CRYSTALLOGRAPHIC PLANES

Subject: Material Science - Lecture #7

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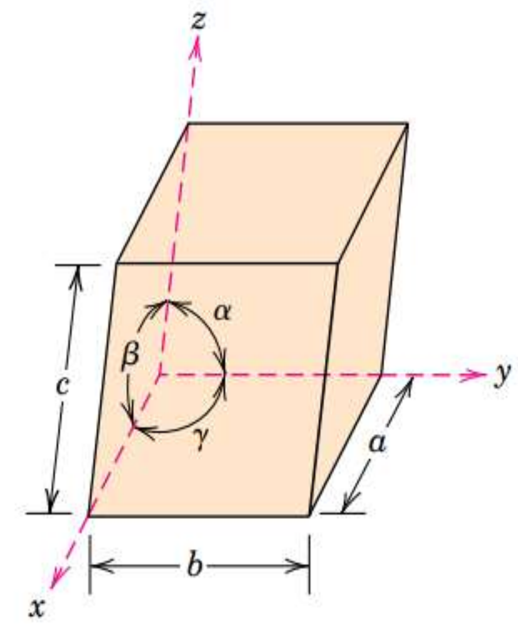
CRYSTALLOGRAPHIC PLANES

- The orientations of planes for a crystal structure are represented in a similar manner. The unit cell is the basis, with the three-axis coordinate system as represented in Figure below
- In all (<u>except the hexagonal</u>) crystal system, crystallographic planes are specified by three **Miller indices** as (hkl).
- Any two planes parallel to each other are equivalent and have identical indices.



The procedure used to determine three **Miller indices**(hkl) is as follows:

1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.

When selecting a new origin, the following procedure is suggested:

- If the crystallographic plane that intersects the origin lies in one of the unit cell faces, move the origin one unit cell distance parallel to the axis that intersects this plane.
- If the crystallographic plane that intersects the origin passes through one of the unit cell axes, move the origin one unit cell distance parallel to either of the two other axes.
- For all other cases, move the origin one unit cell distance parallel to any of the three unit cell axes.

2. At this point, the crystallographic plane either intersects or parallels each of the three axes. The coordinate for the intersection of the crystallographic plane with each of the axes is determined (referenced to the origin of the coordinate system). These intercepts for the $x, y,$ and z axes will be designed by $A, B,$ and C, respectively.

3. The reciprocals of these numbers are taken. A plane that parallels an axis is considered to have an infinite intercept and therefore a zero index.

4. The reciprocals of the intercepts are then normalized in terms of (i.e., multiplied by) their respective a, b, and c lattice parameters. That is,

$$\frac{a}{A} \quad \frac{b}{B} \quad \frac{c}{C}$$

5. If necessary, these three numbers are changed to the set of smallest integers by multiplication or by division by a common factor.

6. Finally, the integer indices, not separated by commas, are enclosed within parentheses, thus: (hkl). The $h, k, \text{and } l$ integers correspond to the normalized intercept reciprocals referenced to the *x*, *y*, and *z* axes, respectively.

In summary, the $h, k, and\ l$ indices may be determined using the following equations:

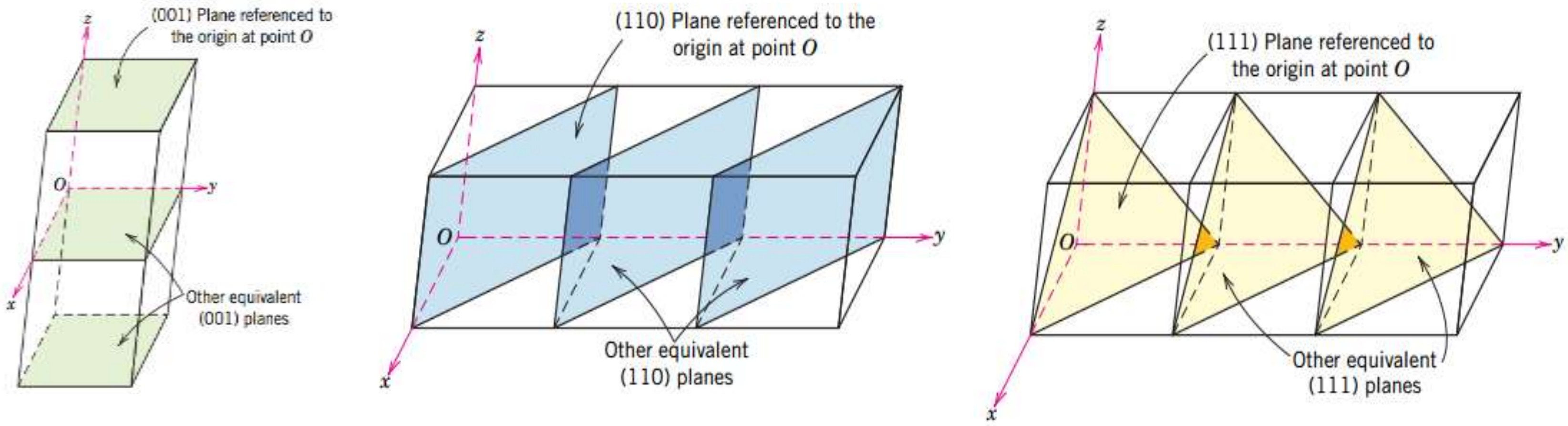
$$h = \frac{na}{A} \quad \dots \dots \dots (3.14a)$$

