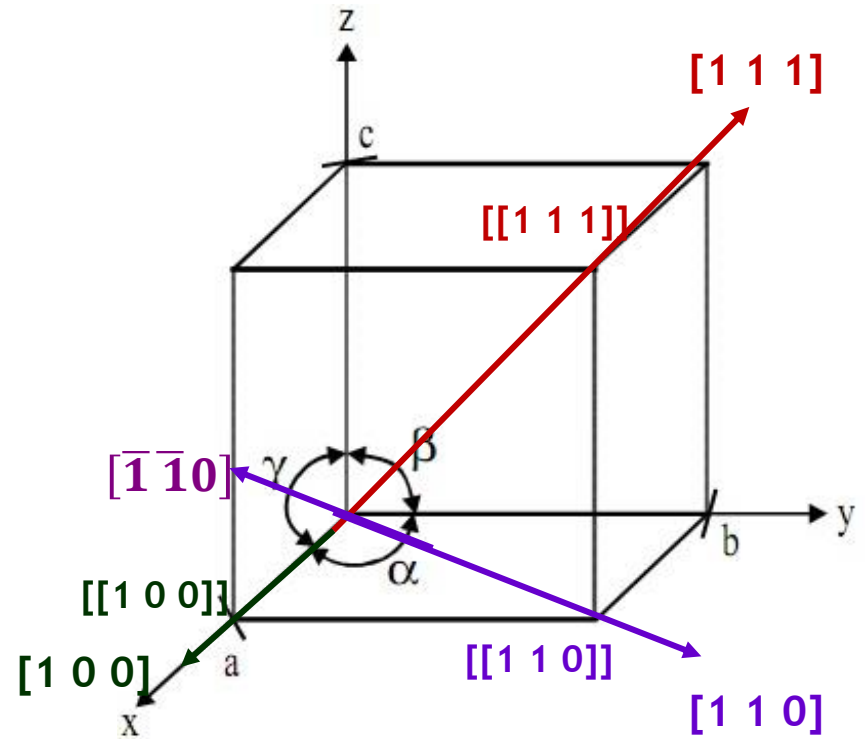# Crystal Directions

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Miller Indices

1. Indices of Site, [[m n p]]
2. Indices of Direction, [m n p]
3. Indices of Plane, (h k l)

* Indices of negative directions are indicated by " ‾ " bar sign.

Example: $[\bar{1}00], [\bar{1}\bar{1}0]$, etc.

* Intercepts of the planes are used describe a plane.

The Families of Crystal Directions

- In a crystal, there are infinite number of directions. Some of the directions form families.

- Some set of directions have identical spacing between the atoms, or we can say same unit translations. These are called equivalent directions.

- These equivalent directions form families of directions denoted as *<hkl>*.

- Example: In cubic crystals, the family <100> comprises of the directions [100], [010], [001], [$\bar{1}$00], [0$\bar{1}$0], [00$\bar{1}$]

