Outline (Chapter 3)

- **Crystal Systems**
- **Crystallographic <u>points</u>, <u>directions</u>, & <u>planes</u>**

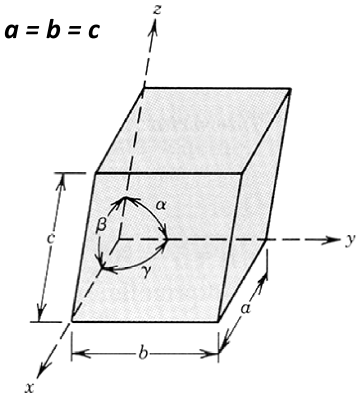
Crystal Systems

- Group crystals depending on shape of Unit Cell.
- **Unit cell** can have different dimensions based on different :

1) Lattice Parameters **(a, b, and c)**
2) Angles **(α, β and γ)**

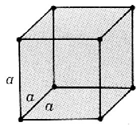
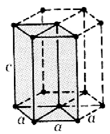
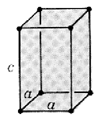
Note: *for the cubic system all sides equal so* ***a = b = c***

SEVEN possible **crystal systems**	
Cubic	most symmetry
…	
…	
Triclinic	least symmetry

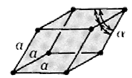
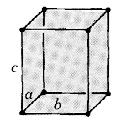
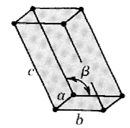
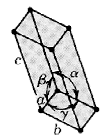


Crystal Systems

Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	

Crystal Systems

Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

Crystallographic points

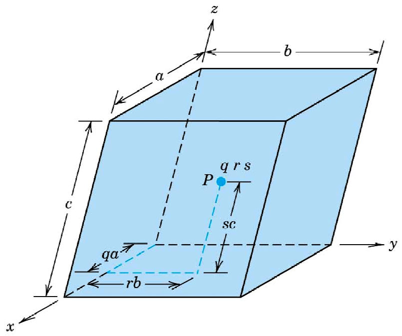
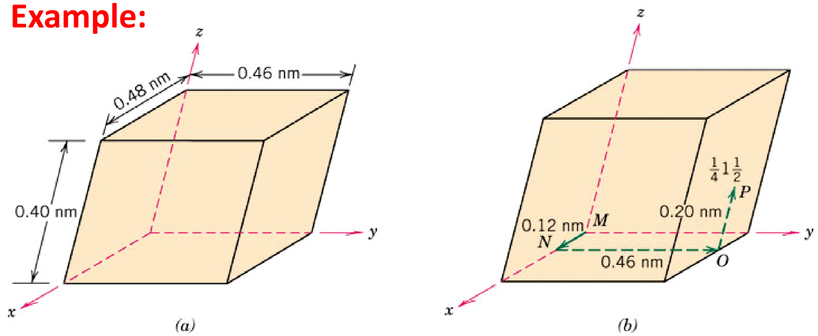


FIGURE 3.5 The manner in which the q, r, and s coordinates at point P within the unit cell are determined. The q coordinate (which is a fraction) corresponds to the distance qa along the x axis, where a is the unit cell edge length. The respective r and s coordinates for the y and z axes are determined similarly.

Crystallographic points

Example:



Find coordinates of point P.

Starting from origin, Point M- coordinates (0,0,0):
Along *x (M-N)*:
Along *y (N-O)*:
Along *z*: *(O-P)*:

Crystallographic Directions

- **Crystallographic Directions:** Line between two points or vector.

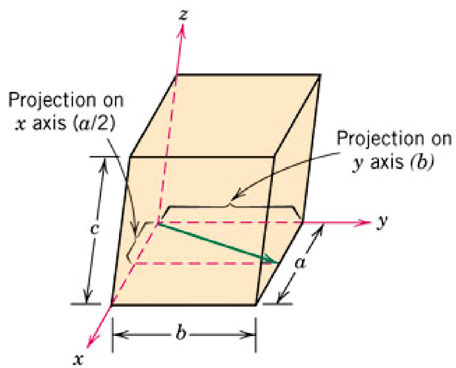
✓ Enclose in SQUARE brackets with no commas **[u v w]**, and minus numbers given by bar **over** number; e.g.

$$[11\bar{2}],\ [111],\ [2\bar{1}2]$$

✓ **In HCP: [u v t w] or [a_1 a_2 a_3 c]**

✓ **Position vector** so that it **passes through origin** (parallel vectors can be translated).
✓ Length of vector projected onto the three axes (*x, y* and *z)* is determined in terms of unit cell dimensions (*a, b* and *c).*
✓ Multiply or divide by common factor to reduce to lowest common integers.

