Crystal Lattice

The specific properties of crystals are due to the symmetry and anisotropy of crystalline medium. A perfect crystal represents in a three-dimensional space the repetition of a small part of a crystalline lattice, which is called the *elementary cell.*

With every point of an elementary cell, a set of atoms called *basis* is associated.

The crystalline structure is formed by motion of a basis in all three directions.

Translation symmetry

In accordance with it, three translations vectors **a**, **b** and **c** can be chosen in such a way that we can define the translation operator as follows:

$$\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$$

n_1, n_2, n_3 are arbitrary integers, **a**, **b,** and **c** are the translation vectors along the sides of elementary parallelepiped cell

The real crystal lattice is formed when the basis is connected with an arbitrary point in identical way. Thus:

Lattice plus basis = the crystalline structure

Vectors of primitive translations are often chosen as orts of *crystallographic* coordinate axes. The minimal quantity needed for determination of the crystalline structure is called the *primitive basis.*

In order to describe the structure of a crystal you are to determine the crystal lattice, to choose crystallographic coordinate axes, to find the basis and a set of symmetry operations, which can produce translation of the crystalline structure.

The set of symmetry transformations relative certain point of a lattice when the late is transformed in it is called the *local group of symmetry* of a crystalline lattice.

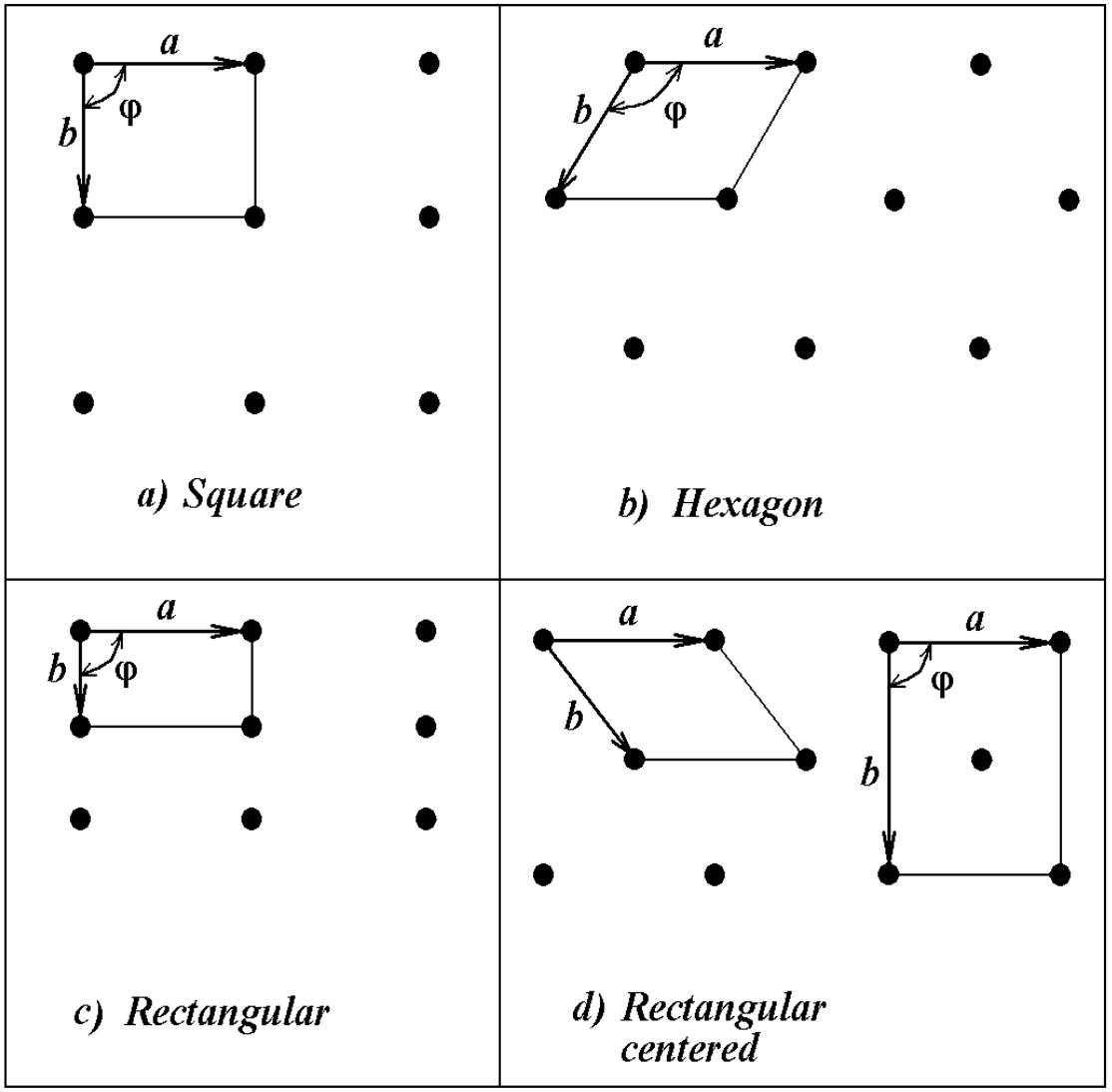
Crystal Lattice

In order to build up the two-dimensional lattice, you have to choose translation vectors **a** and **b** and an angle φ between them. The lengths of translation vectors **a** and **b** and the angle φ between them can be of any magnitude.

The restrictions of the vectors **a** and **b** is due to symmetry requirements and lead to a special type of a crystal lattice.

There are five types of the Bravais lattices.

Basic two-dimensional lattices



Oblique:
Parallelogram
$a \neq b$, $\varphi \neq 90°$

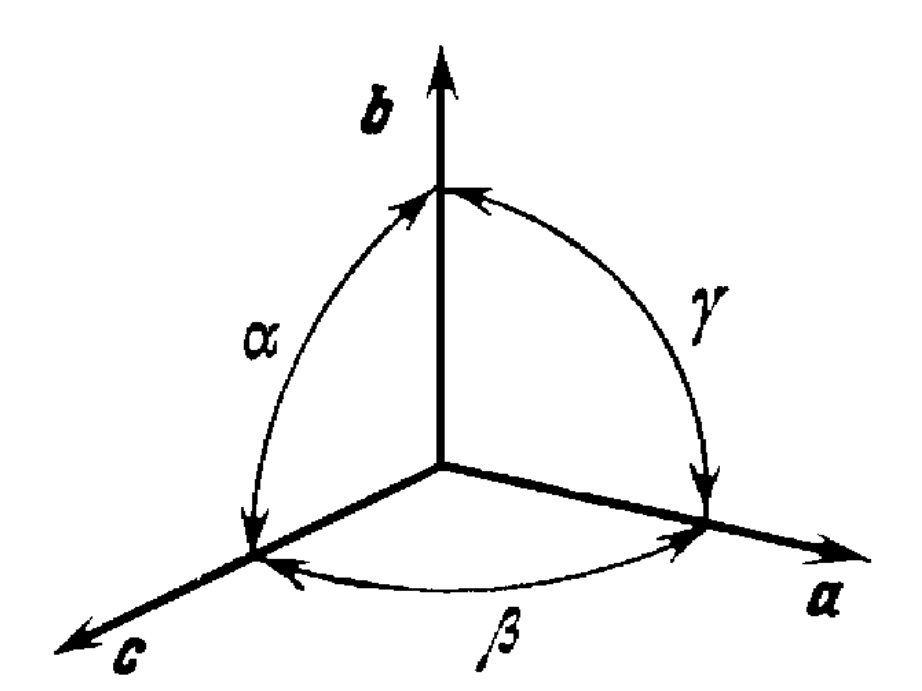
Square: $a = b$, $\varphi = 90°$

Hexagonal:
60°-rhomb $a = b$,
$\varphi = 120°$

Primitive rectangular:
rectangle a $\neq b$, $\varphi = 90°$

Centered rectangular:
rectangle $a \neq b$, $\varphi = 90°$

Tree-Dimensional Crystal Lattice

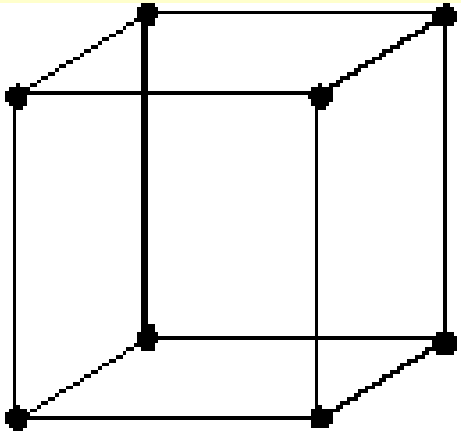


There are fourteen three-dimensional lattices called the **Brave lattices**.

