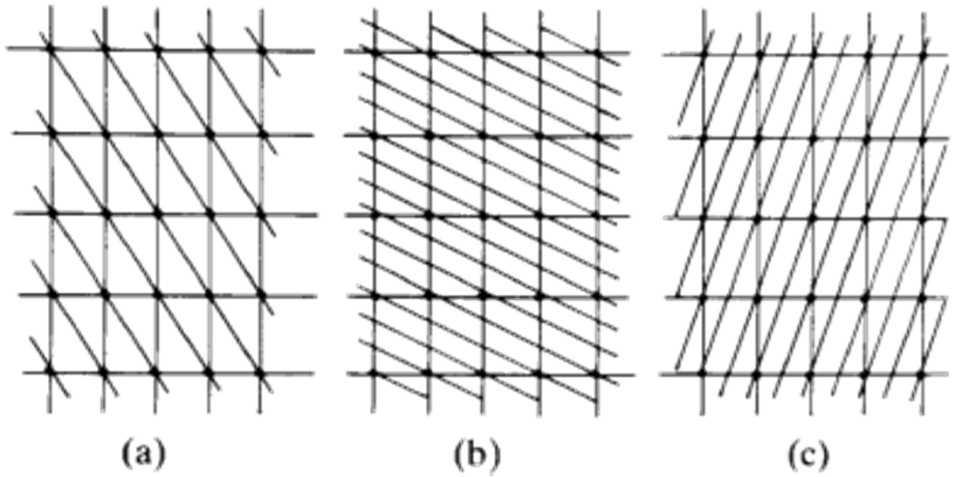
Planes in Lattices and Miller Indices

An essential concept required to understand the diffraction of X-rays by crystal lattices (at least using the Bragg treatment) is the presence of planes and families of planes in the crystal lattice. Each plane is constructed by connecting at least three different lattice points together and, because of the periodicity of the lattice, there will a family (series) of planes parallel passing through every lattice point. A convenient way to describe the orientation of any of these families of plane is with a Miller Index of the form (hkl) in which the plane makes the intercepts with a unit cell of *a*/h, *b*/k and *c*/l. Thus the Miller index indicates the reciprocal of the intercepts.

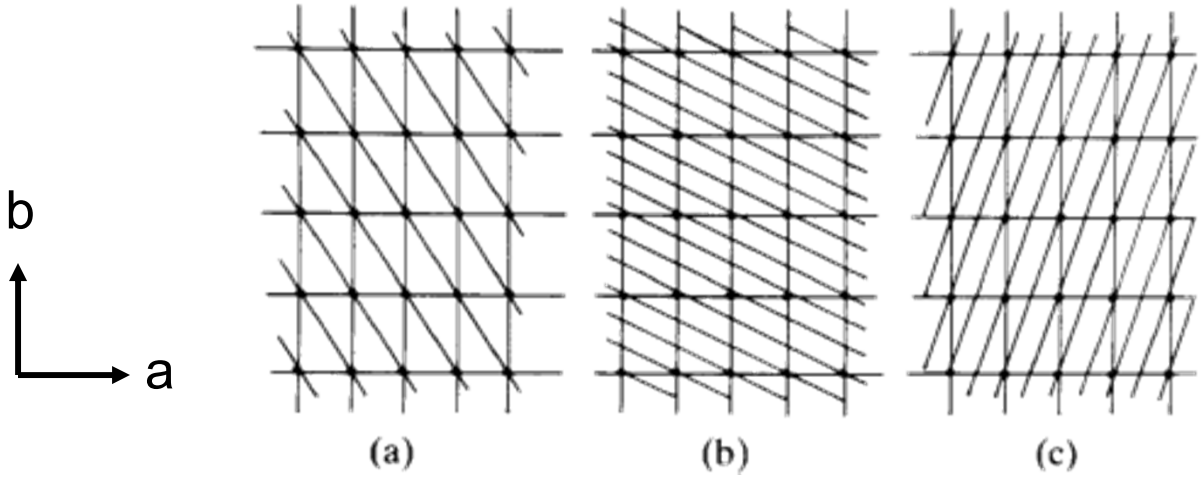


2-D planes

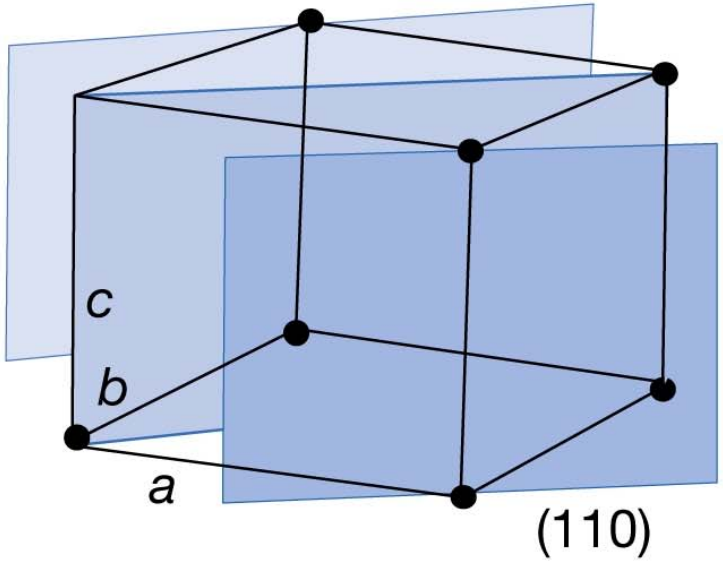
Note: If a plane does not intersect an axis, the intercept would be ∞ and the reciprocal is 0.

