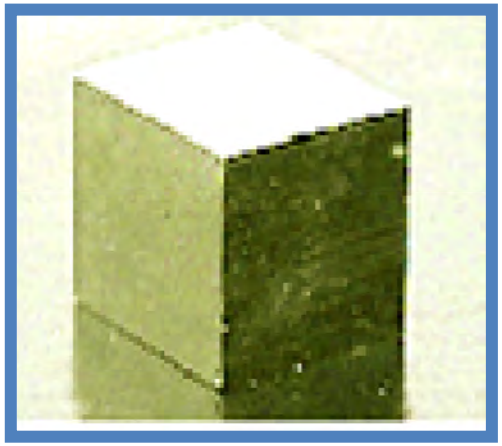
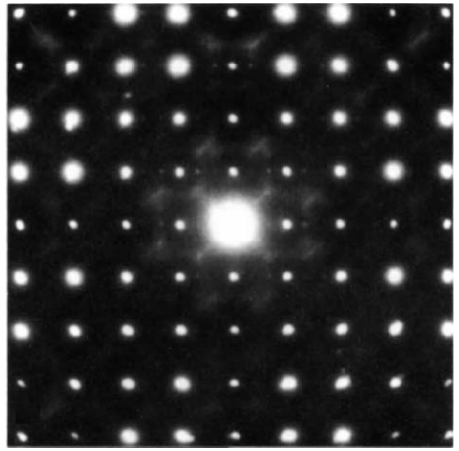
Lecture 4 Jan 16 2013



$$\mathbf{K}\cdot\mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

$$[\mathbf{b_1}\,\mathbf{b_2}\,\mathbf{b_3}]^{\prime\prime} = 2\pi\,[\mathbf{a_1}\mathbf{a_2}\mathbf{a_3}]^{-1}\,.$$



$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

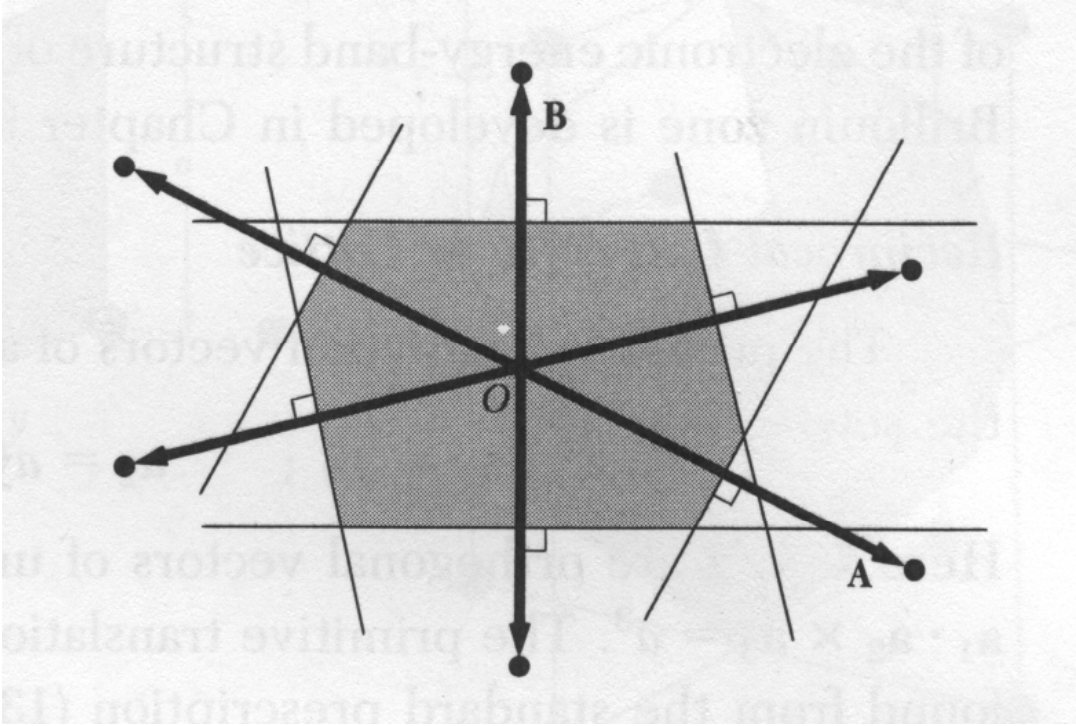
$$\mathbf{K} = k_1\mathbf{b_1} + k_2\mathbf{b_2} + k_3\mathbf{b_3}$$

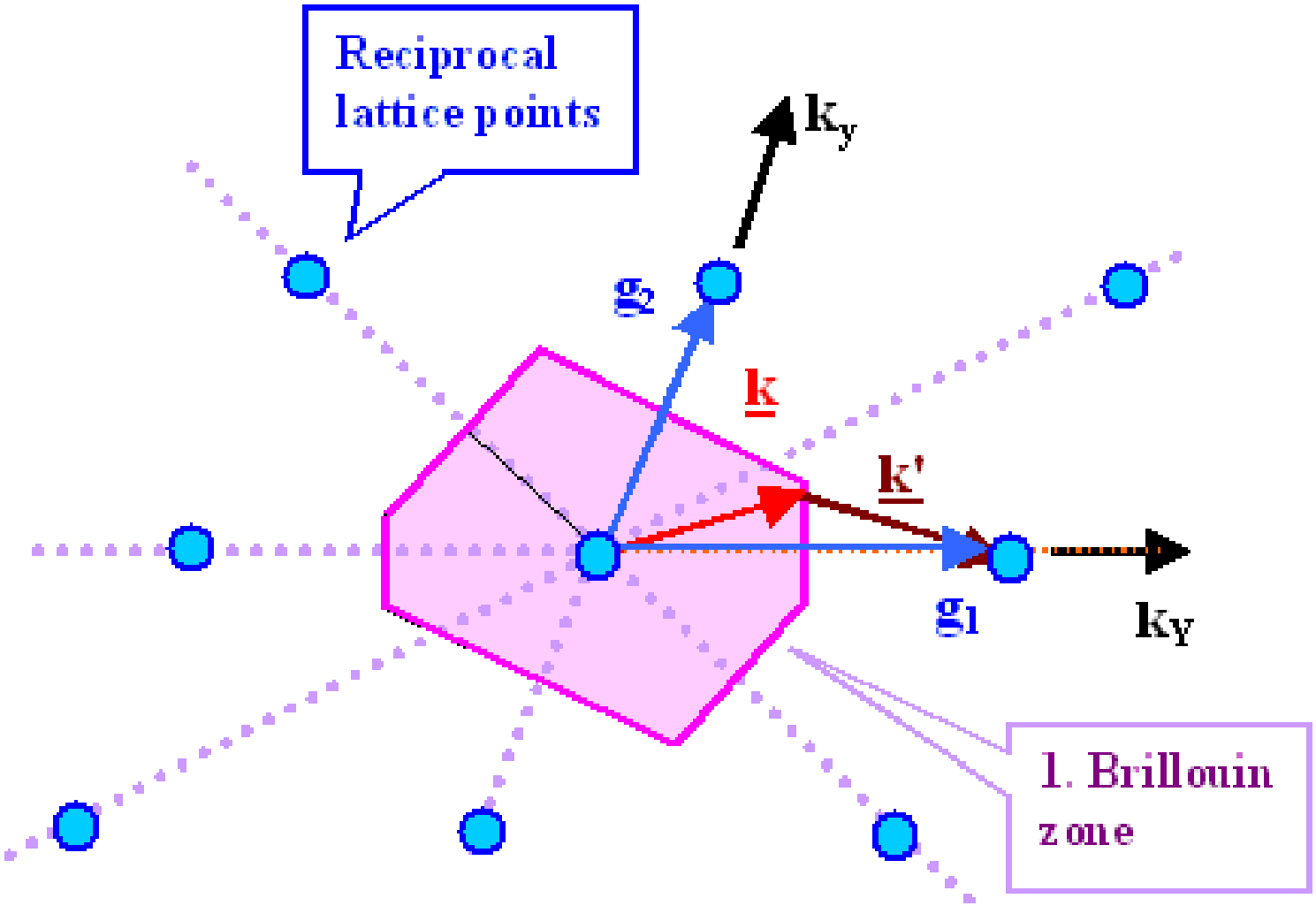
Primitive cell
Wigner-Seitz cell (WS)

