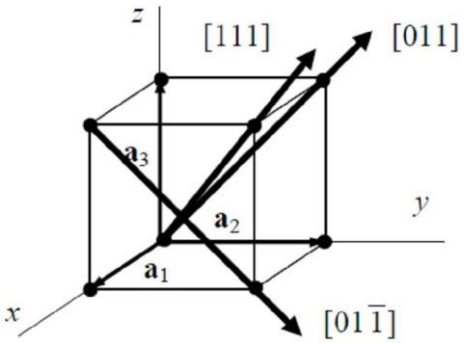
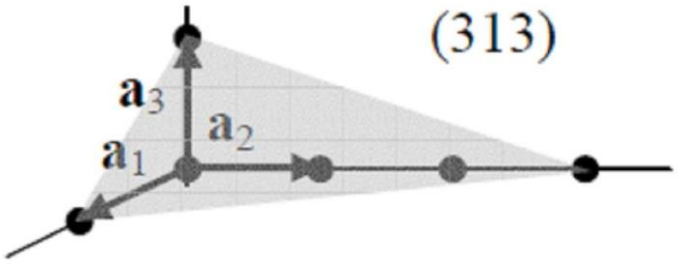
Crystal planes and Miller Indices

Index system for crystal directions and planes

Crystal directions: Any lattice vector can be written as that given by Eq.(1.2). The direction is then specified by the three integers $[n_1 n_2 n_3]$. If the numbers $n_1 n_2 n_3$ have a common factor, this factor is removed. For example, [111] is used rather than [222], or [100], rather than [400]. When we speak about directions, we mean a whole set of parallel lines, which are equivalent due to transnational symmetry. Opposite orientation is denoted by the negative sign over a number. For example:





Crystal planes: The orientation of a plane in a lattice is specified by *Miller indices*. They are defined as follows. We find intercept of the plane with the axes along the primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$. Let's these intercepts be *x*, *y*, and *z*, so that *x* is fractional multiple of a_1, *y* is a fractional multiple of a_2 and *z* is a fractional multiple of a_3. Therefore we can measure *x*, *y*, and *z* in units a_1, a_2 and a_3 respectively. We have then a triplet of integers (*x y z*). Then we invert it (1/*x* 1/*y* 1/*z*) and reduce this set to a similar one having the smallest integers by multiplying by a common factor. This set is called Miller indices of the plane (*hkl*). For example, if the plane intercepts *x*, *y*, and *z* in points 1, 3, and 1, the index of this plane will be (313).

The orientation of a crystal plane is determined by three points in the plane, provided they are not collinear. If each point lay on a different crystal axis, the plane could be specified by giving the co-ordinates of the points in terms of the lattice constants *a, b, c*. A notation conventionally used to describe lattice points (sites), directions and planes is known as Miller Indices.

A crystal lattice may be considered as an assembly of equidistant parallel planes passing through the lattice points and are called lattice planes. In order to specify the orientation one employs the so called Miller indices.

For simplicity, let us start with a two dimensional lattice and then generalized to three dimensional case.

The equation of plane in 2-D and 3D having the intercepts a, b and a, b, c respectively are

$$\frac{x}{a}+\frac{y}{b}=1 \qquad \textit{and} \qquad \frac{x}{a}+\frac{y}{b}+\frac{z}{c}=1$$

Crystal direction is the direction (line) of axes or line from the origin and denoted as [111], [100], [010] etc.

How to find Miller Indices:

To determine the indices for the plane p in Figure 2,

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

-Take reciprocal to this set.

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

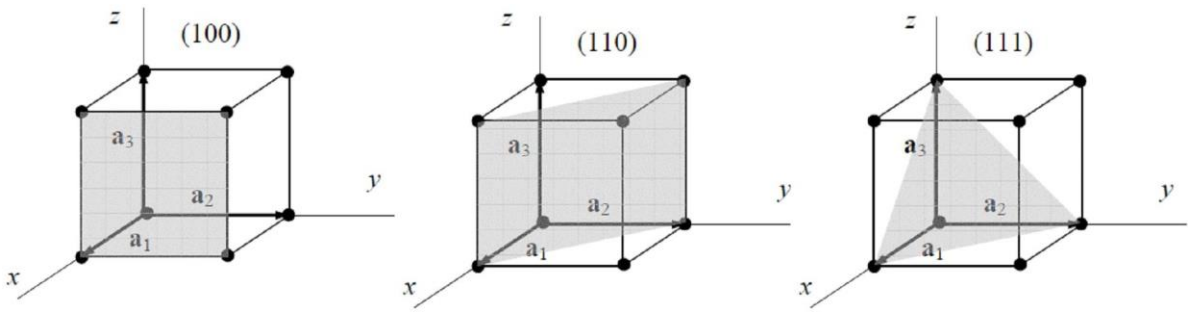
To determine the Miller indices:

(i) Find the intercepts on the axes along the basis vector $\vec{a},\vec{b},\vec{c}$ in terms of the lattice constants *a,b* and *c*. The axes may be those of a primitive or nonprimitive cell.
Let these intercepts be x, y, z. We form the fractional triplet $\left(\frac{x}{a},\frac{y}{b},\frac{z}{c}\right)$.

