Lecture 3
Crystal Structure

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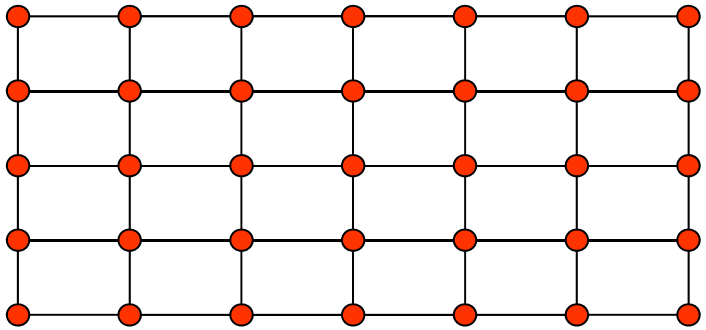
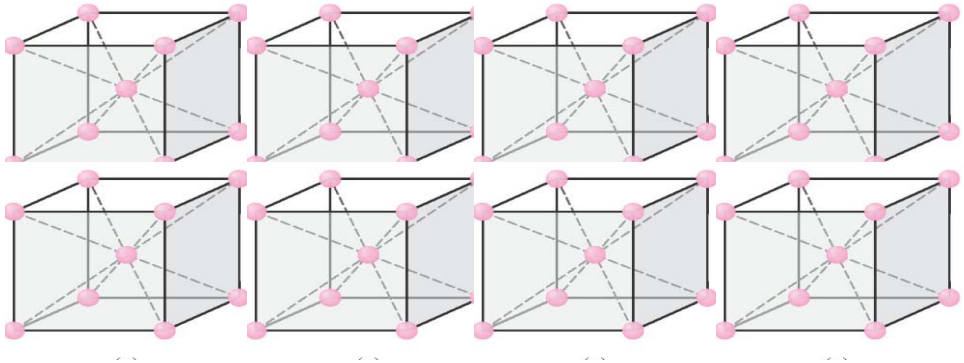
Chapter 4
OR Solid state physics, Kittel (Wiley)

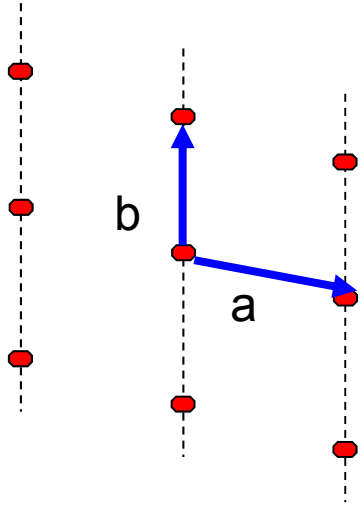
Crystal Planes

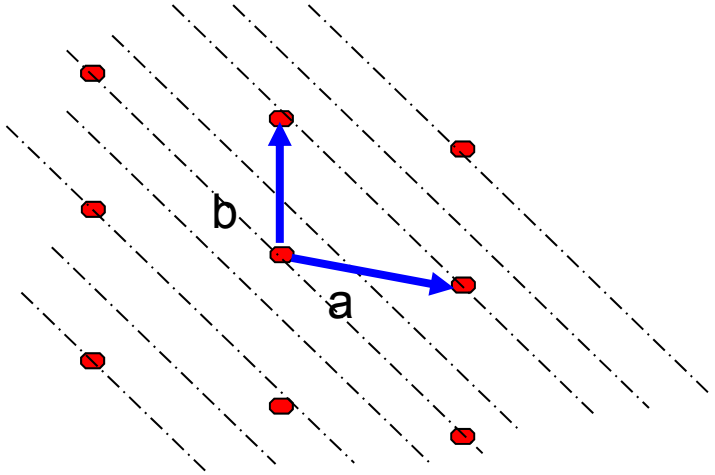




- Within a crystal lattice it is possible to identify sets of equally spaced parallel planes. These are called lattice planes.

The set of planes in 2D lattice.





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.