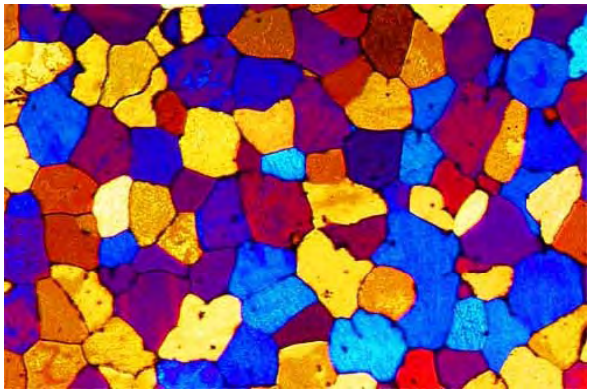
Primitive cell

First Brillouin zone

The Wigner-Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone. (Wigner-Seitz is real space concept while Brillouin zone is a reciprocal space idea).




Reciprocal
lattice points
k_y
g_2
$\underline{k}$
$\underline{k'}$
g_1
k_y
1. Brillouin
zone

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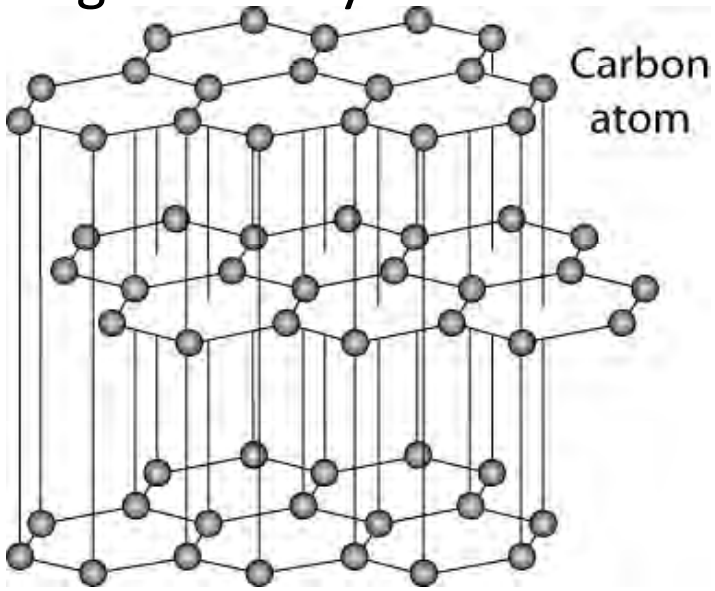
Powder cell

Polymorphic Forms of Carbon

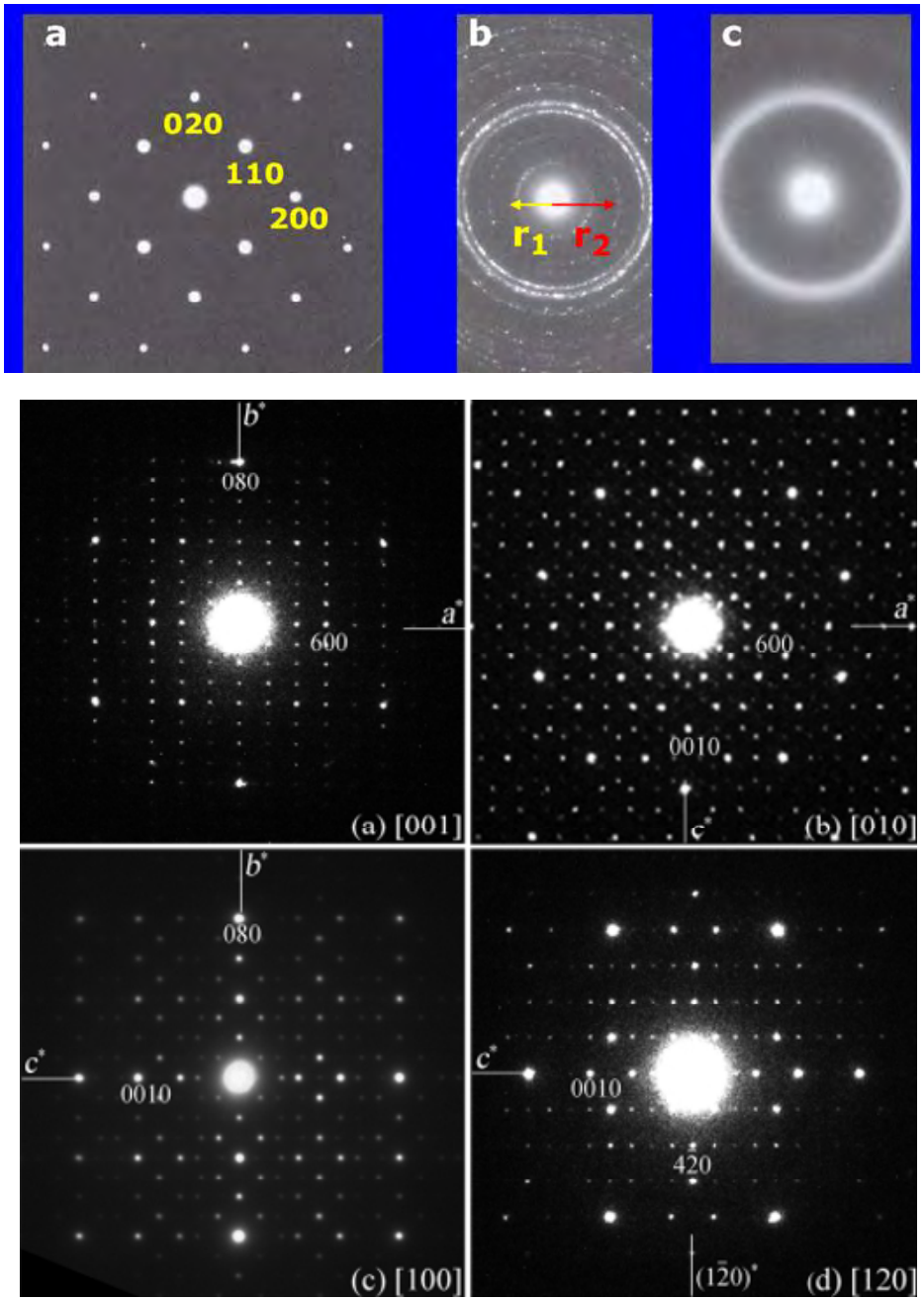
Graphite

– a soft, black, flaky solid, with a layered structure – parallel hexagonal arrays of carbon atoms

