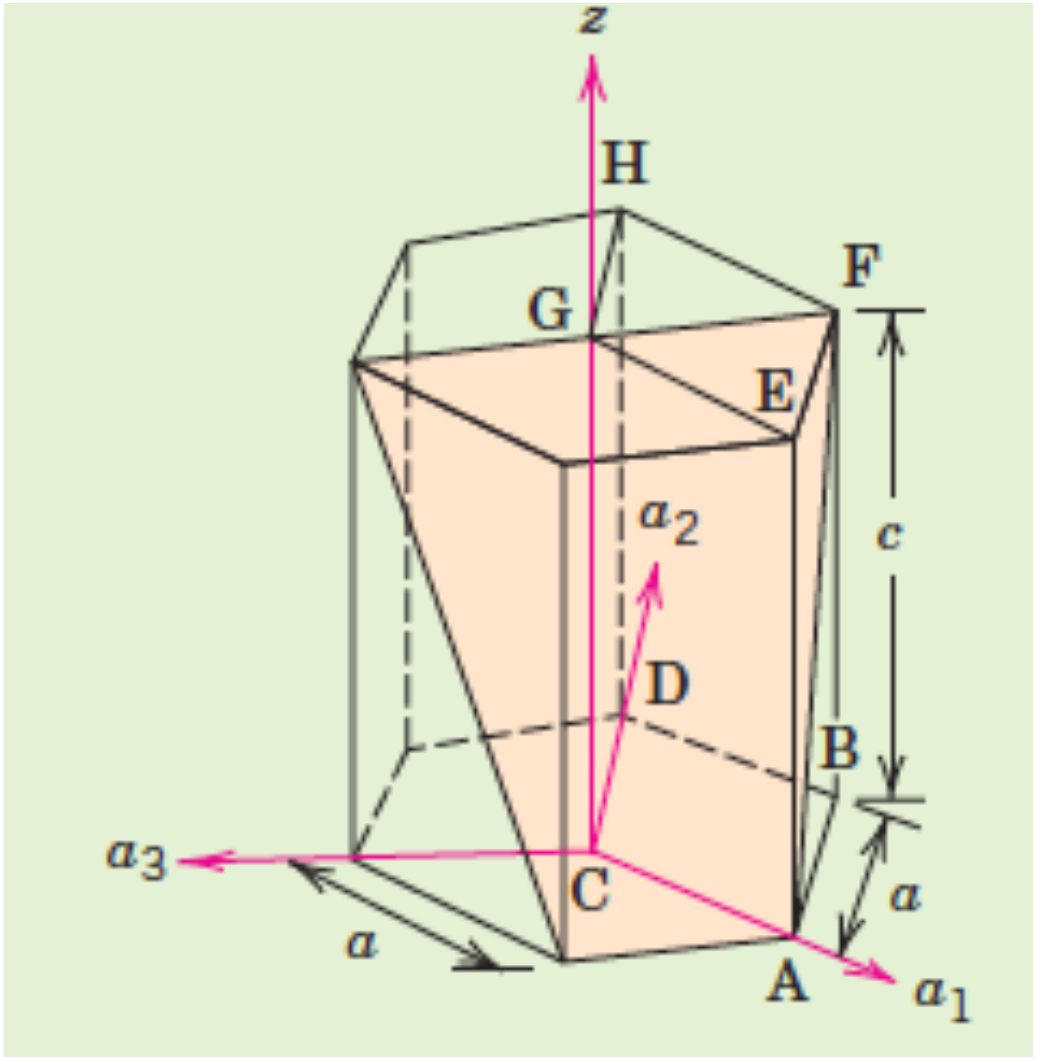


Intercepts: 1 ∞ $\bar{1}$ 1

Reciprocal: 1 0 $\bar{1}$ 1

Plane: $(10\bar{1}\ 1)$

❑ Cont'd: Crystallographic plane in HCP



$(1\bar{1}01)$

Linear &
Planar densities

❑ Linear Density

The number of atoms per unit length for a specific crystallographic direction

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

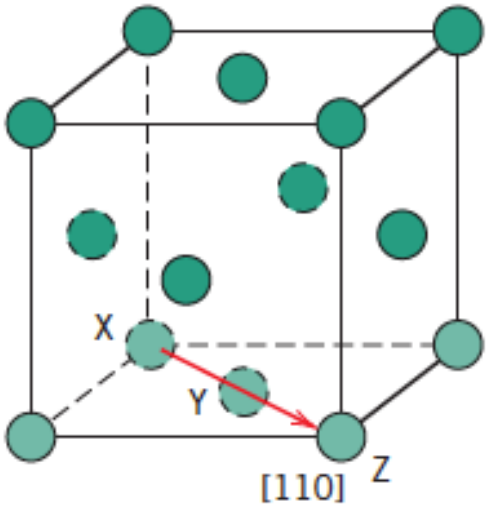
Example:

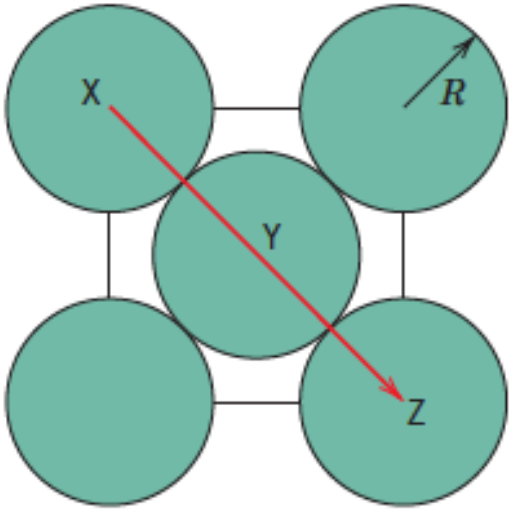
Calculate $LD_{[100]}$, $LD_{[110]}$, &$LD_{[111]}$ for FCC and BCC crystal structures