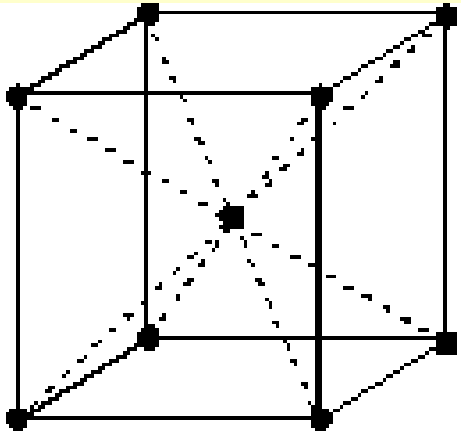
Fourteen Bravais lattices are subdivided into seven systems.

Each system is characterized by axes ***a, b, c,*** and angles α, β, γ

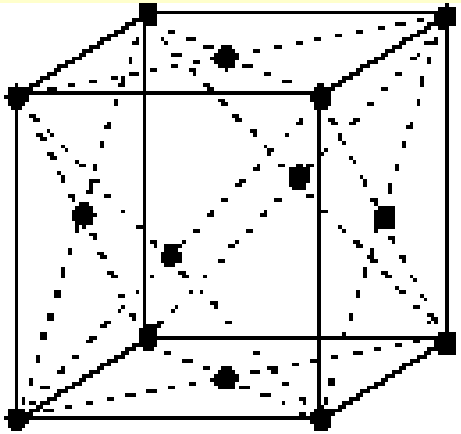
Cubic system



Cubic *P*



Cubic *I*

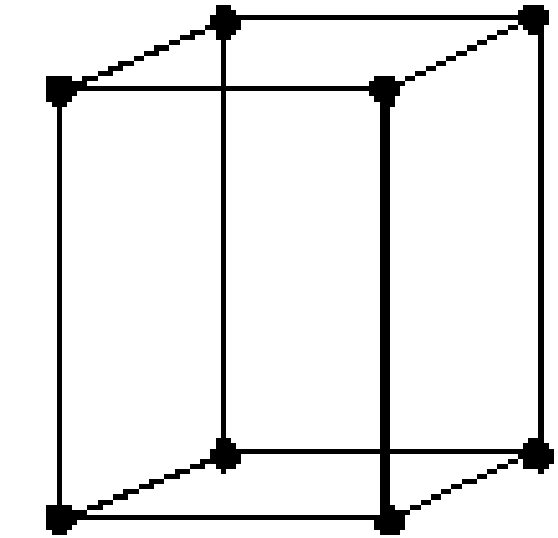


Cubic *F*

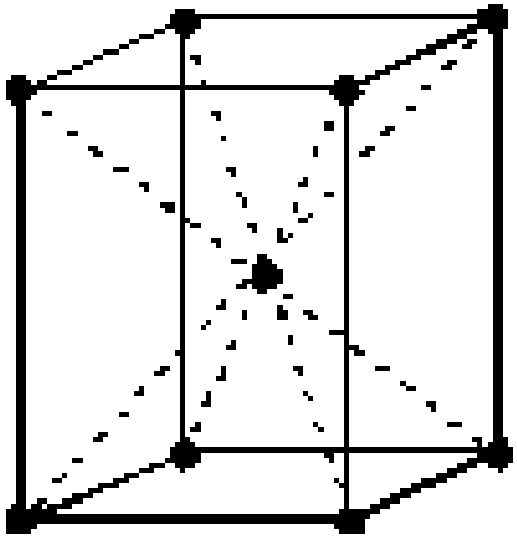
$$a = b = c; \alpha = \beta = \gamma = 90^\circ$$

P – symbol of a primitive lattice,
I – a bulk-centered cell, F – a face-centered cell