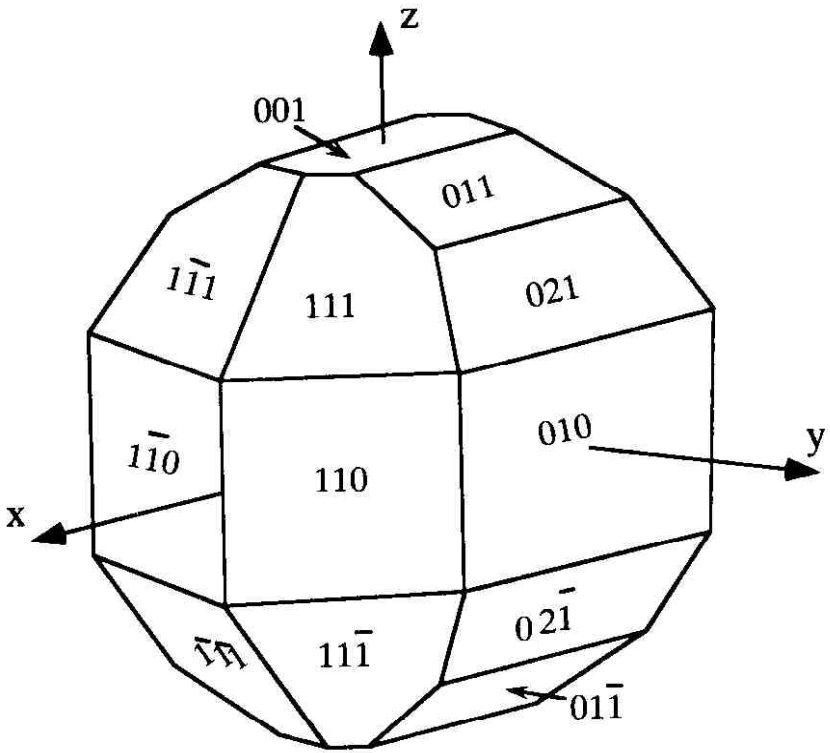


– weak van der Waal's forces between layers

– planes slide easily over one another

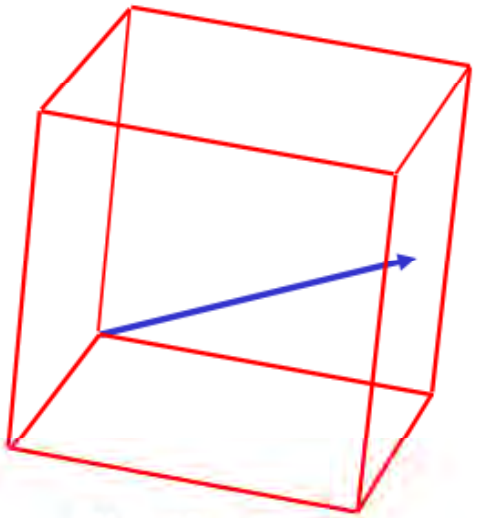

a
020
110
200
b
r1
r2
c
b*
080
a*
600
(a) [001]
a*
600
0010
c*
(b) [010]
b*
080
c*
0010
(c) [100]
c*
0010
420
(1$\bar{2}$0)*
(d) [120]

Miller indices

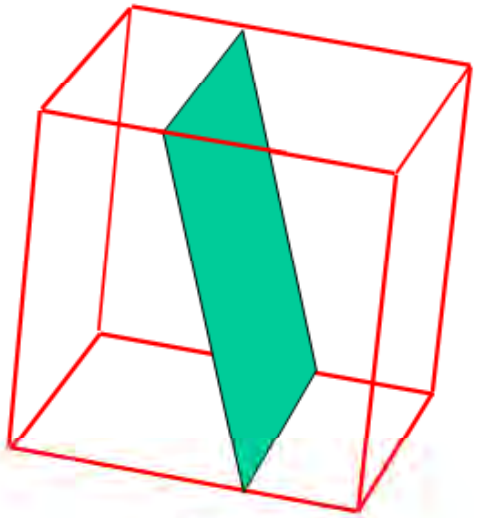


- Miller indices used to express lattice *planes* and *directions*
- x, y, z are the axes (on arbitrarily positioned origin)
- a, b, c are lattice parameters (*length of unit cell along a side*)
- h, k, l are the Miller indices for planes and directions - expressed as planes: (hkl) and directions: [hkl]

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



direction



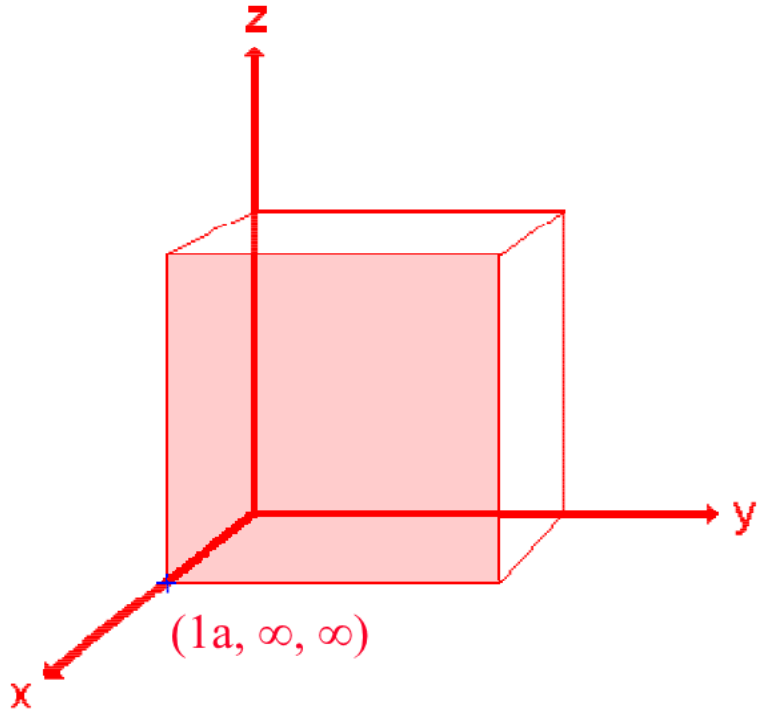
plane

Simple cubic

Miller Indices

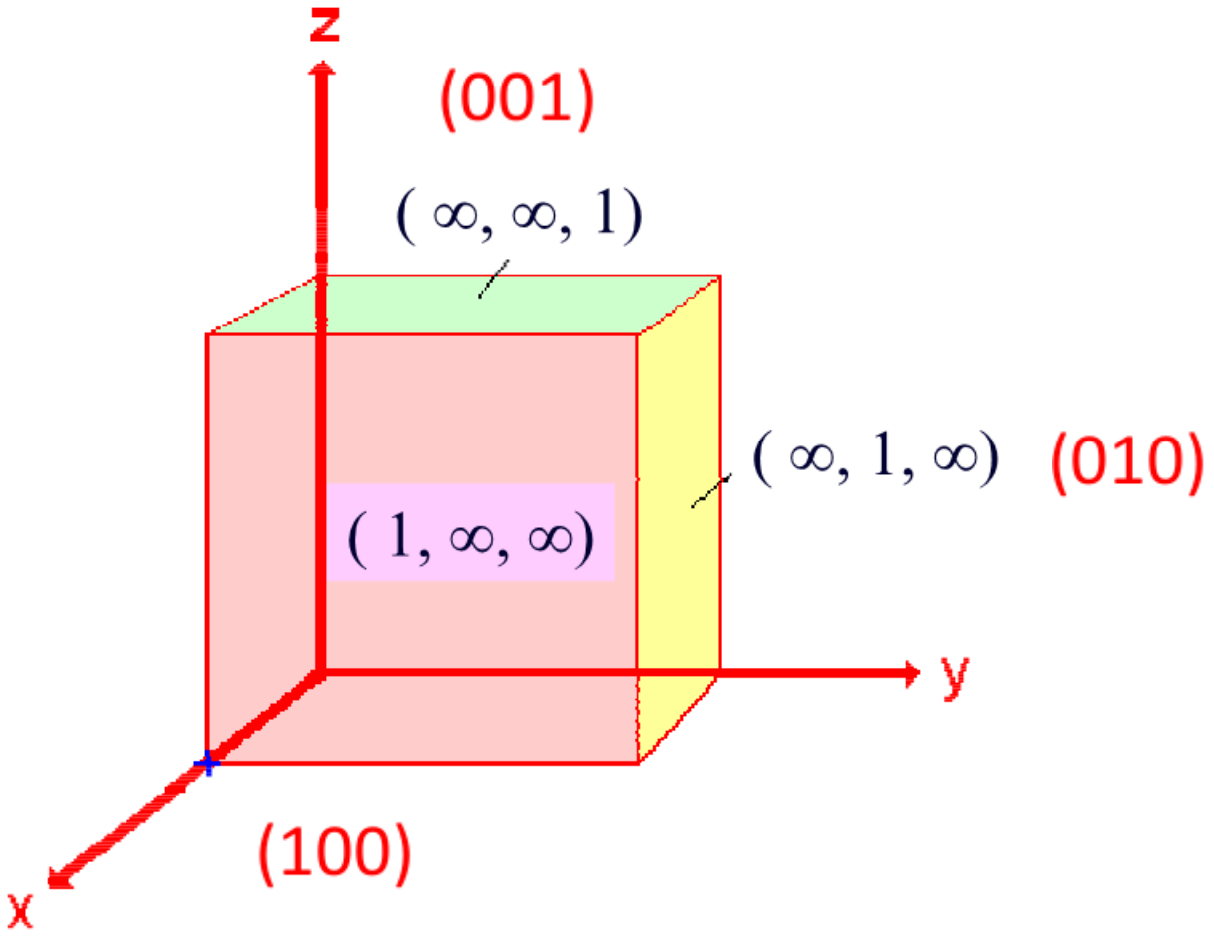
Rules for determining Miller Indices:

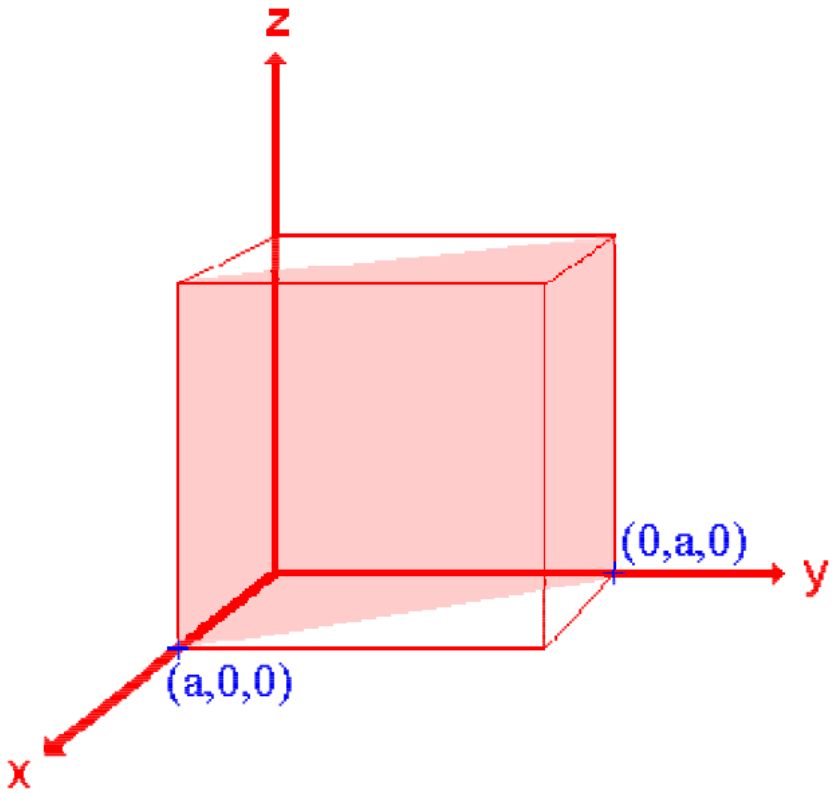
1. Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
2. Take the reciprocals
3. Clear fractions
4. Reduce to lowest terms



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

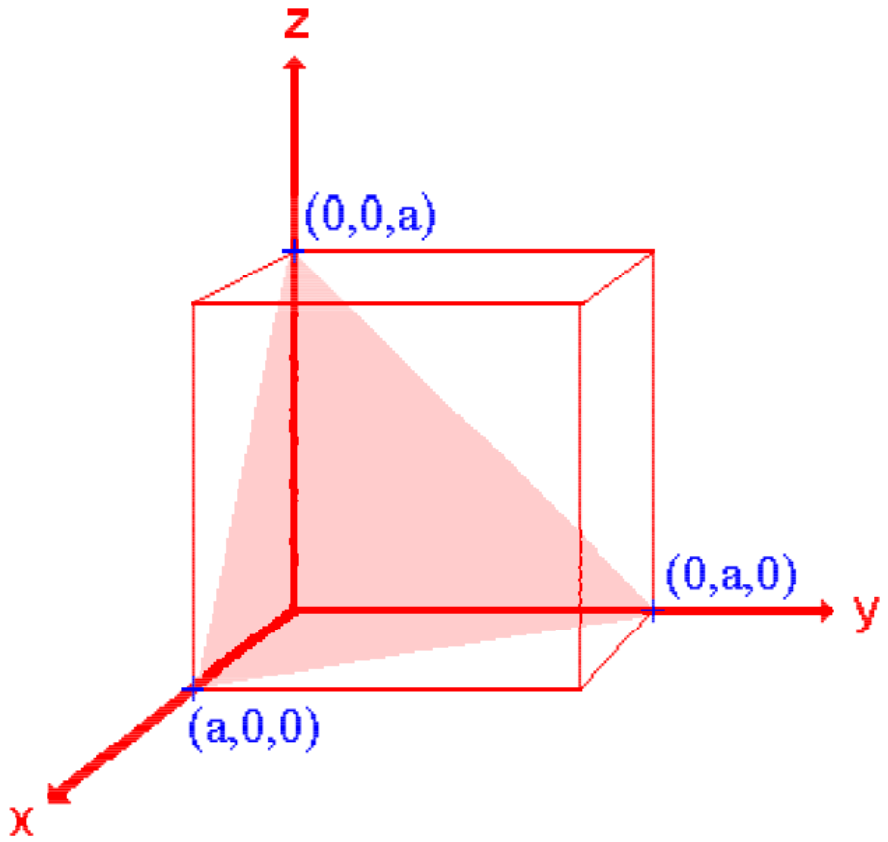
Miller indice (100)


z
(001)
(∞, ∞, 1)
(∞, 1, ∞)
(010)
(1, ∞, ∞)
y
x
(100)



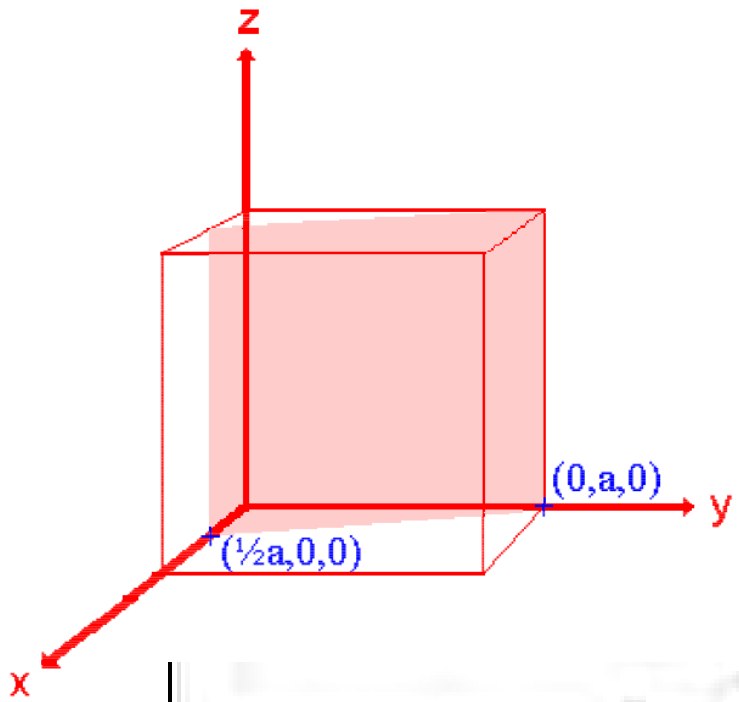
	a	b	c
intercept length	1	1	∞
reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{\infty}$
cleared fraction	1	1	0