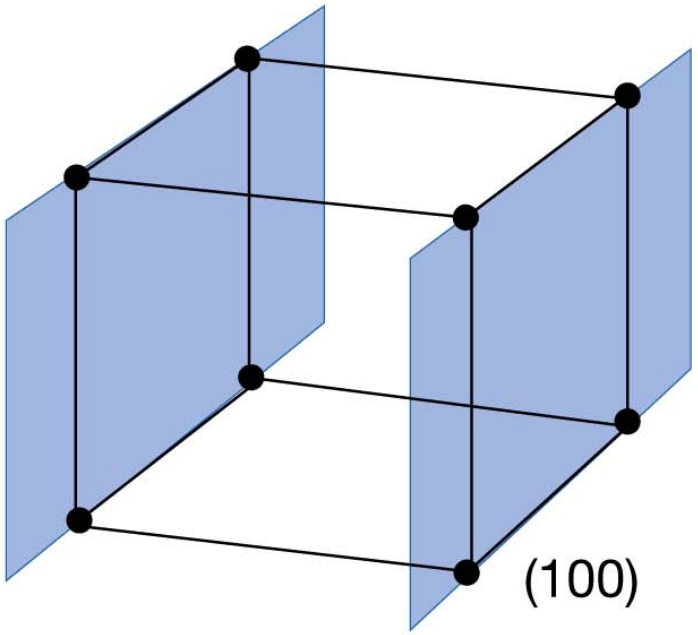
Note: If the reciprocal of the intercept is a fraction, multiply each of the h, k and l values by the lowest common denominator to so that they become integers!

Planes in Lattices and Miller Indices

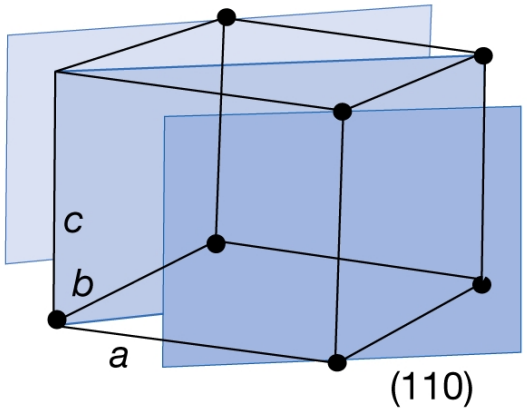


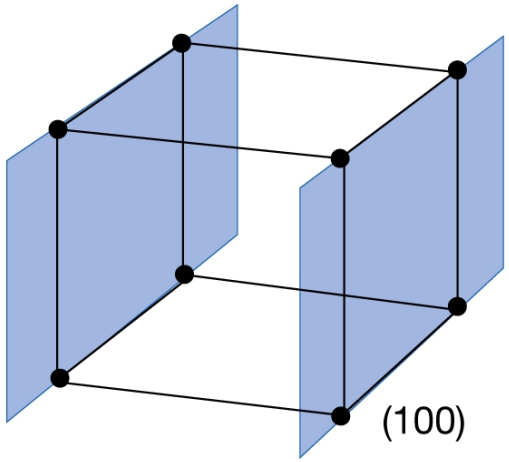
(110) planes **(130) planes** **(-210) planes**

