University of Anbar

College of Science

Department of Physics

فيزياء الحـالة الصلبة
Solid state Physics

المرحلة الرابعة

الكورس الاول

صلبة 1

Syllabus of this course   مفردات الكورس

1- crystal structure
2- x-ray diffraction
3- lattice vibration
4- thermal properties in solids
5- free electron model

Crystal Structure

2.1 Unit cell:

The smallest unit building in the crystal, consisting of atoms, ions, or molecules, whose repetition in space produces a crystal lattice.

The unit cell divided into two types:

a- Primitive unit cell. (خلية وحدة بدائية)

The parallelepiped (متوازي السطوح) shown in the Fig.(1) is called a primitive unit cell . A cell will fill all space by the repetition تكرار of suitable crystal translation operation.

A primitive cell is a minimum – volume cell, there is always one lattice point per primitive cell (or one atom), excluding hexagon باستثناء سداسي الزوايا, which contains two.
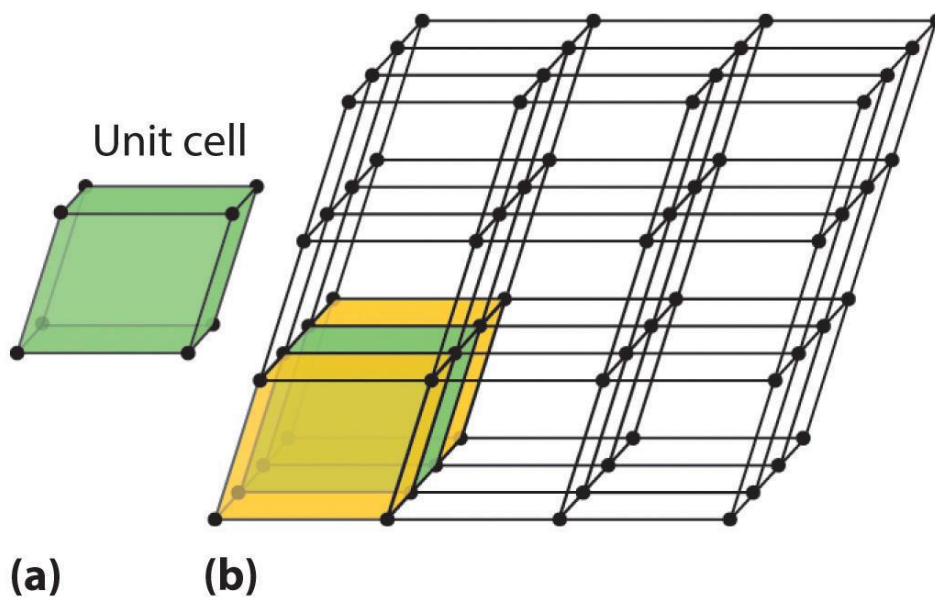

(a)   (b)

Fig. 1 The parallelepiped is a primitive unit cell, the total number of lattice points (or atoms) in the cell is one: 8 x ⅛=1. The volume of a parallelepiped with axes a, b, c is: $V = \vec{a} \times \vec{b}.\vec{c}$

Another way of choosing primitive cell is shown in Fig. (2). This is known as a Wigner-Seitz cell in 2-D.
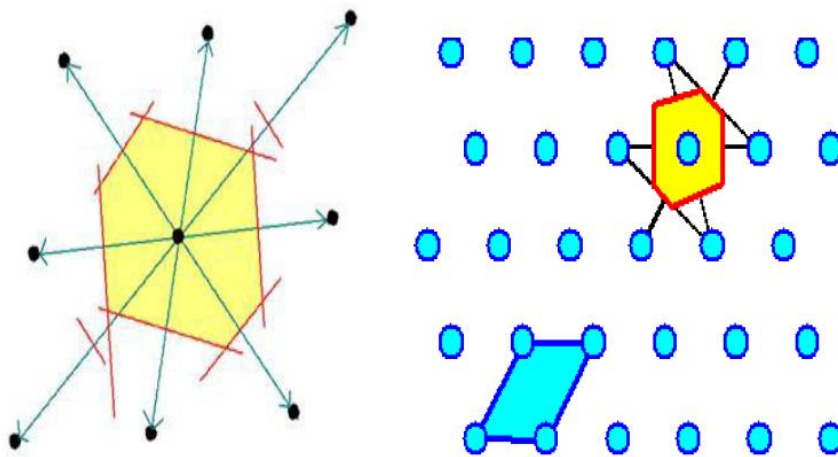
Fig. 2 Wigner-Seitz cell in 2-D (Elementary cell)

b- Non-primitive unit cell.