$$k = \frac{nb}{B} \quad \dots \dots \dots (3.14b)$$

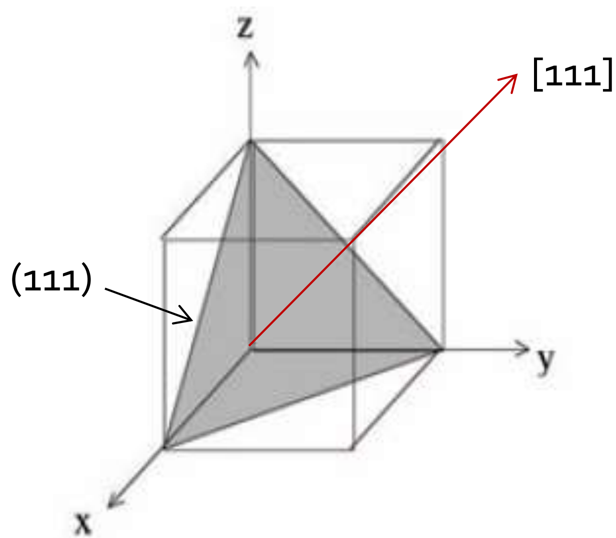
$$l = \frac{nc}{C} \quad \dots \dots \dots (3.14c)$$

In these expressions, n is the factor that may be required to reduce $h, k,$ and l to integers.

- An intercept on the negative side of the origin is indicated by a bar or minus sign positioned over the appropriate index.
- Furthermore, reversing the directions of all indices specifies another plane parallel to, on the opposite side of, and equidistant from the origin.
- Several low-index planes are represented in Figure

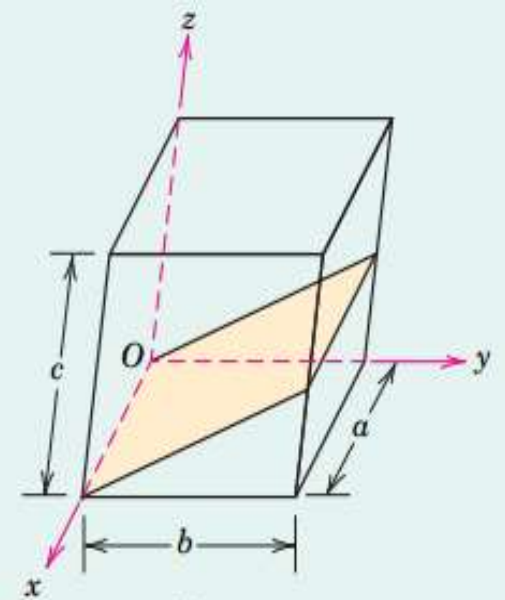


- One interesting and unique characteristic of cubic crystals is that planes and directions having the same indices are perpendicular to one another; however, for other crystal systems there are no simple geometrical relationships between planes and directions
having the same indices.



EXAMPLE PROBLEM
Determination of Planar (Miller) Indices

Determine the Miller indices for the plane shown in the accompanying sketch (*a*).



