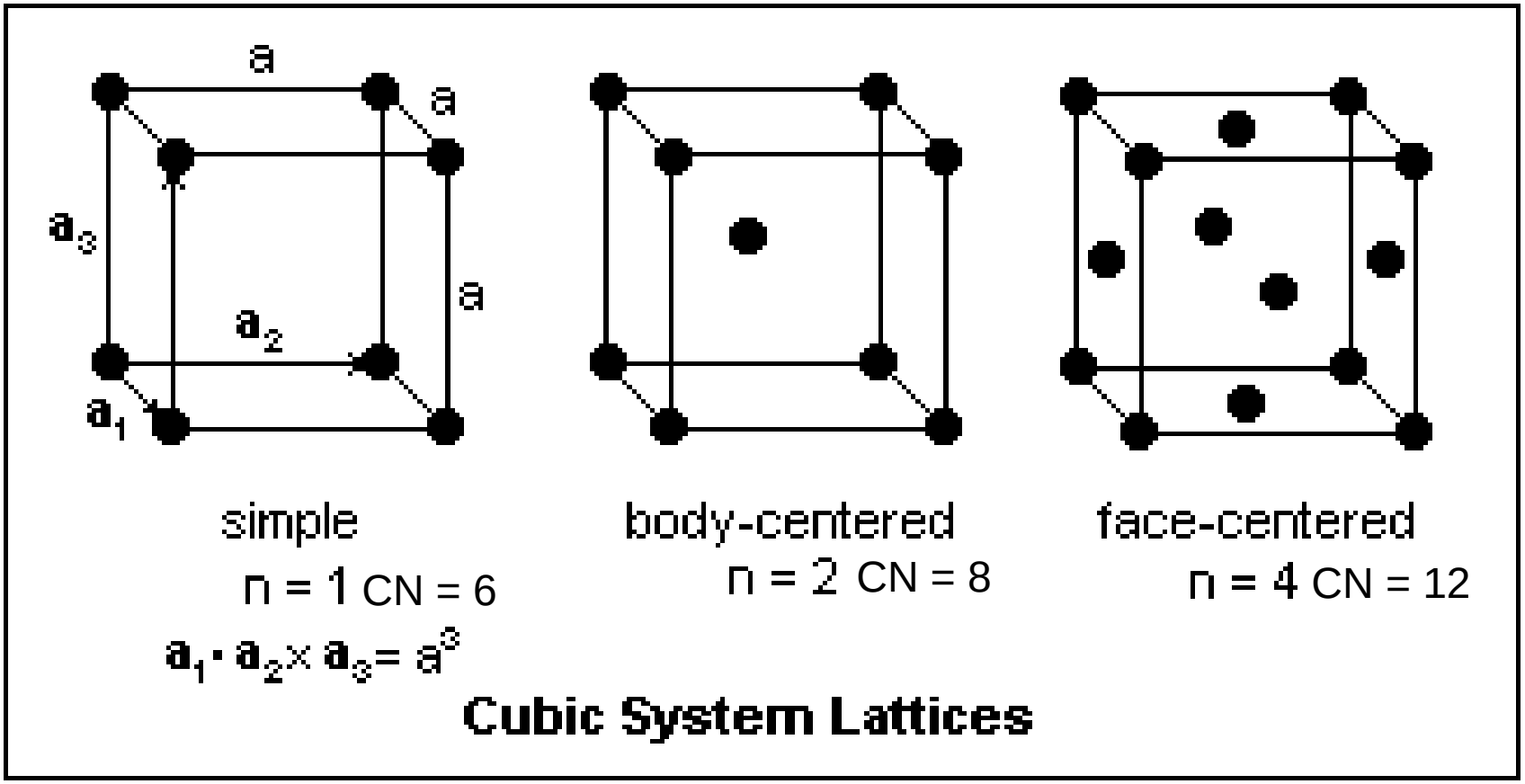
Chapter 3: The Structure of Crystalline Solids (2)

Class Exercise

- Draw the unit cell structure for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) lattices
- Give coordination number (CN) for atoms in each of those structures
- Give the “average” number of atoms in a unit cell for simple cubic, body-centered cubic, and face-centered cubic structures and explain why

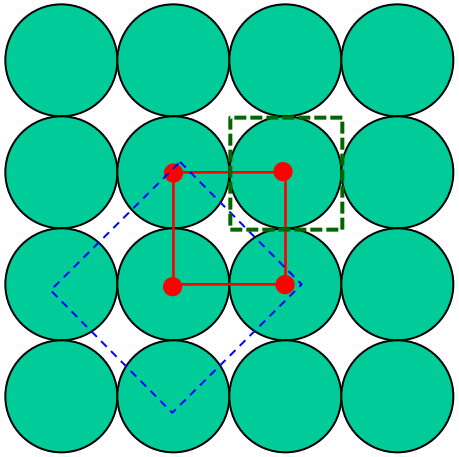
Three Types of Unit Cell Structures for Cubic Crystal Systems