It is consisting of more than one lattice point (or atoms). Fig.(3) shows a group of primitive and non-primitive unit cells in 2 and 3-D:
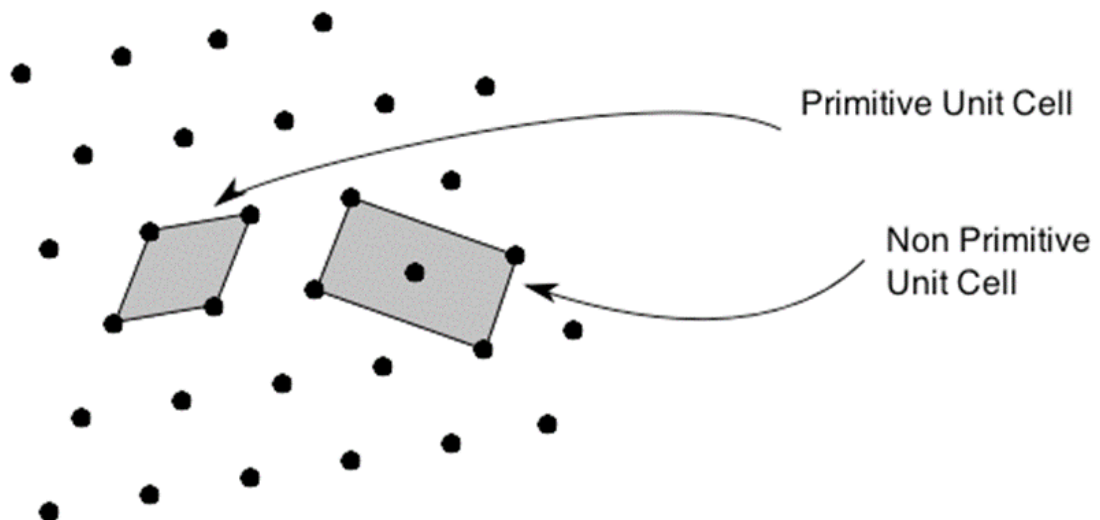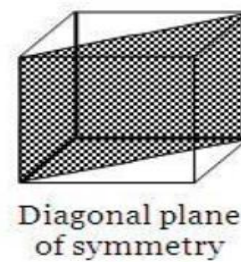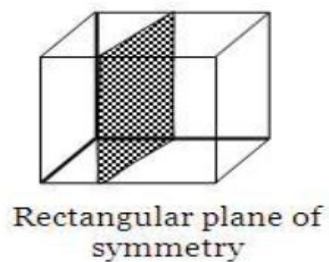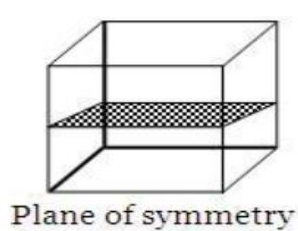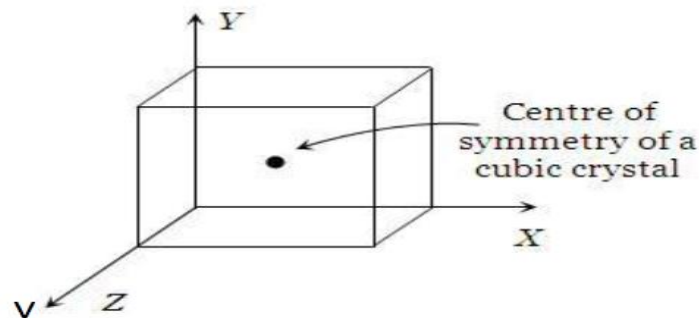

Fig. 3 Primitive and non-primitive unit cells.

2.2 Fundamental type of lattice:

Crystal lattice can be carried into themselves by the lattice translations (T) and by other symmetry operations [Rotation about an axis (1, 2, 3, 4, and 6-fold), Reflection at a plane, and Inversion through a point].

Centre of symmetry of a cubic crystal

Plane of symmetry　　　Rectangular plane of symmetry　　　Diagonal plane of symmetry

The crystal has n-fold axis of rotation if rotation through an angle ($\varnothing=2\pi/n$) carry the lattice into itself. Lattice can be found such that 1, 2, 3, 4, and 6-fold rotation axes carry the lattice into itself, corresponding to rotations by $\varnothing=2\pi$, $2\pi/2$, $2\pi/3$, $2\pi/4$, and $2\pi/6$ radians.