Tetragonal system



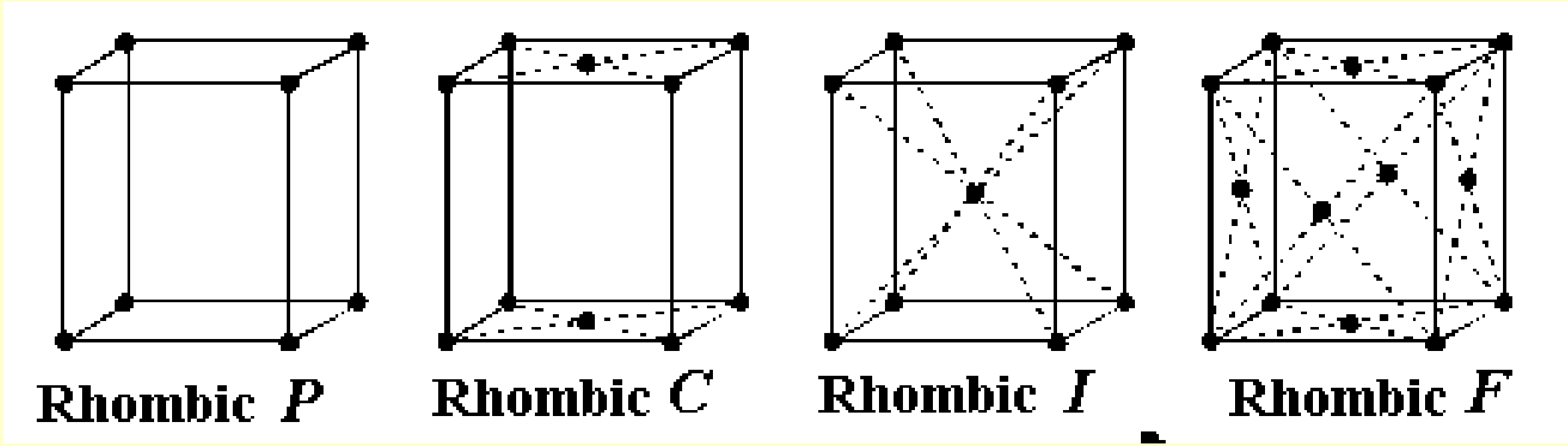
Tetragonal *P*



Tetragonal *I*

$$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$$

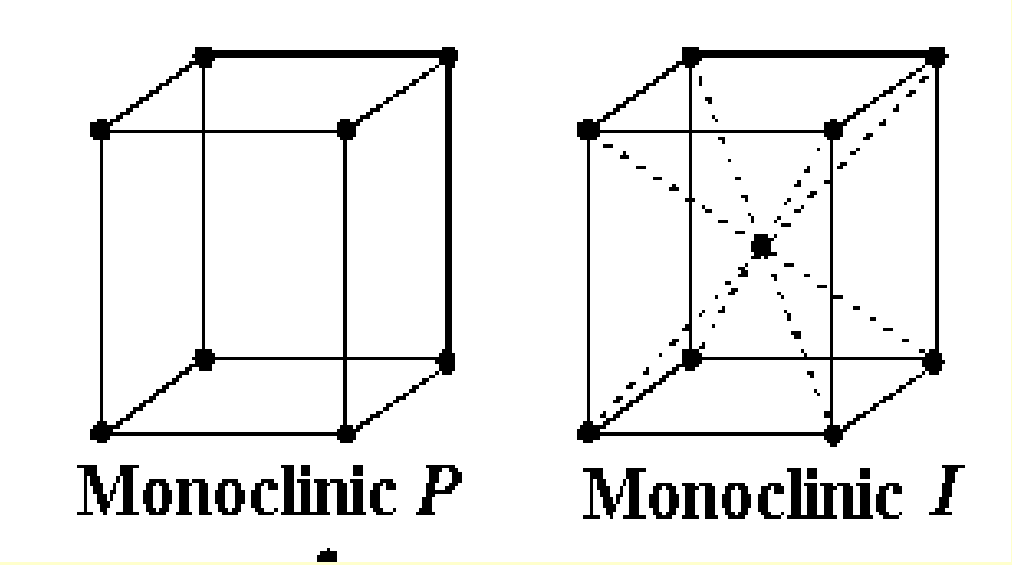
Rhombic system



