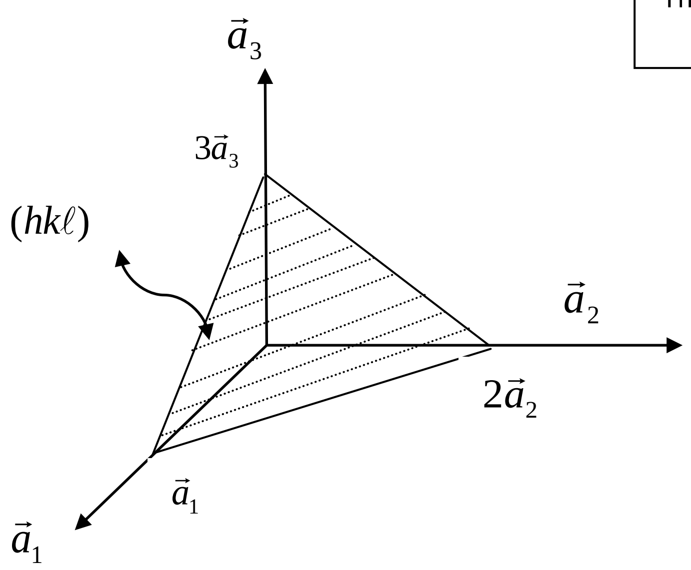
Simple procedure for finding Miller indices of a plane:

- Establish the coordinate axes along the edges of the unit cell
- Note where the plane intersects the axes.
- Divide each intercept by the unit cell length in along the respective coordinate axis.
- Record the normalized intercepts in x, y, z order.
- Compute the reciprocal of each intercept.
- Multiply the intercepts by the smallest overall constants that yield whole numbers. (See figure 33).



The normalized intercept values are 1, 2 and 3,

⇩

The reciprocals are 1, 1/2 and 1/3.

⇩

The multiplier to convert to whole number is 6.

⇩

The Miller indices (*h k l*) for this plane (632)

Figure 33: The Miller indices (*h k l*) for a plane intersecting the crystal axes at 1, 2 and 3.

Representation of a plane and a family of equivalent planes:

A certain plane with Miller indices h, k, ℓ is represented by parentheses as (h, k, ℓ).[e.g. the planes (100), $(\bar{1}00)$, (110), (111), $(2\bar{2}1)$ and (222)]. (See figure 34)

[Note: A bar is placed over the number to indicate the negative intercept].

For a cubic lattice we may have a set of planes which are equivalent to each other; e.g. (001), (010), (100), $(00\bar{1})$, $(0\bar{1}0)$ and

($\bar{1}00$), as shown in figure 35. This six equivalent faces of a cube are collectively designated as {100} where any of the individual set of these six indices will be the representative to the whole set if this set of indices is enclosed in braces { }.