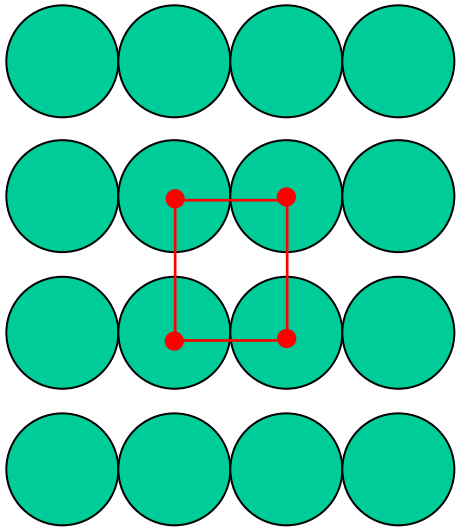
http://mysite.du.edu/~jcalvert/phys/lattice.htm

Class Exercise

Using the concepts for lattice and unit cell, for 2D lattices (of the same atoms) given below, please draw the 2D unit cell and determine the coordination number (CN) and number of atoms per unit cell (n)



See red square for unit cell
CN (# of nearest neighbor) = 4
Average number of atoms per unit cell = 4x1/4 = 1
(The dashed square in blue represents symmetry, but it not the smallest)
(The dotted square in green is smallest, but does not represent symmetry: it can rotate any degree) and does not distinguish from other pattern as on the right)

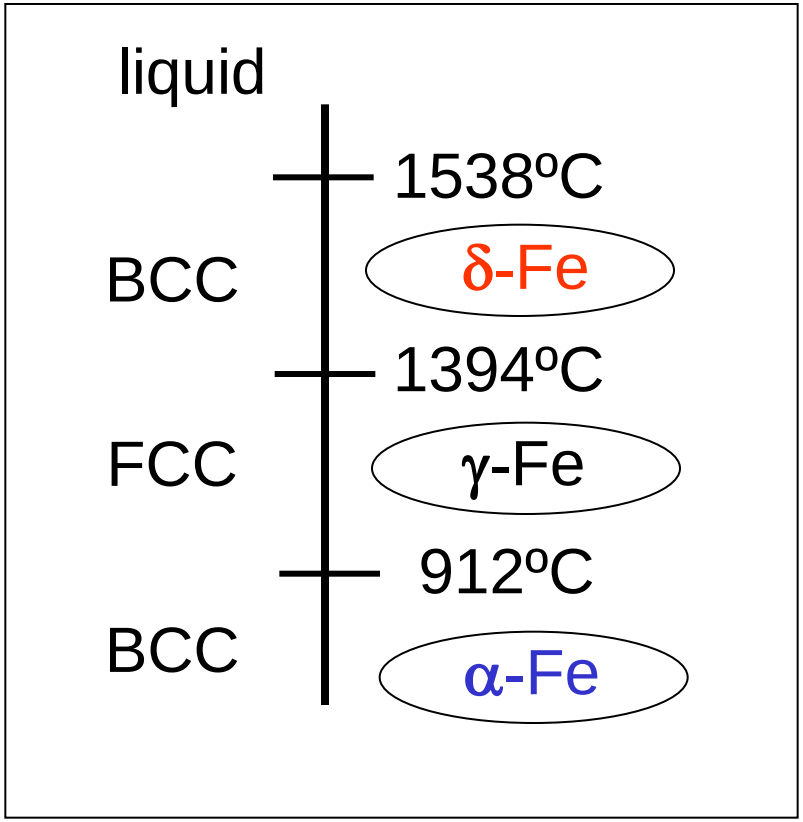


CN = 2
Average number of atoms per unit cell = 4x1/4 = 1

Polymorphism

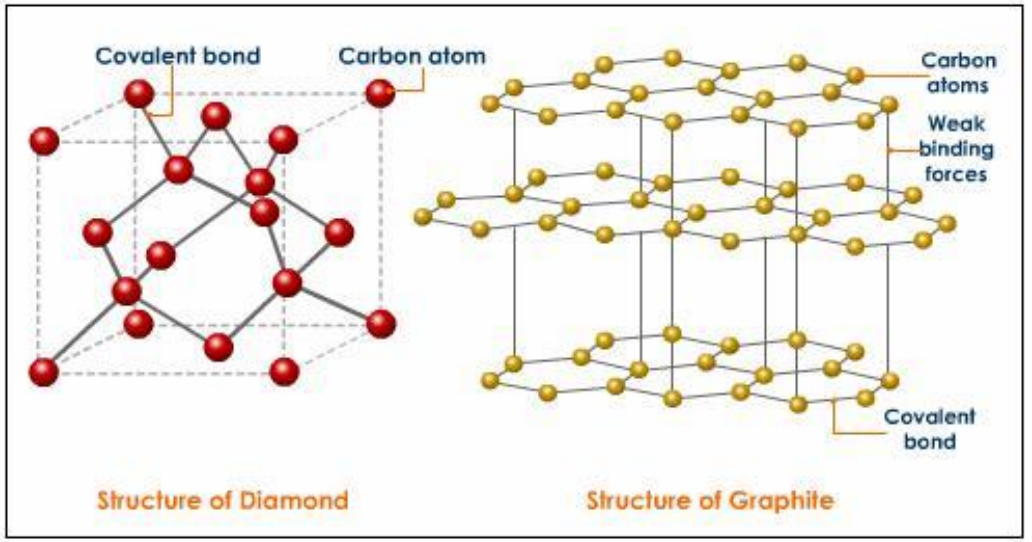
- Two or more distinct crystal structures for the same material (allotropy/polymorphism) in terms of composition