- **Write down the directions from the family <110> and <111>.**

  <110> family has 12 members and <111> family has 8 members

Table: The unit translations for low index directions of a cubic system

Family	Unit translation		
	P	I	F
⟨100⟩	a	a	a
⟨110⟩	$\sqrt{2}a$	$\sqrt{2}a$	$a/\sqrt{2}$
⟨111⟩	$\sqrt{3}a$	$\sqrt{3}a/2$	$\sqrt{3}a$
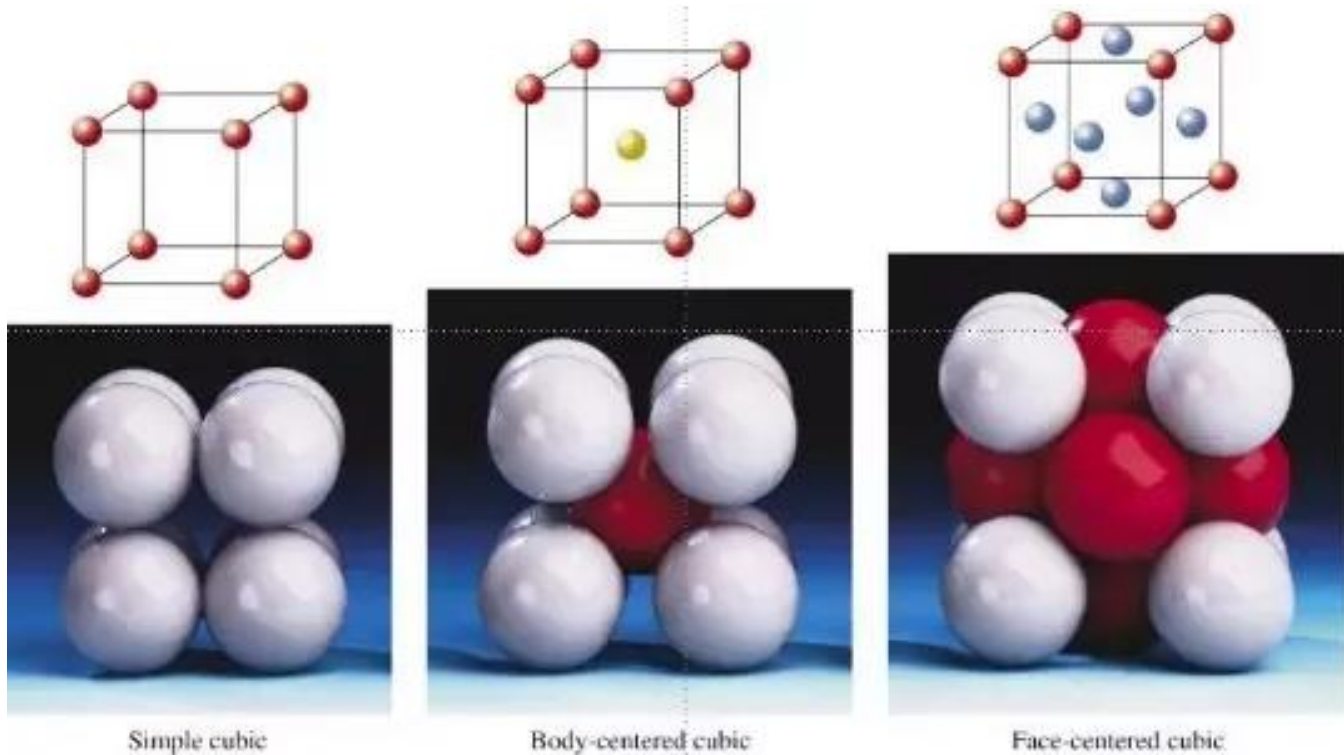
Simple cubic   Body-centered cubic   Face-centered cubic

Angle between Two Crystal Directions in Cubic Structure

Dot product of two directions $[h_1 k_1 l_1]$ and $[h_2 k_2 l_2]$ is used.

$$cos\varphi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{(h_1^2 + k_1^2 + l_1^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}}$$

Determination of angle between [111] and [001] directions in cubic structure

$$cos\varphi = \frac{0+0+1}{(3)^{1/2}(1)^{1/2}} = \frac{1}{\sqrt{3}}$$

$\varphi = 54.75^o$

Problem: Calculate the angle between [111] and $[\bar{1}\bar{1}1]$ directions in cubic structure.
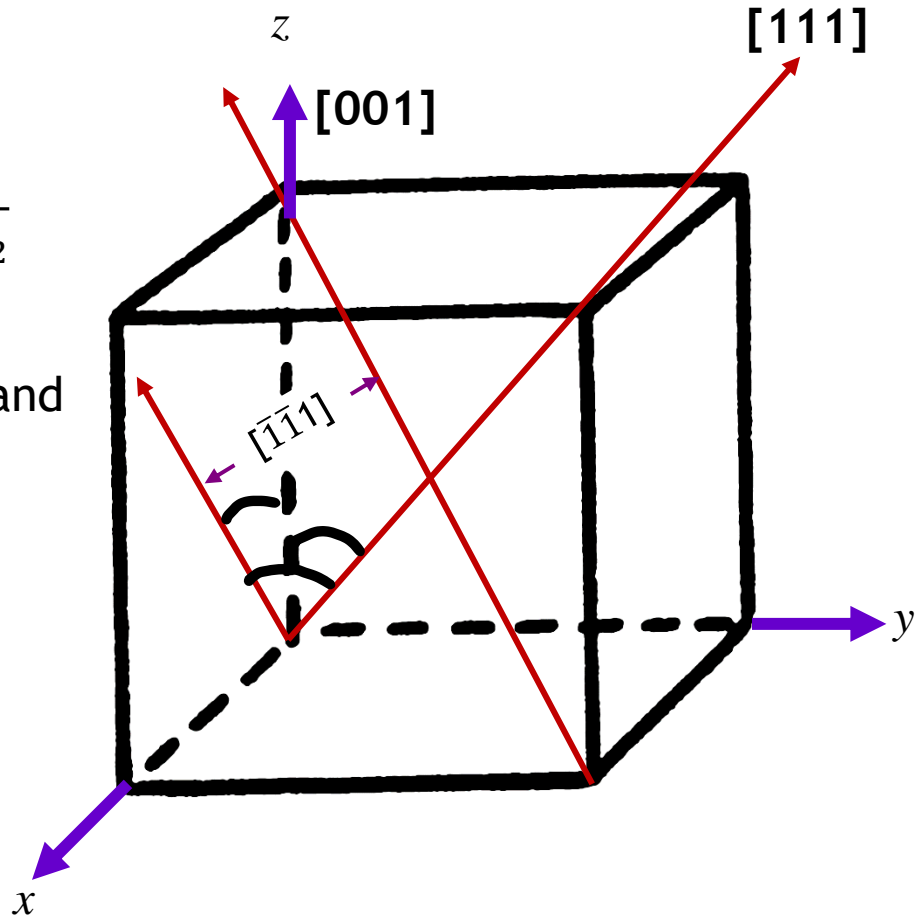
Answer: $\varphi = 109.5^o$