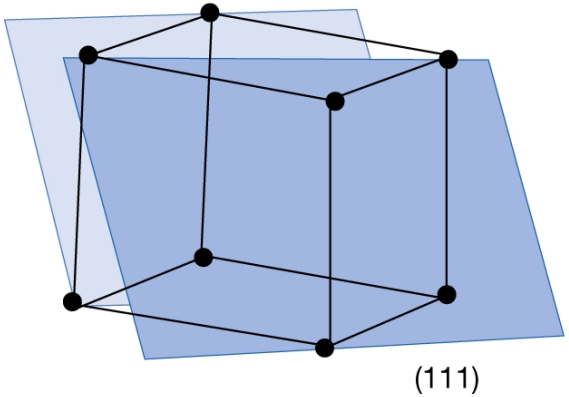


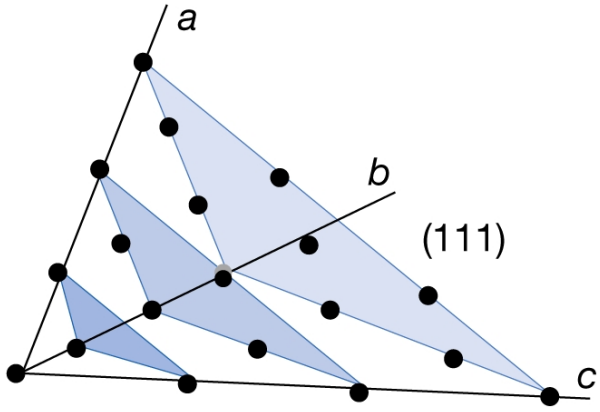


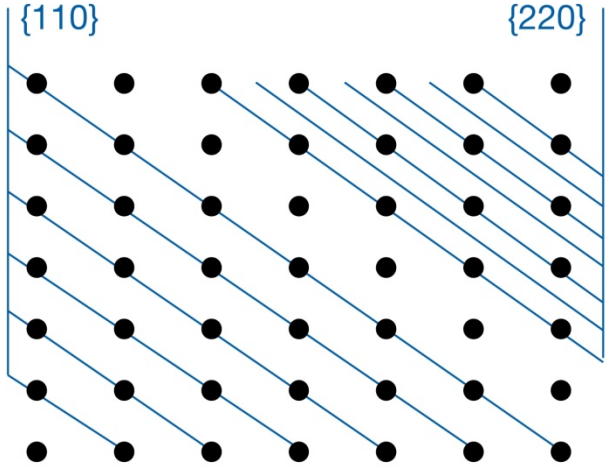
Planes in Lattices and Miller Indices





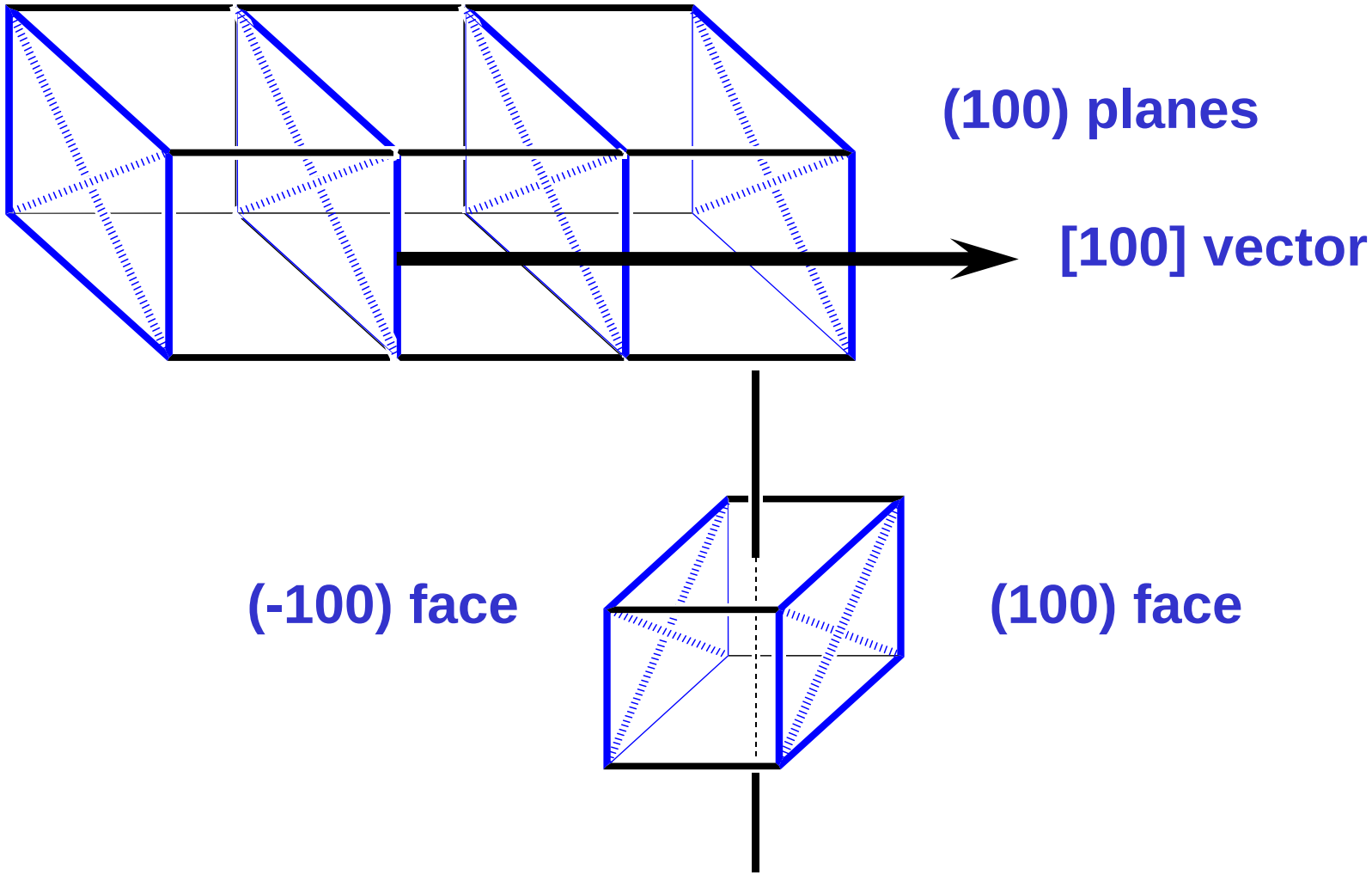






Planes in Lattices and Miller Indices

The orientation of planes is best represented by a vector normal to the plane. The direction of a set of planes is indicated by a vector denoted by square brackets containing the Miller indices of the set of planes. Miller indices are also used to describe crystal faces.