$$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$$

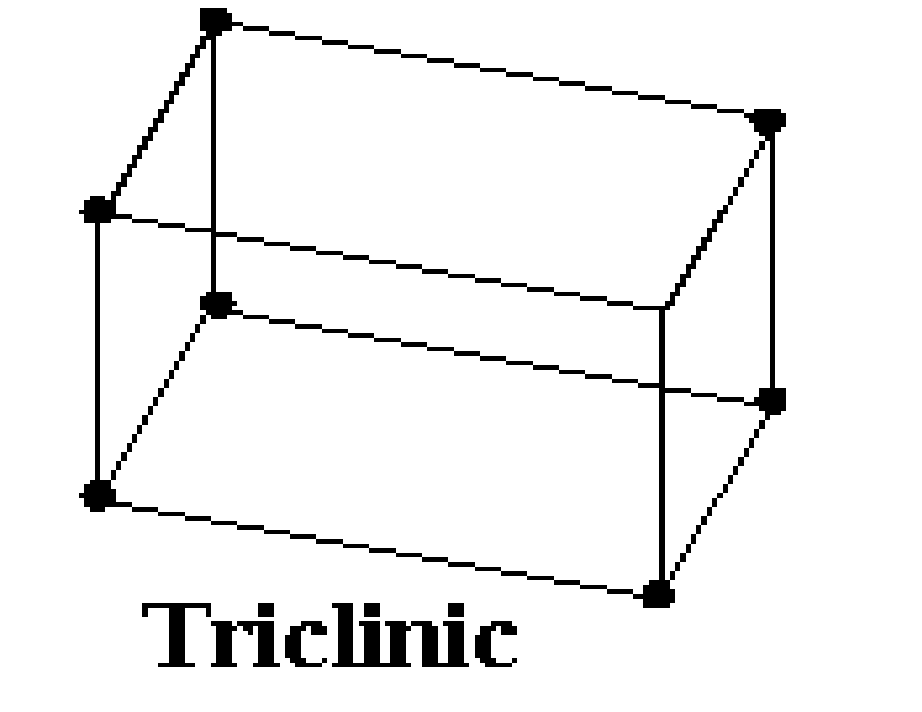
C – a base-centered cell

Monoclinic system



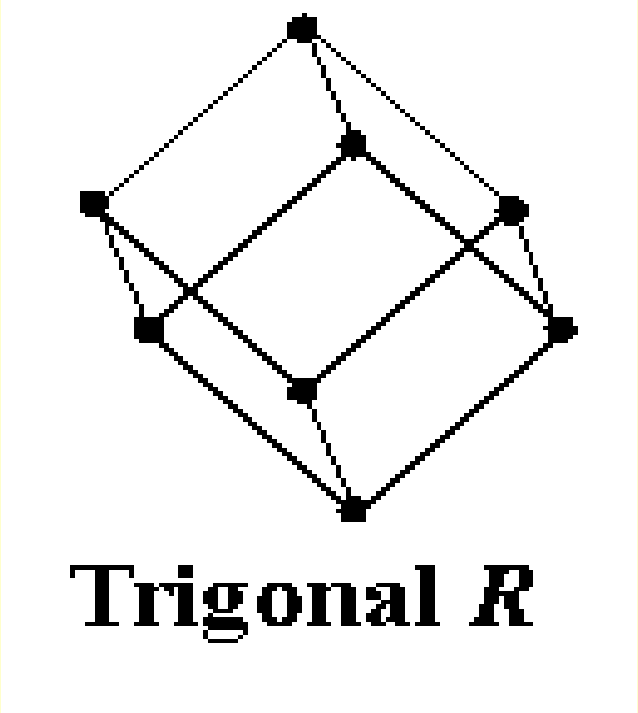
$$a \neq b \neq c; \quad \alpha = \gamma = 90° \neq \beta$$