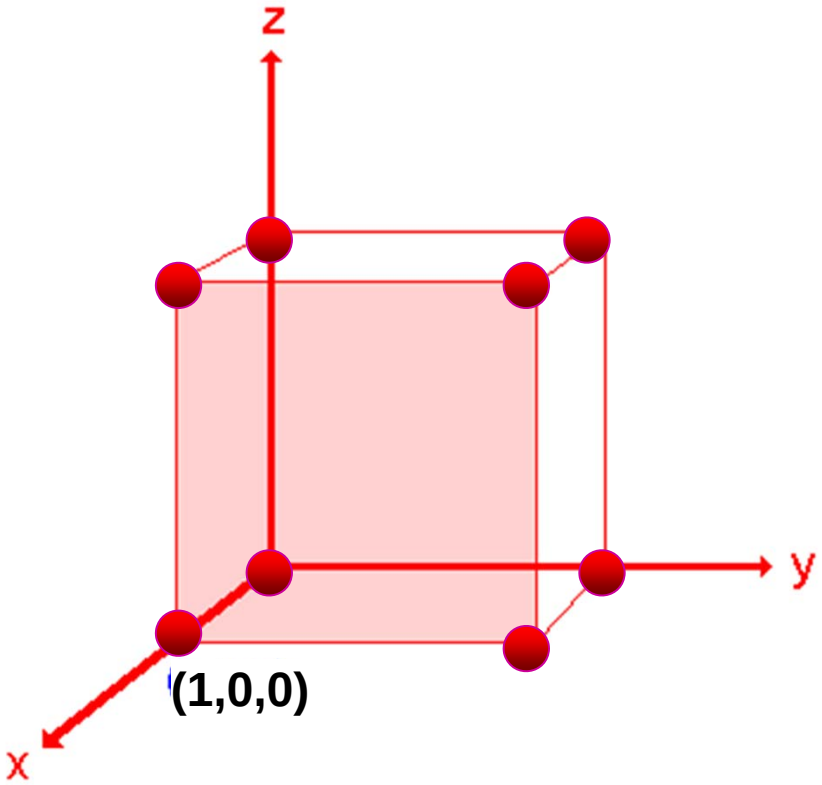
To determine Miller indices of a plane, take the following steps;

1) Determine the intercepts of the plane along each of the three crystallographic directions

2) Take the reciprocals of the intercepts

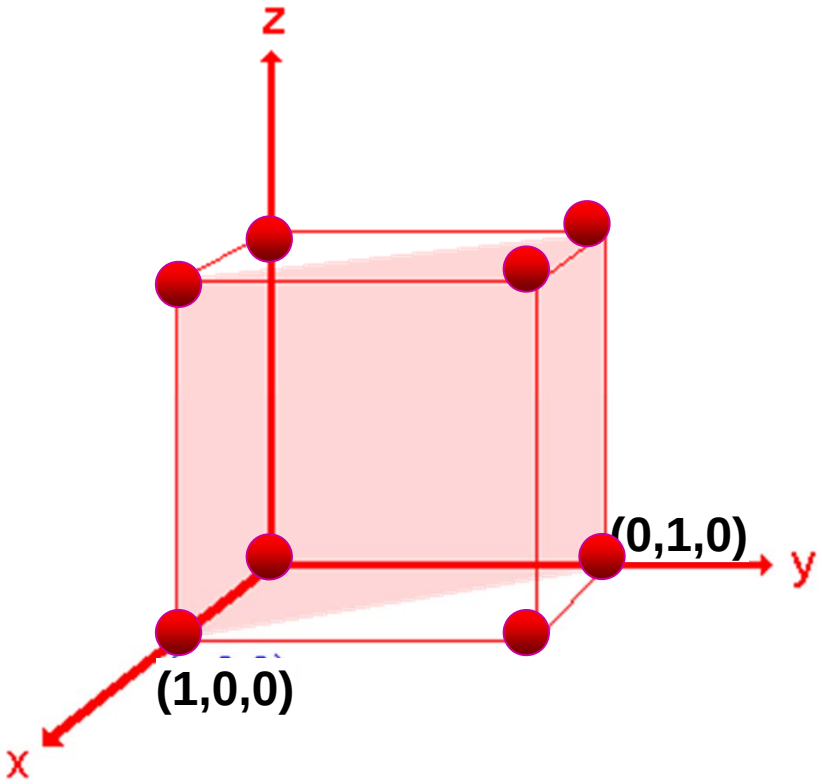
3) If fractions result, multiply each by the denominator of the smallest fraction

Example-1



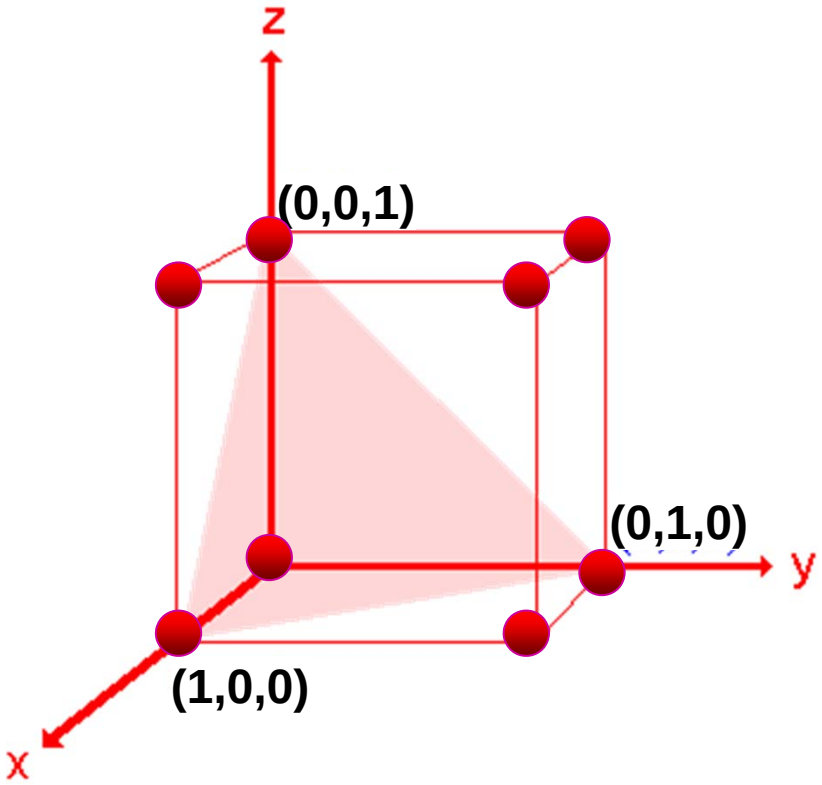
Axis	x	y	z
Intercept points	1	∞	∞
Reciprocals	1/1	1/ ∞	1/ ∞
Smallest Ratio	1	0	0
Miller İndices (100)			

