EC-⑥

Subject : PHYSICS

Topic : Reciprocal Lattice

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Ans. Reciprocal lattice. Every crystal has two lattices associated with it, the crystal lattic direct space lattice) and the reciprocal lattice.

The concept of reciprocal lattice was devised for the purpose of tabulating two impo properties of crystal planes; their *slope* and their *interplanar spacing*.

Each set of parallel planes in a direct lattice can be represented by a *normal* to these pl having length equal to the reciprocal of the interplanar spacing. The normals are drawn reference to any arbitrary origin and points are marked at their ends. *These points form a reg arrangement which is called reciprocal lattice.* Thus each point in a reciprocal lattice representative point of a particular parallel set of planes. It is easier to deal with such points tha deal with set of planes. This is why we use reciprocal lattice.

Thus reciprocal lattice vector is a vector whose magnitude is equal to the reciprocal of inter planar spacing i.e., $\frac{1}{d_{hkl}}$ *and direction is parallel to the normal to (hkl) plane.*

Why reciprocal lattice is so named? The reciprocal lattice is so named because the len assigned to each normal representing the reciprocal lattice is proportional to the reciprocal of interplanar spacing of that plane in ordinary space.

Primitive translation vectors of reciprocal lattice. Let $\vec{a}$, $\vec{b}$, $\vec{c}$ be the primitive transla vectors of a direct space lattice for a crystal forming a primitive unit cell. The volume of this cell is given by

$$V = \vec{a}\cdot(\vec{b}\times\vec{c}) = \vec{b}\cdot(\vec{c}\times\vec{a}) = \vec{c}\cdot(\vec{a}\times\vec{b})$$

The vectors given by

$$\vec{A} = 2\pi\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

$$\vec{B} = 2\pi\frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})}$$

and $$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})}$$

are known as *reciprocal lattice vectors* or *primitive translation vectors of reciprocal lattice.*

Reciprocal lattice vectors are orthogonal to two axis vectors. Each of the reciprocal lattice vectors is *orthogonal* to two of the axis vectors of a direct space lattice of the crystal as proved below.

$$\vec{A} \cdot \vec{a} = 2\pi, \; \vec{A} \cdot \vec{b} = 0 \text{ and } \vec{A} \cdot \vec{c} = 0$$

Thus $\vec{A}$ is normal to $\vec{b}$ and $\vec{c}$.

Similarly $$\vec{B} \cdot \vec{a} = 0, \; \vec{B} \cdot \vec{b} = 2\pi \text{ and } \vec{B} \cdot \vec{c} = 0$$

$\therefore$ $\vec{B}$ is normal to $\vec{a}$ and $\vec{c}$.

Also $$\vec{C} \cdot \vec{a} = 0, \; \vec{C} \cdot \vec{b} = 0 \text{ and } \vec{C} \cdot \vec{c} = 2\pi$$

$\therefore$ $\vec{C}$ is normal to $\vec{a}$ and $\vec{b}$.

Choosing $\vec{A}$, $\vec{B}$ and $\vec{C}$ as the primitive translation vectors of the reciprocal lattice (also known as reciprocal axes) we can construct the reciprocal lattice points or reciprocal lattice vectors given by

$$\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

where *hkl* are integers and define the co-ordinates of the point in the reciprocal space.

The crystal lattice is a lattice in *real or ordinary space* whereas reciprocal lattice is a lattice in the *reciprocal space or associated $\vec{k}$ space or Fourier space.* The wave vector $\vec{k}$ is always drawn in Fourier space. Vectors in the crystal lattice have dimensions of length $[L^1]$ and vectors in the reciprocal lattice have dimensions of 1/Length $[L^{-1}]$.

Construction of reciprocal lattice. A reciprocal lattice to direct lattice is constructed by the following method:

(*i*) Take origin at some arbitrary point.

(*ii*) From the origin draw normals to every set of parallel planes of direct lattice. The direction of the normal specifies the orientation of the plane and thus the two dimensional plane is represented by the normal which has only one dimension.

(*iii*) Take length of each normal equal to or 2π times the reciprocal of the interplanar spacing for the corresponding set of planes.

(*iv*) The terminal points of these normals form the reciprocal lattice because the distances in these lattices are the reciprocal to those in the direct crystal lattice.

As an example, consider a unit cell of a monoclinic crystal in which $a \neq b \neq c$; $\alpha = \gamma = 90°$ and $\beta > 90°$. Orient the unit cell in such a way that the $\vec{b}$ axis is perpendicular to the plane of the paper *i.e.*, the $\vec{a}$ and $\vec{c}$ axes lie in the plane of the paper (Fig. 2.10).