Miller indice (110)

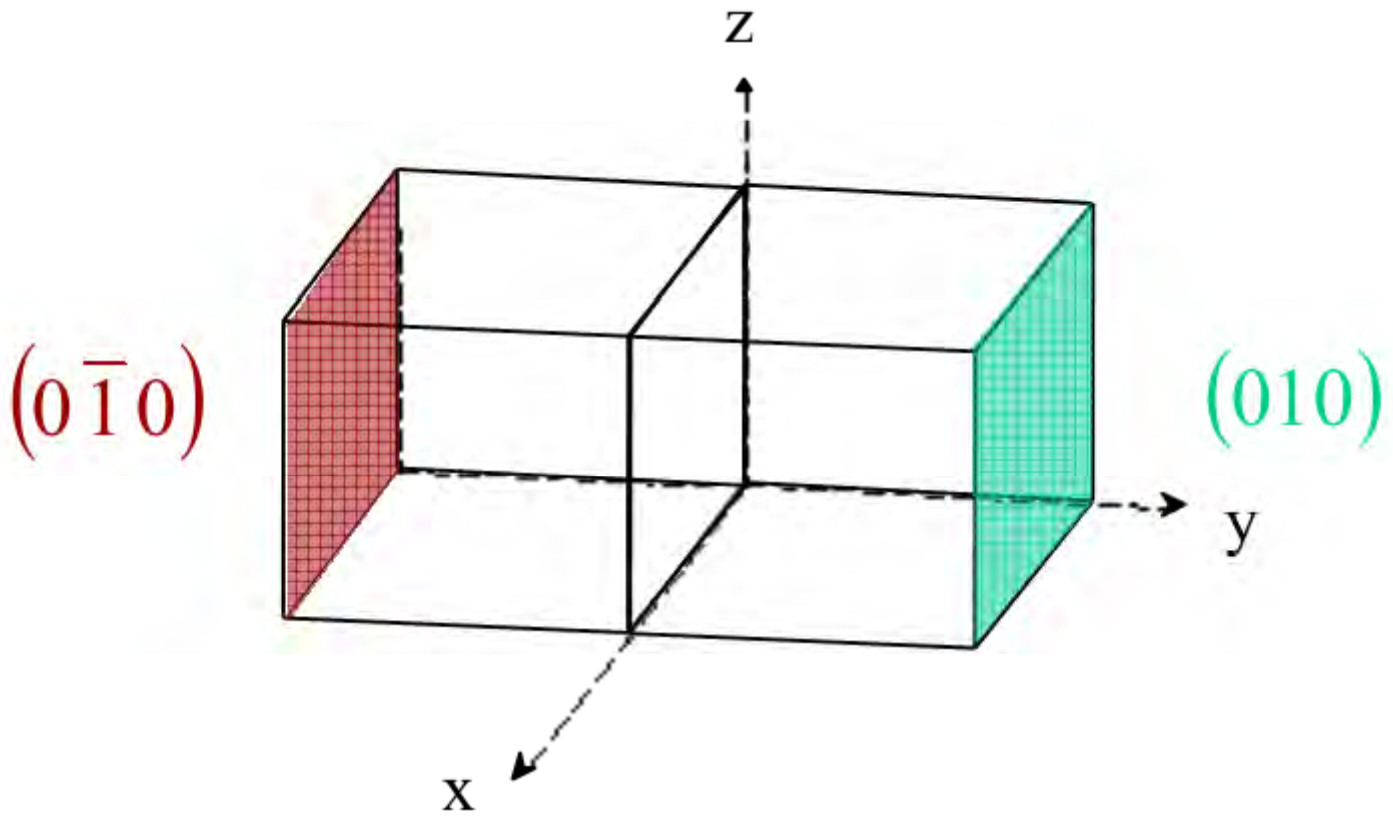


	a	b	c
intercept length	1	1	1
reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{1}$
cleared fraction	1	1	1

Miller indice (111)



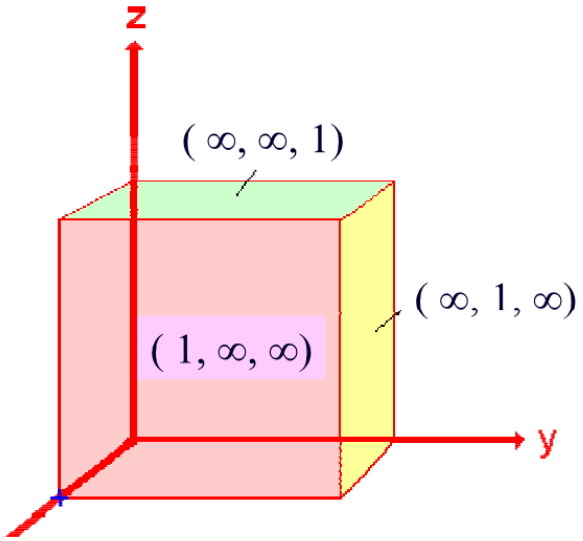
	a	b	c
intercept length	1/2	1	∞
reciprocal	1/(1/2)	1/1	1/∞
cleared fraction	2	1	0
Miller indice	(210)		



– Negative values are expressed with a bar over the number

• *Example: -2 is expressed* $\bar{2}$

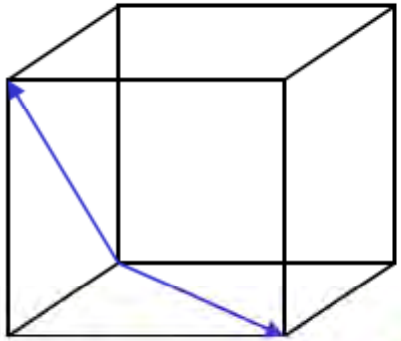
Simple cubic



Index	Members in family for **cubic lattice**
<100>	[100],[$\bar{1}$00],[010],[0$\bar{1}$0],[001],[00$\bar{1}$]
<110>	[110],[$\bar{1}$10],[1$\bar{1}$0],[$\bar{1}\bar{1}$0],[101],[$\bar{1}$01],[10$\bar{1}$],[$\bar{1}$0$\bar{1}$],[011],[0$\bar{1}$1],[01$\bar{1}$],[0$\bar{1}\bar{1}$]
<111>	[111],[$\bar{1}$11],[1$\bar{1}$1],[11$\bar{1}$],[$\bar{1}\bar{1}$1],[$\bar{1}$1$\bar{1}$],[1$\bar{1}\bar{1}$],[$\bar{1}\bar{1}\bar{1}$]

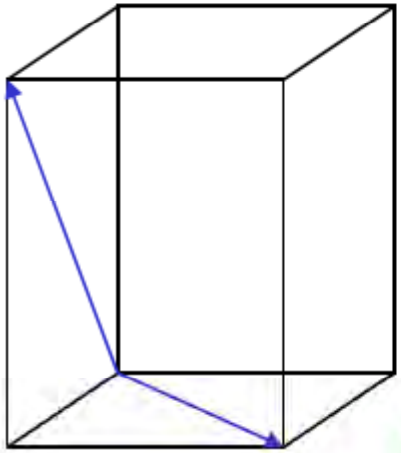
THE ARC.