Iron



Carbon

Diamond vs. Graphite



http://openstudy.com/updates/4eccf97ce4b04e045aed8891

Virtual Materials Science & Engineering (VMSE)

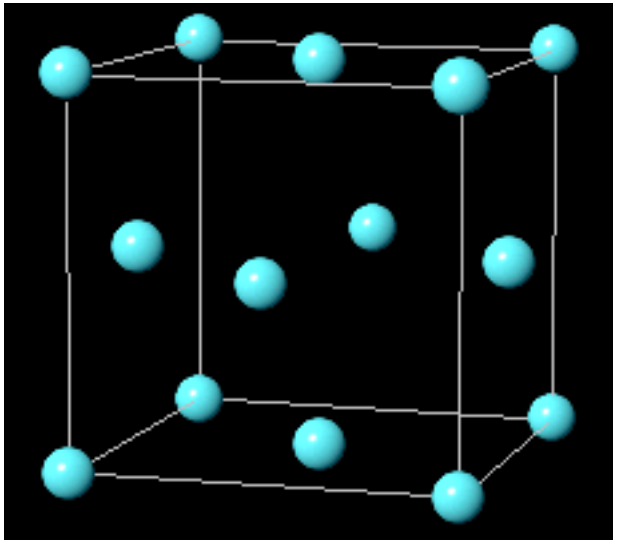
- VMSE is a tool to visualize materials science topics such as crystallography and polymer structures in three dimensions

  - Available in Student Companion Site at http://www.wiley.com/college/callister/CL_EWSTU01031_S/vmse/

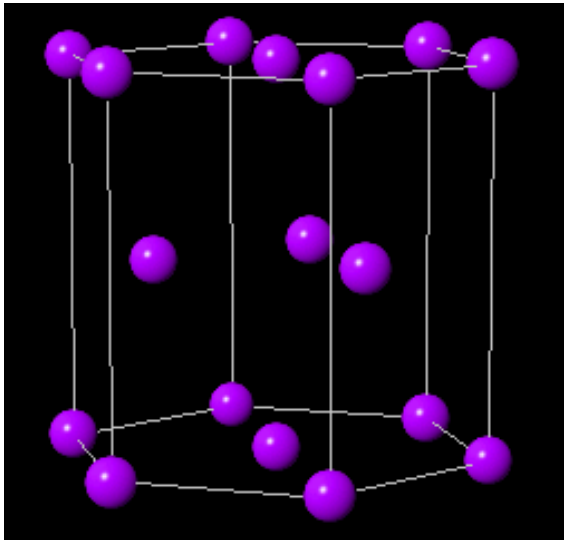
Unit Cells

- VMSE allows you to view the unit cells and manipulate them in three dimensions

- Below are examples of actual VMSE screen shots



FCC Structure



HCP Structure

Other Links

- Flash 3D Atomic Structure Model Viewer
  http://www.dawgsdk.org/crystal/index.en

Crystal Structure Application Problem 2 Estimation of Theoretical Density or Atom Size

$$\text{Density} = \rho = \frac{\text{Total mass of atoms in a unit cell}}{\text{Total volume of a unit cell}}$$

For simple pure element,

If known n = number of atoms/unit cell

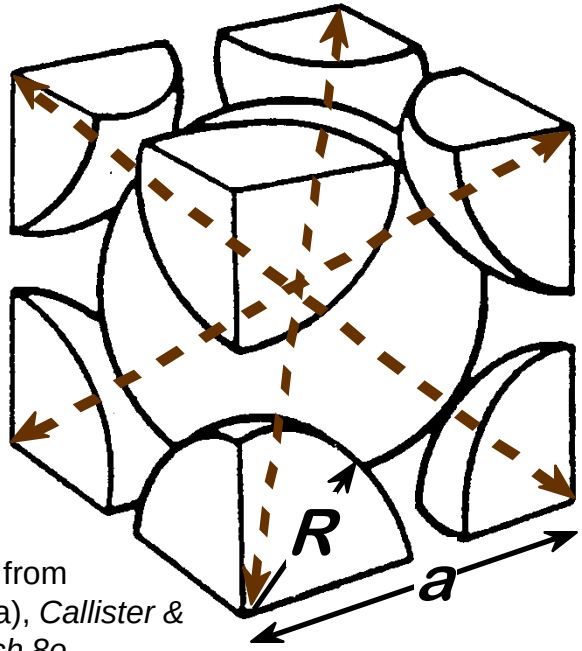
A = atomic weight (in g/mol)