(ii) Take the reciprocals of these numbers.
(iii) Reduce the numbers to three smallest integers by multiplying the numbers with the same integral multipliers.

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

The Miller indices specify not just one plane but an infinite set of equivalent planes. Note that for cubic crystals the direction [hkl] is perpendicular to a plane (hkl) having the same indices, but this is not generally true for other crystal systems. Examples of the planes in a cubic system:



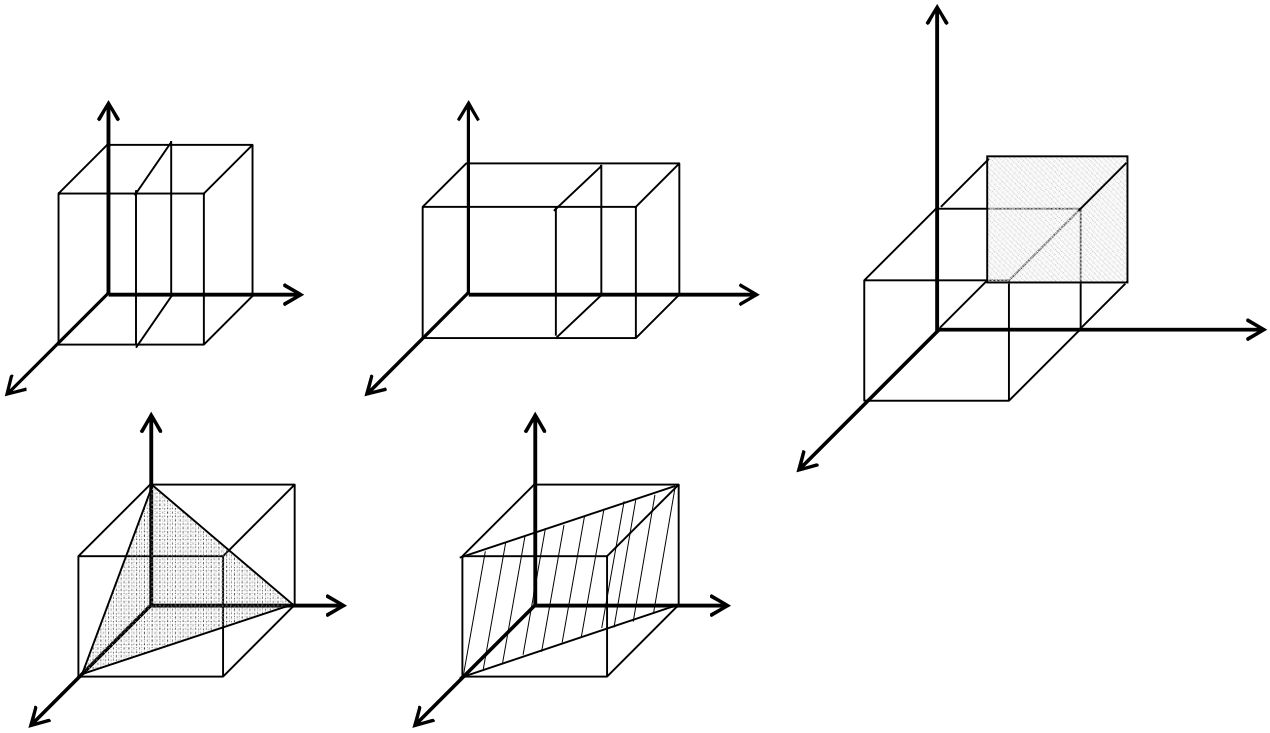
Example: Let the intercepts are x = 2a, y = 3/2b, z – c.

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

Then invert it $\left(\frac{1}{2},\frac{2y}{3},1\right)$

and finally multiply by a common (factor) denomenator. Which is 6, to obtain the miller indices (3 4 6).

Exercise: x = 2a, y = 3b, z = 6c $\Rightarrow$ (321).