Example-2



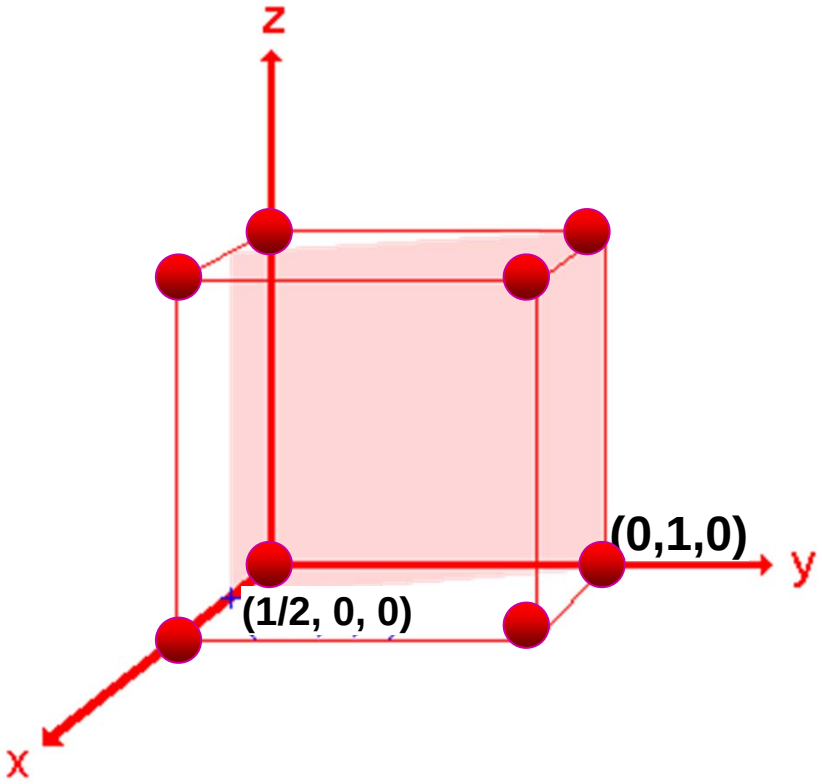
Axis	x	y	z
Intercept points	1	1	∞
Reciprocals	1/1	1/ 1	1/ ∞
Smallest Ratio	1	1	0
Miller İndices (110)			

Example-3



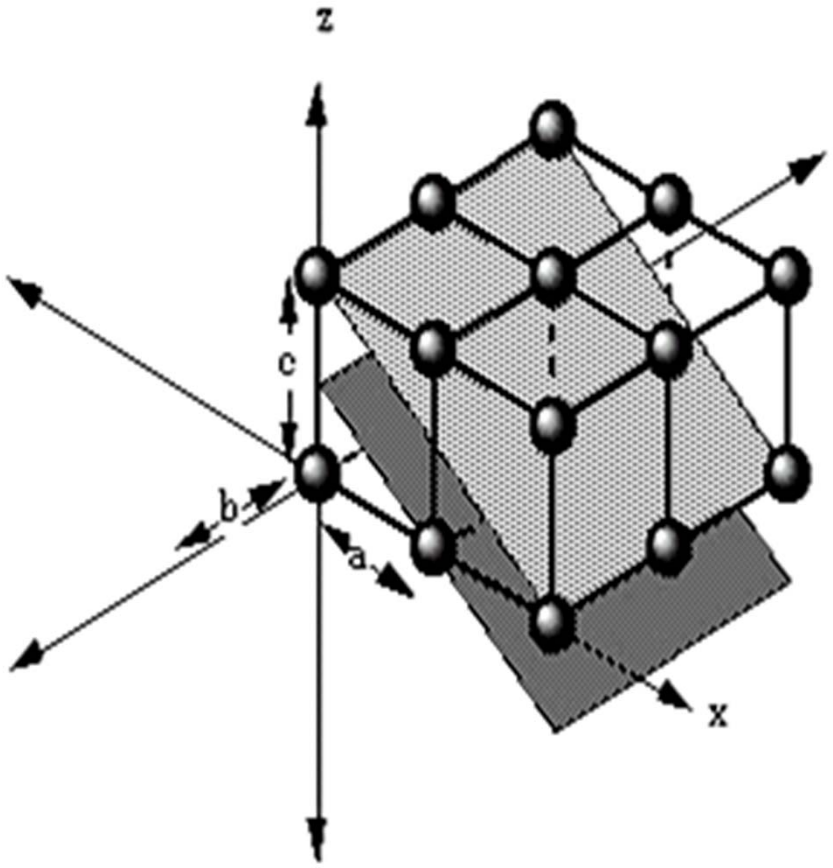
Axis	x	y	z
Intercept points	1	1	1
Reciprocals	1/1	1/ 1	1/ 1
Smallest Ratio	1	1	1
Miller İndices (111)			