❑ Cont'd: Linear Density

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

Example: $LD_{[110]}$ for FCC crystal structure





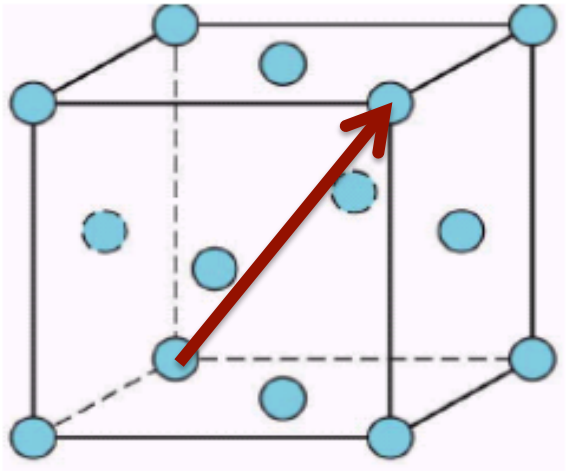
$LD_{[110]/FCC}$ = 2 atoms/√2 *a

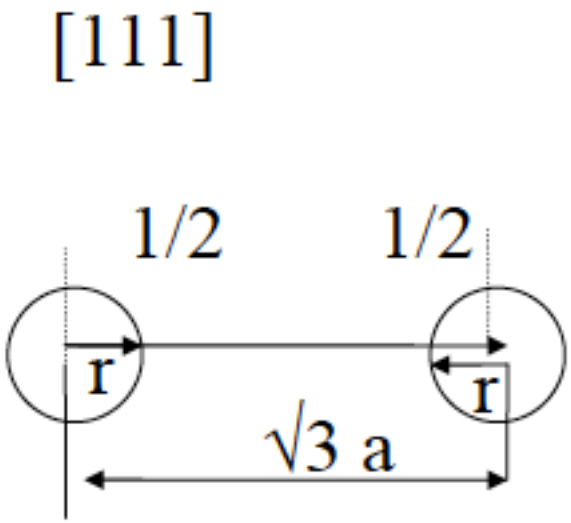
= √2 / a

❑ Cont'd: Linear Density

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

Example: $LD_{[111]}$ for FCC crystal structure





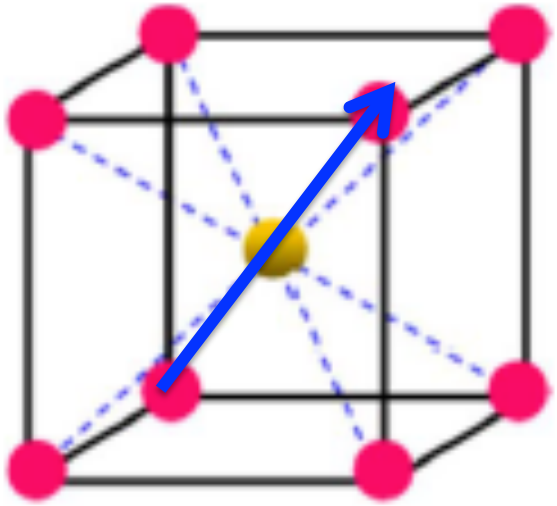
$LD_{[111]/FCC}$ = 1 atom/√3 *a

= 1/√3 a

❑ Cont'd: Linear Density

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

Example: $LD_{[111]}$ for BCC crystal structure



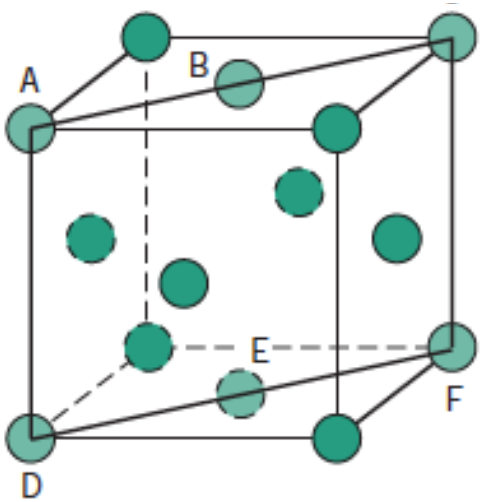
$LD_{[111]/BCC}$ = 2 atoms/√3 *a
= 2/√3 a

