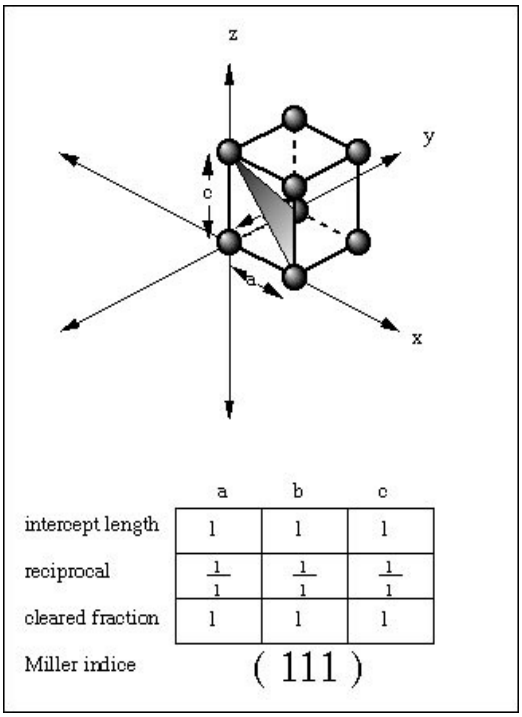
Crystallography: Miller Indices

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 method by which indices are determined is best shown by example. Recall, that there are three axes in crystallographic systems (*except sometimes in the hexagonal system adopts a convention where there are four axes). Miller indices are represented by a set of 3 integer numbers.

Example of the (111) plane:



	a	b	c
intercept length	1	1	1
reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{1}$
cleared fraction	1	1	1
Miller indice	(111)		

If you want to describe the orientation of a crystal face or a plane of atoms within a crystal lattice, then there are series of steps that will lead you to its notation using Miller indices.

1. The first thing that must be acertained are the fractional intercepts that the plane/face makes with the crystallographic axes. In other words, how far along the unit cell lengths does the plane intersect the axis. In the figure above, the plane intercepts each axis at exact one unit length.

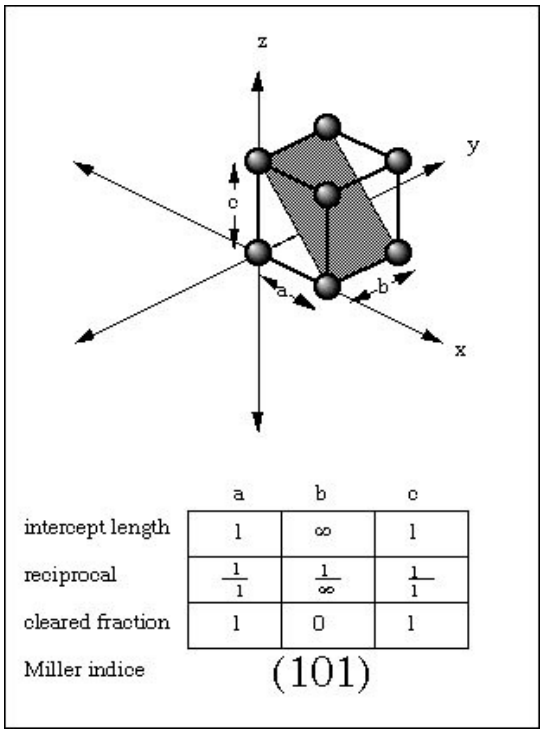
2. Step two involves taking the reciprocal of the fractional intercept of each unit length for each axis. In the figure above, the values are all 1/1.

3. Finally the fractions are cleared (*i.e.,* make 1 as the common denominator).

4. These integer numbers are then parenthetically enclosed and designate that specific crystallographic plane within the lattice. Since the unit cell repeats in space, the notation actually represents a family of planes, all with the same orientation. In the figure above, the Miller indice for the plane is (111)

Why go through all of these operations?

Example of the (101) plane:



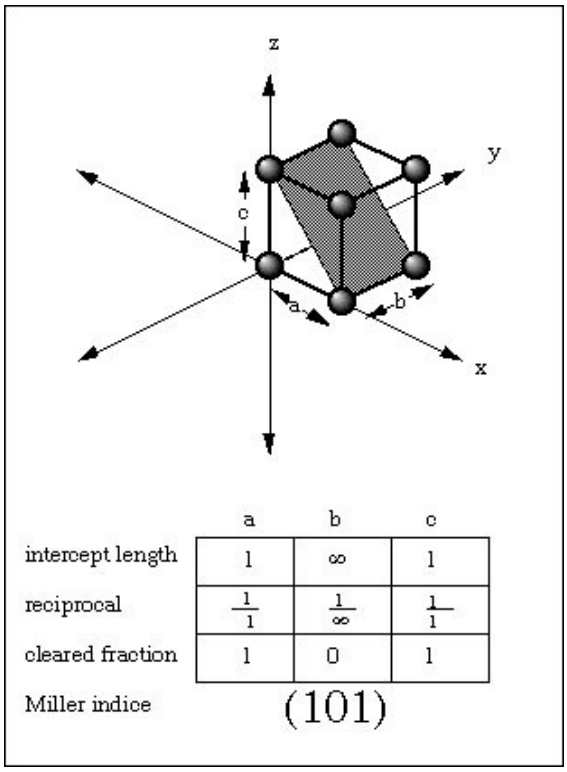
	a	b	c
intercept length	1	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	1