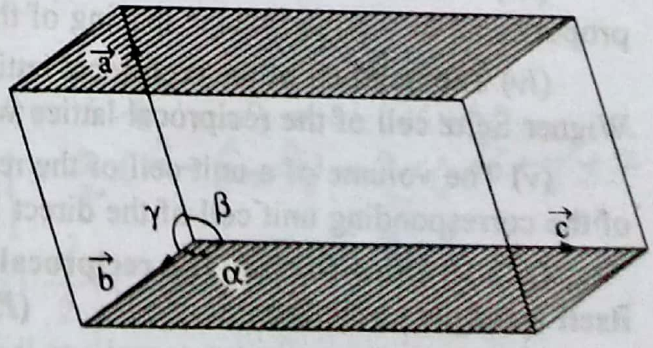

Fig. 2.10

Consider planes of the type (*h*0*l*) which are parallel to $\vec{b}$ axis (Fig. 2.11) and hence perpendicular to the plane of the paper. Therefore, the normal to these planes lies in the plane of the paper. The planes ($h0l$) being perpendicular to the plane of the paper are represented by lines. Th the line (101) in fact means the plane (101) and so on. (Fig. 2.11)

Taking the point of intersection of the three axes as the origin draw normals to the pla ($h\ 0\ l$) and take their lengths equal to $\frac{1}{d_{h0l}}$ where d_{h0l} is the interplanar spacing for the planes.

We know that (200) planes have half the interplanar spacing as compared to (100) planes, & reciprocal lattice point (200) is, therefore, twice as far away from the origin as the point (100). I this manner if we draw normals to the ($h\ k\ l$) planes, we get a three dimensional reciprocal lat

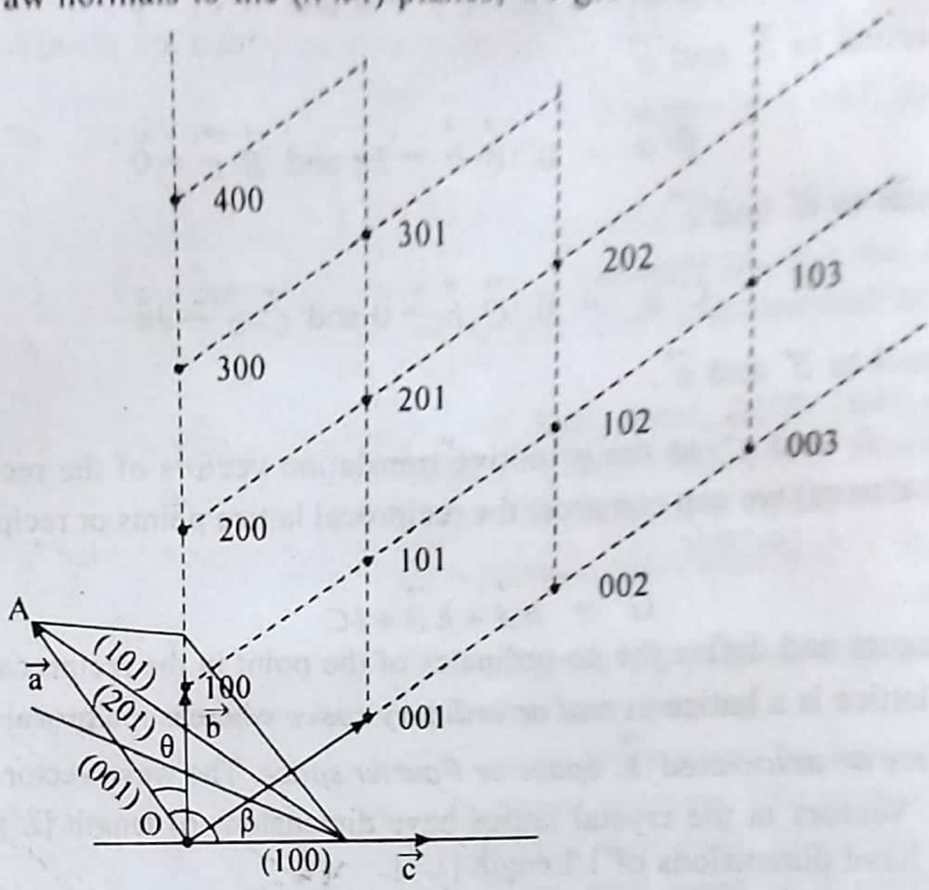

Fig. 2.11

Properties of reciprocal lattice. (*i*) The direct lattice is the reciprocal lattice to its ow reciprocal lattice. Simple cubic lattice is *self reciprocal* whereas *bcc* and *fcc* lattices are recipro of each other.

(*ii*) Each point in a reciprocal lattice corresponds to a particular set of parallel planes of th direct lattice.

(*iii*) The distance of a reciprocal lattice point from an arbitrarily fixed origin is inverse proportional to the interplanar spacing of the corresponding parallel planes of the direct lattice.

(*iv*) The unit cell of the reciprocal lattice is not necessarily a parallelopiped. We deal with th Wigner Seitz cell of the reciprocal lattice which constitutes the *Brillouin zone*.

(*v*) The volume of a unit cell of the reciprocal lattice is inversely proportional to the volum of the corresponding unit cell of the direct lattice.