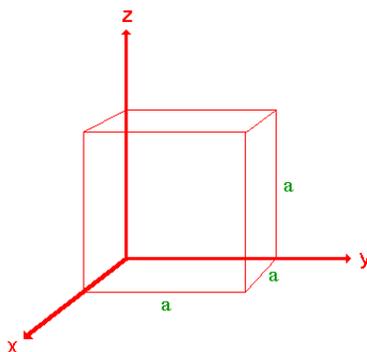


31.2: The Orientation of a Lattice Plane is Described by its Miller Indices

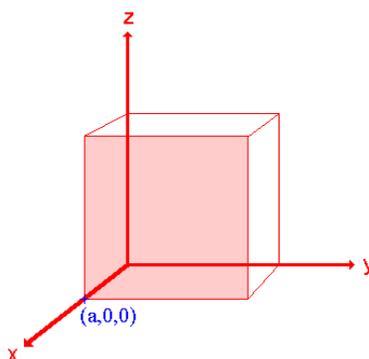
The orientation of a surface or a crystal plane may be defined by considering how the plane (or indeed any parallel plane) intersects the main crystallographic axes of the solid. The application of a set of rules leads to the assignment of the Miller Indices (hkl), which are a set of numbers which quantify the intercepts and thus may be used to uniquely identify the plane or surface.

Assigning Miller Indices for a cubic crystal system

The following treatment of the procedure used to assign the Miller Indices is a simplified one (it may be best if you simply regard it as a "recipe") and only a **cubic** crystal system (one having a cubic unit cell with dimensions $a \times a \times a$) will be considered.



The procedure is most easily illustrated using an example so we will first consider the following surface/plane:



Step 1: Identify the intercepts on the x -, y - and z - axes.

In this case the intercept on the x -axis is at $x = a$ (at the point $(a,0,0)$), but the surface is parallel to the y - and z -axes - strictly therefore there is no intercept on these two axes but we shall consider the intercept to be at infinity (∞) for the special case where the plane is parallel to an axis. The intercepts on the x -, y - and z -axes are thus

Intercepts: a, ∞, ∞

Step 2: Specify the intercepts in fractional co-ordinates

Co-ordinates are converted to fractional co-ordinates by dividing by the respective cell-dimension - for example, a point (x,y,z) in a unit cell of dimensions $a \times b \times c$ has fractional co-ordinates of $(x/a, y/b, z/c)$. In the case of a cubic unit cell each co-ordinate will simply be divided by the cubic cell constant, a . This gives

Fractional Intercepts: $a/a, \infty/a, \infty/a$ i.e. $1, \infty, \infty$

Step 3: Take the reciprocals of the fractional intercepts

This final manipulation generates the Miller Indices which (by convention) should then be specified without being separated by any commas or other symbols. The Miller Indices are also enclosed within standard brackets (...) when one is specifying a unique surface such as that being considered here.

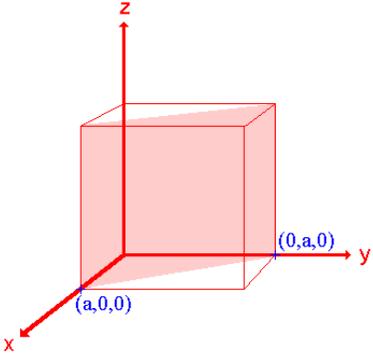
The reciprocals of 1 and ∞ are 1 and 0 respectively, thus yielding

Miller Indices: **(100)**

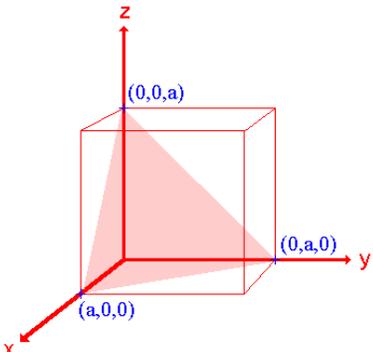
So the surface/plane illustrated is the (100) plane of the cubic crystal.