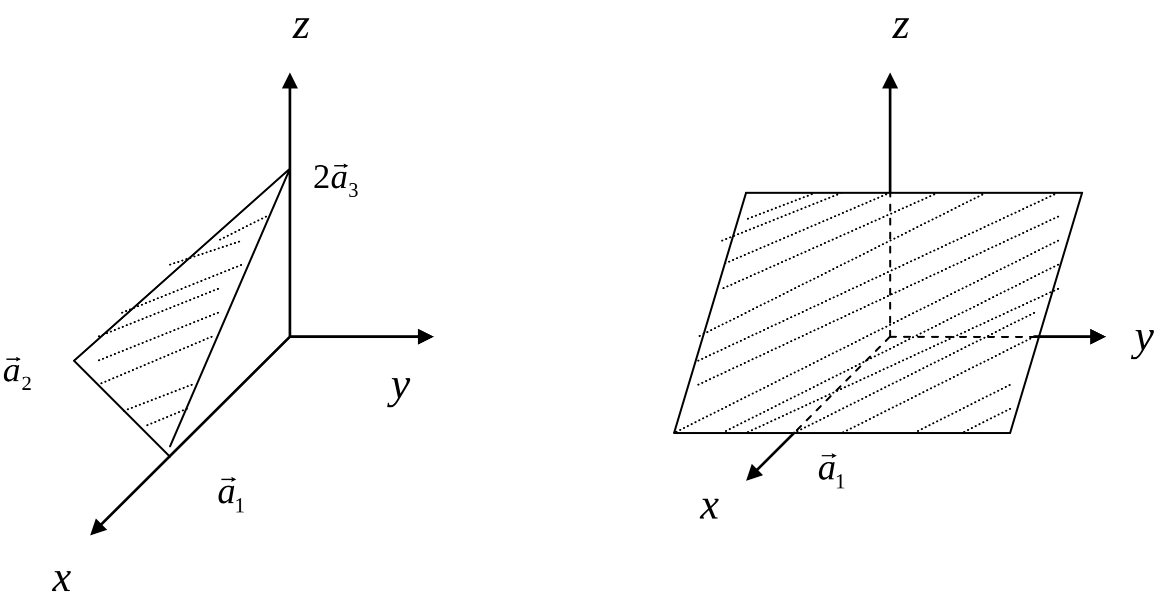


Figure 34:

a) The Miller indices (*h k l*) for this plane ($2\bar{2}1$)

b) The Miller indices (*h k l*) for this plane (100)

Simple procedure for finding Miller indices of a vector (or a direction):

- Establish the coordinate axes along the edges of the unit cell.
- Draw a vector in the direction of interest.
- Decompose the vector into components by projecting it onto the coordinate axes.
- Record the components in x, y, z order.
- Multiply the components by the smallest overall constant that yields whole numbers.
- Miller indices of a vector are enclosed in brackets [ ].
- A plane has the same Miller indices as its normal vector.
- A family of equivalent vectors is enclosed in angle brackets < >.

Again for a cubic lattice we may have a set of vectors which are equivalent to each other, e.g. $[001]$, $[010]$, $[100]$, $[00\bar{1}]$, $[0\bar{1}0]$ and $[\bar{1}00]$. This six equivalent vectors perpendicular to the faces of a cube are collectively designated as $<100>$ where any of the individual set of these six indices will the representative to the whole set if this set of indices is enclosed in braces < >.

Notes:

1) In cubic lattices a direction $[h\ k\ \ell]$ is perpendicular to the plane $(h\ k\ \ell)$. This is convenient in analyzing lattices with cubic unit cells, but it should be remembered that it is not necessarily true in the case of non-cubic systems.
2) In most cases, directions and planes are indexed in terms of conventional rather than primitive lattice vectors.

The angle between two crystallographic directions for a cubic lattice:

When two crystallographic directions denoted by [$h_1\ k_1\ \ell_1$] and [$h_2\ k_2\ \ell_2$] or a plane ($h_1\ k_1\ \ell_1$) and another plane ($h_2\ k_2\ \ell_2$), the angle between them can be obtained from the relation:

$$\cos\theta = \frac{h_1 h_2 + k_1 k_2 + \ell_1 \ell_2}{(h_1^2 + k_1^2 + \ell_1^2)^{1/2}(h_2^2 + k_2^2 + \ell_2^2)^{1/2}}$$ (prove it?)