Planes in Lattices and Miller Indices

A summary of notation that you will see in regard to planes and/or crystal faces:

(hkl) denotes a set of planes

[hkl] designates a vector (the direction of the planes)

{hkl} set of faces made equivalent by the symmetry of the system, thus:

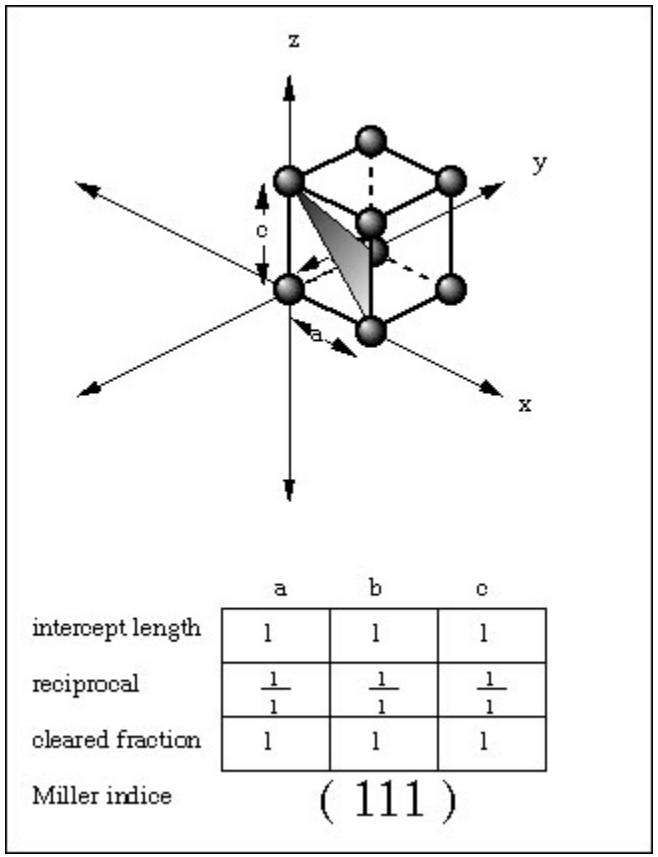
{100} for point group 1 this refers only to the (100) face

{100} for point group -1 this refers to (100) and (-100) faces

for mmm {111} implies
(111),(11-1),(1-11),(11-1),(-1-11),(-11-1),(1-1-1),(-1-1-1)