Fig. Angle between [111] and $[\bar{1}\bar{1}1]$ directions in cubic structure

How to find Miller Indices

1. First we have to find the intercepts with the axes along the basis vector $\vec{a}$, $\vec{b}$ and $\vec{c}$. Let these intercepts of the plane be x, y, z. We form the fractional triplet $\left(\frac{x}{a}, \frac{y}{b}, \frac{z}{c}\right)$.

2. Take reciprocal to this set $\left(\frac{a}{x}, \frac{b}{y}, \frac{c}{z}\right)$.

3. Then reduce this set to a similar one having the smallest integers multiplying by common factor.

4. This last set is enclosed in parentheses (h k l), is called the index of the plane or Miller Indices.

Example:

1. Let the intercepts are x = 2a, y = 3b/2, z = c.

2. We first form the set, $\left(\dfrac{x}{a}, \dfrac{y}{b}, \dfrac{z}{c}\right) = \left(\dfrac{2a}{a}, \dfrac{3b}{2b}, \dfrac{c}{c}\right) = \left(2, \dfrac{3}{2}, 1\right)$

3. Taking the reciprocal, $\left(\dfrac{1}{2}, \dfrac{2}{3}, 1\right)$

4. Finally, multiply by a common (factor) denominator. Which is 6, to obtain the miller indices (h k l) = (3 4 6).
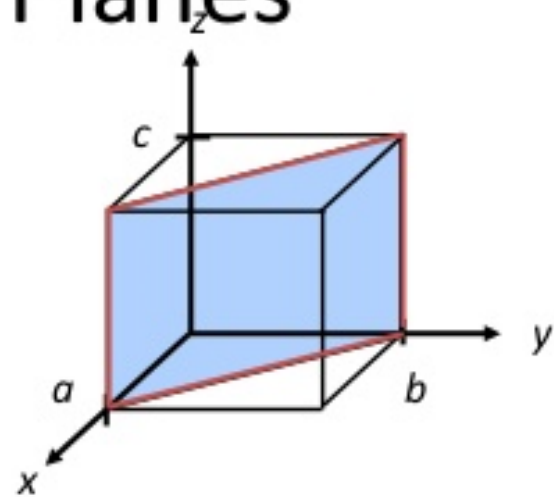

