Al-Mustaqbal University College

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Mathematical Notation of Crystal Planes

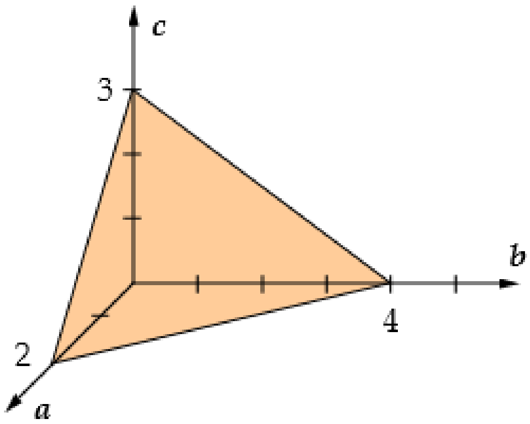
To define a particular plane of atoms in a crystal we use a mathematical notation known as Miller indices

(i)Find the intercepts of the plane with the 3 crystal directions or axes in terms of primitive vectors a , b , c

(ii)Take the reciprocals

(iii)Multiply the resulting 3 numbers by the smallest number that makes the result equal to 3 integers h, k, l

The plane is then defined by the notation (h k l)



Thus, in the above example:

intercepts= 2 , 4 , 3

reciprocals= 1/2 , 1/4 , 1/3

x 12 = 6 , 3 , 4

and so the plane is (6 3 4)

Note that negative index is written as h(-)

In a crystal with true cubic symmetry the choice of which of the three axes to label the x-axis, and which the y and the z, is entirely arbitrary. Thus the (100) plane is physically equivalent to the mathematically distinct (010) and (001) planes.

This leads to the grouping of various numbers of planes into sets, or families

Crystallography: Miller Indices

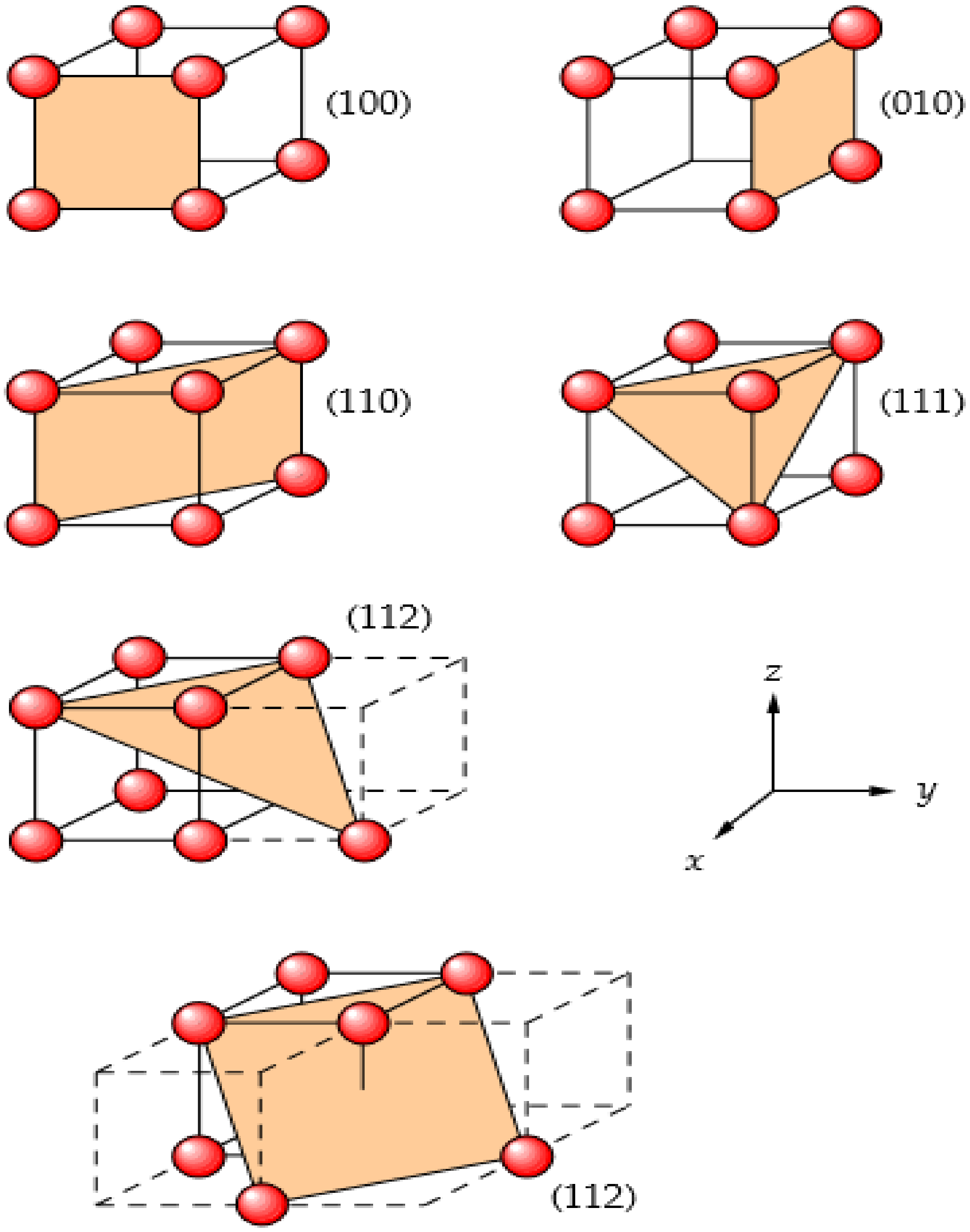
Miller Indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals of the fractional intercepts which the plane makes with the crystallographic axes.

The sets of planes are denoted { h k l.{

For directions in a crystal, take components (or projections) on axes a , b and c. For example, the direction whose components are 2a, 3b, 2c is denoted [2 3 2]. Directions also occur in sets, and are denoted <h k l>

For a cubic lattice, the direction [h k l] is perpendicular to the plane (h k l). In non-cubic systems, this is not necessarily true!

The Miller indices for hexagonal crystals are a special case (not considered here).



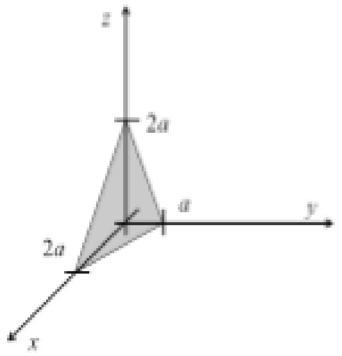
Miller indices

Solved problems

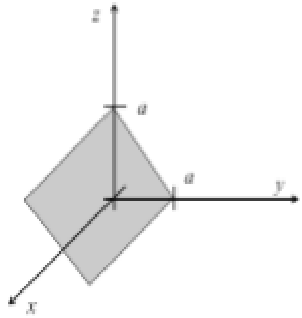
Find the intercepts with the x, y, z, axes: 2, 1, 2 (in units of *a*)
invert the intercepts: 1/2, 1, 1/2
multiply by 2 to produce integers: 1, 2, 1
put in parentheses to denote a plane (1, 2, 1)
direction normal to this plane is [1, 2, 1]

(1 2 1) plane
[1 2 1] normal to the plane

a)



b)



Find the intercepts with the x, y, z, axes: infinity, 1, 1 (in units of *a*)
invert the intercepts: 0, 1, 1
multiply by 1 to produce integers: 0, 1, 1
put in parentheses to denote a plane (0, 1, 1)
direction normal to this plane is [0, 1, 1]

(0 1 1) plane
[0 1 1] normal to the plane