Triclinic system



$$a \neq b \neq c; \alpha \neq \beta \neq \gamma$$

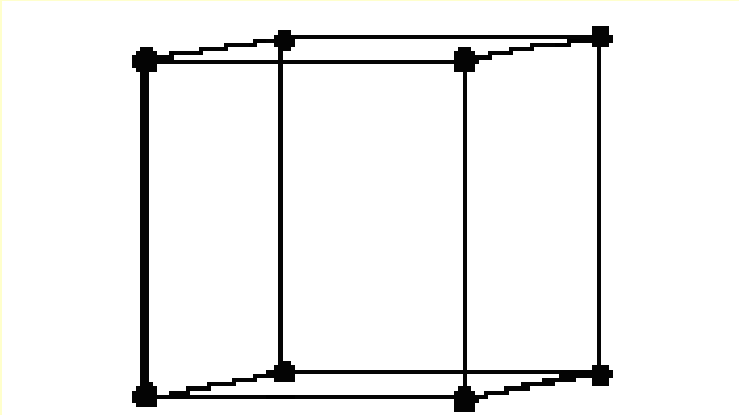
Trigonal system



$$a = b = c; \alpha = \beta = \gamma < 120°, \neq 90°$$

Rhombohedral *R*

Hexagonal system

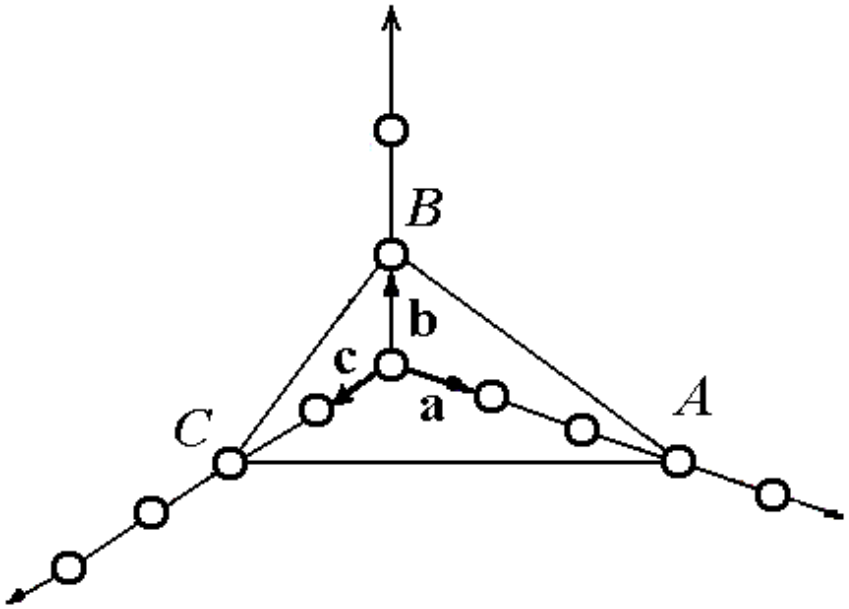


$$a = b \neq c;\ \alpha = \beta = 90^\circ, \gamma = 120^\circ$$

Labeling crystal planes

To describe the orientation of crystallographic planes and direction in a crystal,
the *Miller indices* are used.

Having described what is meant by the crystal lattice, how can we use this concept to label a crystal plane?
A general prescription, first suggested
By William Miller in 1839, is as follows:

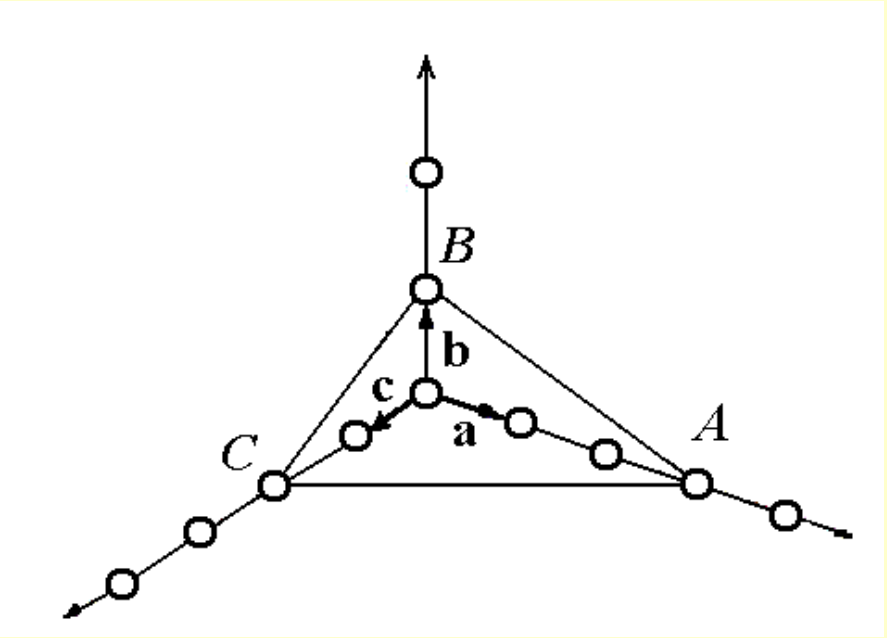


The position of the planes ABC is given by the integers ***h, k, l,*** which are determined as follows

$$h : k : l = \frac{1}{n_1} : \frac{1}{n_2} : \frac{1}{n_3}$$

h, k, and *l* are the minimal integers that satisfy this equation. The plane that is chosen in accordance with that condition is designated by the *Miller indices (hkl).*

A general prescription, first suggested By William Miller in 1839, is as follows:

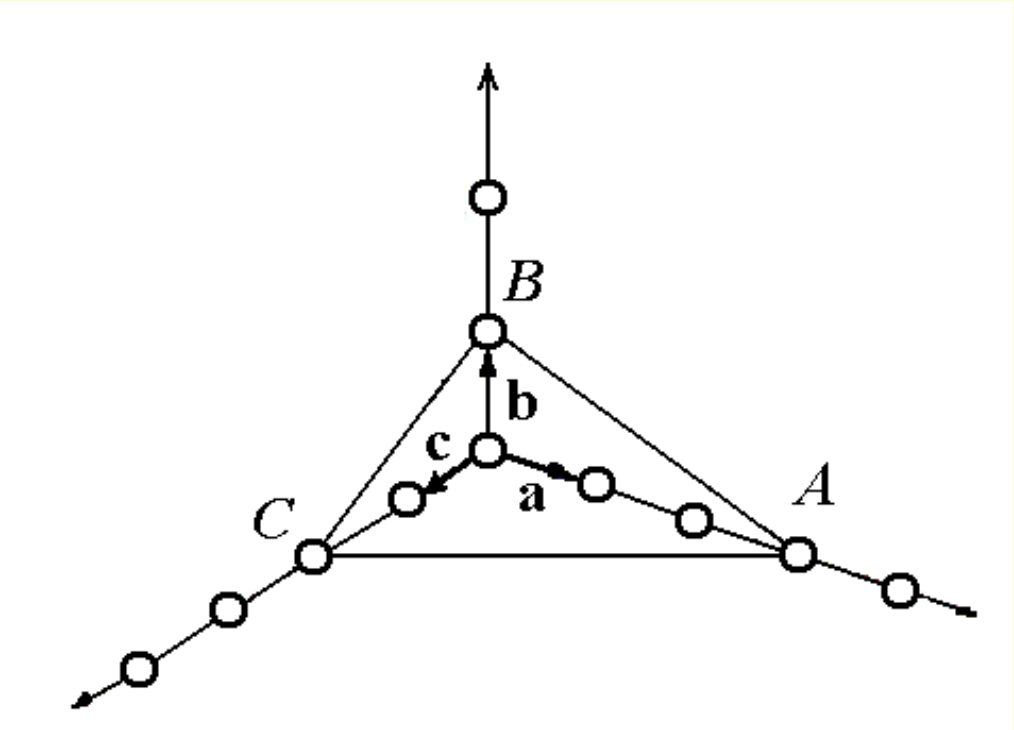


(1) determine the intercepts on the axes in units of the primitive vectors **a, b** and **c**;

(2) take the reciprocal of each number;

(3) reduce these numbers to the three smallest integers *h*, *k* and *l*, having the same ratio;

(4) the values *h, k* and *l* are called the Miller indices and are enclosed in parentheses (*hkl*) to denote a crystal plane.



Determine the Miller indices for the plane shown in Fig.