Example-4



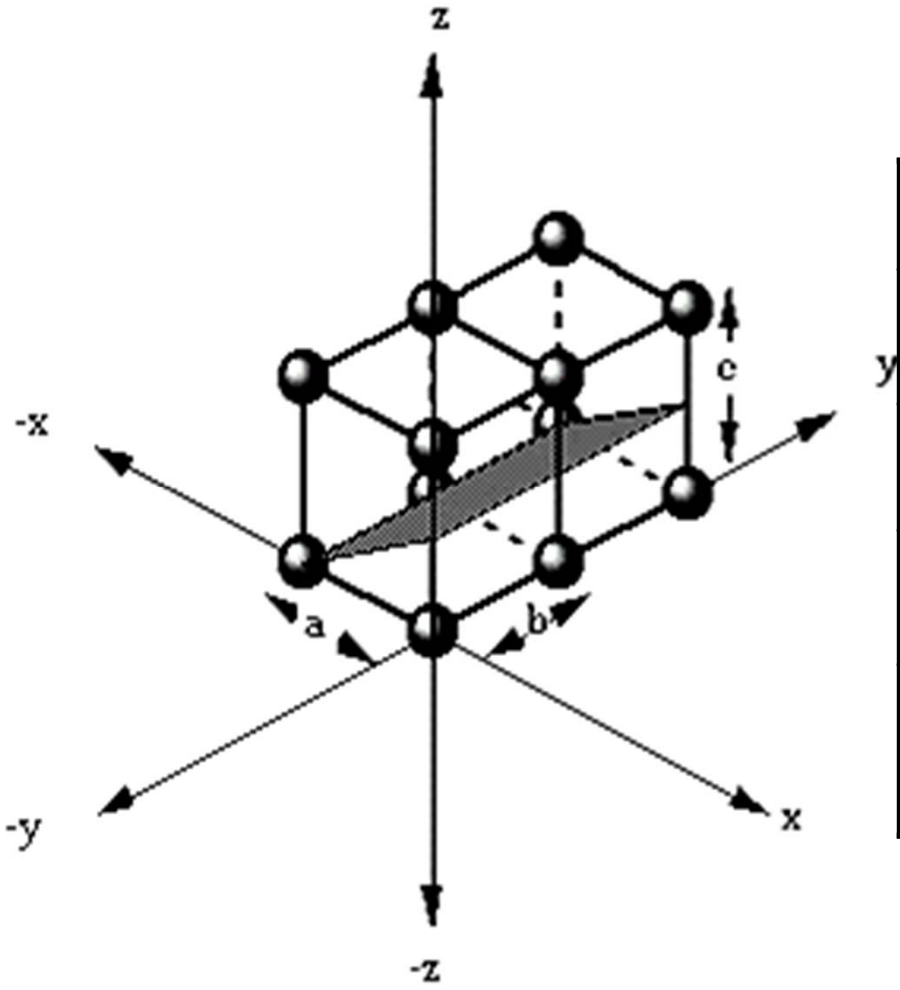
Axis	x	y	z
Intercept points	1/2	1	∞
Reciprocals	1/(½)	1/ 1	1/ ∞
Smallest Ratio	2	1	0
Miller İndices (210)			

Example-5



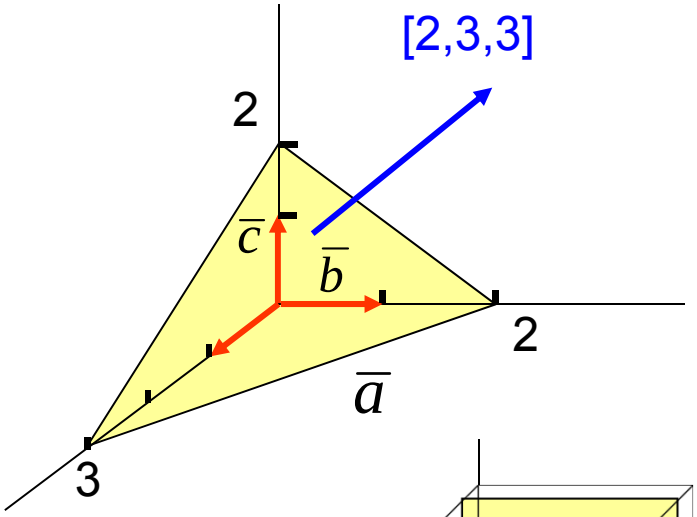
Axis	a	b	c
Intercept points	2	∞	1
Reciprocals	**1/2**	**1/ ∞**	**1**
Smallest Ratio	1	0	2
Miller İndices (102)			