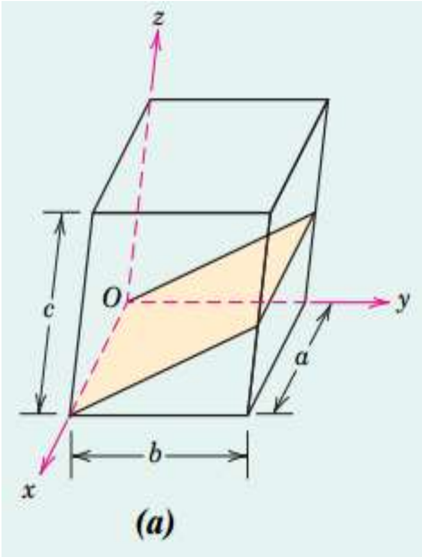
(a)

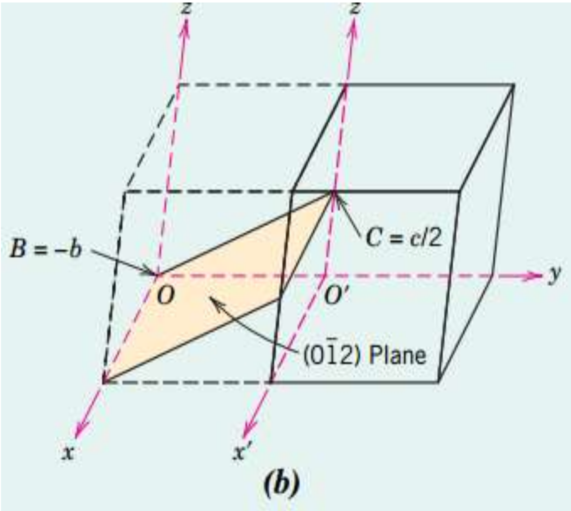
Solution

Because the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell.

In choosing this new unit cell, we move one unit-cell distance parallel to the y-axis, as shown in sketch (*b*).

(If the crystallographic plane that intersects the origin passes through one of the unit cell axes, move the origin one unit cell distance parallel to either of the two other axes)





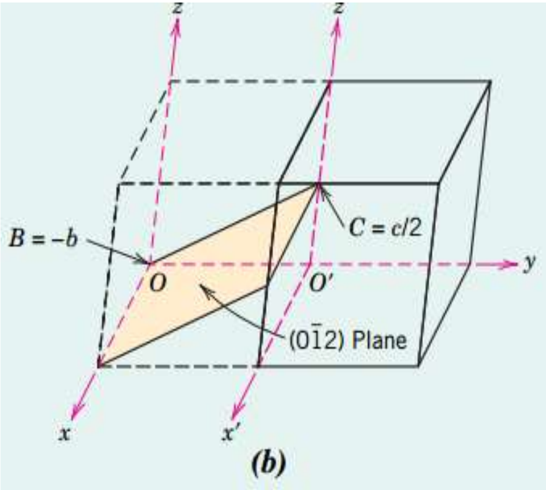
Thus $x' - y - z'$ is the new coordinate axis system having its origin located at O'.

Because this plane is parallel to the x'- axis its intercept is ∞a—that is,

$A = \infty a$

intersections with the y and z' axes are as follows:

$B = -b \quad ; \quad C = \dfrac{c}{2}$



use Equations 3.14a–3.14c to determine values of $h, k,$ and l.

$$h = \frac{na}{A} = \frac{1a}{\infty a} = 0$$

$$k = \frac{nb}{B} = \frac{1b}{-b} = -1$$

$$l = \frac{nc}{C} = \frac{1c}{c/2} = 2$$

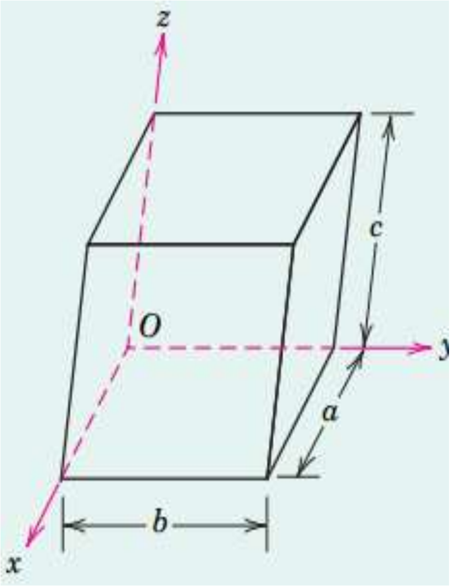
And finally, enclosure of the 0, -1, and 2 indices in parentheses leads to $(0\bar{1}2)$

This procedure is summarized as follows:

	x	y	z
Intercepts (A, B, C)	∞a	$-b$	$c/2$
Calculated values of h, k, and l (Equations 3.14a–3.14c)	$h = 0$	$k = -1$	$l = 2$
Enclosure		$(0\bar{1}2)$	

EXAMPLE PROBLEM
Construction of a Specified Crystallographic Plane

Construct a (101) plane within the following unit cell.



Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order.

$$h = 1 \quad ; \quad k = 0 \quad ; \quad l = 1$$

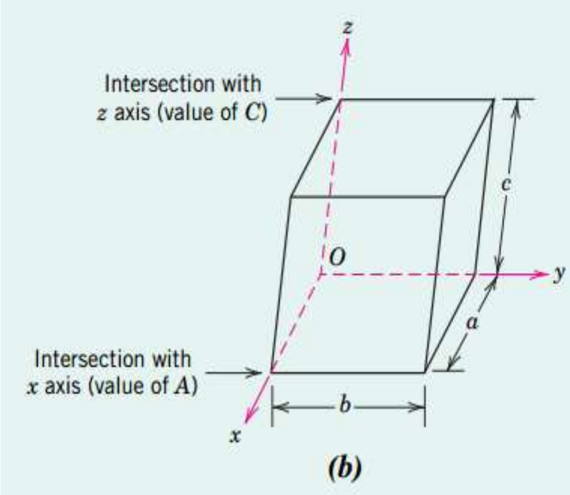
we want to solve for the values of A, B, and C using rearranged forms of Equations 3.14a–3.14c.

Taking the value of $n = 1$ because these three Miller indices are all integers—leads to the following:

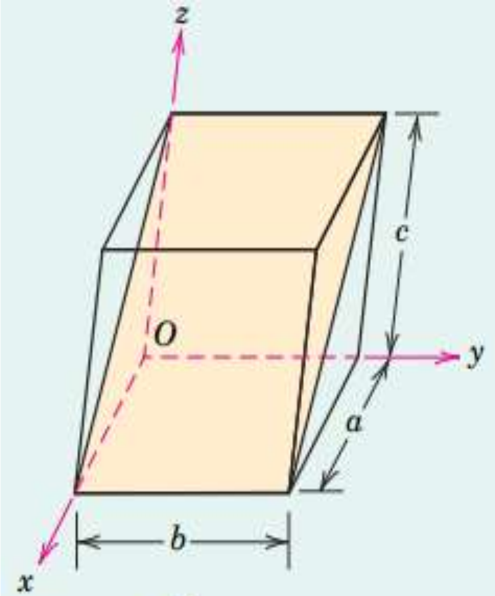
$$A = \frac{na}{h} = \frac{1a}{1} = a$$

$$B = \frac{nb}{k} = \frac{1b}{0} = \infty b$$

$$C = \frac{nc}{l} = \frac{1c}{1} = c$$



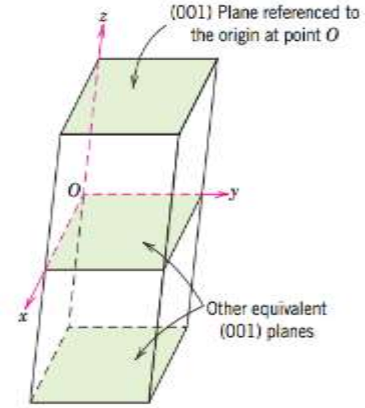
- Thus, this (101) plane intersects the x axis at a (because $A = a$), it parallels the y axis (because $B = b$), and intersects the z axis at c.



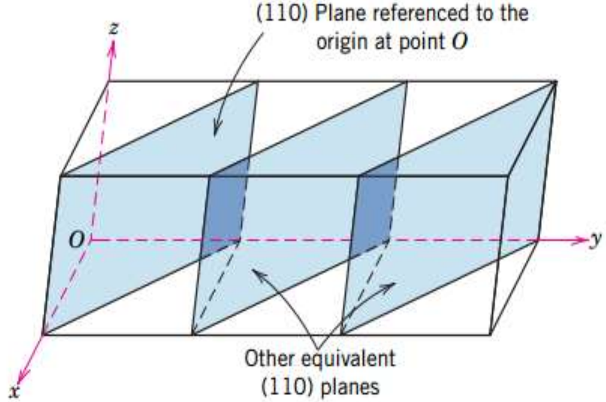
(c)