V_C = Volume of unit cell, Vc = a^3 for cubic structure

N_A = Avogadro's number = 6.022×10^{23} atoms/mol

$$\rho = \frac{n\,(A/N_A)}{V_C}$$

Crystal Structure Application Problem 2 Estimation of Theoretical Density or Atom Size



Adapted from Fig. 3.2(a), *Callister & Rethwisch 8e.*

- Ex: Cr (BCC unit cell)

  Atom mass: A = 52.00 g/mol

  Atom radius: R = 0.125 nm

  n = 2 atoms/unit cell

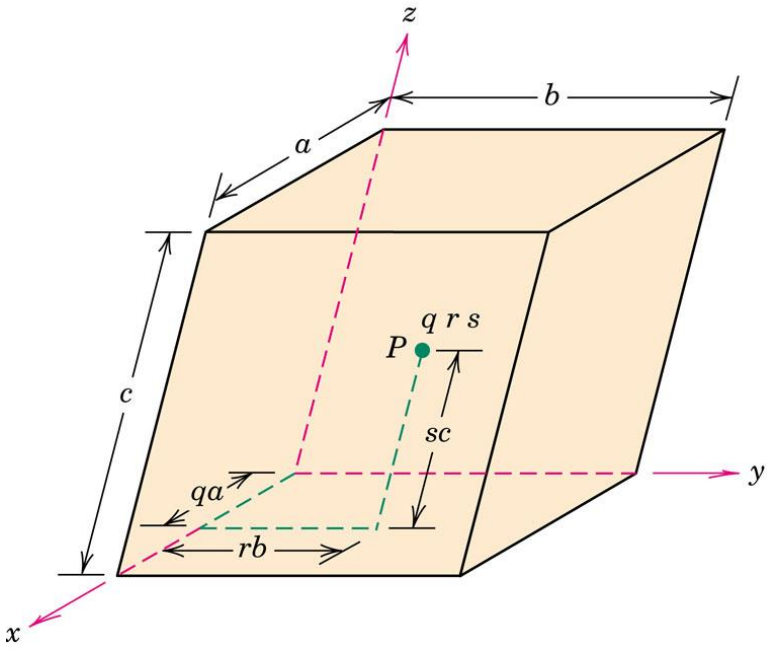
  $a = 4R/\sqrt{3}$ = 0.2887 nm

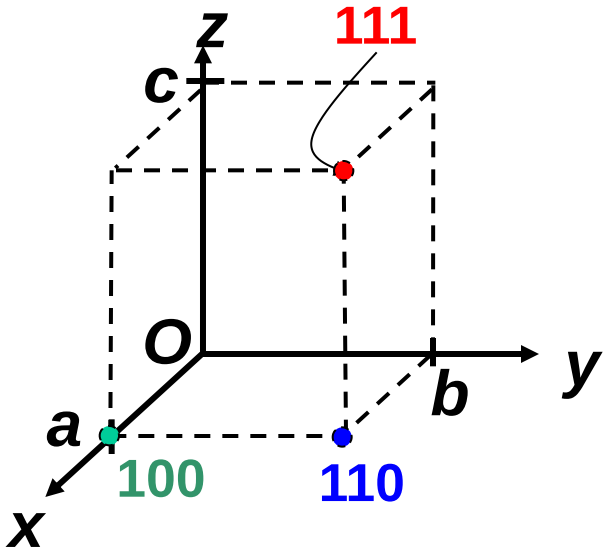
$$\rho = \frac{\text{\# of atoms per unit cell} \times \text{Mass per mole of atoms}}{\text{Volume of a unit cell} \times \text{\# of atoms per mole}} = \frac{2 \times 52.00}{a^3 \times 6.022 \times 10^{23}}$$

$\rho_{theoretical}$ = 7.18 g/cm^3

$\rho_{measured}$ = 7.19 g/cm^3

Point Coordinates in Crystal Structure





- **Unit cell** – repeating unit that reflects crystal symmetry
- **Point coordinates**:
  - Specified in terms of its coordinates (fractional length in "projection") with respect to the three edges of the unit cell,
    Example:
    Point P, with *q* reflecting the projection of the point to *x* axis, *r* reflecting projection to *y* axis, and *s* reflecting project onto *z* axis (x, y, z axis along a, b, c edge of the unit cell, with unit length of a, b, c, respectively), coordinate of
    qrs
- Axes may or may not be orthogonal to each other
- In some cases, some points are (geometrically) equivalent