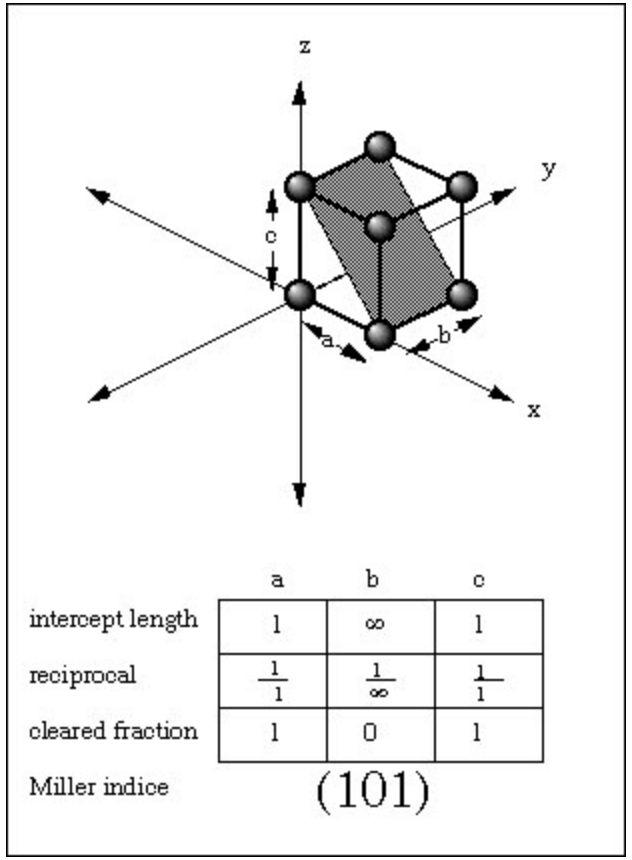
Planes in Lattices and Miller Indices

Pictures from: http://www.gly.uga.edu/schroeder/geol6550/millerindices.html



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

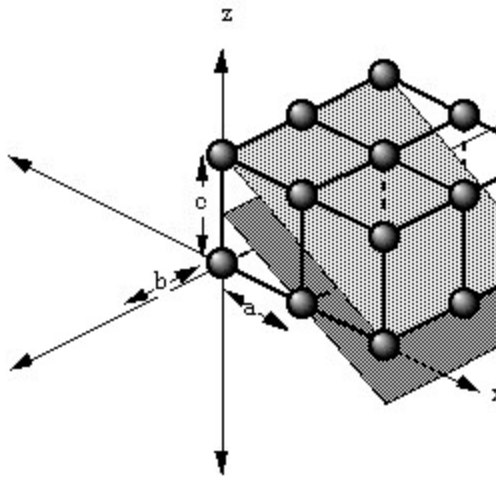
Miller indice (111)



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

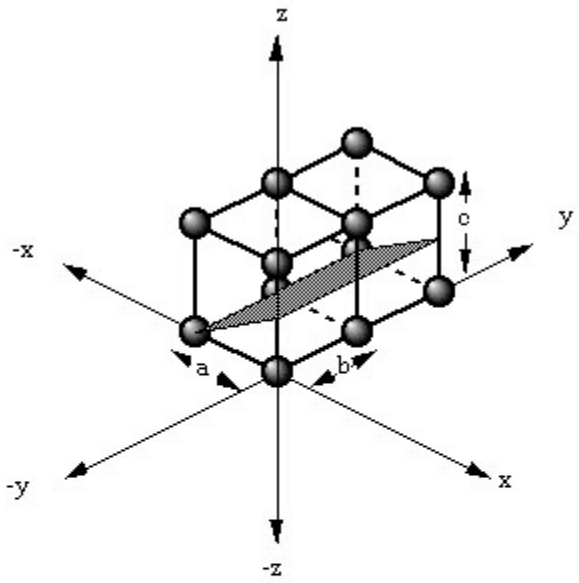
Miller indice (101)

Planes in Lattices and Miller Indices



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

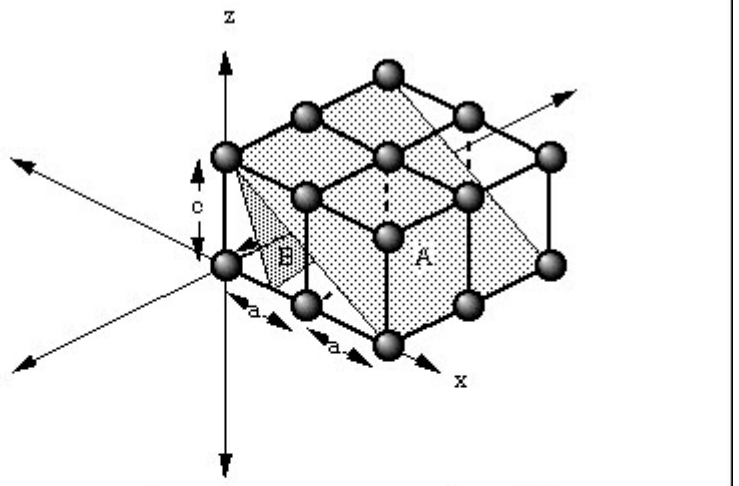
Miller indice (102)