- Equivalence of directions



[101] = [110]

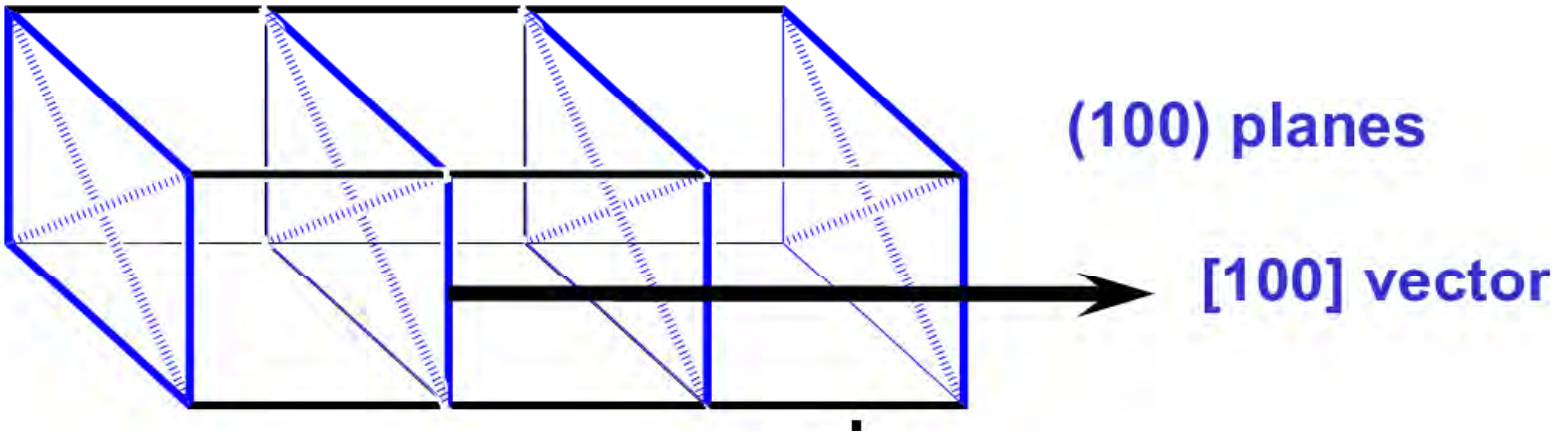
cubic



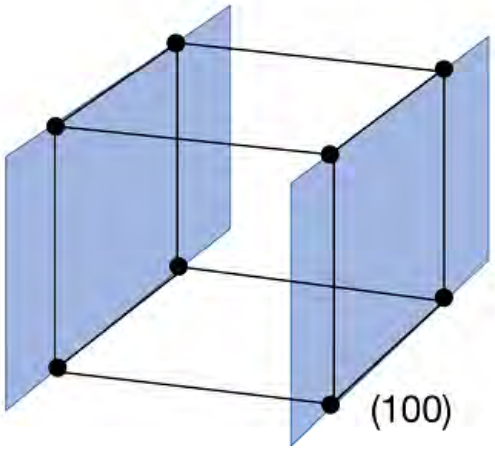
[101] ≠ [110]

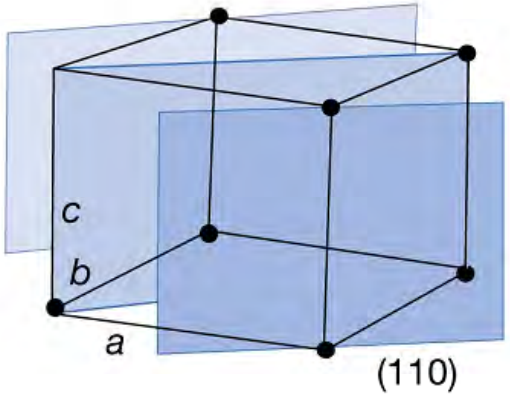
tetragonal

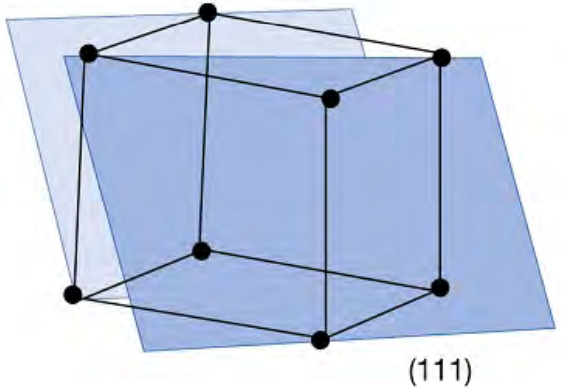
The orientation of planes is best represented by a vector normal to the plane. The direction of a set of planes is indicated by a vector denoted by square brackets containing the Miller indices of the set of planes. Miller indices are also used to describe crystal faces.



- [hkl] represents a direction
- <hkl> represents a family of directions
- (hkl) represents a plane
- {hkl} represents a family of planes





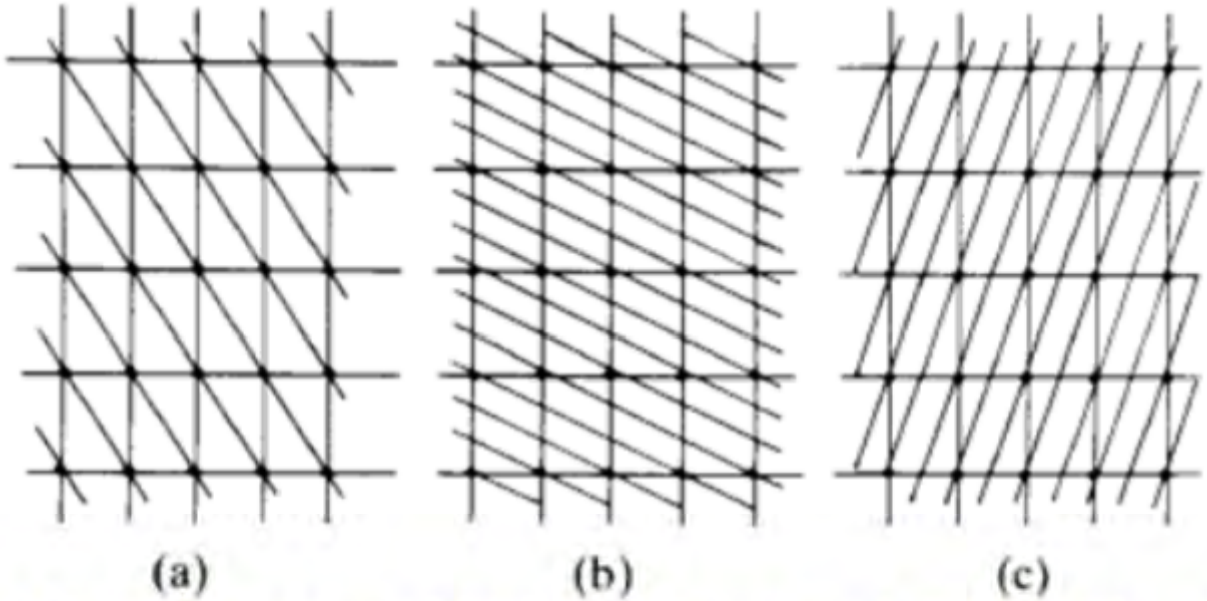


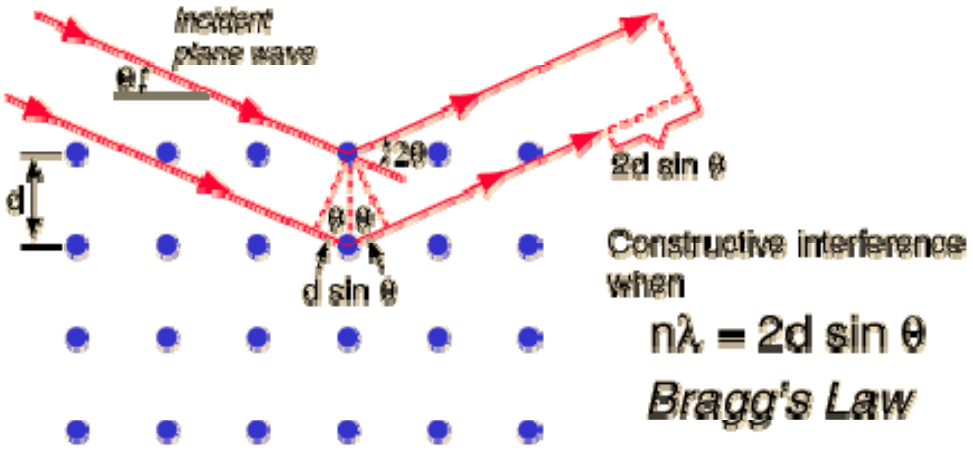
$$d_{hkl}^2\left(\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right)=1$$

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

d_{100}=?