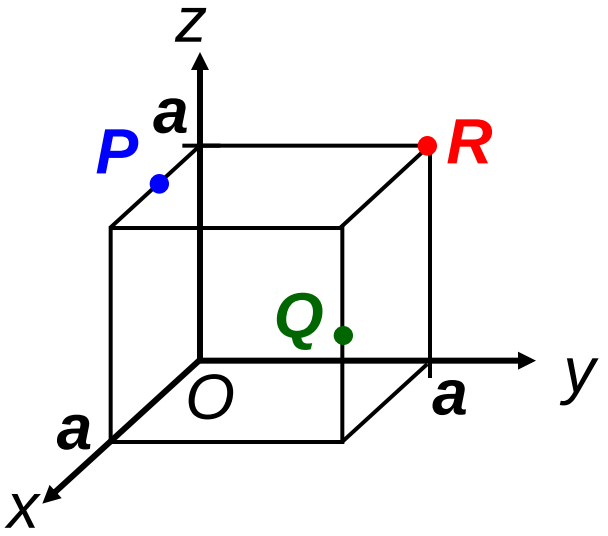
Class Exercise – Coordinates of Points

- Specify the coordinates for three points as labeled in the graph for a (simple) cubic unit cell

  P ½ 0 1

  Q 1 1 ½

  R 0 1 1

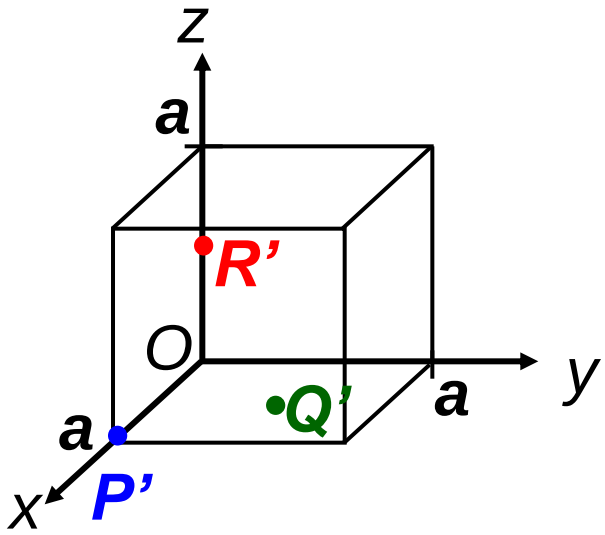


- Label the points based on the coordinates given for a cubic unit cell

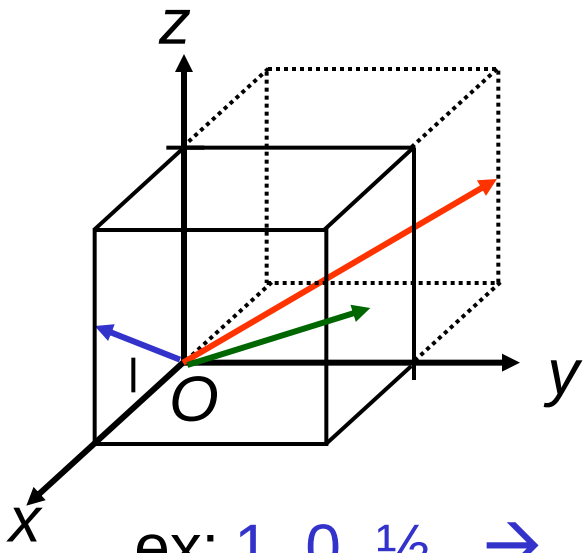
  P’ 1 0 0

  Q’ ½ ½ 0

  R’ 0 0 ½



Directions in Crystal Structure



1. Vector repositioned (if necessary) with starting point to pass through origin *O*.
2. Read off projections of the end point of the vector in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas **[*uvw*]**

ex: 1, 0, ½ → 2, 0, 1 → [201] direction

½, 1, ½ → 1, 2, 1 → [121] direction

-1, 1, ½ → -2, 2, 1 → [$\bar{2}$21] direction

overbar represents a negative index

For some crystal systems, some directions are equivalent

→ families of directions, designated in the form of **<*uvw*>**

e.g., for simple cubic, [100], [010], [001], [100], [010], [00$\bar{1}$] directions are all equivalent, as <100> family

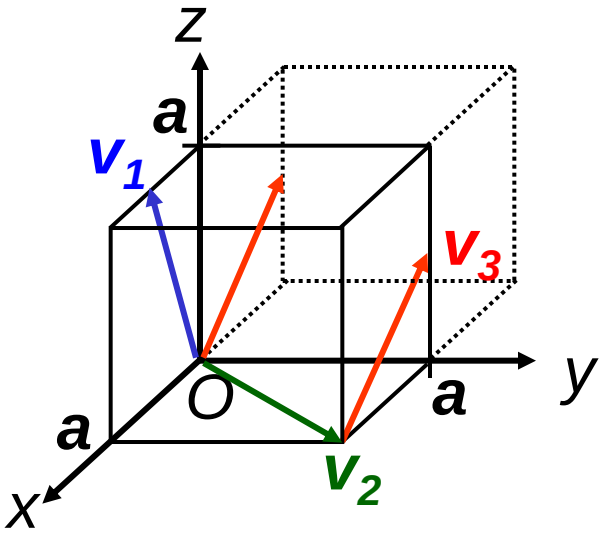
Class Exercise – Directional Indices

- Specify the directional indices for the crystallography directions as labeled in the graph

  v1 [102]

  v2 [110]

  v3 [$\bar{2}$01]