In general

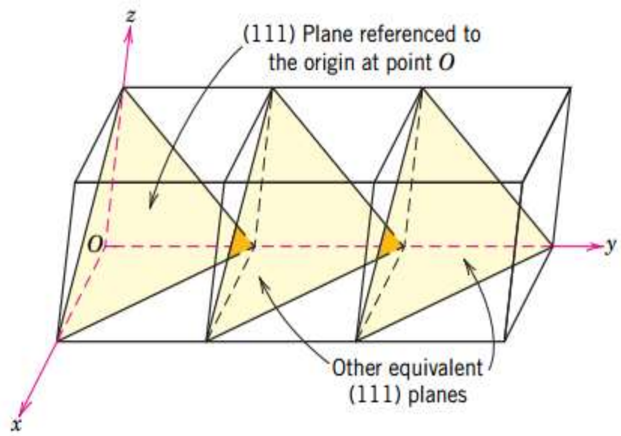
- If two of the $h, k,$ and l indices are zeros [as with (100)], the plane will parallel one of the unit cell faces



- If one of the indices is a zero [as with (110)], the plane will be a parallelogram, having two sides that coincide with opposing unit cell edges (or edges of adjacent unit cells)

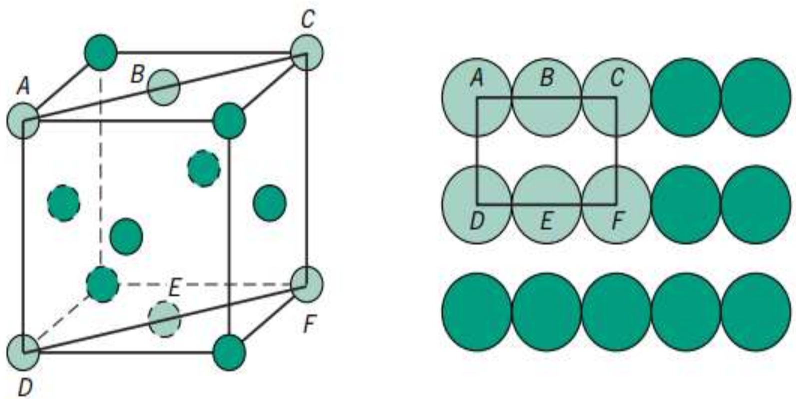


- If none of the indices is zero [as with (111)], all intersections will pass through unit cell faces

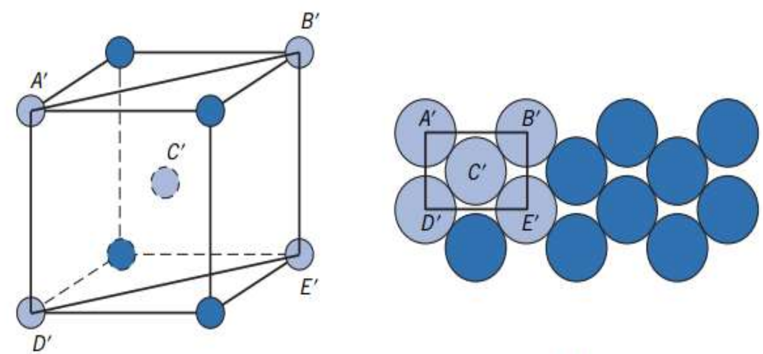


Atomic Arrangements

- The atomic arrangement for a crystallographic plane, which is often of interest, depends on the crystal structure.
- The (110) atomic planes for FCC and BCC crystal structures are represented in Figures 3.12 and 3.13, respectively.
- Note that the atomic packing is different for each case.