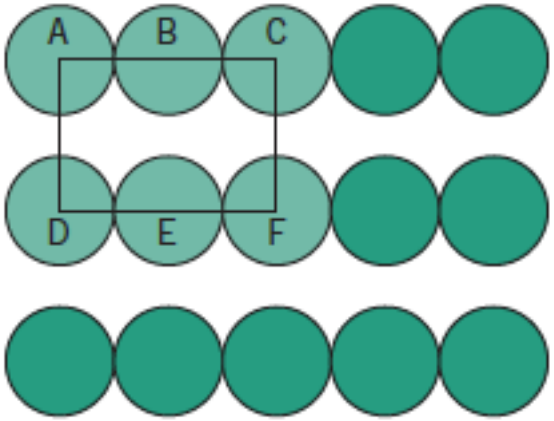
❑ Planar Density

The number of atoms per unit area for a particular crystallographic plane

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

Example: $PD_{(110)/FCC}$ for FCC crystal structure





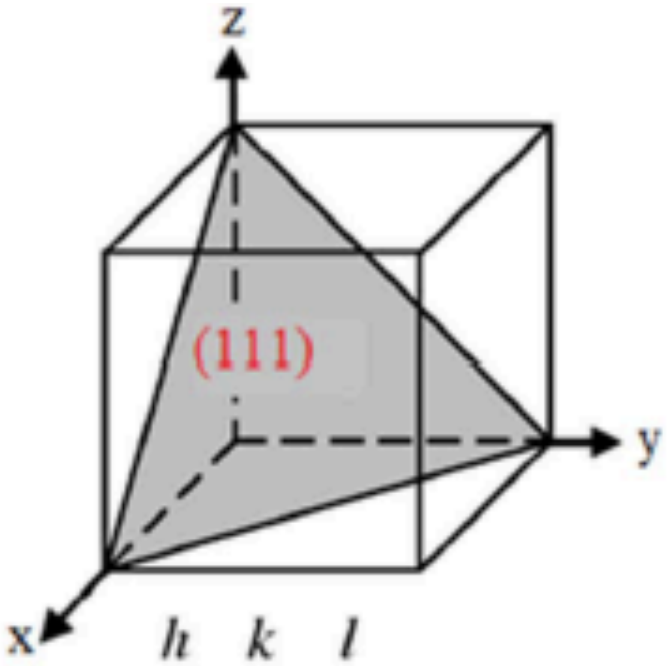
$PD_{(110)/FCC}$ = 2 atoms/(√2 a * a)

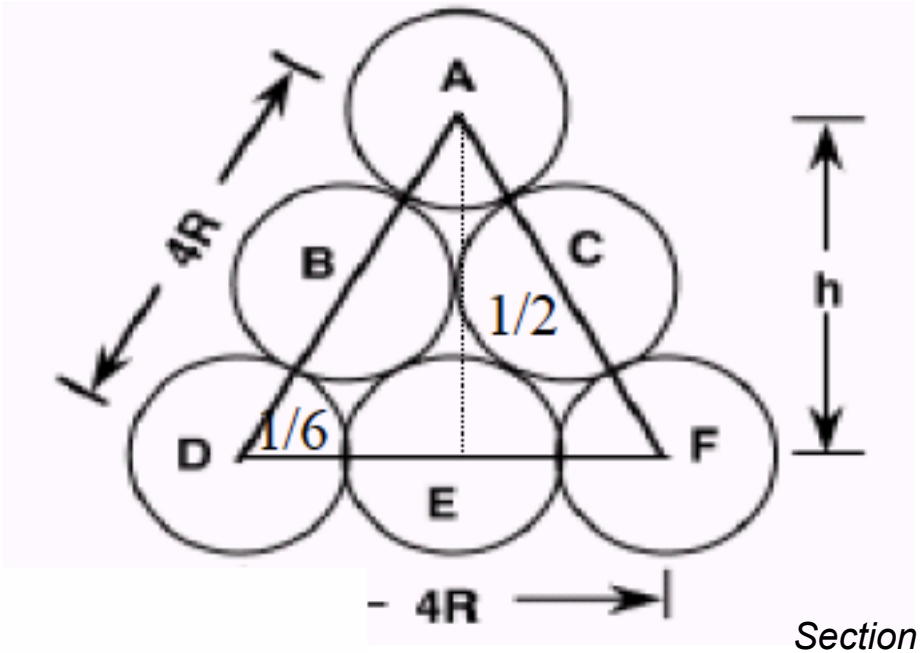
= √2 / a^2

❑ Cont'd: Planar Density

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

Exercise: $PD_{(111)/FCC}$ for FCC crystal structure ?!





❑ Why studying linear and planar densities?!

"Slip occurs on the most densely packed crystallographic planes and, in those planes, along directions having the greatest atomic packing".

e.g. FCC: (111) [110]

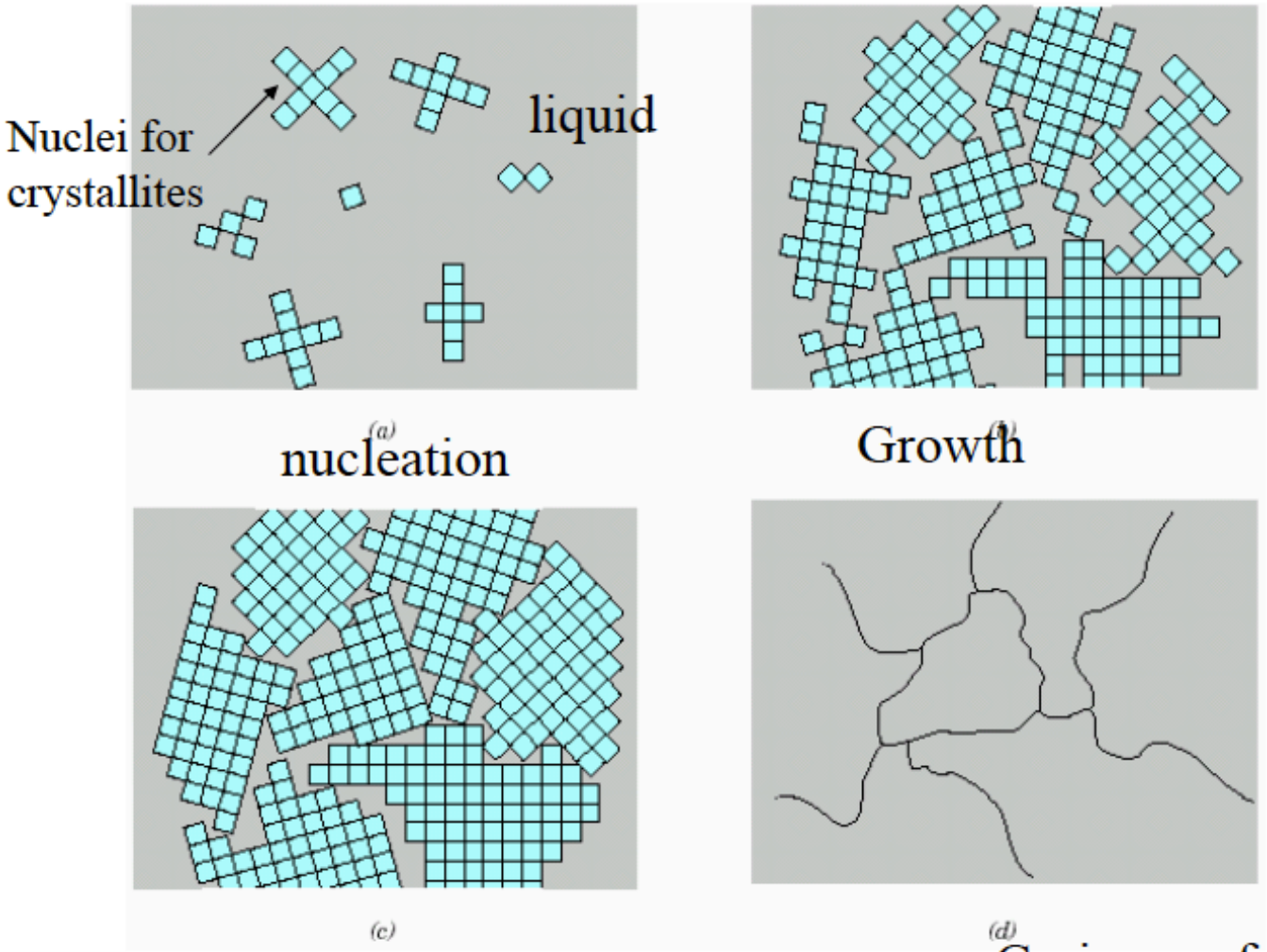
Slip is the main plastic deformation mechanism for most metals