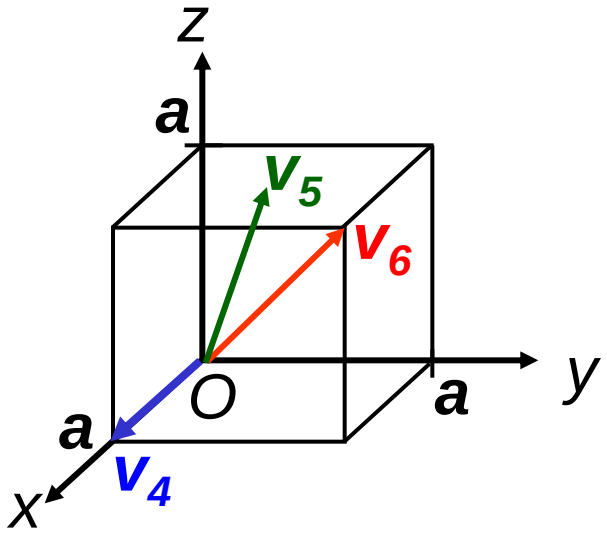


- Draw the crystallography directions based on directional indices given below

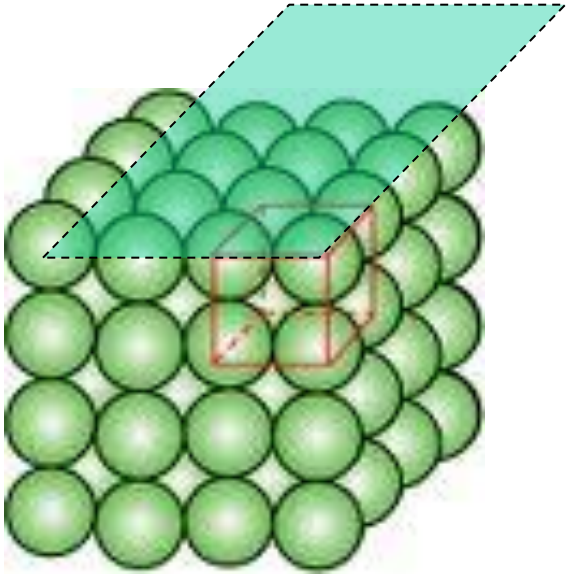
  v4 [100]

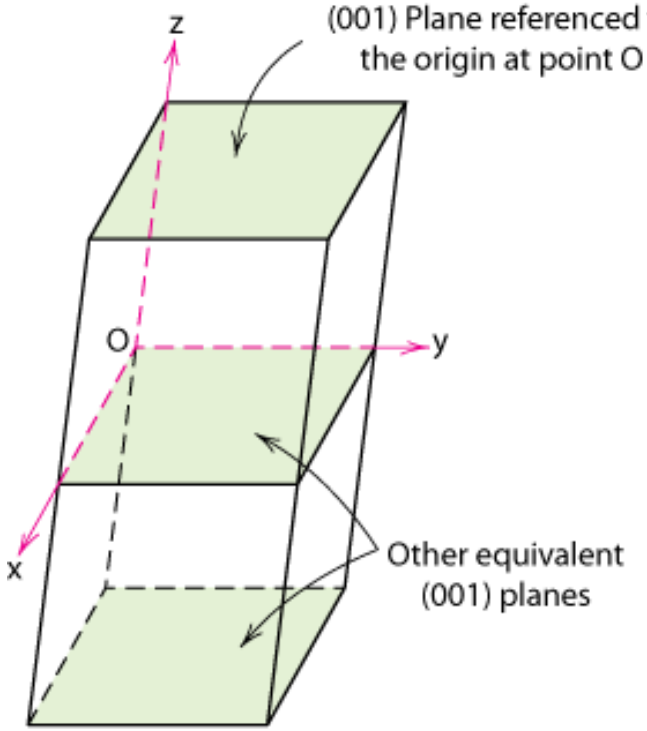
  v5 [112]

  v6 [111]