Following the procedure outlined above:

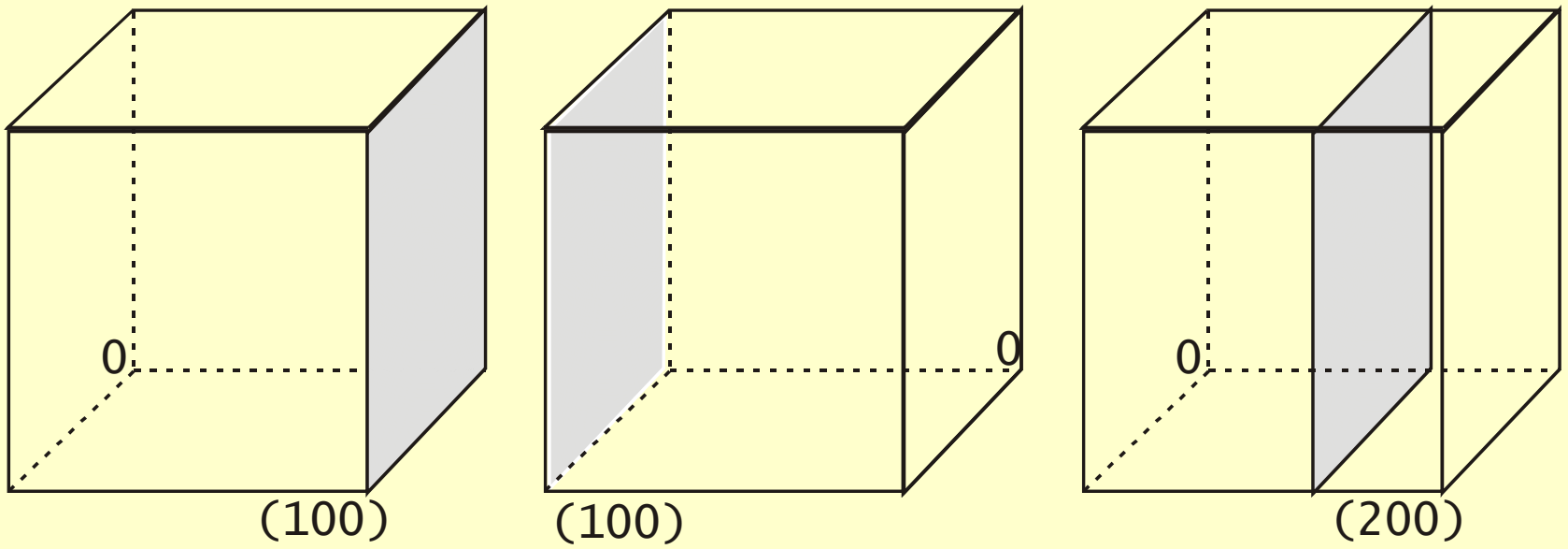
(1) The intercepts on the axes in units of **a, b** and **c** are 3, 1 and 2, respectively.

(2) The reciprocals are

$$h:k:l=\frac{1}{3}:\frac{1}{1}:\frac{1}{2}=2:6:3$$

(3) The smallest set of integers with the same common ratio are 2, 6, 3.

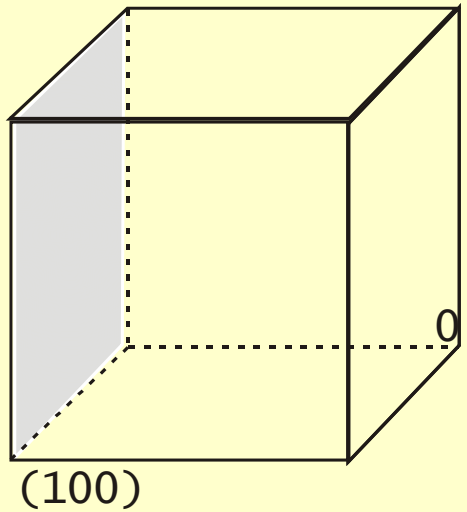
(4) Consequently, we can label the plane a (263) plane.



If a plane is parallel to a particular axis, the corresponding Miler index is zero. (In effect, we are saying that the intercept with the axis occurs at infinity and the reciprocal of infinity is zero.)

If a plane intercepts an axis at a negative value, this is denoted by placing a bar over the corresponding Miler index, i.e.

$(\bar{1}00)$



The Miller indices *(hkl)* do not actually denote a single plane but a set of parallel planes.