	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 $(\bar{1}02)$

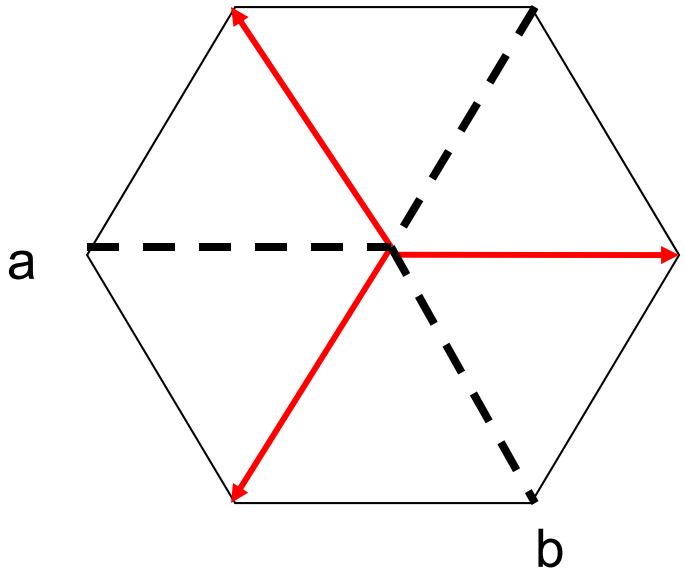
Planes in Lattices and Miller Indices

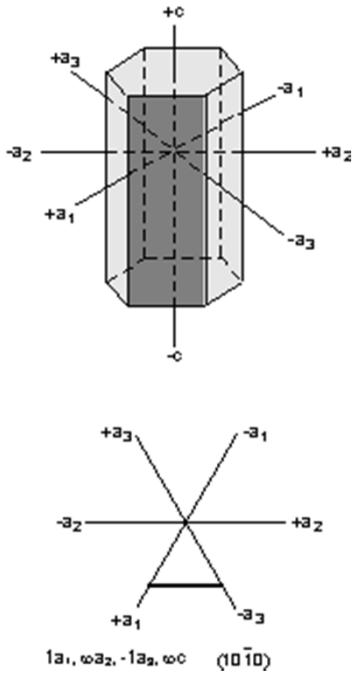


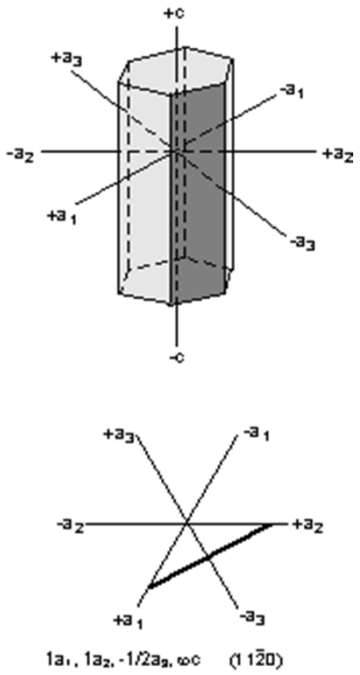
	plane A			plane B		
	a	b	c	a	b	c
intercept length	1	∞	$\frac{1}{2}$	$\frac{1}{2}$	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1/2}$	$\frac{1}{1/2}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	2	2	0	1
Miller indice	(102)			(201)		

Planes in Lattices and Miller Indices

Note that for hexagonal systems, the Miller-Bravais indices are often used instead. These have the form (hkil), where h, k, and i are the reciprocals of the plane intercepts for the three co-planar vectors indicated below and l is the reciprocal for the intercept in the c direction. Note that h, k and i are not linearly independent so the rule **h+k+i = 0** must always be obeyed.







Planes in Lattices and Bragg's Law

We are interested in the planes in a crystal lattice in the context of X-ray diffraction because of Bragg's Law:

$$n\lambda = 2\,d\,\sin(\theta)$$

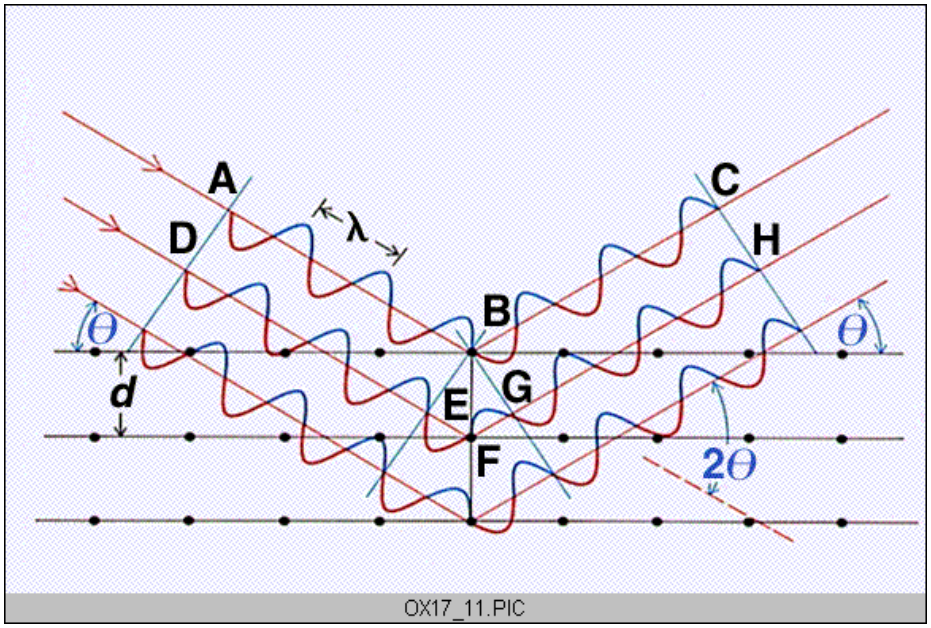
Where:

n is an integer

λ is the wavelength of the X-rays

d is distance between adjacent *planes* in the lattice

θ is the incident angle of the X-ray beam



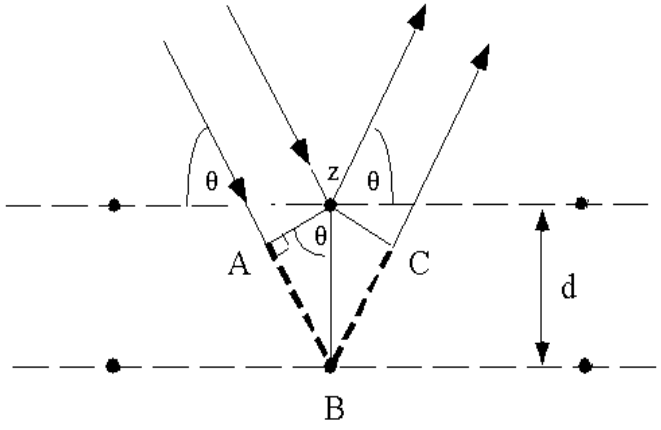
Bragg's law tells us the conditions that must be met for the reflected X-ray waves to be in phase with each other (constructive interference). If these conditions are not met, destructive interference reduces the reflected intensity to zero!

W.H.Bragg and son W.L.Bragg were awarded the Nobel prize in 1915.

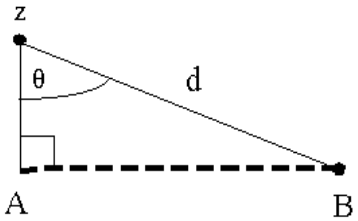
Simple derivation of Bragg's Law

Bragg's Law can be derived using simple geometry by considering the distances traveled by two parallel X-rays reflecting from adjacent planes. The X-ray hitting the lower plane must travel the extra distance AB and BC. To remain in phase with the first X-ray, this distance must be a multiple of the wavelength thus:

$n\lambda = AB+BC = 2AB$
(since the two triangles are identical)



The distance AB can be expressed in terms of the interplanar spacing (d) and incident angle (θ) because d is the hypotenuse of right triangle *zAB* shown at right.
Remember sin = opposite/hypotenuse



$\sin(\theta) = AB/d$ thus $AB = d \sin(\theta)$

Therefore:

$$n\lambda = 2\, d \sin(\theta)$$

Note: d and $\sin(\theta)$ are inversely proportional (reciprocal). This means that smaller values of d diffract at higher angles – this is the importance of "high angle" data!

Diffraction of X-rays

You may wonder why to X-rays reflect in this way and what is causing them to "reflect" in the first place. The actual interaction is between the X-rays and the **ELECTRONS** in the crystal and it is a type of elastic scattering. The oscillating electric field of the X-rays causes the charged particles in the atom to oscillate at the same frequency. Emission of a photon *at that frequency* (elastic) returns the particles in the atom to a more stable state. The emitted photon can be in any direction and the intensity of the scattering is given by the equation:

$$I(2\theta) = I^o \left[(n\, e^4)/(2\, r^2\, m^2\, c^4)\right] \left[(1 + \cos^2(2\theta))/2\right]$$

$I(2\theta)$ = observed intensity
I^o = incident intensity
n = number of scattering sources
r = distance of detector from scattering source
m = mass of scattering source
c = speed of light, e = electron charge, $[(1 + \cos^2(2\theta))/2]$ is a polarization factor

Note that the mass of the scattering particle (m) is in the denominator – this means that the scattering that we see is attributable only to the electrons (which have masses almost 2000 times less than that of a proton).

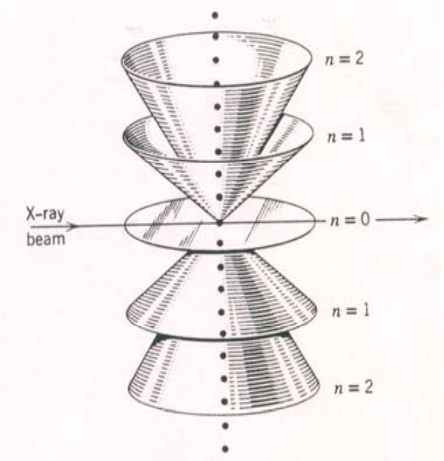
Laue's interpretation

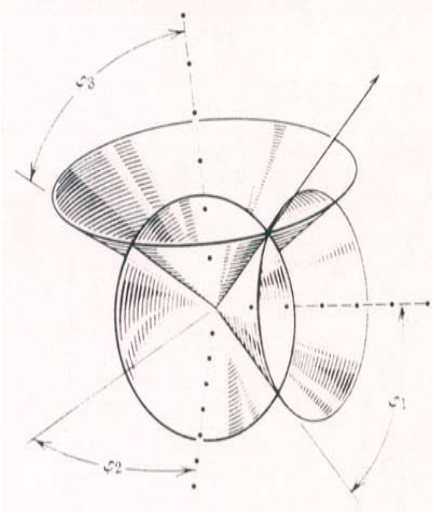
Max von Laue derived a different set of equations describing the "in phase" diffraction of X-rays by a line of scattering objects (note that the n in the diagram below is the integer corresponding to the integer n in the Bragg equation). Each line of objects generates cones of "in phase" scattering that follow the equations:

$a(\cos \Psi_1 - \cos \varphi_1) = \lambda h$ (for a line in the *a* direction)
$b(\cos \Psi_2 - \cos \varphi_2) = \lambda k$ (for a line in the *b* direction)
$c(\cos \Psi_3 - \cos \varphi_3) = \lambda l$ (for a line in the *c* direction)

Where Ψ is the angle between the incident beam and the line and φ is the angle between the cone and the line of scatterers. In three dimensions, a reflection will only be observed at the intersection of the cones in all three directions (all three equations are satisfied).