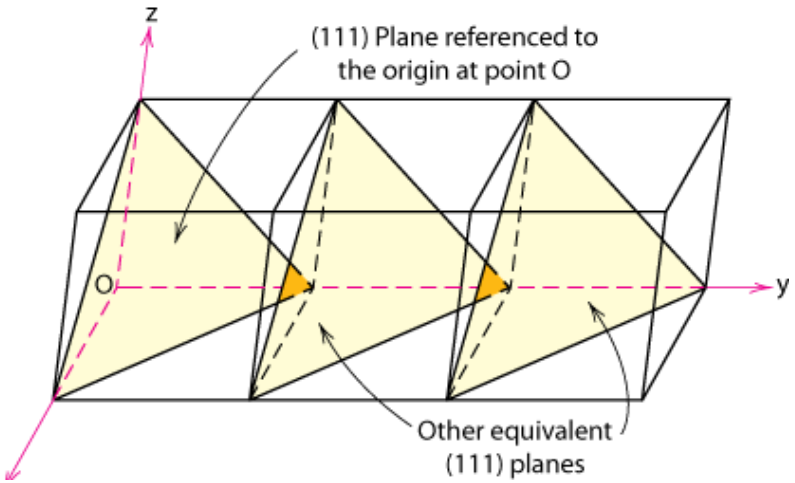


Planes in Crystal Structure (1)





(a)



apted from Fig. 3.10,
llister & Rethwisch 8e.

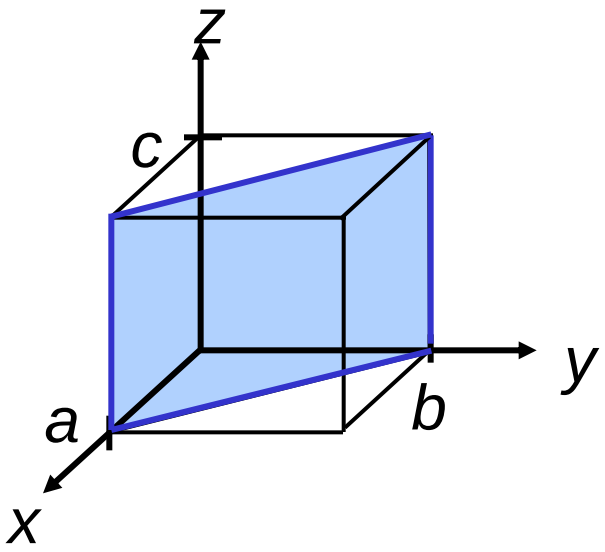
Planes in Crystal Structure (2)

- **Miller Indices**: Indices given to describe crystal planes - Reciprocals of the (three) axial intercepts for a plane, cleared of fractions
- Method
  1. *If a crystal plane **not** passing through origin, r*ead off the intercepts of that plane with three axes of the unit cell in terms of edge length *a*, *b*, *c (Otherwise a parallel plane or alternative origin has to be chosen so that the plane does NOT pass through the origin)*
  2. Take reciprocals for each of the three intercepts, respectively
  3. If contains non-integer, reduce to smallest integer set by multiplying a common integer, when applicable
  4. Enclose in parentheses, no commas i.e., **(*hkl*)**

Planes in Crystal Structure (4)

example

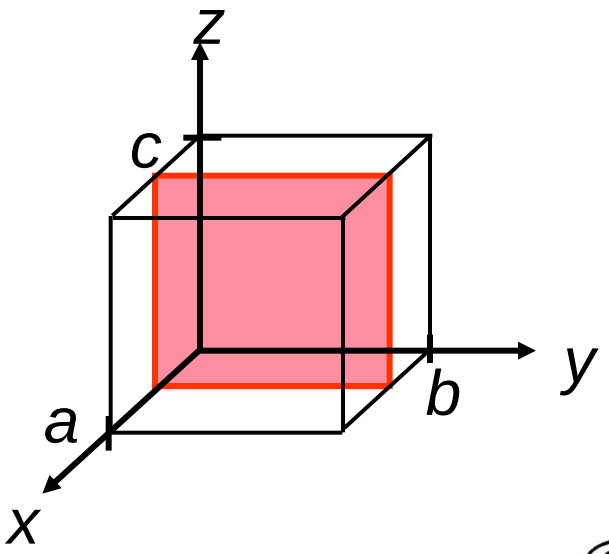
		x	*y*	z
1.	Intercepts	1a	1b	∞c
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Miller Indices	(110)		



example

		x	*y*	*z*
1.	Intercepts	1/2a	∞b	∞c
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Miller Indices	(200)		

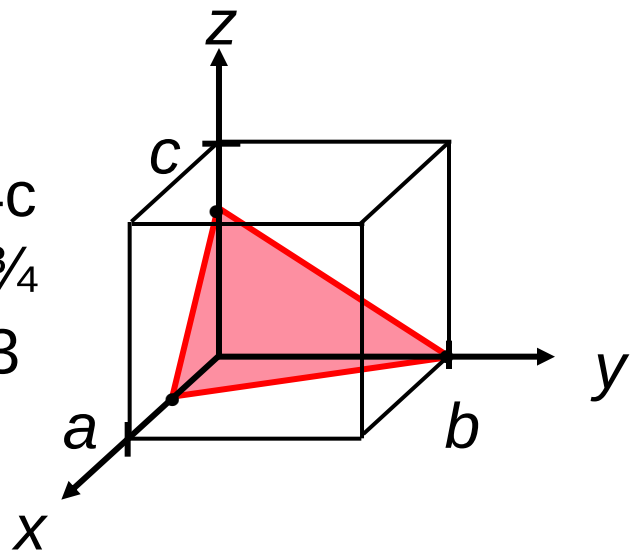
DO NOT reduce to (100)