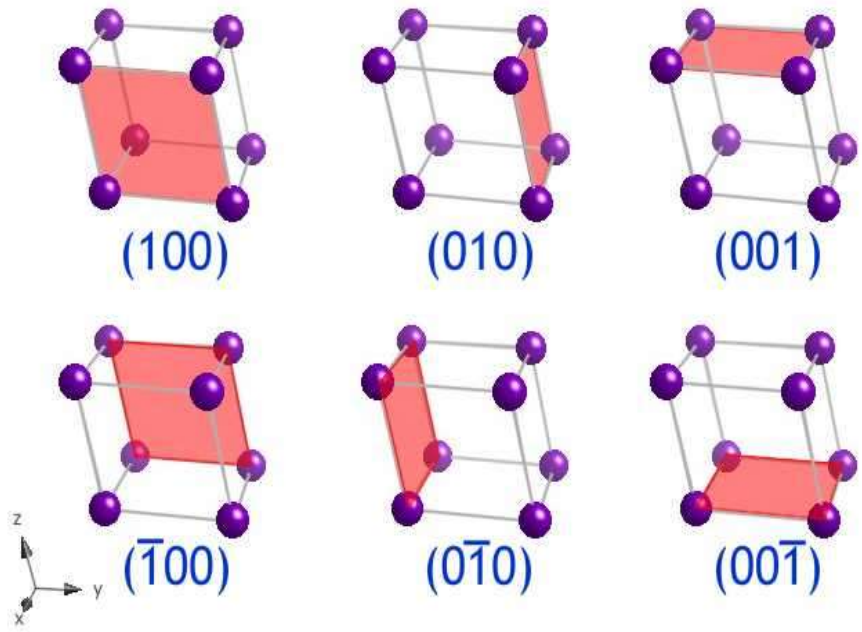
(a) FCC *(b)*



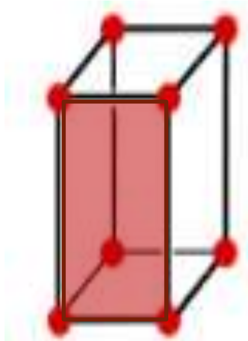
(a) BCC *(b)*

- A “family” of planes contains all planes that are *crystallographically equivalent*— that is, having the <u>same atomic packing.</u>
- A family is designated by indices enclosed in braces—such as {100}.

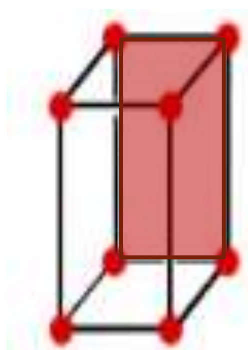
For example, in cubic crystals, the $(100), (010), (001), (\bar{1}00), (0\bar{1}0)$ and $(00\bar{1})$ planes all belong to the {100} family.



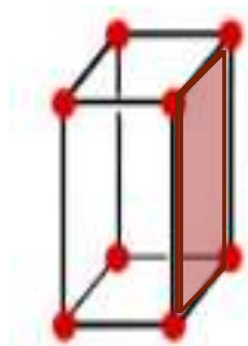
- However, for <u>tetragonal</u> crystal structures, the {100} family contains only the $(100), (\bar{1}00), (010)$, and $(0\bar{1}0)$ planes because the (001) and $(00\bar{1})$ planes are not crystallographically equivalent.



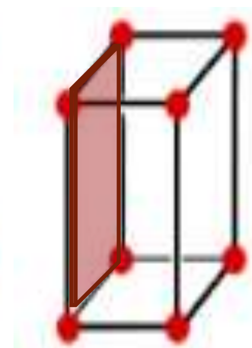
(100)



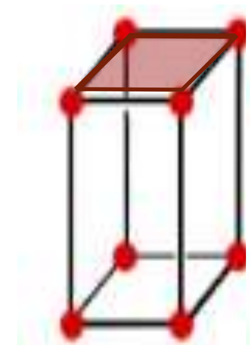
$(\bar{1}00)$



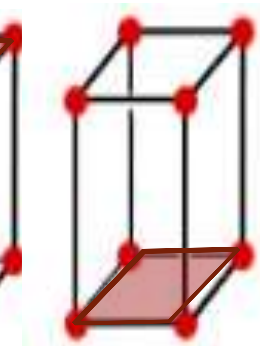
(010)



$(0\bar{1}0)$



(001)