Axis of two fold symmetry　　　Axis of three fold symmetry
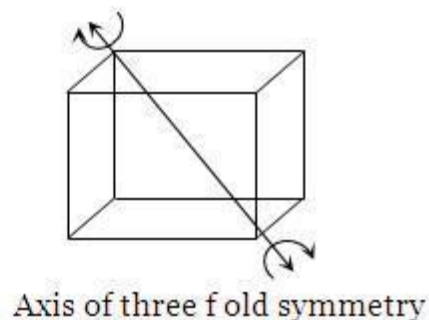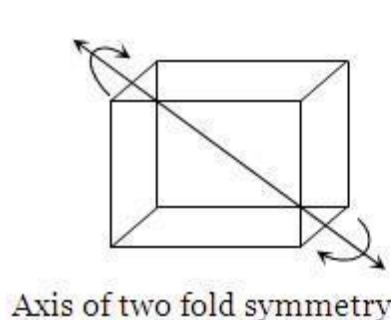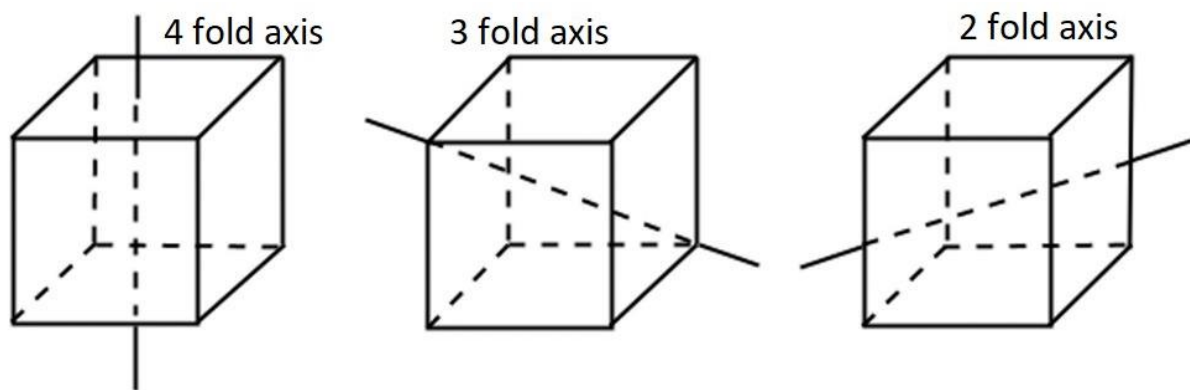
2.3 Three- dimensional lattice type: (the fourteen Bravais lattices and the seven crystal systems)

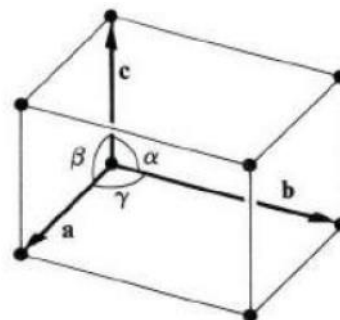There are only l4 different Bravais lattices in 3-D listed in Table (1). The general lattice is triclinic and 13 special lattices.

Unit cell specified محدد by the lengths of basis vectors a, b, and c; also by the angles between the vectors.

The 14 lattices (or crystal classes) are grouped into seven crystal systems as shown in figure 4, each specified by the shape and symmetry of the unit cell. These systems are the triclinic, monoclinic, orthorhombic, tetragonal, cubic, hexagonal, and the trigonal (or rhombohedral). In every case the cell is a parallelepiped whose sides are the bases a, b, c. The $\alpha, \beta,$ and $\gamma,$ opposite angles are called.