Crystallographic Directions



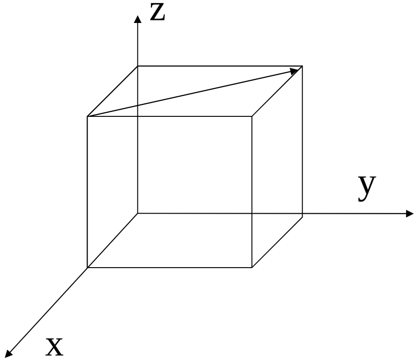
Example (green vector):

✓ **Step one:**
on x: **½ a**, y: **1b,** z: **0c**

✓ **Step two:**
Reduce to common integer:
(multiply by 2) **1, 2, 0**

✓ **Step three:**
Place in square brackets: **[1 2 0]**

Crystallographic Directions



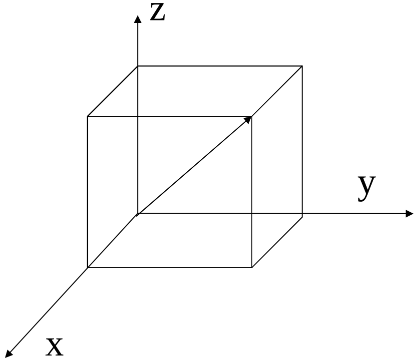
Problem Review 1:

1)
on x: , y: , z: ,
2)
Reduce to common integer:

3)
Place in square brackets: [ ]

✓Find out the opposite:
By having the directions how to draw the vector!

Crystallographic Directions



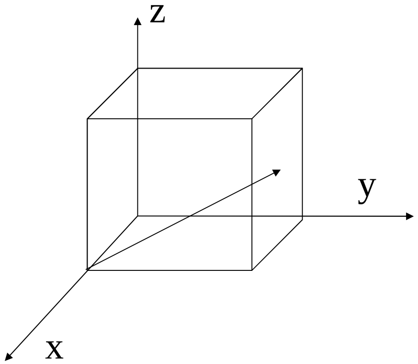
Problem Review 2:

1)
on x: , y: , z: ,
2)
Reduce to common integer:

3)
Place in square brackets: [ ]

✓Find out the opposite:
By having the directions how to draw the vector!

Crystallographic Directions



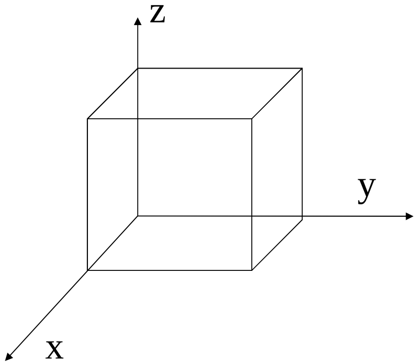
Problem Review 3:

1)
on x: , y: , z: ,
2)
Reduce to common integer:

3)
Place in square brackets: [ ]

✓Find out the opposite:
By having the directions how to draw the vector!

Crystallographic Directions



Problem Review 4:

Draw [1 1 $\bar{2}$] and [$\bar{1}$ $\bar{1}$ $\bar{1}$]

Crystallographic Directions

• Parallel vectors have same indices.
Changing sign of **all** indices gives opposite direction.

• If directions are similar:
(i.e., same atomic arrangements - for example, the edges of a BCC cube)
they belong to a **FAMILY of directions**:

$$[100], [\bar{1}00],\ [010],\ [0\bar{1}0], [001], [00\bar{1}] = <100>$$

Note: **only in cubic** systems because in a cube a=b=c

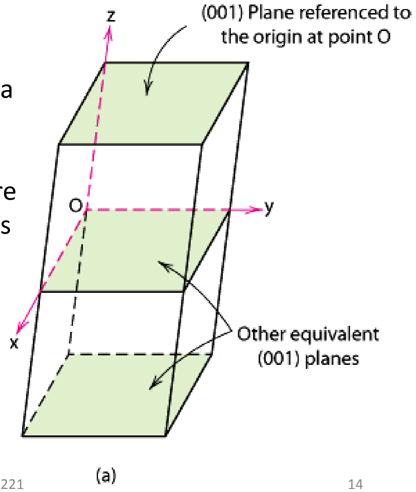
i.e. with < > brackets can change order and sign of integers.		
e.g.	**cube internal diagonals**	**<111>**
	cube face diagonals	**<110>**

Crystallographic Planes

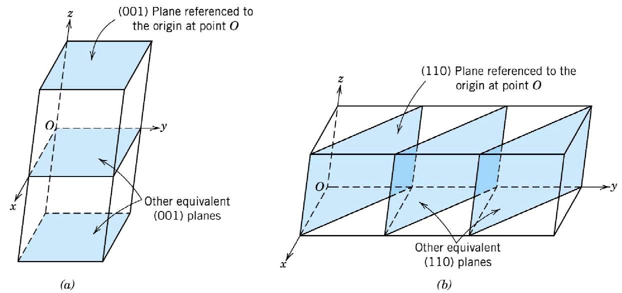
➢ **Crystal Planes specified by Miller Indices (*h k l*) (Reciprocal Lattice).**

➢ Used to describe a plane (or surface) in a crystal e.g., plane of maximum packing.