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


(a)
(b)
(c)
(110) planes
(130) planes
(-210) planes


Incident plane wave
θ
2θ
d
θ θ
d sin θ
2d sin θ
Constructive interference when
nλ = 2d sin θ
Bragg's Law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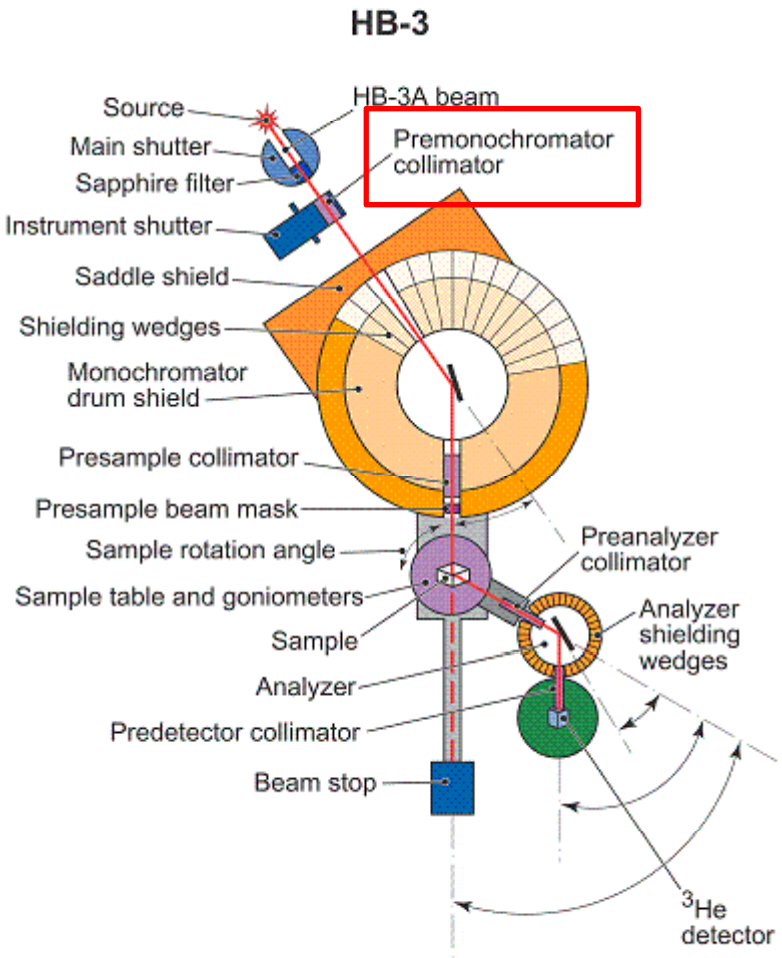
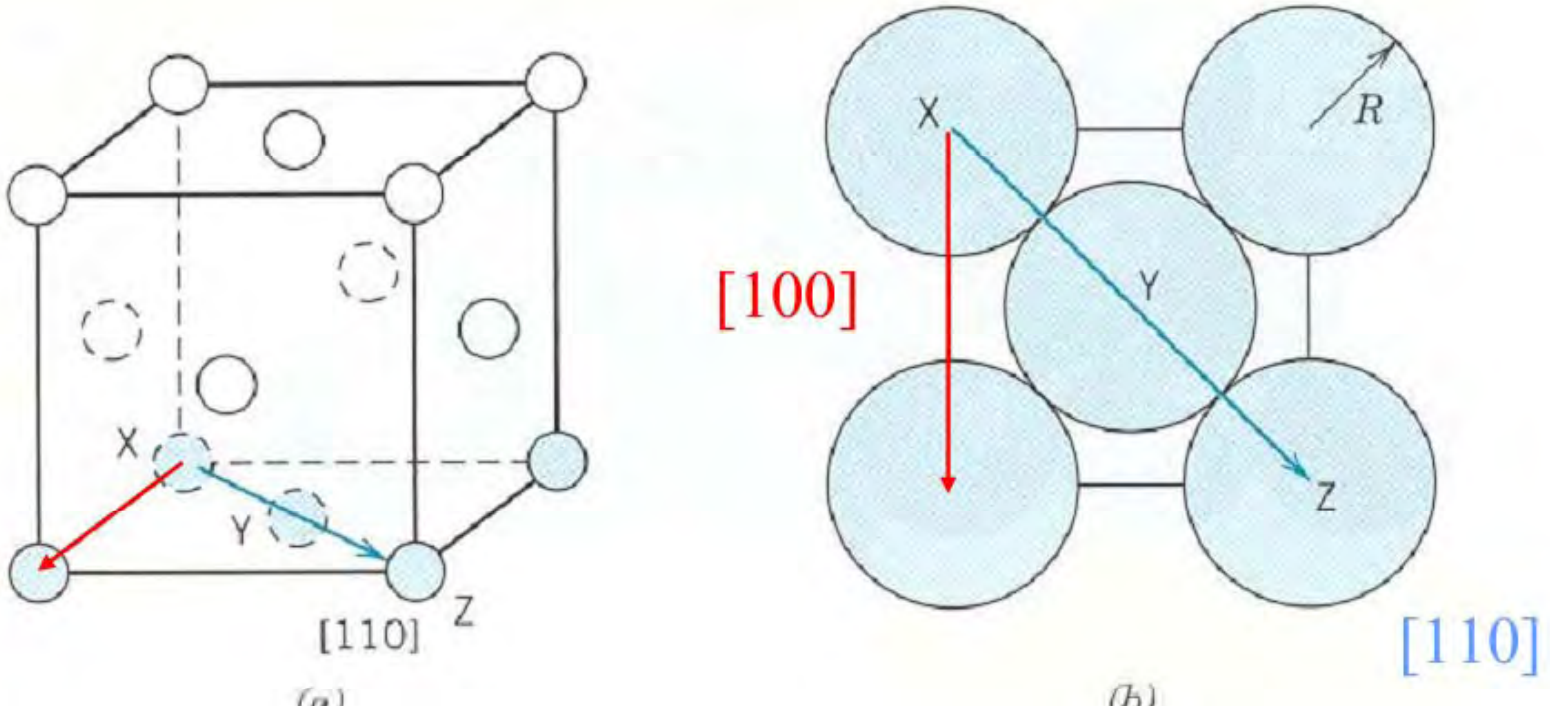
ORNL 2003-02834/dgc





Speed of sound along directions

- Slip (deformation in metals) depends on linear and planar density
- Slip occurs on planes that have the greatest density of atoms in direction with highest density (*we would say along closest packed directions on the closest packed planes*)

$$v = \sqrt{\frac{\text{elastic property}}{\text{inertial property}}} = \sqrt{\frac{B}{\rho}}$$ where B = bulk modulus, ρ = density

Linear and Planar density

- Linear Density

– Number of atoms per length whose centers lie on the direction vector for a specific crystallographic direction.

$$LD = \frac{\#\text{ of atoms centered on a direction vector}}{\text{length of direction vector}}$$

- Planar Density

– Number of atoms per unit area that are centered on a particular crystallographic plane.

$$PD = \frac{\#\text{ of atoms centered on a plane}}{\text{area of plane}}$$

Where does a protein crystallographer see the Miller indices?