Example-6



Axis	a	b	c
Intercept points	-1	∞	½
Reciprocals	**1/-1**	**1/ ∞**	**1/(½)**
Smallest Ratio	-1	0	2
Miller İndices $(\bar{1}02)$			

Miller Indices

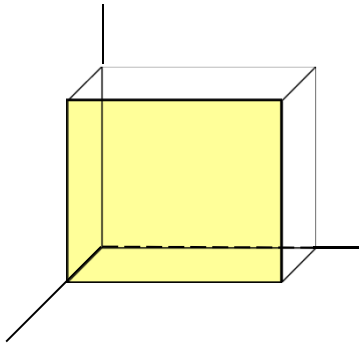


Plane intercepts axes at $3\bar{a}, 2\bar{b}, 2\bar{c}$

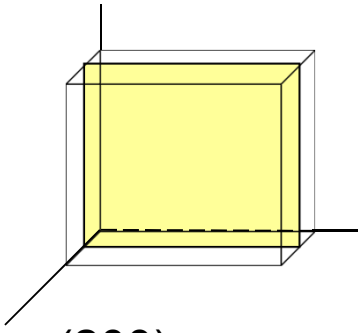
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Indices of the plane (Miller): (2,3,3)

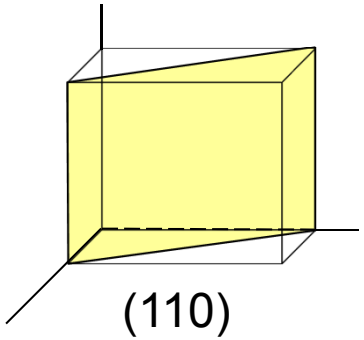
Indices of the direction: [2,3,3]



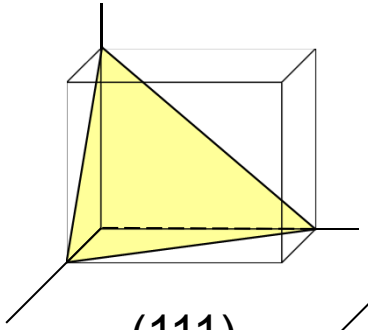
(100)



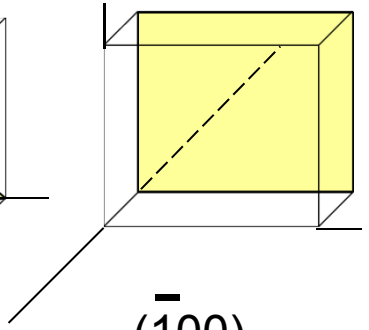
(200)



(110)