Trielinic

Simple monoclinic

Base-centered monoclinic

Simple orthorhombic

Base-centered orthorhombic

Body-centered orthorhombic

Face-centered orthorhombic

Simple tetragonal

Body-centered tetragonal

Simple cubic

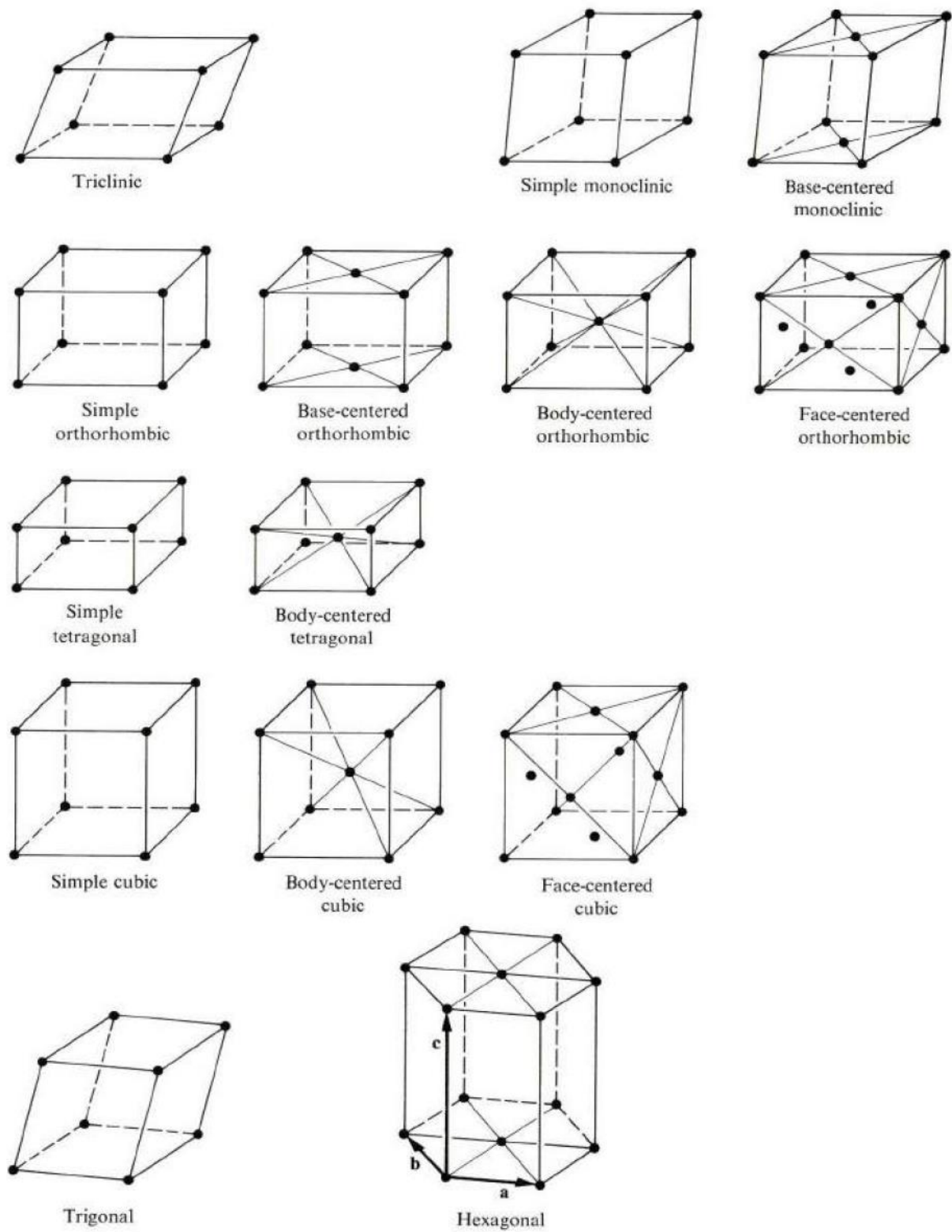Body-centered cubic

Face-centered cubic

Trigonal

Hexagonal

Figure　4 of the 14 Bravais lattices grouped into the 7 crystal systems

Table (1) **The Seven Crystal Systems And Fourteen Bravais Lattices In Three Dimensions**

System	Restrictions on Conventional Unit Cell Dimensions and Angles	Bravais Lattices in the System
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	P (primitive)
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	P (primitive) I (body-centered)
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	P (primitive) C (base-centered) I (body-centered) F (face-centered)
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	P (primitive) I (body-centered)
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	P (primitive or simple cubic) I (body-centered) F (face-centered)
Trigonal	$a = b = c$ $120° > \alpha = \beta = \gamma \neq 90°$	R (rhombohedral primitive)
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	P (primitive rhombohedral)

Fig.(5) shows the cubic space lattices. The characteristics of cubic lattices listed in Table (2).

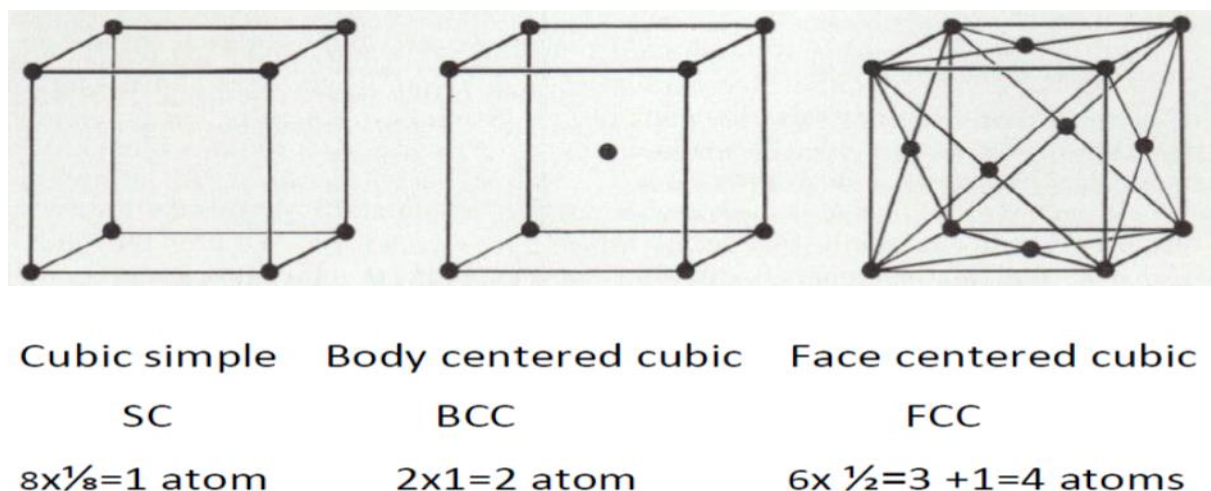Cubic simple   Body centered cubic   Face centered cubic