➢ Any two planes parallel to each other are equivalent and have identical Miller indices



Crystallographic Planes



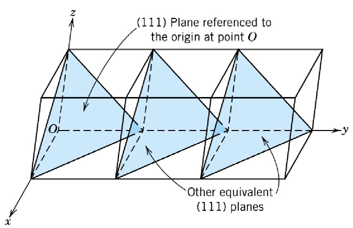


FIGURE 3.9 Representations of a series each of (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes.

Crystallographic Planes

- **How To find Miller Indices (planer indices) of a plane:**

o If the plane passes through the selected origin, construct a parallel plan in the unit cell or select an origin in another unit cell.

1. Determine where plane intercepts axes. (if no intercept i.e.., **plane is parallel to axis, then ∞**)

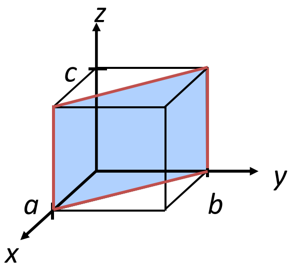
e.g., axis	x	y	z
intercept	**a**	**b**	**c**

2. **Take reciprocals** of intercepts (assume reciprocal of ∞ is 0):
1/a 1/b 1/c

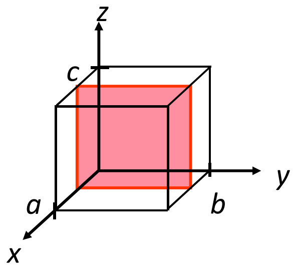
3. Multiply or divide to clear fractions (reduction): **h k l**
4. Enclose in curved brackets: **(h k l)**

Crystallographic Planes

example	*a*	*b*	*c*
Step 1: Intercepts	1	1	∞
Step 2: Reciprocals	1/1	1/1	1/∞
	1	1	0
Step 3: Reduction	1	1	0
Step 4: Miller Indices	(110)		

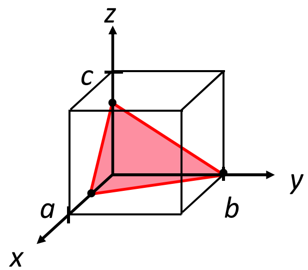


example	*a*	*b*	*c*
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/½	1/∞	1/∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(100)		



Crystallographic Planes

example	*a*	*b*	*c*
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



Crystallographic Planes

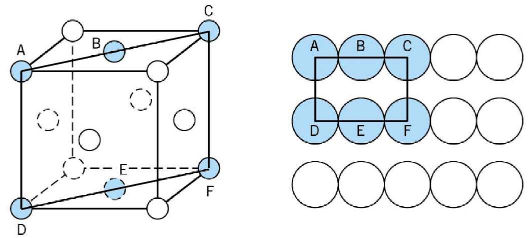
Family of Planes: {*hkl*}

✓ These planes are crystallographically similar (same atomic arrangements)
e.g., for cube faces: {100}

$$(100), (\bar{1}00), (010), (0\bar{1}0), (001), (00\bar{1}) = \{100\}$$

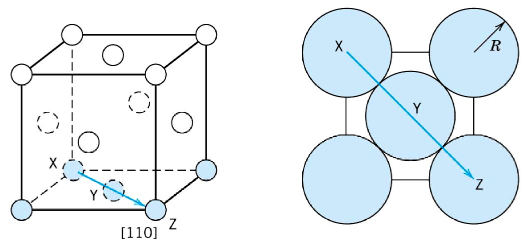
NOTE:
In CUBIC system only, directions are perpendicular to planes with same indices.
e.g., [111] direction is perpendicular to the (111) plane.

Crystallographic Planes



(*a*) (*b*)

FIGURE 3.10 (*a*) Reduced-sphere FCC unit cell with (110) plane. (*b*) Atomic packing of an FCC (110) plane. Corresponding atom positions from (*a*) are indicated.



(*a*) (*b*)

FIGURE 3.12 (*a*) Reduced-sphere FCC unit cell with the [110] direction indicated. (*b*) The bottom face-plane of the FCC unit cell in (*a*) on which is shown the atomic spacing in the [110] direction, through atoms labeled X, Y, and Z.