Miller indice (101)

This becomes immediately apparent when we consider the case of the (101). In this case the plane intercepts the *a* axis at one unit length and also the *c* axis at one unit length. The plane however, never intersects the *b* axis. In other words, it can be said that the intercept to the *b* axis is infinity. The intercepts are then designated as 1,infinity,1. The reciprocals are then 1/1, 1/infinity, 1/1. Knowing 1/infinity = 0 then the indices become (101).

Look at worked examples for the (010) and (201) and (bar-201).

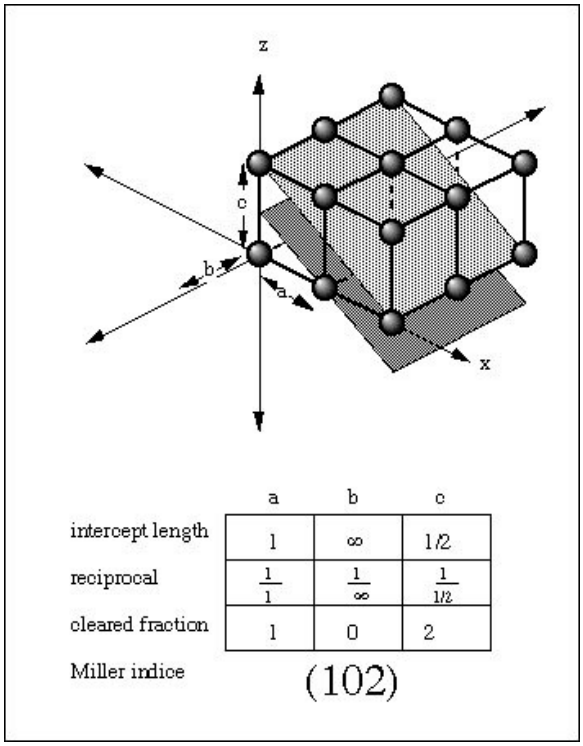
Example of the (101) plane:



	a	b	c
intercept length	1	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	1

Miller indice (101)

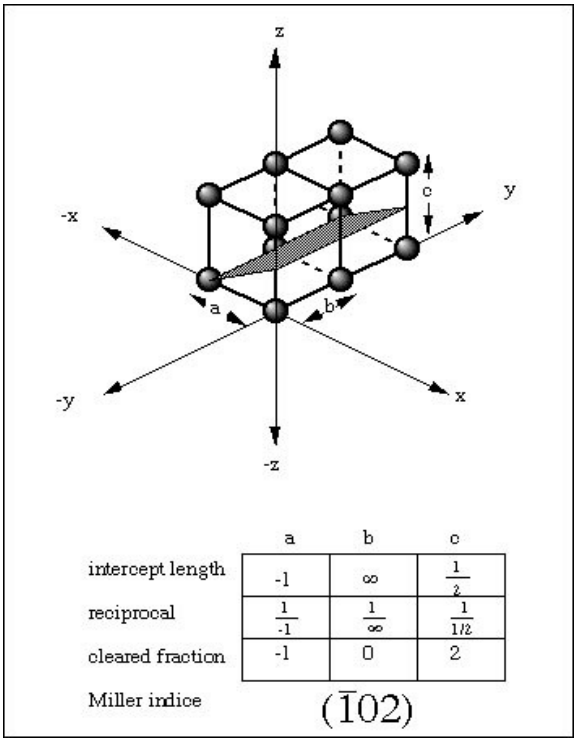
Example of the (102) plane:



	a	b	c
intercept length	1	∞	1/2
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1/2}$
cleared fraction	1	0	2

Miller indice (102)