SC   BCC   FCC

$8 \times \frac{1}{8} = 1$ atom $2 \times 1 = 2$ atom $6 \times \frac{1}{2} = 3 + 1 = 4$ atoms

Figure 5 of Cubic space lattices.

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Table (2) Characteristics of cubic lattices.

	BCC I	SC p	FCC F
Volume unit cell	a^3	a^3	a^3
Number of lattice points per unit cell	2	1	4
Number of lattice points per volume	$\dfrac{2}{a^3}$	$\dfrac{1}{a^3}$	$\dfrac{4}{a^3}$
Number of points neighboring first class	8	6	12
Distance between adjacent points of first class	$\dfrac{\sqrt{3}}{2}a$	a	$\dfrac{1}{\sqrt{2}}a$
Number of points neighboring second-class	6	12	6
Distance between adjacent points of first class	a	$\sqrt{2}a$	a
Filling factor	0.68	0.52	0.74

simple cubic   body-centered cubic   face-centered cubic
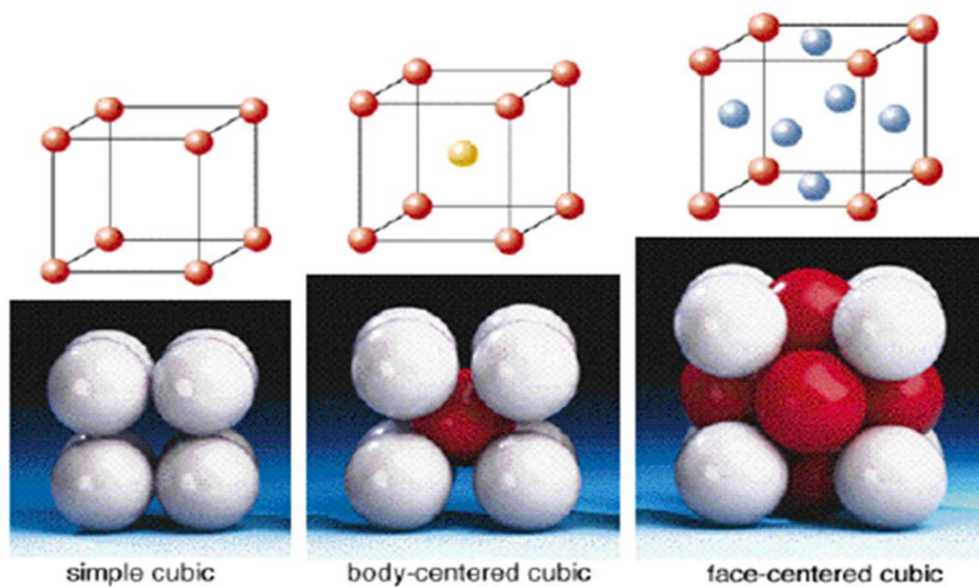
2.4 Index systems for crystal planes:

There are several methods to represent the crystalline planes ones intercepts method and Miller method (Miller indices are used to specify directions and planes in lattices or in crystals). The plane in Fig(6) intercepts the main crystallographic axes of the solid a,b,c at 3a,2b,2c.The reciprocals متبادل of these numbers are ⅓,½,½. The smallest three integers are 2,3,3 .The result, in closed in parentheses أقواس (hkl) and thus the indices of the plane are (233).
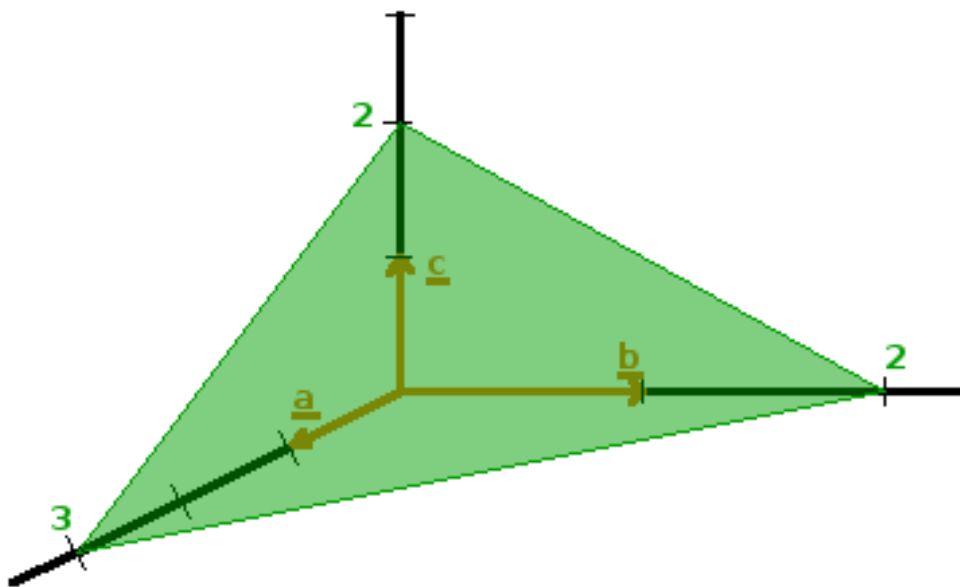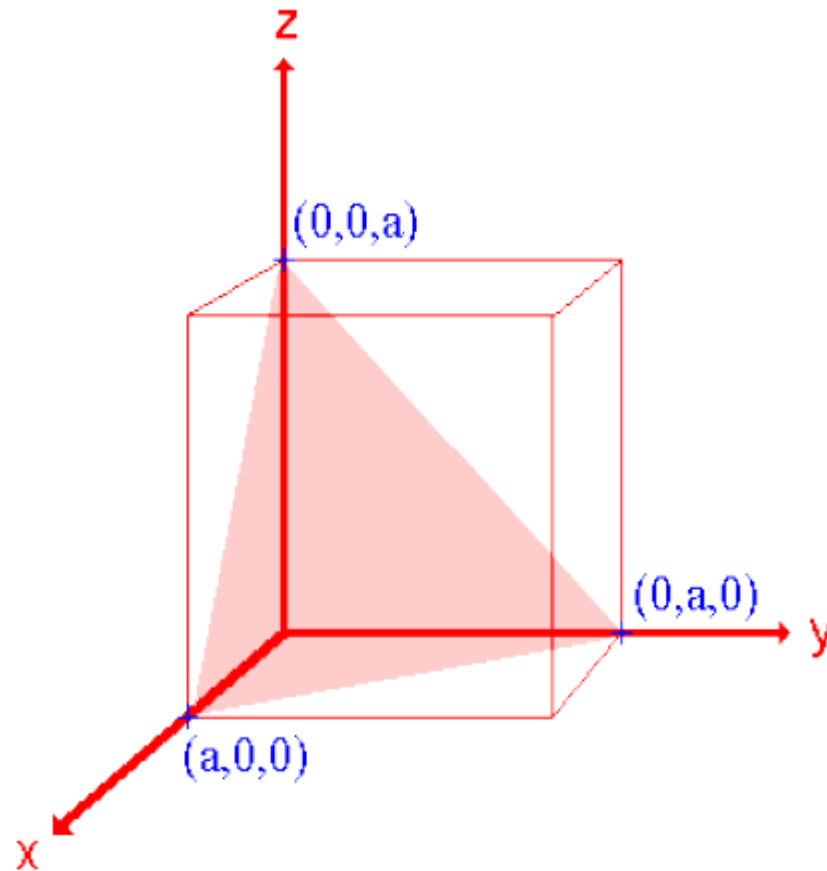

Fig. 6 Intercepts on the axes in terms of a,b,c

Notes

• (hkl) represents a plane

• {hkl} represents a family of planes or set of faces made equivalent by the symmetry of the system.

• [hkl] represents a direction

• <hkl> represents a family of directions
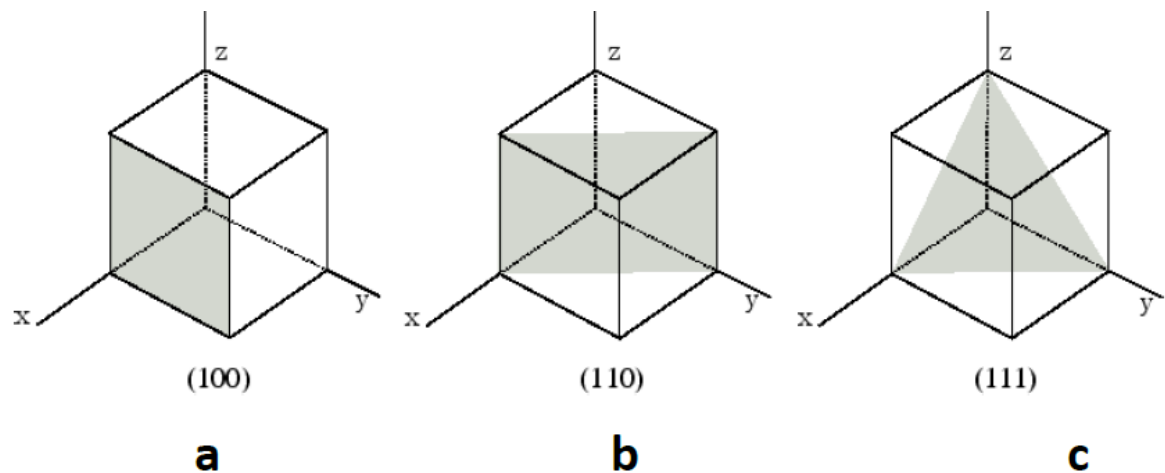
What's the Miller Index of this plane?