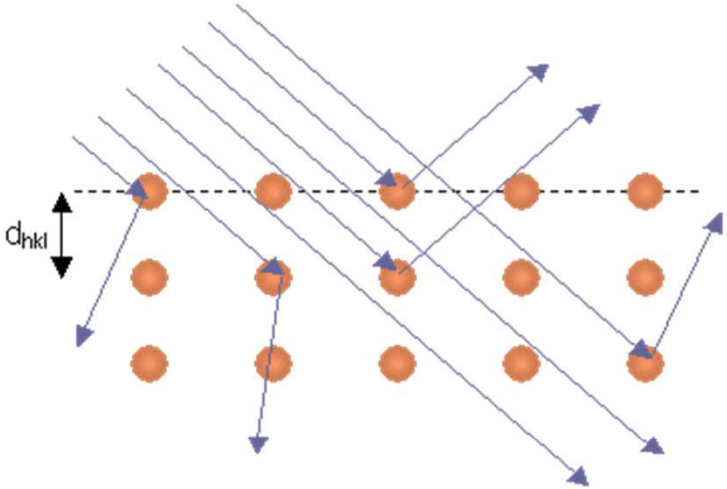
With a little geometry (see Ladd and Palmer 3.4.3), it can be shown that this treatment is equivalent to Bragg's law.

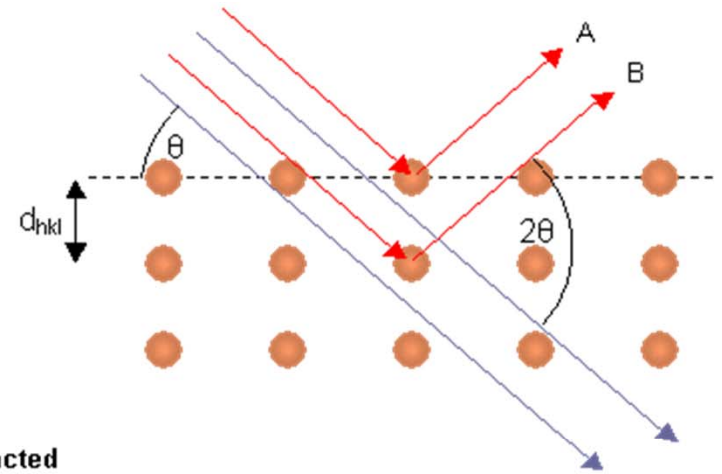


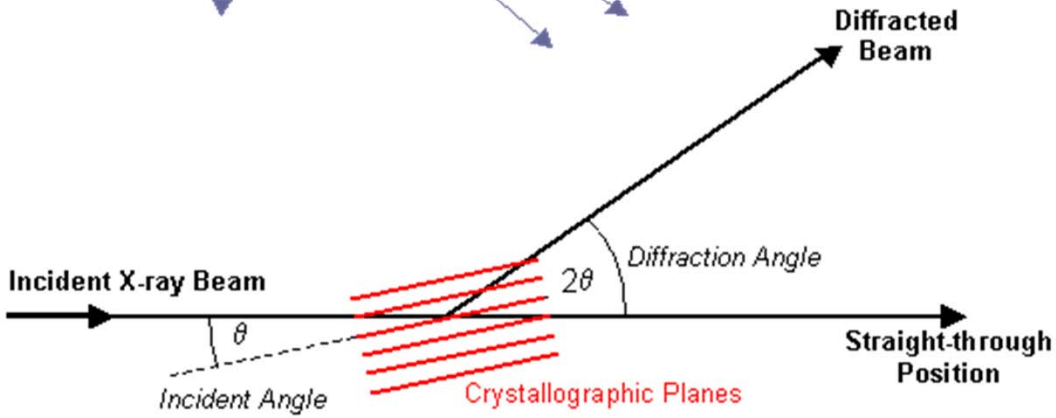


Summary of Diffraction by Planes

If they interact with electrons in the crystal, incident X-rays will be scattered. Only the X-rays that scatter “in phase” (constructive interference) will give rise to *reflections* we can observe. We can use Bragg’s Law to interpret the diffraction in terms of the distance between lattice planes in the crystal based on the incident and diffraction angle of the reflection.







Note: The diffraction angle is generally labeled 2θ because of the geometric relationship shown on the left.