- **Common crystal faces are parallel to lattice planes**

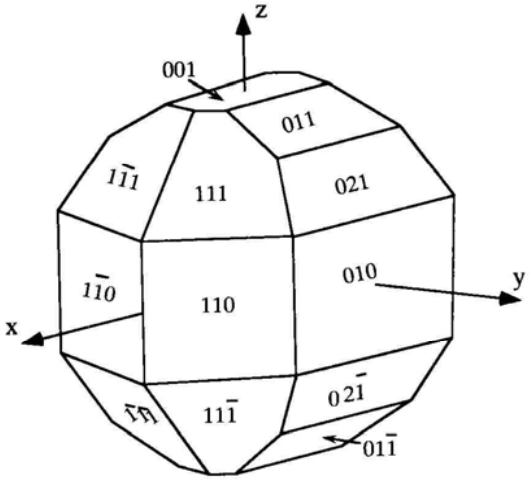
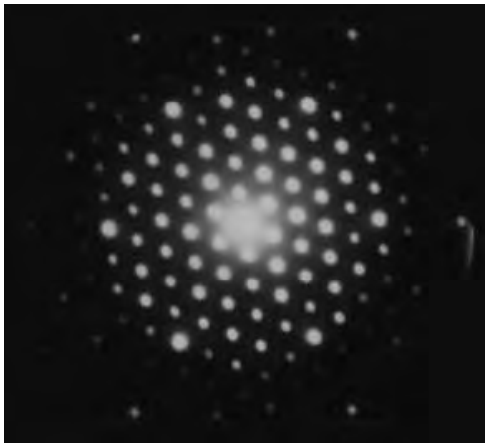


Figure 3.7. A crystal showing several faces.

- **Each diffraction spot can be regarded as a X-ray beam reflected from a lattice plane, and therefore has a unique Miller index.**



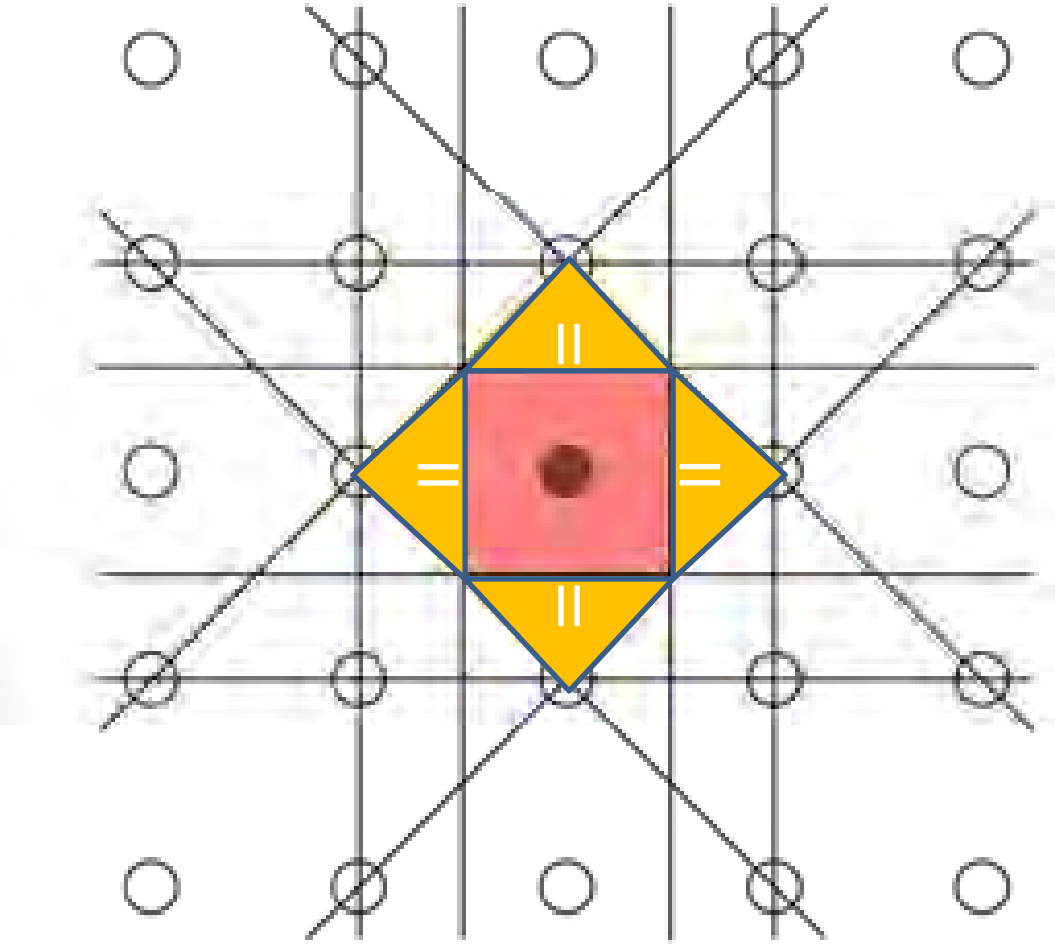
Miller indices

A Miller index is a series of coprime integers that are inversely proportional to the intercepts of the crystal face or crystallographic planes with the edges of the unit cell.

It describes the orientation of a plane in the 3-D lattice with respect to the axes.

The general form of the Miller index is (h, k, l) where h, k, and l are integers related to the unit cell along the a, b, c crystal axes.

Irreducible brillouin zone

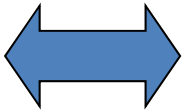


Reciprocal lattice

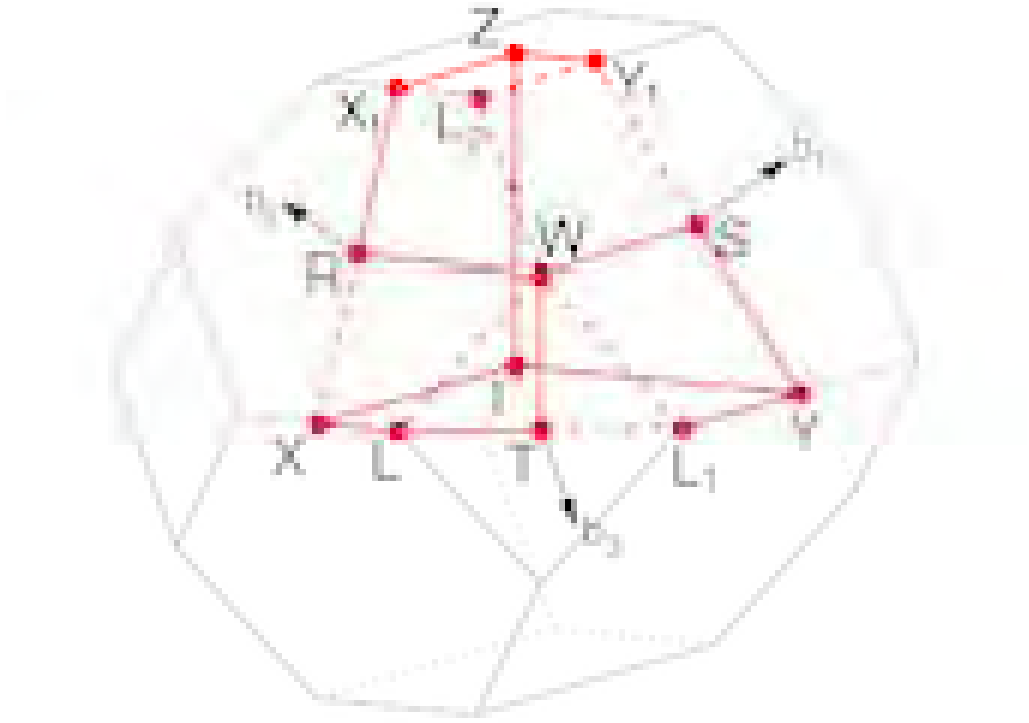
$$\vec{g} = h\vec{a}' + k\vec{b}' + l\vec{c}'$$

The Bravais lattice after Fourier transform

real space	reciprocal lattice
normals to the planes(vectors)	points
spacing between planes	1/distance between points (actually, 2p/distance)
l (distance, wavelength)	2p/l=k (momentum, wave number)
Bravais cell	Wigner-Seitz cell



Brillouin zone



ORCI path: Γ-X-L-T-W-R-X_1-Z-Γ-Y-S-W|L_1-Y|Y_1-Z

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]