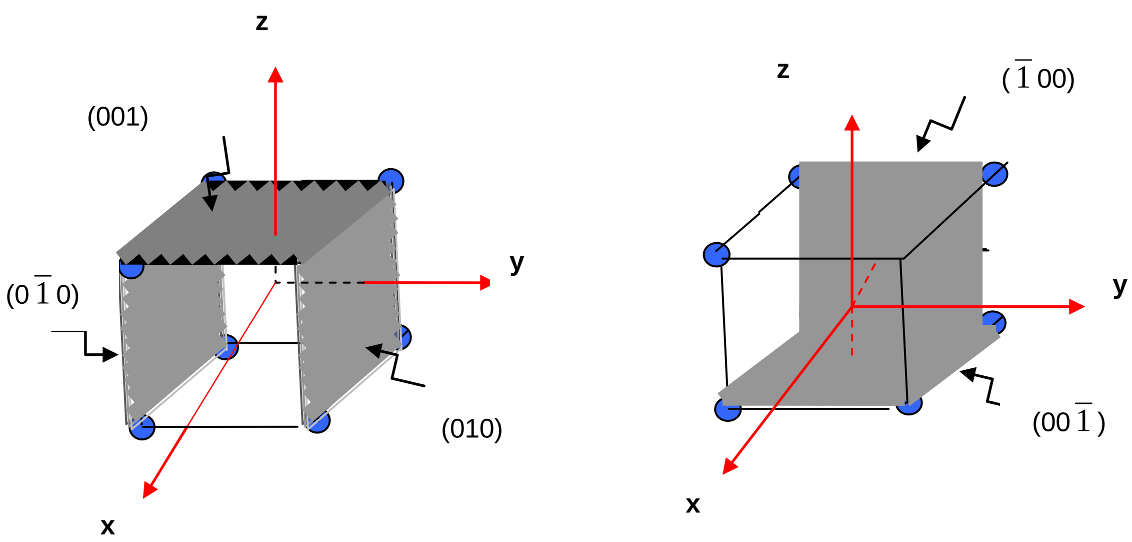


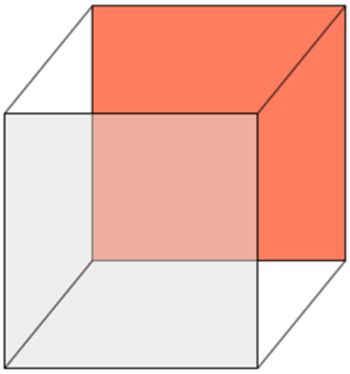
Figure 35: A family of lattice planes in a simple cubic lattice

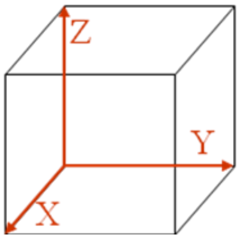
a) The faces with Miller indices (001), (010) and (0 $\bar{1}$ 0)

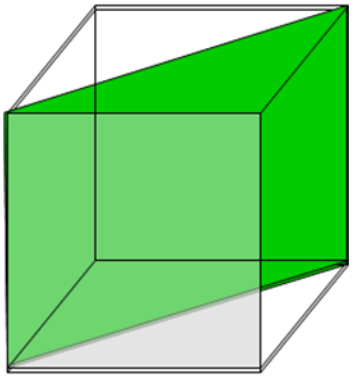
b) The faces with Miller indices ($\bar{1}$ 00) and (00 $\bar{1}$)

Important Note: Different crystal planes have different atomic structures which lead to different chemical and electrical properties of these surfaces.

Examples: Cubic lattice



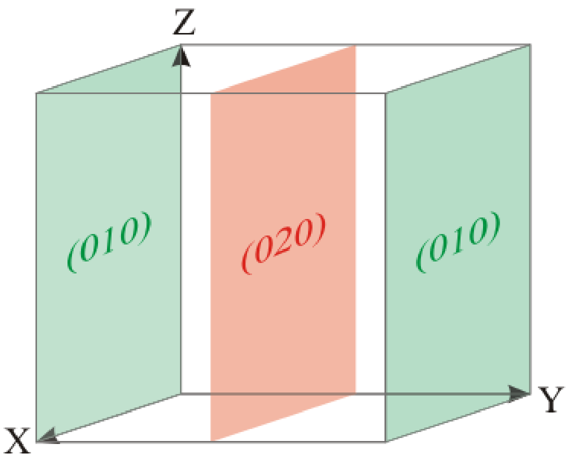




Intercepts → 1 ∞ ∞
Plane → (100)
Family → {100} → 6

Intercepts → 1 1 ∞
Plane → (110)
Family → {110} → 6

❑ What about planes passing through fractional lattice spacings?