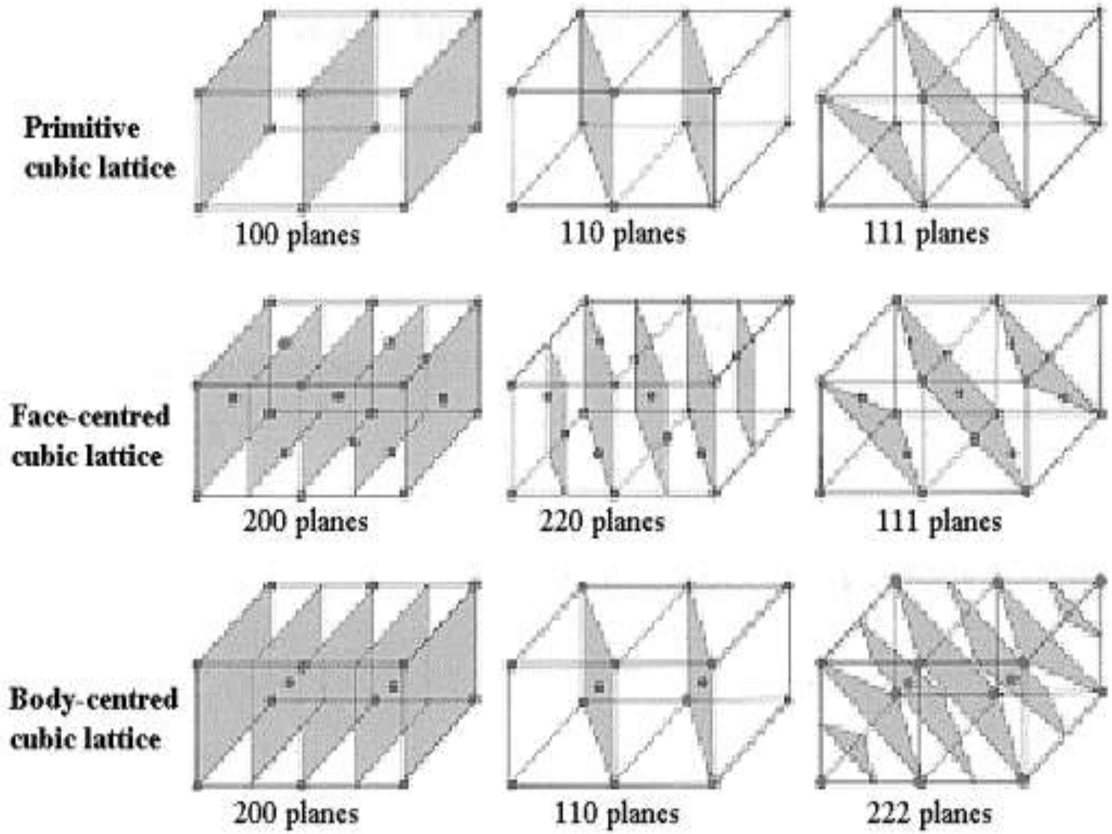


$(00\bar{1})$

- <u>in the cubic system only</u>, planes having the same indices, irrespective of <u>order</u> and <u>sign</u>, are equivalent. For example, both $(1\bar{2}3)$ and $(3\bar{1}2)$ belong to the {123} family.

{123} family have 48 sets of planes in total

(321), $(\bar{3}\bar{2}\bar{1})$; $(\bar{3}21)$, $(3\bar{2}\bar{1})$; $(3\bar{2}1)$, $(\bar{3}2\bar{1})$; $(32\bar{1})$, $(\bar{3}\bar{2}1)$,
(213), $(\bar{2}\bar{1}\bar{3})$, $(\bar{2}13)$, $(2\bar{1}\bar{3})$, $(2\bar{1}3)$, $(\bar{2}1\bar{3})$, $(21\bar{3})$, $(\bar{2}\bar{1}3)$,
(132), $(\bar{1}\bar{3}\bar{2})$, $(\bar{1}32)$, $(1\bar{3}\bar{2})$, $(1\bar{3}2)$, $(\bar{1}3\bar{2})$, $(13\bar{2})$, $(\bar{1}\bar{3}2)$,
(312), $(\bar{3}\bar{1}\bar{2})$, $(\bar{3}12)$, $(3\bar{1}\bar{2})$, $(3\bar{1}2)$, $(\bar{3}1\bar{2})$, $(31\bar{2})$, $(\bar{3}\bar{1}2)$,
(231), $(\bar{2}\bar{3}\bar{1})$, $(\bar{2}31)$, $(2\bar{3}\bar{1})$, $(2\bar{3}1)$, $(\bar{2}3\bar{1})$, $(23\bar{1})$, $(\bar{2}\bar{3}1)$,
(123), $(\bar{1}\bar{2}\bar{3})$, $(\bar{1}23)$, $(1\bar{2}\bar{3})$, $(1\bar{2}3)$, $(\bar{1}2\bar{3})$, $(12\bar{3})$, $(\bar{1}\bar{2}3)$,



Miller indices for three types of cubic lattices.

Thank you for your attention

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