Other Examples

1. The (110) surface

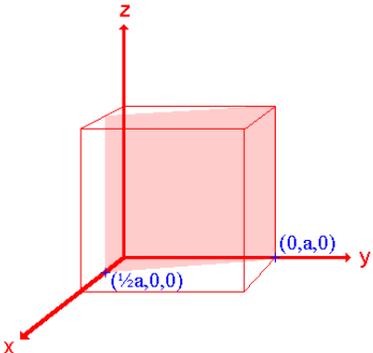
	<p><i>Assignment</i> Intercepts: a, a, ∞ Fractional intercepts: $1, 1, \infty$ Miller Indices: (110)</p>
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2. The (111) surface

	<p><i>Assignment</i> Intercepts: a, a, a Fractional intercepts: $1, 1, 1$ Miller Indices: (111)</p>
--	---

The (100), (110) and (111) surfaces considered above are the so-called **low index surfaces** of a cubic crystal system (the "low" refers to the Miller indices being small numbers - 0 or 1 in this case). These surfaces have a particular importance but there are an infinite number of other planes that may be defined using Miller index notation. We shall just look at one more ...

3. The (210) surface

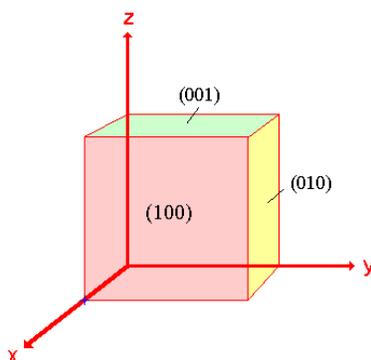
	<p><i>Assignment</i> Intercepts: $\frac{1}{2} a, a, \infty$ Fractional intercepts: $\frac{1}{2}, 1, \infty$ Miller Indices: (210)</p>
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Further notes:

- i. in some instances the Miller indices are best multiplied or divided through by a common number in order to simplify them by, for example, removing a common factor. This operation of multiplication simply generates a parallel plane which is at a different distance from the origin of the particular unit cell being considered. e.g. (200) is transformed to (100) by dividing through by 2 .
- ii. if any of the intercepts are at negative values on the axes then the negative sign will carry through into the Miller indices; in such cases the negative sign is actually denoted by overstriking the relevant number. e.g. (00 -1) is instead denoted by (00 $\bar{1}$).
- iii. in the *hcp* crystal system there are four principal axes; this leads to four Miller Indices e.g. you may see articles referring to an *hcp* (0001) surface. It is worth noting, however, that the intercepts on the first three axes are necessarily related and not completely independent; consequently the values of the first three Miller indices are also linked by a simple mathematical relationship.

What are symmetry-equivalent surfaces?

In the following diagram the three highlighted surfaces are related by the symmetry elements of the cubic crystal - they are entirely equivalent.



In fact, there are a total of 6 faces related by the symmetry elements and equivalent to the (100) surface - any surface belonging to this set of symmetry-related surfaces may be denoted by the more general notation {100} where the Miller indices of one of the surfaces is instead enclosed in curly-brackets.

Final important note: in the cubic system the (*hkl*) plane and the vector [*hkl*], defined in the normal fashion with respect to the origin, are normal to one another **but** this characteristic is unique to the cubic crystal system and does **not** apply to crystal systems of lower symmetry.

The perpendicular distance between planes

The symbol *d* is used to designate the perpendicular spacing between adjacent planes. Table 31.2.1 shows the equations for calculating the value of *d* for four of the seven crystal systems.

Table 31.2.1: Equations for calculating the spacing between adjacent planes, *d*

System	Equation for <i>d</i>
cubic	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$
tetragonal	$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$
hexagonal	$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$
orthorhombic	$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$

✓ Example 31.2.1

If a tetragonal unit cell has dimensions $a = b = 501$ pm and $c = 451$ pm, calculate the perpendicular distance between the 111 planes.

Solution

For a tetragonal unit cell

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}.$$

Thus,

$$\begin{aligned}\frac{1}{d^2} &= \frac{1 + 1}{(501 \text{ pm})^2} + \frac{1}{(451 \text{ pm})^2} \\ &= 1.29 \times 10^{-5} \text{ pm}^{-2}.\end{aligned}$$

Then $d = 279$ pm

Contributors and Attributions

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