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المحاضرة السادسة / مرحلة ثانية / علم المواد/ 2021-2022

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Out lines:-

Reciprocal Lattice

The geometrical structure factor

Introduction:-

There are two type of lattice are extremely important :

1. Reciprocal lattice .
2. Direct lattice (which is the Bravais lattice that determines a given reciprocal lattice).

• The diffraction pattern that is generated in X-ray diffraction is a representation of a "reciprocal lattice"

• X-ray diffraction results from scattering of atoms within any set of parallel planes in a crystal , it is practically difficult to trace the source of each scattering due to the overlap between levels in crystal.

• In order to know the source of each scattering, the reciprocal lattice can be used .

•The reciprocal lattice is of fundamental importance when considering periodic structures and processes in a crystal lattice where momentum is transferred (e.g. diffraction)

• The reciprocal lattice can be defined as an indefinite number of points arranged regularly and periodically in a three- dimensional space.

•The separation of the reciprocal lattice points (magnitude of the vector) is proportional to the reciprocal of the real separation between planes, i.e.

$$|\boldsymbol{G}| = \frac{\boldsymbol{2\pi}}{\boldsymbol{d}}$$

Definition of reciprocal lattice vectors :-

● The primitive translation vectors $\boldsymbol{a1}$,$\boldsymbol{a2}$,$\boldsymbol{a3}$ represent the direct lattice.

● The reciprocal lattice vectors, $\boldsymbol{b1}$,$\boldsymbol{b2}$,$\boldsymbol{b3}$, are defined as follows:

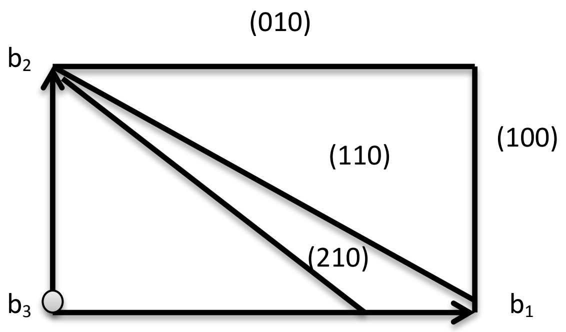
$$b_1=2\pi \frac{a_2 \times a_3}{a_1 . a_2 \times a_3}$$

$$b_2=2\pi \frac{a_3 \times a_1}{a_1 . a_2 \times a_3}$$

$$b_3= 2\pi \frac{a_1 \times a_2}{a_1 . a_2 . a_3}$$

● Construction of reciprocal lattice :-

Each set of parallel planes in a crystal is represented by vectors at the origin point of a reciprocal lattice, and each vector is perpendicular to the group of planes it represents, and its length is inversely proportional to the distance between (d). To construct or draw a reciprocal lattice, we suppose that there is a set of straight lines drawn in two dimensions that represent atomic levels in a cubic cell unit as in the figure below :



In order to set the reciprocal lattice points corresponding to these levels, we do the following :-

1.From the common origin , we draw the coordinates of the crystal .

2. We find the value of 1/d for each set of parallel planes .

3. The points drawn on the column represent the points of reciprocal lattice .

The Geometrical structure factor:-

● The intensity of the different wave reflections depends on the position of the atoms in the unit cell, as well as on the electronic distribution.

● It was found that the amplitude of the scattered wave is proportional to a physical quantity called the " Geometrical structure factor".

● The Geometrical structure factor plays an important role to giving information on or not the phenomenon of diffraction and is done through its account for any level of hkl coordinates in a well- known cell positions for example F.C.C., B.C.C.

● The Geometrical structure is defined as the ratio between the amplitude of the wavelength of all the actual electrons of atoms in a unit cell and the amplitude of the wavelength of a single electron located at a point.

● The Geometrical structure (S_{hkL}) is written in the following form :

$$lS_{hkL}l^2 = [\Sigma_j f_j \cos 2\pi(hx_j + ky_j + LZ_j)]^2 + [\Sigma_j f_j \sin 2\pi(hx_j + ky_j + LZ_j)]^2$$

f_j :- The atomic scattering factor .

Example :-

Calculate the Geometrical structure factor of a body – centered cubic lattice that the cell contains two atoms from their events o,o,o and 1/2, 1/2, 1/2 ?

$$lS_{hkL}l^2 = [\Sigma_j f_j \cos 2\pi(hx_j + ky_j + LZ_j)]^2 + [\Sigma_j f_j \sin 2\pi(hx_j + ky_j + LZ_j)]^2$$

$$lS_{hkL}l^2 = [\Sigma_j f_j \cos 2\pi(0 + 0 + 0)]^2 + [\Sigma_j f_j \sin 2\pi(0 + 0 + 0)]^2$$

$$+[\Sigma_j f_j \cos 2\pi(h1/2 + 1/2\,k + 1/2\,L)]^2 + [\Sigma_j f_j \sin 2\pi(1/2\,h + 1/2\,k + 1/2\,L)]^2$$

$$lS_{hkL}l^2 = f^2 + [f \cos \pi(h+k+l)]^2 = f^2 [1 + \cos \pi(h+k+l)]^2$$

• If the sum of (h+k+l) is an odd number, then $lS_{hkL}l^2 = 0$, This means that levels that have a sum (h+k+l) individually do not reflect the ray Thus, it does not appear spots or anything on the film.

• If the sum of (h + k + L) is an even number, then $lS_{hkL}l^2 = 4f^2$

This means that the process of reflection occurs and black spots appear on the film.