Single crystal vs. polycrystalline materials

Sections 3.13-3.15

Solidification of a polycrystalline metal

liquid	nucleation	growth	Grain with different lattice orientations

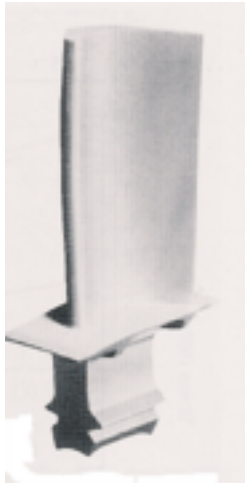


Sections 3.13-3.15

CRYSTALS AS BUILDING BLOCKS

Single crystal: All unit cells have the same orientations

--turbine blades



--diamond single crystals for abrasives

POLYCRYSTALS

- ***Most*** **engineering materials are polycrystals.**

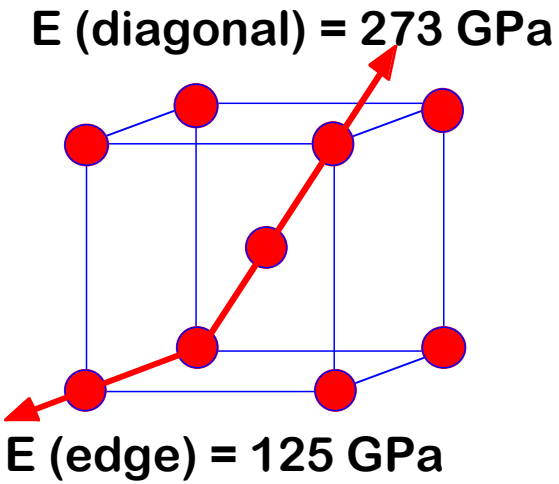
- **Each "grain" is a single crystal.**
- **If crystals are randomly oriented,**
  overall component properties are not directional.
- **Crystal sizes typ. range from 1 nm to 2 cm**

SINGLE VS POLYCRYSTALS

- Single Crystals

  -Properties vary with direction: anisotropic.

  -Example: the modulus of elasticity (E) in BCC iron:



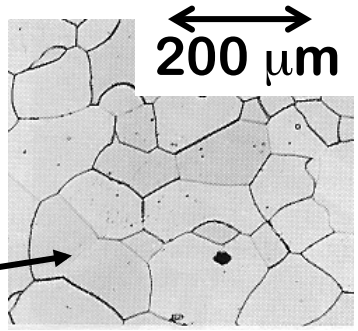
- Polycrystals

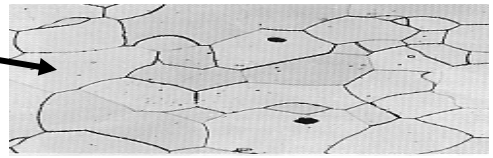
  -Properties may/may not vary with direction.

  -If grains are randomly oriented: isotropic.

  ($E_{poly\ iron}$ = 210 GPa)

  -If grains are textured, anisotropic.





•Different grains have different orientations of atoms separated by grain boundaries.

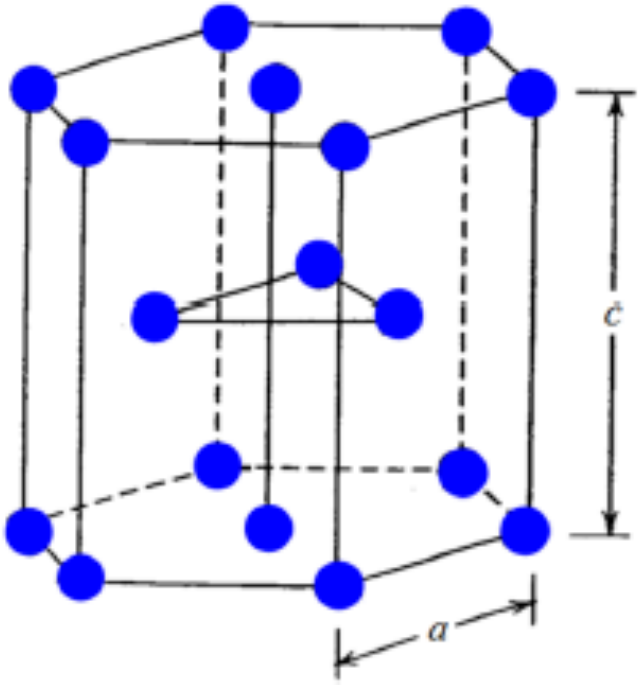
• Anistropy: Properties depend on crystallographic direction.