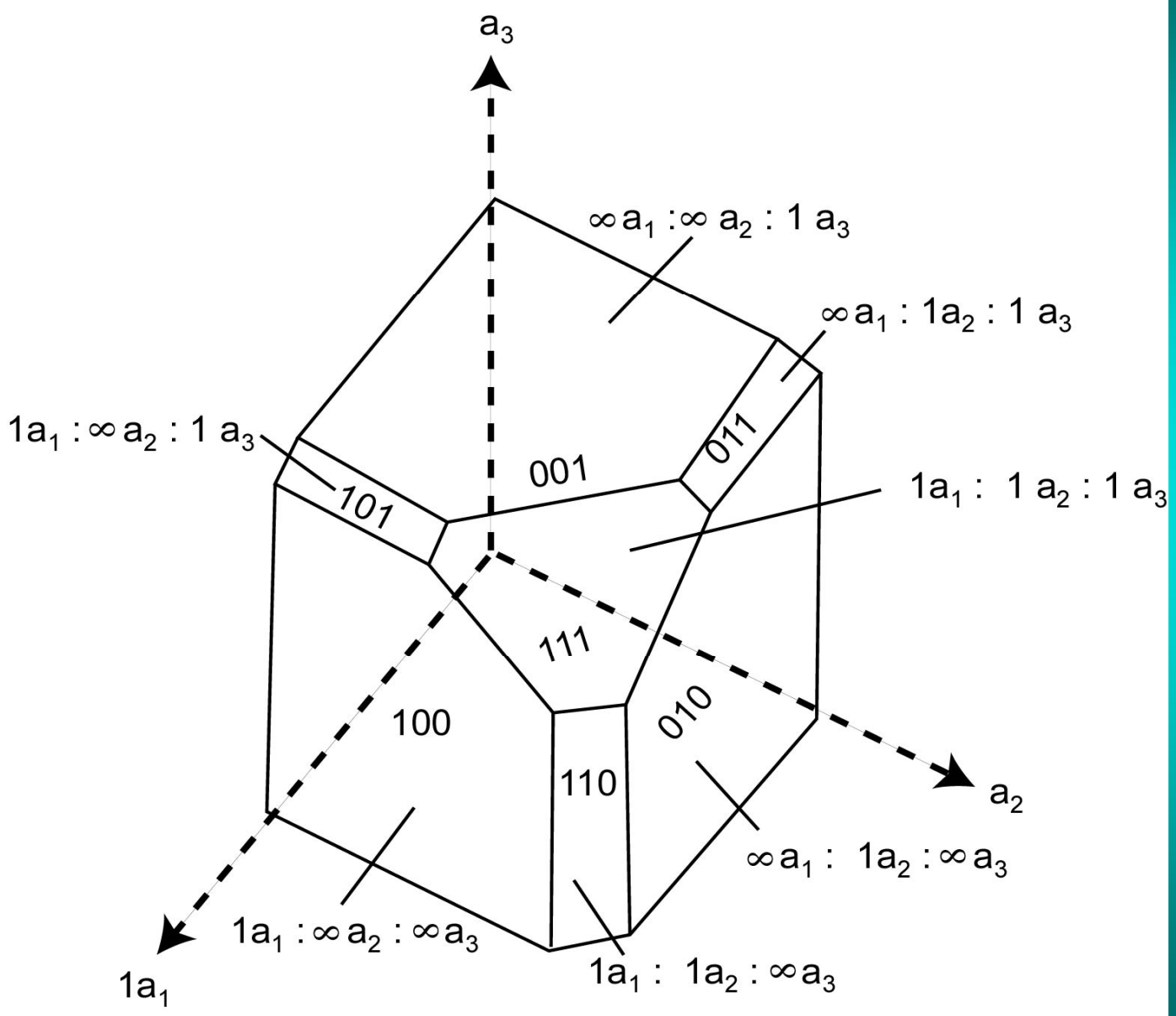


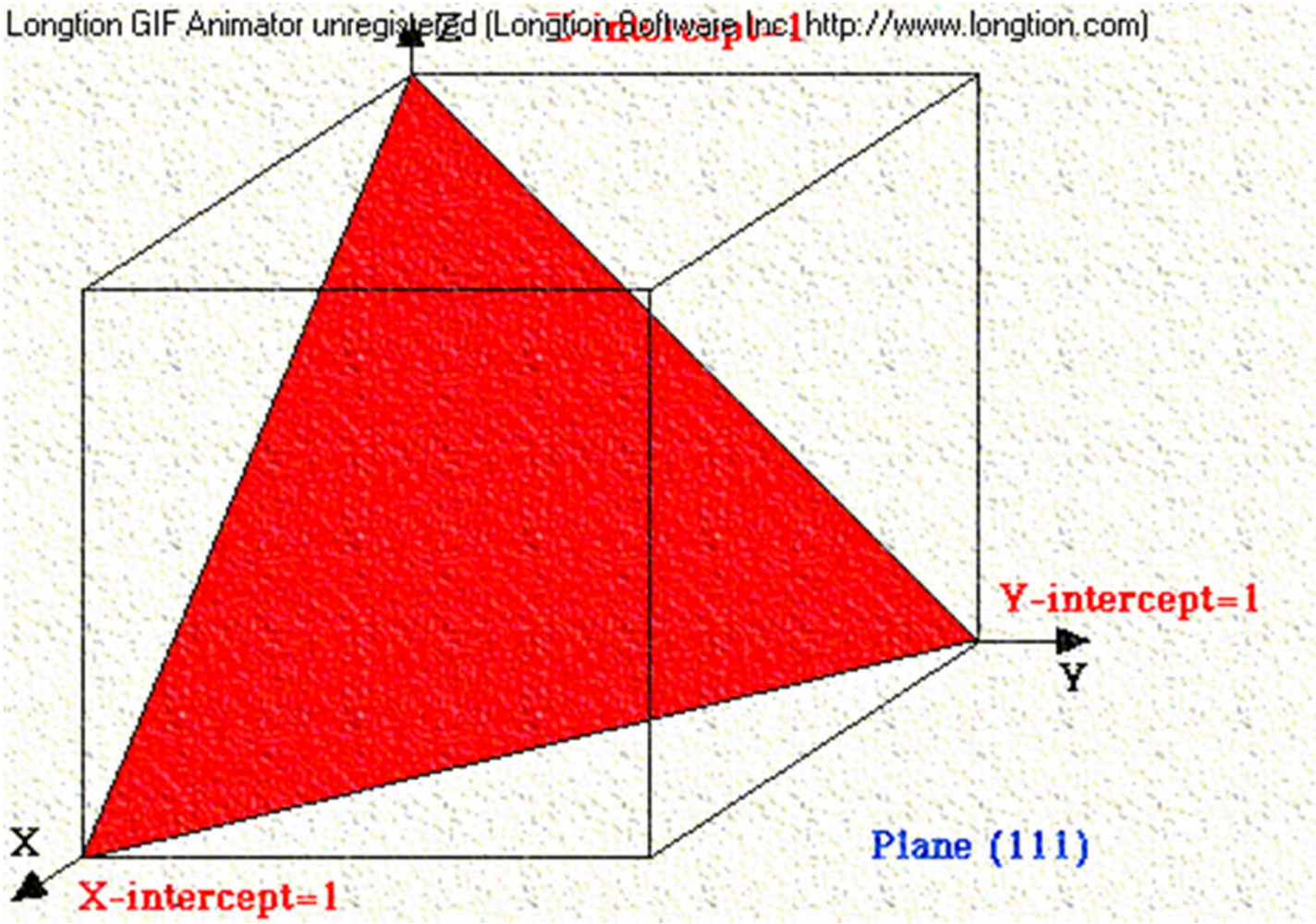
(111)