Planes in Crystal Structure (5)

example

		x	*y*	*z*
1.	Intercepts	1/2a	1b	3/4c
2.	Reciprocals	1/½	1/1	1/¾
		2	1	4/3
3.	Multiply integer of 3	6	3	4
4.	Miller Indices	(634)		



For some crystal systems, some planes are equivalent

Family of Planes {*hkl*}. For example

Cubic: {100} family includes (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$ planes

Class Exercise (5) – Plane Miller Indices

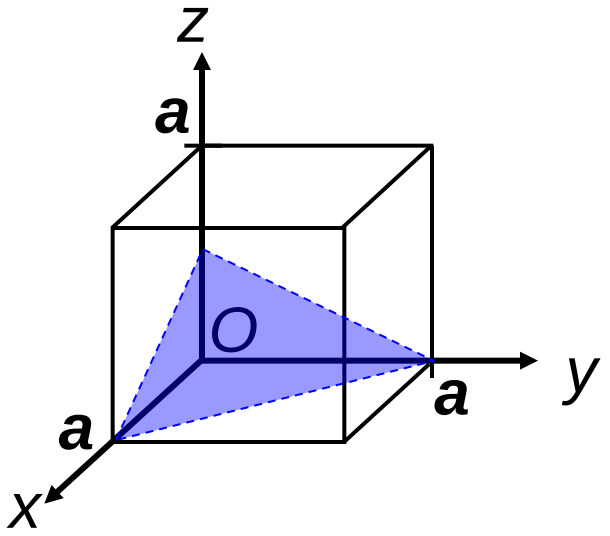
- Specify the Miller indices for the crystallography planes as labeled in the graph

  Axis *x* *y* *z*

  Intercepts a a ½ a

  Reciprocal 1 1 2

  Miller indices (112)



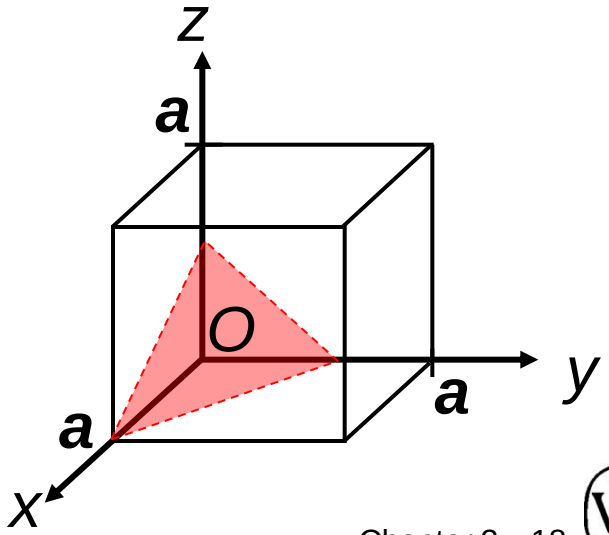
- Draw the crystallography (122) plane

  Miller indices (122)

  Reciprocal 1 ½ ½

  Axis *x* *y* *z*

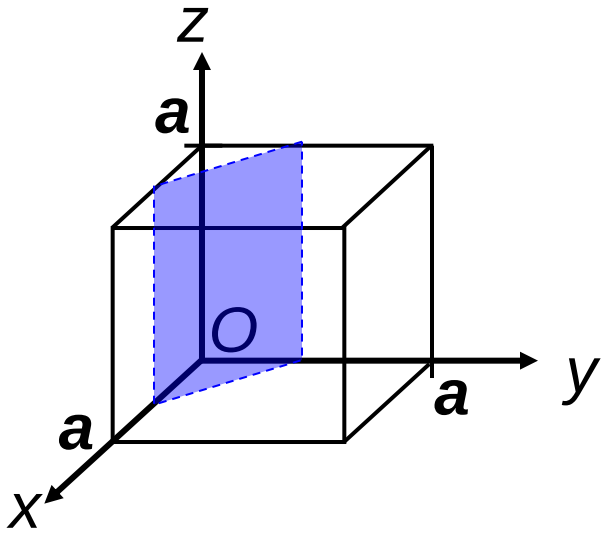
  Intercepts a ½ a ½ a



Class Exercise (6) – Plane Miller Indices

- Specify the Miller indices for the crystallography planes as labeled in the graph

Axis	*x*	*y*	*z*
Intercepts	½a	½a	∞
Reciprocal	2	2	0
Miller indices		(220)	



- Draw the crystallography (101) plane

Miller indices		(101)	
Reciprocal	1	∞	1
Axis	*x*	*y*	*z*
Intercepts	a	∞	a