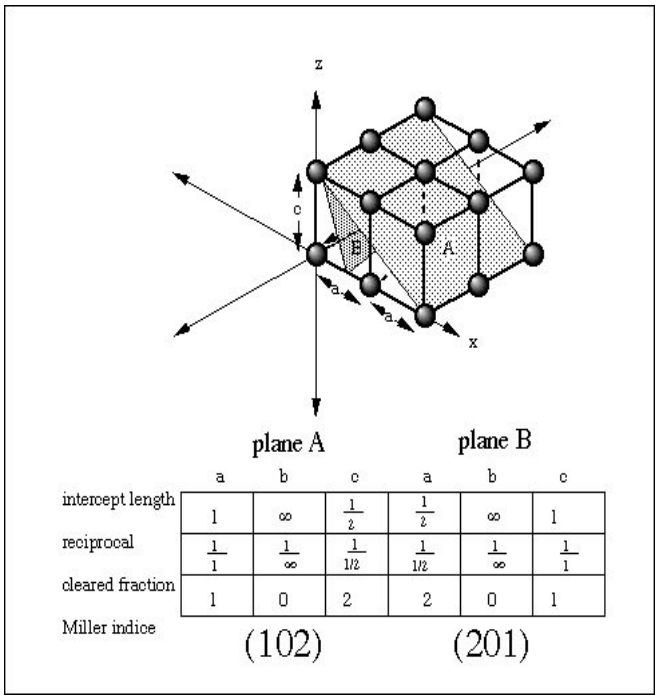
Example of the (-102) plane:



	a	b	c
intercept length	-1	∞	$\frac{1}{2}$
reciprocal	$\frac{1}{-1}$	$\frac{1}{\infty}$	$\frac{1}{1/2}$
cleared fraction	-1	0	2

Miller indice $(\bar{1}02)$

Examples of the (102) and (201) planes:



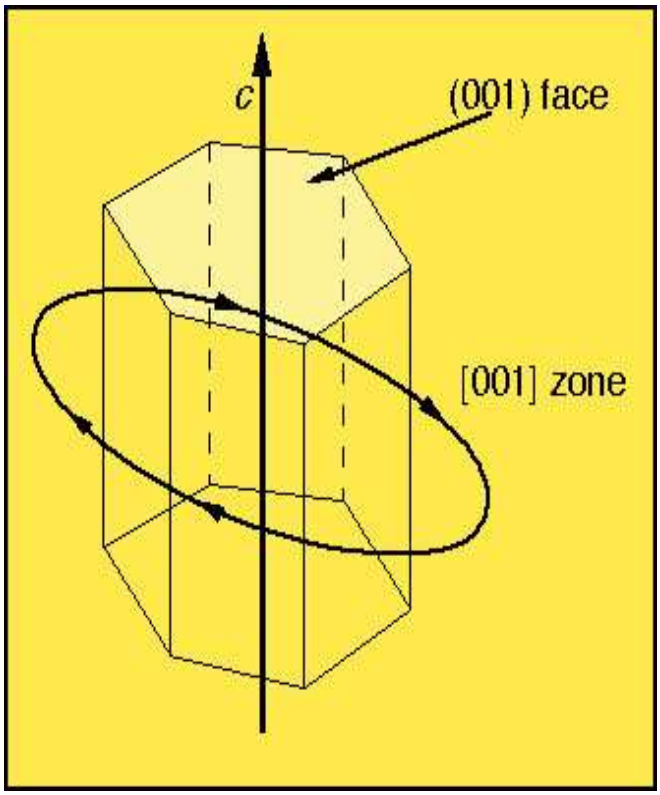
	plane A			plane B		
	a	b	c	a	b	c
intercept length	1	∞	$\frac{1}{2}$	$\frac{1}{2}$	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1/2}$	$\frac{1}{1/2}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	2	2	0	1
Miller indice	(102)			(201)		

Closures for crystallographics indices

(*hkl*) = parenthesis designate a **crystal face** or a **family of planes** throughout a crystal lattice.

Directions are presented by the three integers *uvw*. [*uvw*] = square brackets designate a direction in the lattice from the origin to a point. Used to collectively, they include all the faces of a crystals whose intersects (i.e., edges) parallel each other. These are referred to as crystallographic **zones** and they represent a direction in the crystal lattice.

Zone axis concept



Only in the isometric systems are the same integers used to relater the perpendicular to a family of planes (*hkl*) to the directions [*uvw*].

{*hkl*} = "squiggly" brackets designate a set of face planes that are equivalent by the symmetry of the crystal. The set of face planes results in the **crystal form**. {100} in the isometric class includes (100), (010), (001), (-100), (0-10) and (00-1), while for the triclinic {100} only the (100) is included.

d-spacing is defined as the distance between adjacent planes. When X-rays diffract due to interference amongst a family of similar atomic planes, then each diffraction plane may be reference by its indice d_{hkl}

Fractional coordinates also come sets of three. *x, y, z* denote the locations of atoms within the unit cell. These are real numbers.