($\bar{1}$00)

Miller indices and intercepts




Longtion GIF Animator unregistered (Longtion Software Inc http://www.longtion.com)
Z
Z-intercept=1
Y-intercept=1
Y
X
X-intercept=1
Plane (111)

Indices of a Family or Form

- Sometimes when the unit cell has rotational symmetry, several nonparallel planes may be equivalent by virtue of this symmetry, in which case it is convenient to lump all these planes in the same Miller Indices, but with curly brackets.

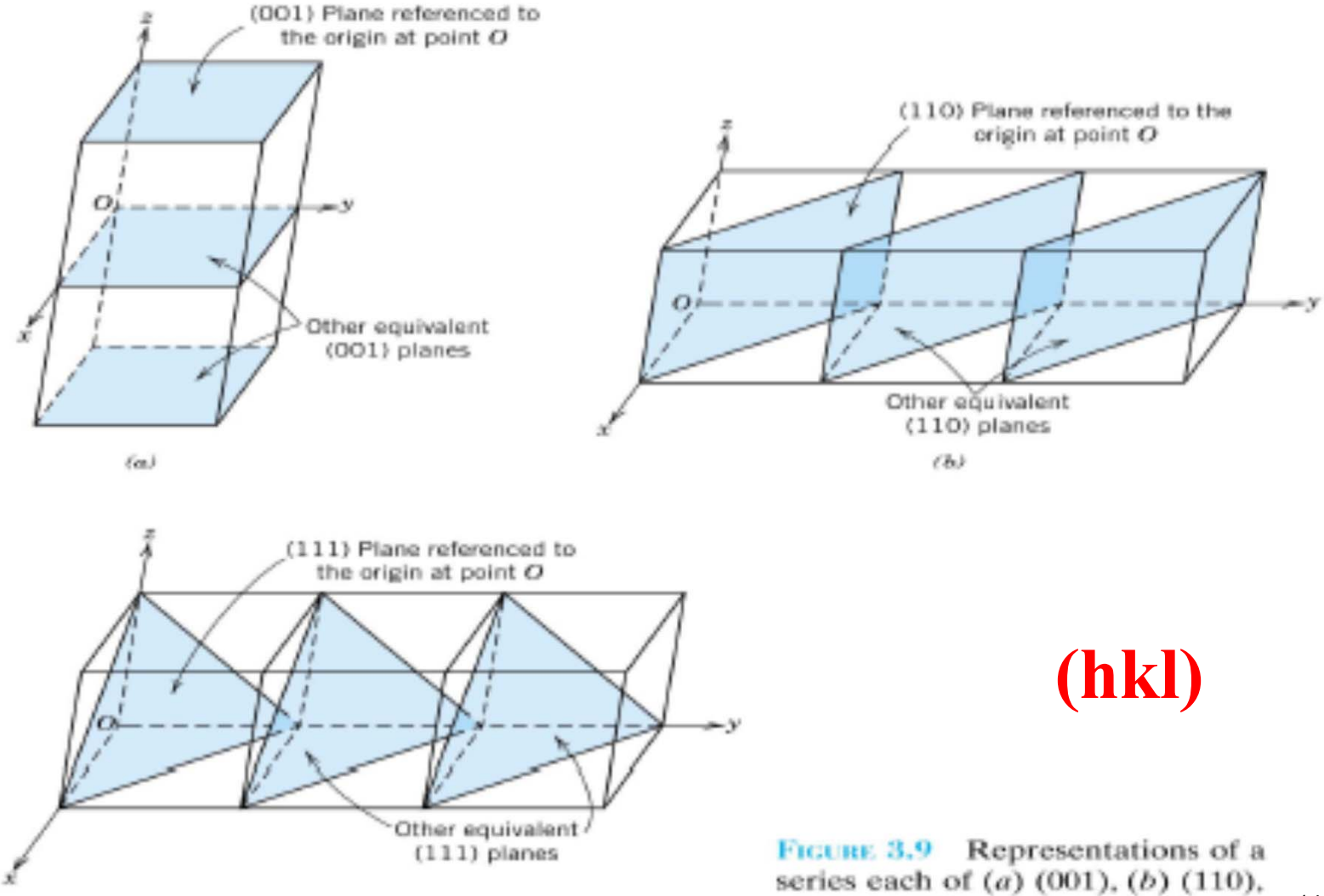
$$\{100\} \equiv (100),(010),(001),(0\,\bar{1}\,0),(00\,\bar{1}),(\bar{1}\,00)$$

$$\{111\} \equiv (111),(11\,\bar{1}),(1\,\bar{1}\,1),(\bar{1}\,11),(\bar{1}\;\bar{1}\;\bar{1}),(\bar{1}\;\bar{1}\,1),(\bar{1}\,1\,\bar{1}),(1\,\bar{1}\;\bar{1})$$

Thus indices {h,k,l} represent all the planes equivalent to the plane (hkl) through rotational symmetry.

