Ans. (*a*) Miller indices and their calculation. The position and orientation of a crystal plane are determined by any three points in the plane provided the points are not collinear. If each point lies on a crystal axis, the plane can be specified by giving the position of the points along the axes in terms of the lattice constants. For example, if the points have the co-ordinates (2, 0, 0) (0, 3, 0) (0, 0, 1) relative to axis vectors from some origin as shown in Fig. 1.29, the plane may be specified by three numbers 2, 3, 1.

However, in crystal structure analysis it is more useful to specify the orientation of a plane in accordance with the following rules.

(*i*) Find the intercepts of the plane on the crystal axes $\vec{a}$, $\vec{b}$ and $\vec{c}$ in terms of the lattice constant. The axes may be primitive or non-primitive.

(*ii*) Take the reciprocals of these numbers and then reduce to the *smallest* three integers having the same ratio. Denote the result as (*h k l*) enclosed in parentheses.

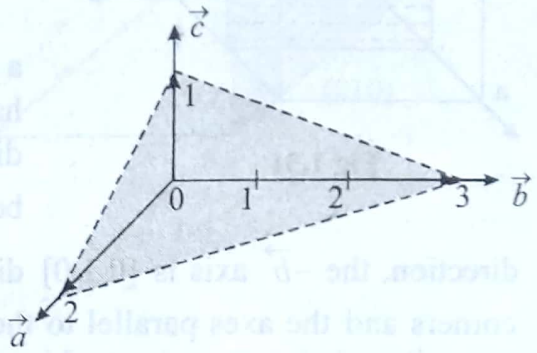

Fig 1.29

The three integers *h*, *k* and *l* are called **Miller indices.**

Orientation of a plane by Miller indices. The Miller indices (*h k l*) may denote a single plane or a set of parallel planes. If a plane cuts an axis on the **negative** side of the origin, the index is

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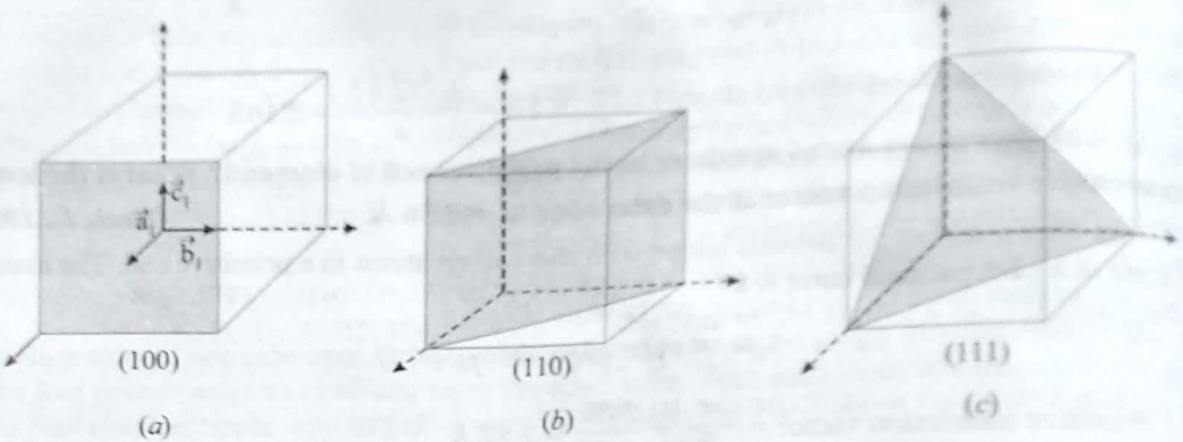
negative and denoted as $(h\,\bar{k}\,l)$ by placing a minus (–) sign above the corresponding index (in this case $\bar{k}$). For an intercept at infinity the corresponding index is **zero**. For the crystal plane having intercepts $2a$, $3b$ and c on the crystal axes $\vec{a}$, $\vec{b}$ and $\vec{c}$, the reciprocals of the numbers 2, 3 and 1 are $\frac{1}{2}$, $\frac{1}{3}$ and 1. The smallest three integers having the same ratio are 3, 2 and 6. The plane is, therefore, referred to as (3 2 6) plane.



(*a*) (*b*) (*c*)

Fig 1.30

The six faces of a cubical crystal are (1 0 0) (0 1 0) (0 0 1) $(\bar{1}\,0\,0)$ $(0\,\bar{1}\,0)$ $(0\,0\,\bar{1})$. From a crystallographic point of view many planes in a lattice are equivalent *i.e.*, a plane with given Miller indices can be shifted about in the lattice simply by a choice of the position and orientation of the unit cell. The indices of such equivalent planes are enclosed in braces {} instead of in parenthesis ( ). For example, all the six cube faces are crystallographically equivalent because the unit cell can be rotated in various directions and still appear the same. The six equivalent faces are collectively designated as {1 0 0}.

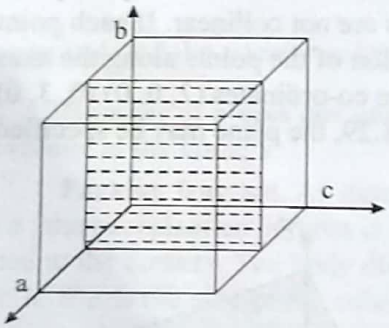


Fig 1.31

The faces (1 0 0) (1 1 0) and (1 1 1) of a cubic crystal are shown in Fig. 1.30 (*a*), (*b*) and (*c*) respectively. The plane shown in Fig. 1.31 is (2 0 0) plane. It is parallel to (1 0 0) and $(\bar{1}\,0\,0)$ plane. Its intercepts on crystal axes $\vec{a}$, $\vec{b}$ and $\vec{c}$ are $\frac{1}{2}a$, ∞ and ∞ respectively.

Miller indices of a direction. The *indices of a direction* in a crystal are expressed as the set of the smallest integers which have the same ratio as the components of a vector in the desired direction referred to the axes vectors. The integers are written between square brackets as [*h k l*]. The $\vec{a}$ axis is the [1 0 0] direction, the $-\vec{b}$ axis is [0 $\bar{1}$ 0] direction. In a cubic crystal if we take the origin at one of the corners and the axes parallel to the edges, the body diagonal would be represented as [1 1 1]. Similarly the $\vec{a}$ axis is [1 0 0] direction, the $\vec{b}$ axis [0 1 0] direction and the $\vec{c}$ axis [0 0 1] direction. In a cubic crystal the direction [*h k l*] is always perpendicular to a plane (*h k l*) having the same indices.

Important features. (*i*) If a plane is parallel to a co-ordinate axis, then the intercept of this plane is *infinity* and hence its Miller index is *zero*.

(*ii*) A plane passing through the origin is defined in terms of a parallel plane having non-zero intercept.

(*iii*) Parallel planes equally spaced have the same index numbers.

(*iv*) It is the ratio of the indices which is important and determines a plane. For example, (2 4 6) and (1 2 3) represent the same plane.

(*v*) The direction $[h\ k\ l]$ is perpendicular to the plane $(h\ k\ l)$. [For proof see **Q 1.23**].

(*b*) **Purpose of taking reciprocals.** The purpose of taking reciprocals to find Miller indices is to bring all the planes inside a single unit cell so that we can discuss all crystal planes in terms of the planes passing through the single unit cell. As the entire crystal can be generated from a single unit cell, the unit cell is studied as a representative of the whole crystal. The unit cell is equivalent to the molecule. Just as we write the chemical equation for a single molecule and this equation applies to the whole sample, similarly the study of the single unit cell gives the characteristics of the whole crystal.