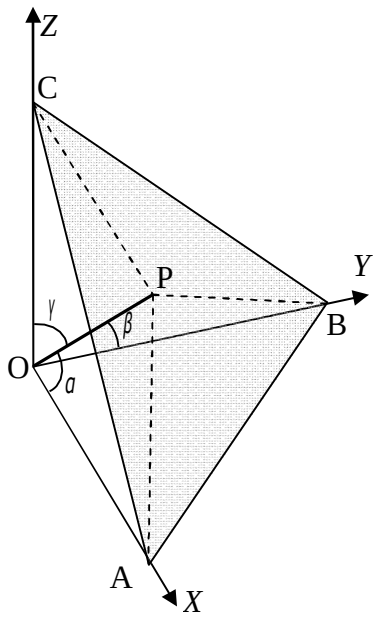


The indices of some important planes in a cubic crystal

Relation between interplanar spacing and Miller indices:

Let us consider three mutually perpendicular coordinate axis, OX, OY, and Oz and assume that a plane (hkl) parallel to the plane passing through the origin makes intercepts a/h, b/k and c/l on the three axes at A. B and C respectively as shown in figure.

Let OP = d_{hkl}, the interplaner spacing be normal to the plane drawn from the origin and makes angle α, β, and γ with the three axes respectively.



Therefore, $OA = \frac{a}{h}, OB = \frac{b}{k}, OC = \frac{c}{l}$

From ΔOPA we get, $\cos\alpha = \frac{OP}{OA} = \frac{d_{hkl}}{a/h}$

Similarly, from ΔOPB we get $\cos\beta = \frac{OP}{OB} = \frac{d_{hkl}}{b/k}$

and from ΔOPC we get $\cos\gamma = \frac{OP}{OC} = \frac{d_{hkl}}{c/l}$

But, for a rectangular coordinate system, using directional cosine we have

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1 \qquad (1)$$

Substituting the values of cosα, cosβ and cosγ in Eq.1 we get,

$$d_{hkl}^2\left(\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right)=1$$

$$\therefore d_{hkl} = \frac{1}{\sqrt{h^2/a^2 + k^2/b^2 + l^2/c^2}} \qquad (2)$$

This is the general formula and is applicable to the primitive lattice of orthorhombic, tetragonal and cubic systems.

i) Orthorhombic system: $a \neq b \neq c$

$$d_{hkl}\frac{1}{\left(\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right)}$$

ii) Tetragonal system: $a = b \neq c$

$$\therefore \quad d_{hkl} = \frac{1}{\sqrt{\left(\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}\right)}}$$

 # a = b = 2.42Å and c = 1.74Å
then d_{101} = 1.41Å

ii) Cubic system: $a = b = c$

$$\therefore \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$a = 2$Å, $d_{111} = 2\sqrt{3}$Å

$a = 421$Å , $d_{321} = 1.01$ Å

$d_{100} = a$, $d_{110} = \frac{a}{\sqrt{2}}$ Å $d_{111} = \frac{a}{\sqrt{3}}$ Å

$\therefore d_{100} : d_{110} : d_{111} = 1: \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}}$

For bcc $\Rightarrow$ $d_{100} = \frac{1}{2}(d_{100,sc}) = \frac{a}{2}$

$d_{110} = (d_{110,sc}) = \frac{a}{\sqrt{2}}$

$d_{111} = \frac{1}{2}(d_{111,sc}) = \frac{a}{2\sqrt{3}}$

and $d_{100} : d_{110} : d_{111} = 1:\sqrt{2}:\frac{1}{\sqrt{3}}$

For bcc $\Rightarrow$ $d_{100} = \frac{1}{2}(d_{100,sc}) = \frac{a}{2}$

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and $d_{100} : d_{110} : d_{111} = 1:\frac{1}{\sqrt{2}}:\frac{2}{\sqrt{3}}$

Ex: Determine the Miller Indices of a plane which is parallel to x-axis and cuts intercepts of 2 and $\frac{1}{2}$, respectively along y and z axes.

Solution:

i) Intercepts	∞	2b	$\frac{1}{2}c$
ii) Division by unit translation	$\frac{\infty}{a} = \infty$	$\frac{2b}{b} = 2$	$\frac{3c}{2c} = \frac{1}{2}$
iii) Reciprocals	$\frac{1}{\infty}$	$\frac{1}{2}$	2
iv) After clearing fraction	0	1	4

Therefore the required Miller indices of the plane (014)

Ex: Determine the M. I. of a plane theat makes intercepts of 2Å, 3 Å, 4 Å on the co-ordinate axes of an orthorhombic crystal with a:b:c = 4:3:2

Solution:

Here the unit translations are a = 4, b = 3 and c = 2 following the same procedure

i) Intercepts	2	3	4
ii) Division by unit translation	$\frac{2}{4}=\frac{1}{2}$	$\frac{3}{3}=1$	$\frac{4}{2}=2$
iii) Reciprocals	2	1	$\frac{1}{2}$
iv) After clearing fraction	4	2	1

Therefore the Miller indices of the plan is (421)