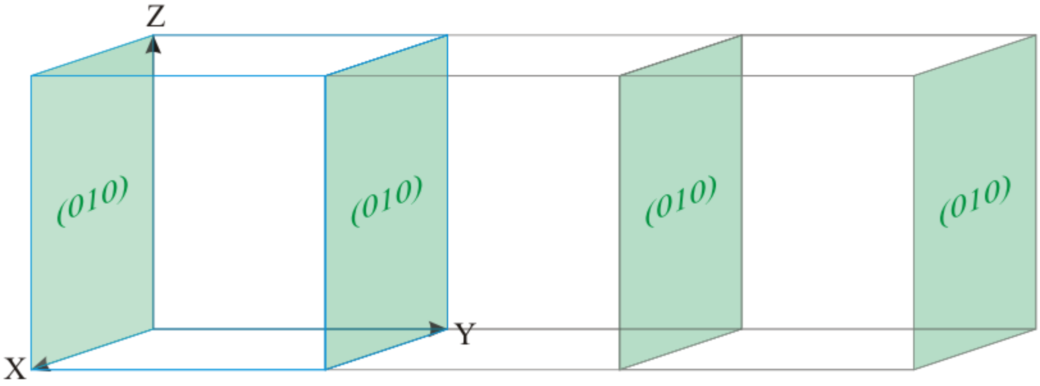
$$d_{010}^{\text{cubic lattice}} = \frac{a}{\sqrt{0^2 + 1^2 + 0^2}} = a$$

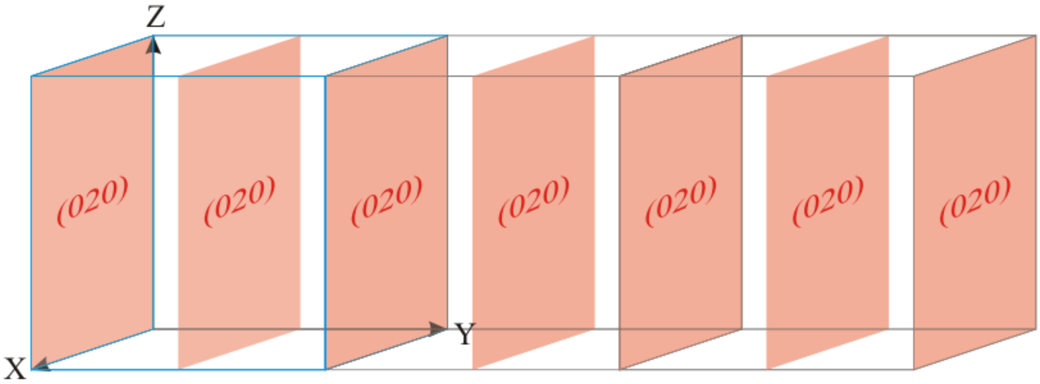
$$d_{020}^{\text{cubic lattice}} = \frac{a}{\sqrt{0^2 + 2^2 + 0^2}} = \frac{a}{2}$$

$$d_{020} = \frac{d_{010}}{2}$$

Intercepts → ∞ ½ ∞
Plane → (0 2 0)

Note: Actually (020) plane has half the spacing as (010) planes





Linear and Planar density

• Linear Density

– Number of atoms per length whose centers lie on the direction vector for a specific crystallographic direction.

$$Linear-Density=\frac{Number-of-atoms-centered-on-adirectional-vector}{Length-of-directional-vector}$$

• Planar Density

– Number of atoms per unit area that are centered on a particular crystallographic plane.

$$Planar-Density=\frac{Number-of-atoms-centered-on-aplane}{Area-of-the-plane}$$

Why do we care about linear and planar densities?

– Properties, in general, depend on linear and planar density.

• Examples:

1. Electrical conductivity depends on planar density

2. Speed of sound along directions

– Slip (deformation in metals) depends on linear and planar density

– Slip occurs on planes that have the greatest density of atoms in direction with highest density