(3 4 6) plane
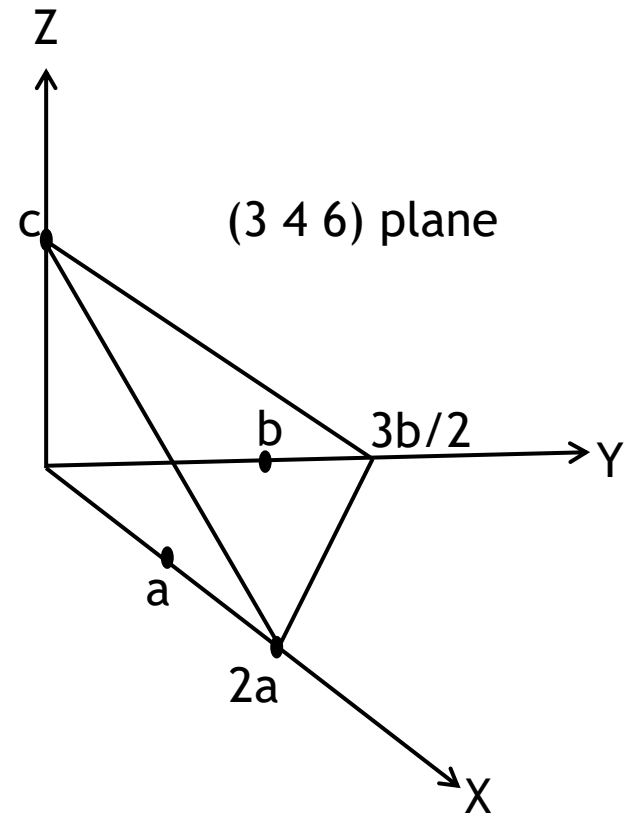
Crystallographic Planes

example		a	b	c
1.	Intercepts	1/2	1	3/4
2.	Reciprocals	$1/\frac{1}{2}$	1/1	$1/\frac{3}{4}$
		2	1	4/3
3.	Reduction	6	3	4
4.	Miller Indices	(634)		
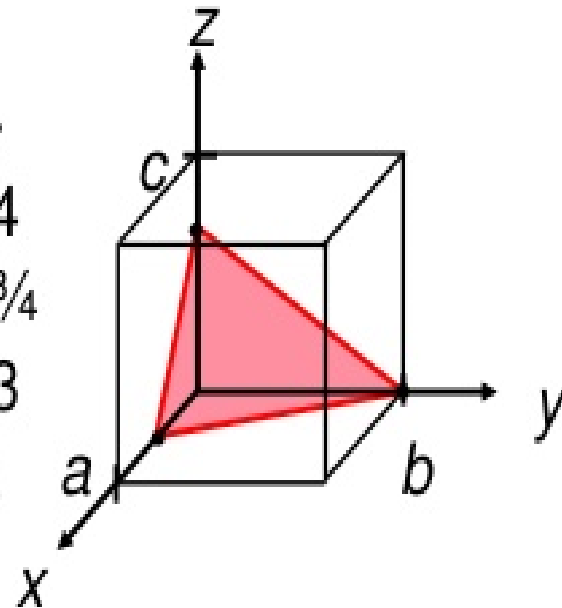
Crystallographic Planes

example	a	b	c
1. Intercepts	1	1	∞
2. Reciprocals	1/1	1/1	1/∞
	1	1	0
3. Reduction	1	1	0
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	(200)		
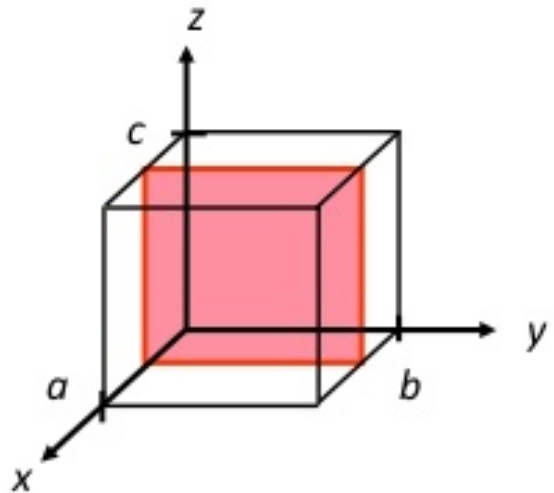
Miller Indices to Intercepts

1. Form a set: $\frac{1}{h}:\frac{1}{k}:\frac{1}{l}=p:q:r$

2. Multiply with unit translation: $pa:qb:rc$

3. Eliminate fraction to form a set $l_1: l_2: l_3$

Here, l_1, l_2 and l_3 are the intercepts along X, Y and Z axes, respectively.

Example: (hkl)=(112)	Example: (hkl)=(301)
Step-1: $p:q:r=\frac{1}{1}:\frac{1}{1}:\frac{1}{2}$	Step-1: $p:q:r=\frac{1}{3}:\frac{1}{0}:\frac{1}{1}$
Step-2: $pa:qb:rc=\frac{a}{1}:\frac{b}{1}:\frac{c}{2}$	Step-2: $pa:qb:rc=\frac{a}{3}:\frac{b}{0}:\frac{c}{1}=\frac{a}{3}:\infty:\frac{c}{1}$
Step-3: $l_1: l_2: l_3$ = 2a:2b:c (after multiplying by lcm)	Step-3: $l_1: l_2: l_3$ = a:∞:3c (after multiplying by lcm)

Sample Problems

- In a crystal, a plane cuts intercepts of $2a$, $3b$ and $6c$ along the three crystallographic axes. Determine the Miller indices of the plane. [Answer: (321)]

- Determine the Miller indices of a plane which is parallel to x-axis and cuts intercepts of 2 and ½ respectively along y and z-axes. [Answer: (014)]

- An orthorhombic crystal whose primitive translations are $a=1.21$ Å, $b=1.84$ Å and $c=1.97$ Å. If a plane $(23\bar{1})$ cuts an intercept of 1.21 Å along x-axis, find the length of intercepts along other two axes. [Answer: *1.23 Å, - 3.94 Å*]

- Determine the Miller indices of plane that make the intercepts of 2 Å, *3 Å and 4 Å* on the coordinate axes of the orthorhombic crystal with *a:b:c=4:3:2.* [Answer: (421)]

- Find the Miller indices of a plane that makes intercepts on *a, b* and *c* axes equal to 3 Å, *4 Å and 3 Å* in a tetragonal crystal with *c/a* ratio 1.5. [Answer: (436)]

- Worked out problems in the book "Solid State Physics" by M. A. Wahab, 2nd ed, Page no. 25 – 27. Practice the problems in the exercise of the mentioned chapter.