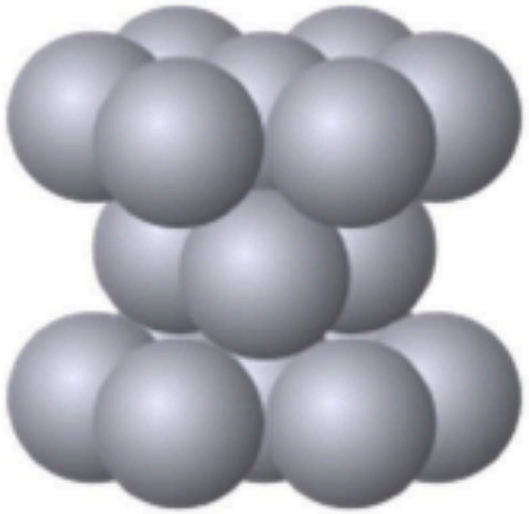
• Isotropic: Properties are independent of directions.

Problems

Show that the APF for HCP (ideal) is 0.74?

c/ a
=1.633
(ideal)





Show that the APF for HCP (ideal) is 0.74?

APF for HCP:

$$APF = \frac{volume\ of\ atoms\ in\ the\ unit\ cell}{Volume\ of\ the\ unit\ cell}$$

1) *volume of atoms in the unit cell*:

$$volume\ of\ atoms\ in\ the\ unit\ cell = no.\ of\ atoms * volume\ of\ sphere$$

$$no.\ of\ atoms = 12\ (corners) * \frac{1}{6} + 2(top\ and\ bottom\ ) * \frac{1}{2} + 3\ (inside) = 6$$

$$volume\ of\ atoms\ in\ the\ unit\ cell = 6 * \underbrace{\frac{4}{3}\ \pi\ \ R^3}_{vol.of\ sphere}$$

$$= 8\,\pi\ \ R^3 = 8\,\pi\ \ (\frac{a}{2})^3 = \pi\ \ a^3$$

Cont'd:

2) *Volume of the unit cell*

$$Volume\ of\ the\ unit\ cell = volume\ of\ the\ hexagonal$$
$$= Area\ of\ base * Height\ of\ the\ unit\ cell$$

$$Area\ of\ base = Area\ of\ six\ triangles = 6 * area\ of\ one\ triangle$$

$$area\ of\ one\ triangle = \frac{1}{2} * base * height\ of\ the\ triangle$$

$$base = a = 2R$$
$$height\ of\ the\ triangle = a \sin 60$$
$$\Longrightarrow Area\ of\ base = 6\ \frac{1}{2}\ a^2 \sin 60 = 3\ a^2 \sin 60$$

$$\Longrightarrow Volume\ of\ the\ unit\ cell = Area\ of\ base * Height\ of\ the\ unit\ cell$$
$$= 3a^2 \sin 60 * c$$
$$= 3a^2 \sin 60 * 1.633\ a$$
$$= 3 * 1.633\ a^3 \sin 60$$

Cont'd:

From (1) and (2)

$$APF = \frac{volume\ of\ atoms\ in\ the\ unit\ cell}{Volume\ of\ the\ unit\ cell}$$

$$APF = \frac{\pi \quad a^3}{3*1.633\ a^3 \sin 60} = 0.74$$

Density Computations

3.7 Molybdenum has a BCC crystal structure, an atomic radius of 0.1363 nm, and an atomic weight of 95.94 g/mol. Compute and compare its theoretical density with the experimental value found inside the front cover.

3.8 Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm^3, and an atomic weight of 106.4 g/mol.

3.9 Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3, and an atomic weight of 180.9 g/mol.

Use the following:

atoms/unit cell

Atomic weight (g/mol)

$$\rho = \frac{n A}{V_C N_A}$$

Volume/unit cell (cm^3/unit cell)

Avogadro's number (6.023×10^{23} atoms/mol)