Exercise: What's the Miller Index of below planes?

Solution: These planes cuts all 3 crystallographic axes.

a• Intercepts = $(1, \infty, \infty) \rightarrow (100)$

b• Intercepts = $(1, 1, \infty) \rightarrow (110)$

c• Intercepts = $(1, 1, 1) \rightarrow (111)$

(100)   (110)   (111)

a   **b**   **c**

The indices (hkl) may denote a single plane or a set of crystal planes (see right below), when we speak of the (222) plane we mean a plane parallel to (111) but cutting the x,y,z (or a,b,c) axes at ½,½,½.

The indices of some important planes in cubic crystal are illustrated by Fig. 7.

$$\frac{1}{1/_2}, \frac{1}{1/_2}, \frac{1}{1/_2} = (222) = (111)$$

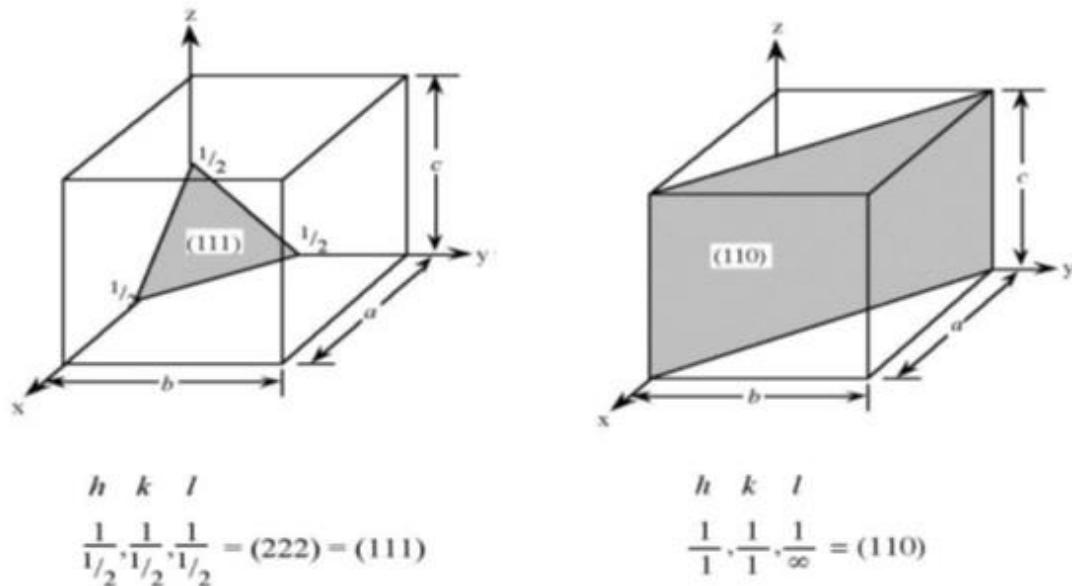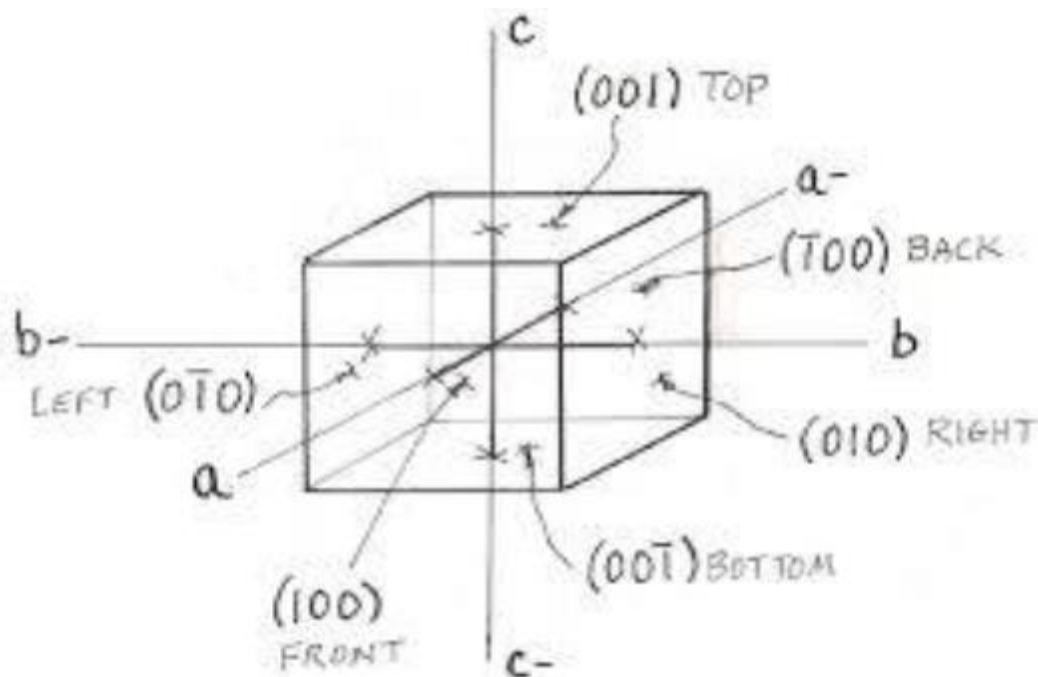$$\frac{1}{1}, \frac{1}{1}, \frac{1}{\infty} = (110)$$