THREE IMPORTANT CRYSTAL PLANES

- Parallel planes are equivalent



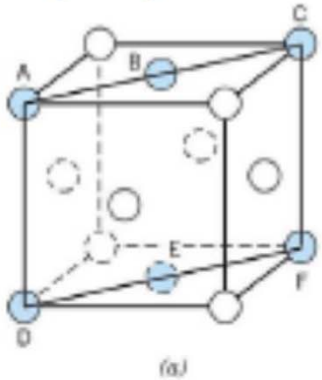
(hkl)

FIGURE 3.9 Representations of a series each of (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes.

FCC & BCC CRYSTAL PLANES

(Consider (110) plane)

- Atomic packing different in the two cases
- Family of planes: all planes that are crystallographically equivalent—that is having the same atomic packing, indicated as {hkl}
  - For example, {100} includes (100), (010), (001) planes
  - {110} includes (110), (101), (011), etc.



(a)

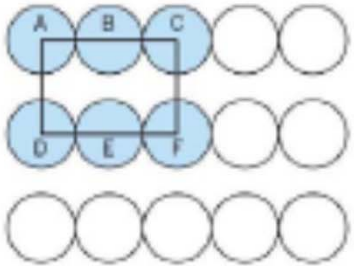
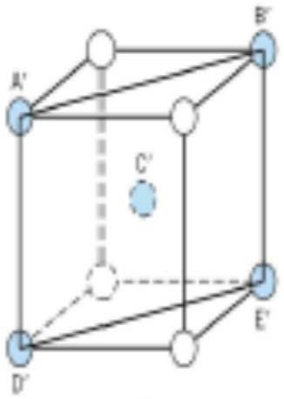
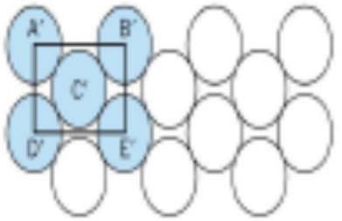


FIGURE 3.10 (*a*) Reduced-sphere FCC unit cell with (110) plane. (*b*) Atomic packing of an FCC (110) plane. Corresponding atom positions from (*a*) are indicated.

FIGURE 3.11 (*a*) Reduced-sphere BCC unit cell with (110) plane. (*b*) Atomic packing of a BCC (110) plane. Corresponding atom positions from (*a*) are indicated.



(a)



(b)

LINEAR & PLANAR DENSITIES

- Linear density (LD) = number of atoms centered on a direction vector / length of direction vector
  - LD (110) = 2 atoms/(4R) = 1/(2R)
- Planar density (PD) = number of atoms centered on a plane / area of plane
  - PD (110) = 2 atoms / [(4R)(2R√2)] = 2 atoms / ($8R^2\sqrt{2}$) = $1/(4R^2\sqrt{2})$
- LD and PD are important considerations during deformation and "slip"; planes tend to slip or slide along planes with high PD along directions with high LD

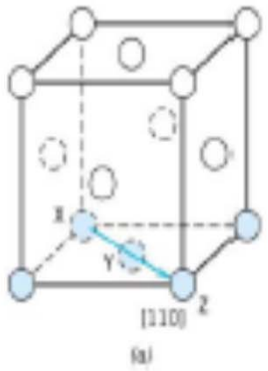


FIGURE 3.12 (*a*) Reduced-sphere FCC unit cell with the [110] direction indicated. (*b*) The bottom face-plane of the FCC unit cell in (*a*) on which is shown the atomic spacing in the [110] direction, through atoms labeled X, Y, and Z.

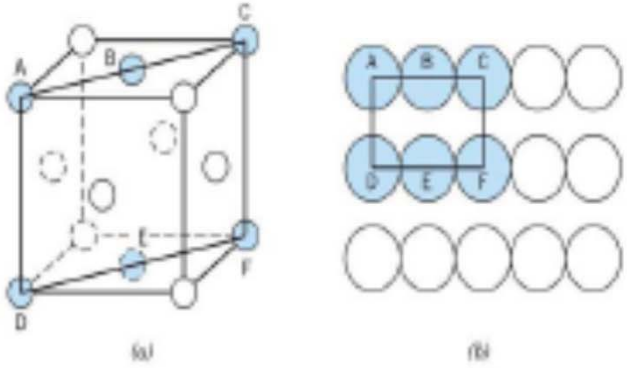


FIGURE 3.10 (*a*) Reduced-sphere FCC unit cell with (110) plane. (*b*) Atomic packing of an FCC (110) plane. Corresponding atom positions from (*a*) are indicated.