$a_{FCC} = 2 * \sqrt{2} * R$

$$R = \left(\frac{nA_{Ir}}{16\rho N_A \sqrt{2}} \right)^{1/3}$$

For FCC

$a_{BCC} = 4 * R / \sqrt{3}$

$$R = \left(\frac{3n\sqrt{3}A_V}{64\rho N_A} \right)^{1/3}$$

For BCC

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2nd Semester 1426/27

1st Mid-term exam

6/3/1427

Grade	
1st	
2nd	
3rd	
4th	
Total /40	

Problem 2

a) Sketch the following direction and plane within a cubic unit cell

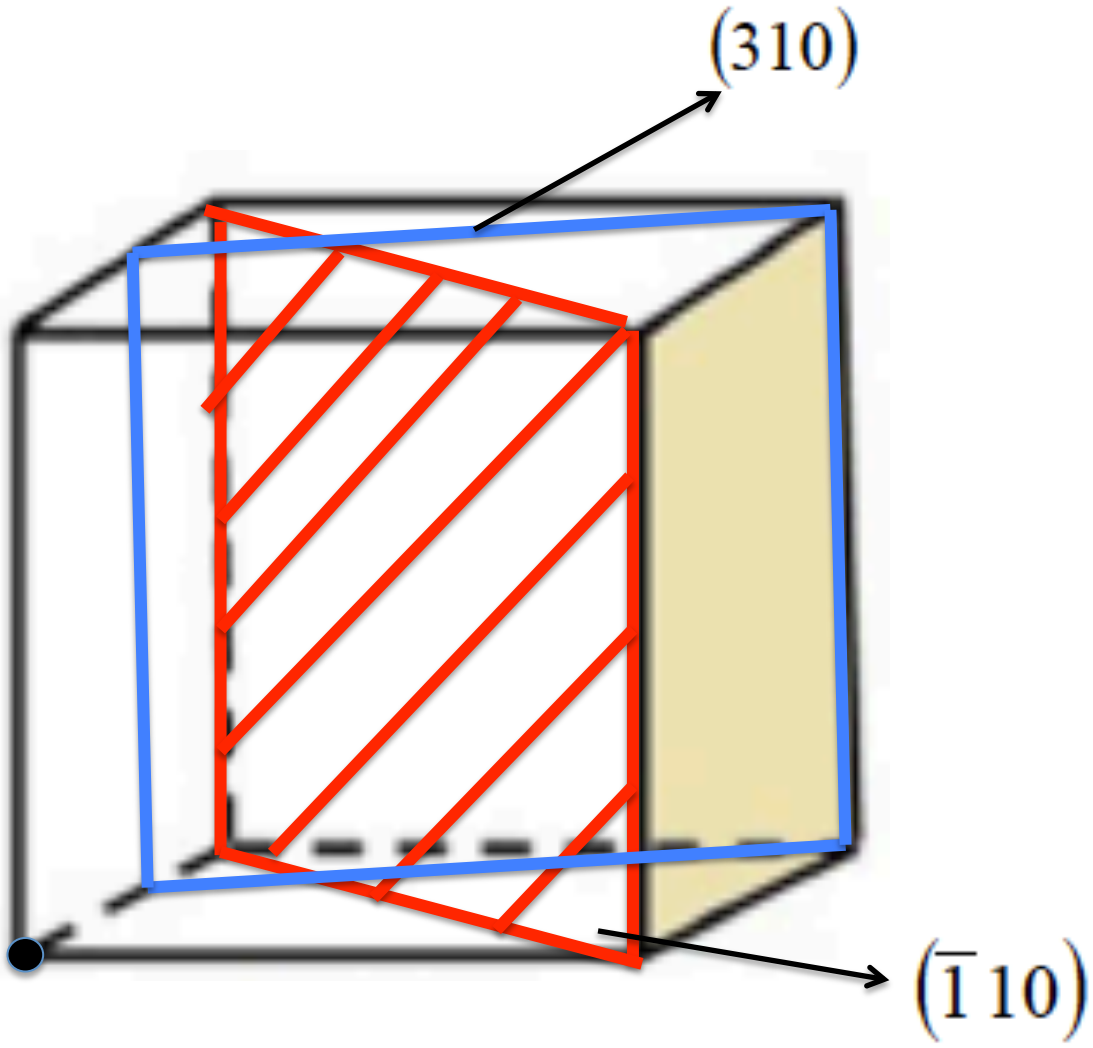
$[\bar{1}10]$ $(\bar{1}10)$

$[\bar{1}20]$ (310)

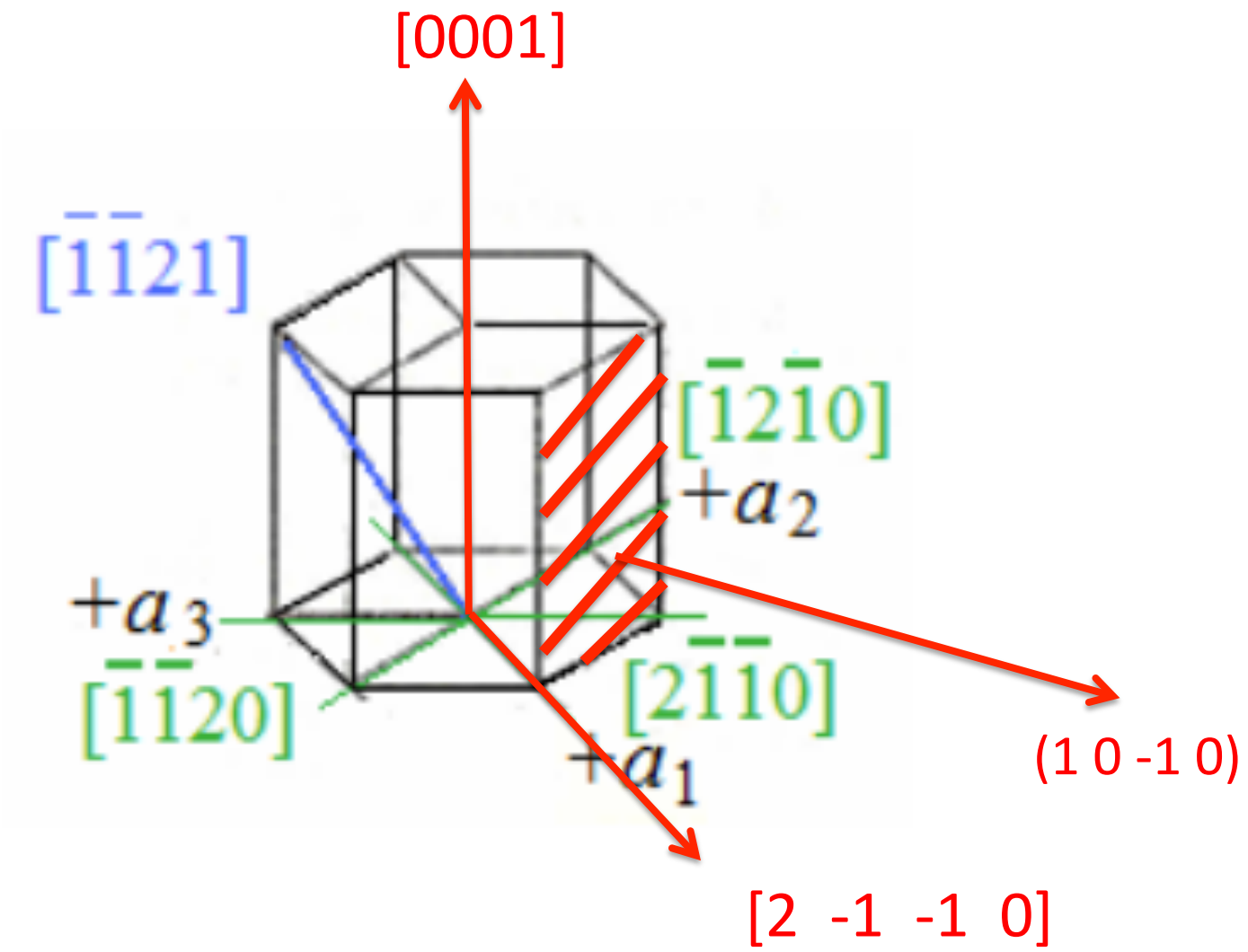
b) Sketch the following planes and directions in a hexagonal unit cell:

$(0001), (10\bar{1}0), [0001], [2\bar{1}\bar{1}0]$

Problem 2. a



Problem 2. b



(0001) is the basal plane

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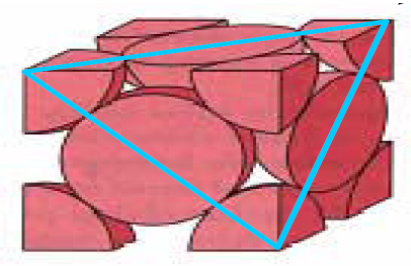
c)Gold (Au) has FCC unit cell and a lattice constant of 0.408 nm, Find

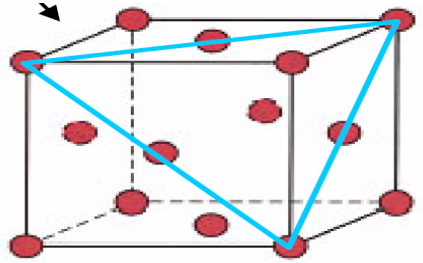
1- The linear density LD_{110} in atoms/m

2- Planar density PD_{111} in atoms/m^2

Show the atom arrangements in both cases.

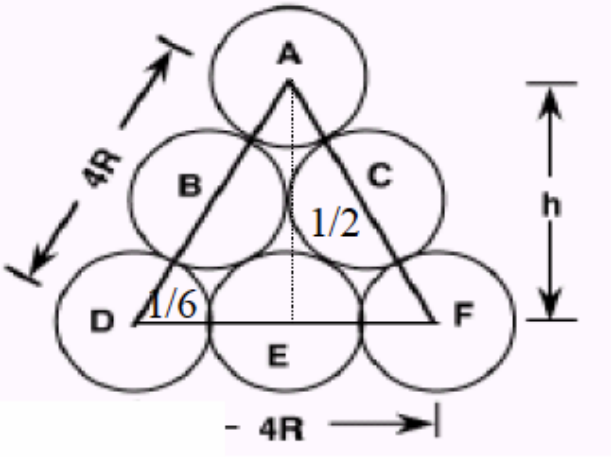
Prob. 2c





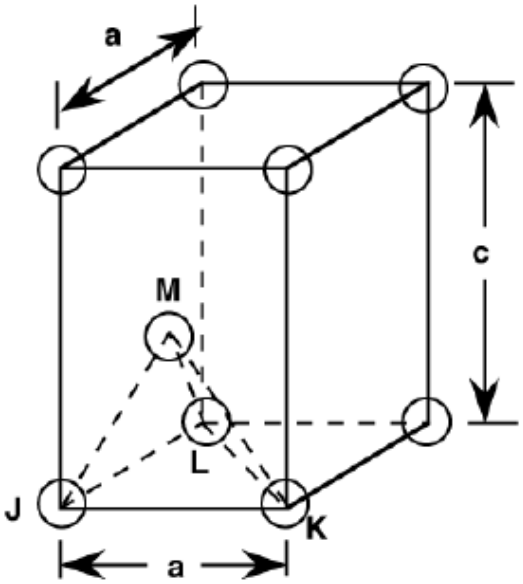
$$LD_{[110]} = \frac{2\ atoms}{\sqrt{2}\ a} = 3.4662\ x\ 10^{9}\ atoms/m$$

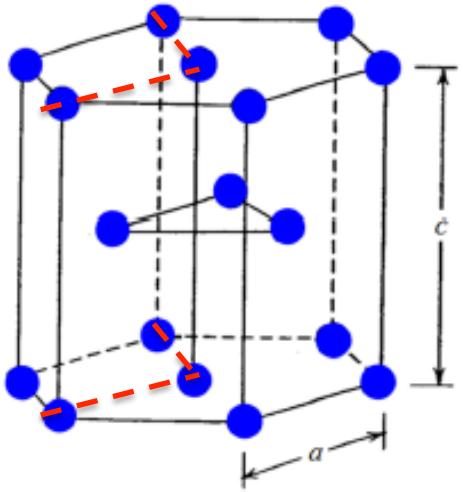
$$PD_{(111)} = \frac{3*\frac{1}{6}+3*\frac{1}{2}}{Area\ of\ (111)\ plane}$$