Figure 7

The Miller indices are defined by

$$h = n\frac{a}{x}, \quad k = n\frac{b}{y}, \quad l = n\frac{c}{z}$$

Family of planes for cubic lattice

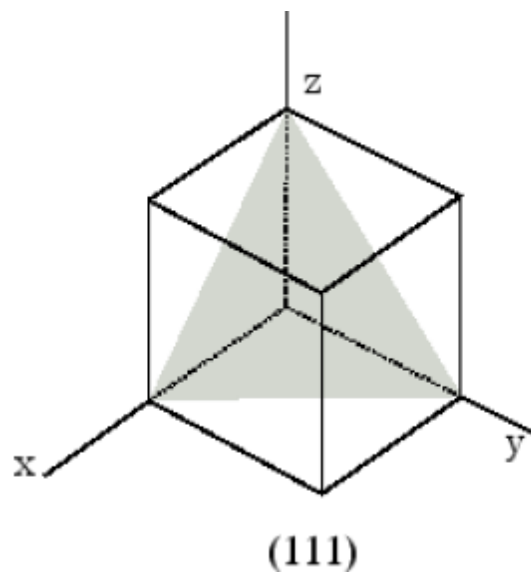$\{100\} = (100),(100), (010),(0\bar{1}0), (00\bar{1}), (001).$

Exercise: Draw the plane (111) in cubic unit cell. `

Solution: 1-Draw the cube and select the three axes and the origin

2- Take the inverted of miller indices

$$\frac{1}{1}, \quad \frac{1}{1}, \quad \frac{1}{1},$$

x=1 , y =1 , z= 1 as shown

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(111)

Homework(1): Draw the plane ($\bar{1}00$) in cubic unit cell.?

2.5 Angle between two planes:

To find the angle between two planes you must know Miller indices for each plane of indices

To find a relationship symbolized the first plane

$\vec{A}=h_1u_1+k_1v_1+l_1w_1$ and for 2nd plane
$\vec{B}=h_2u_2+k_2v_2+l_2w_2$

$\vec{A}.\vec{B}=|A||B|\cos\theta$

Taking into account that:

$u_1.u_2= v_1.v_2= w_1.w_2=1$

$u_1.v_2 = u_1.w_2= v_1.u_2 = v_1.w_2= w_1.u_2=w_1.v_2 = 0$

We find

$\cos\theta = h_1h_2+k_1k_2+l_1l_2 \; / \; [(h_1{}^2+k_1{}^2+l_1{}^2)(h_2{}^2+k_2{}^2+l_2{}^2)]^{\frac{1}{2}}$

Homework(2): Calculate the angle between the planes (100), (010).

Note: The general relation between inter planar spacing d_{hkl} and Miller indices (hkl) is :

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

Exercise:
Find the inter planar distance for a plane (100) in SC , if a=b=c=4A^0

Solution:

The inter planar distance for SC become:

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

$$\frac{1}{d_{hkl}^2} = \frac{1^2}{4^2} + \frac{0^2}{4^2} + \frac{0^2}{4^2} \quad , \quad \therefore \frac{1}{d_{hkl}^2} = \frac{1}{4^2} \quad , \text{Then}$$

$$d=4$$

References

1-　Charles Kittel - Introduction to Solid State Physics-Wiley (2005)
2-　 J. S. Blakemore - Solid State Physics-Cambridge University Press (1985)
3-　M. A. OMAR Elementary-solid-state-physics