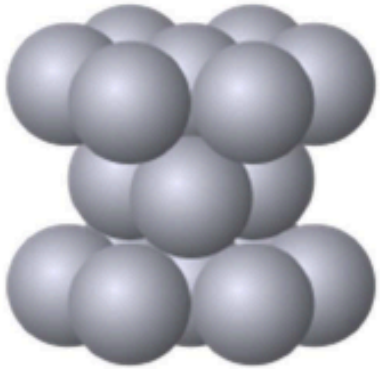


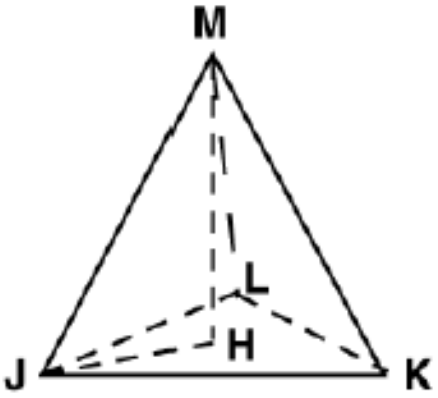
$$= \frac{3*\frac{1}{6}+3*\frac{1}{2}}{\frac{1}{2}*base*height} = \frac{3*\frac{1}{6}+3*\frac{1}{2}}{\frac{1}{2}*\sqrt{2}\ a*\frac{\sqrt{3}}{\sqrt{2}}a} = 13.87\ x\ 10^{18}\ atoms/m2$$

3.4 For the HCP crystal structure, show that the ideal c/a ratio is 1.633.







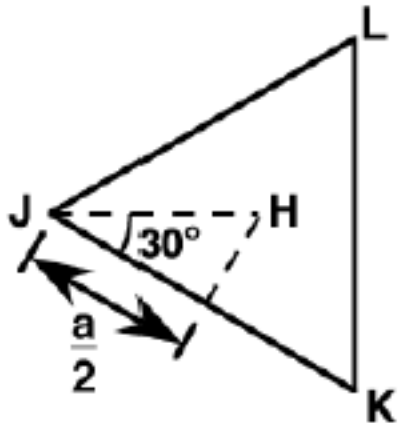


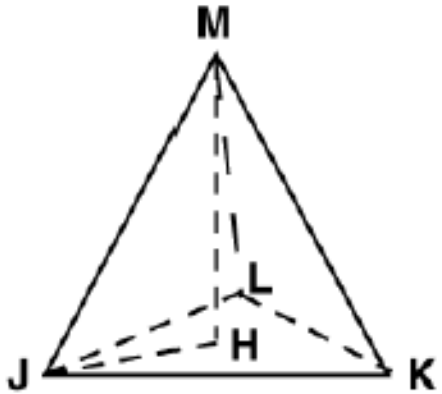
$$\overline{JM} = \overline{JK} = 2R = a$$

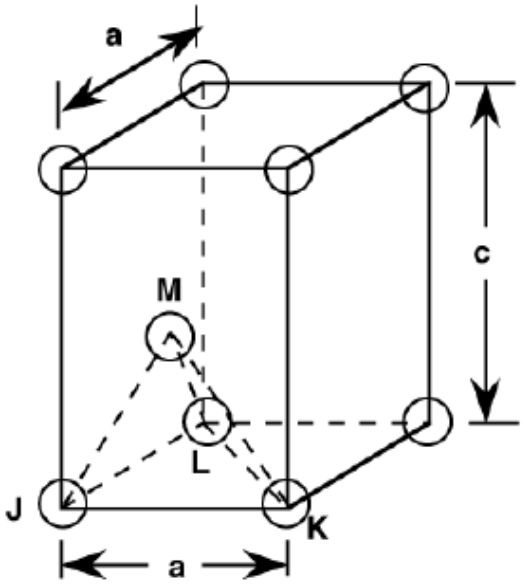
$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2, \text{ or}$$

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

3.4 For the HCP crystal structure, show that the ideal c/a ratio is 1.633.







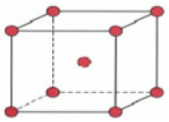
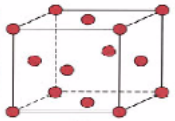
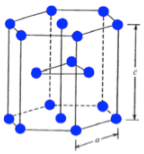
$$\cos 30^\circ = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}, \text{ and}$$

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4} \quad \Rightarrow \quad \frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

Review: Chapter 3

- Crystalline vs. amorphous materials
- lattice, unit cell, lattice parameters → 7 Crystal system
- BCC, FCC, HCP
  - Close packed direction (relate a to R)
  - Coordination number (touching atoms)
  - # of atoms/unit cell (corner, face, inside)
  - APF = $\frac{n * 4/3\ \pi R^3}{\text{Volume of unit cell}}$

		Close packed direction	Coordination # (Z)	# of atoms/unit cell	**APF**
BCC		Cube diagonal $a=4R/\sqrt{3}$	8	2	0.68
FCC		Face diagonal $a=4R/\sqrt{2}$	12	4	0.74
HCP		Edge $a=2R$	12	6	0.74

Cont'd:

- Theoretical Density

  Calculate density or R from the density

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

- Crystal direction: Cubic [uvw] & HCP [uvtw]
- Crystal planes: Cubic (hkl) & HCP (hktl)

- Linear density, $LD_{[xxx]}$

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

- Planar density, $PD_{(xxx)}$

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

- Single crystal vs. polycrystalline materials

Main relations (Chapter 3)

$$APF = \frac{n * 4/3\,\pi R^3}{\text{Volume of unit cell}}$$

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

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

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