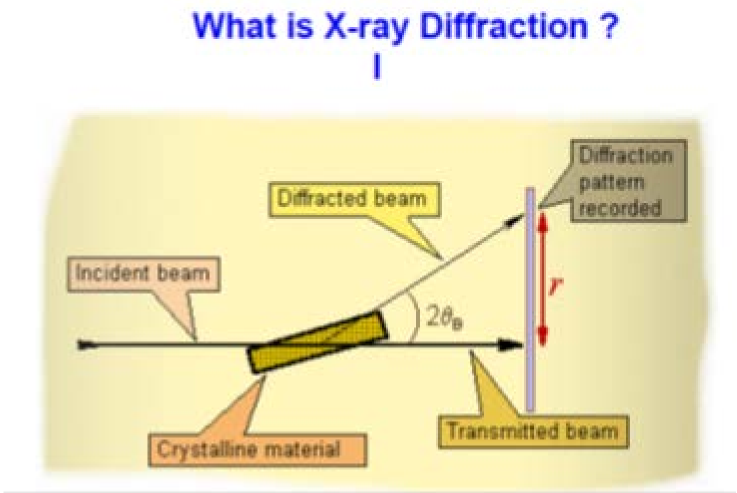
Lecture (5)

X-Ray Diffraction(Bragg's Law)

X-rays are electromagnetic radiation of wavelength about 1 Å (10-10 m), which is about the same size as an atom.

The discovery of X-rays in 1895 enabled scientists to probe crystalline structure at the atomic level. X-ray diffraction has been in use in two main areas, for the fingerprint characterization of crystalline materials and the determination of their structure. We can determine the size and the shape of the unit cell for any compound most easily using X-ray diffraction. X-ray Diffraction Structural Analysis



- ✓ X-ray diffraction provides most definitive structural information
- ✓ .Interatomic distances and bond angles X - rays
- ✓ To provide information about structures we need to probe atomic distances this requires a probe wavelength of 1 x 10^{-10} m ~Angstroms

Bragg's Law

$$n\lambda = 2d\sin\theta$$

BRAGG LAW

$$2d(\sin\theta) = \lambda_0$$

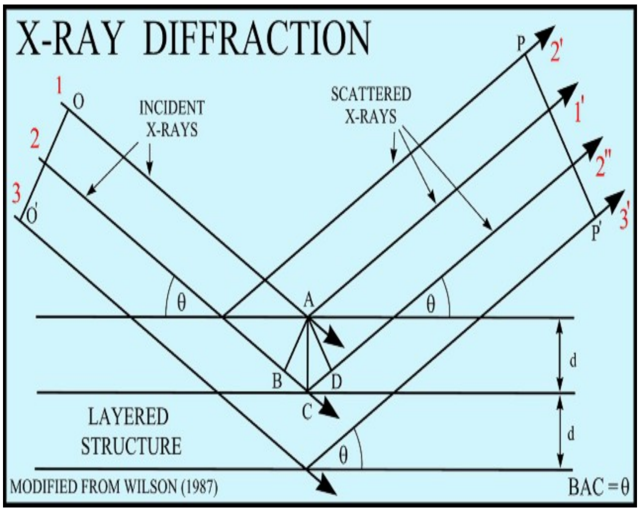
where:

d = lattice interplanar spacing of the crystal

θ = x-ray incidence angle (Bragg angle)

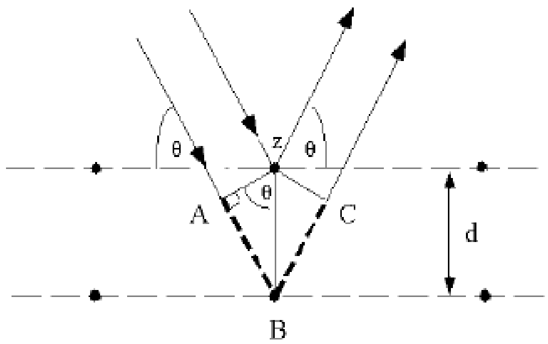
λ = wavelength of the characteristic x-rays

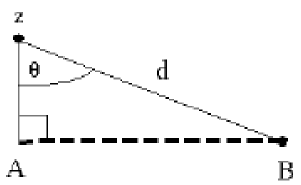
English physicists Sir W.H. Bragg and his son Sir W.L. Bragg developed a relationship in 1913 to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence (theta, θ). The variable *d* is the distance between atomic layers in a crystal, and the variable lambda λ is the **wavelength** of the incident X-ray beam; n is an integer. This observation is an example of X-ray **wave interference** (Roentgenstrahlinterferenzen), commonly known as X-ray diffraction (XRD), and was direct evidence for the periodic atomic structure of crystals postulated for several centuries.



Derivation of Bragg's Law

Bragg's Law can be derived using simple geometry by considering the distances traveled by two parallel X-rays reflecting from adjacent planes. The X-ray hitting the lower plane must travel the extra distance AB and BC. To remain in phase with the first X-ray, this distance must be a multiple of the wavelength thus:





$n\lambda = AB+BC = 2AB$
(since the two triangles are identical)

The distance AB can be expressed in terms of the interplanar spacing (d) and incident angle (θ) because d is the hypotenuse of right triangle *zAB* shown at right.

$\sin(\theta) = AB/d$ thus $AB = d \sin(\theta)$

Therefore:
$n\lambda = 2 d \sin(\theta)$

Why XRD?

- Measure the average spacings between layers or rows of atoms
- Determine the orientation of a single crystal or grain
- Find the crystal structure of an unknown material
- Measure the size, shape and internal stress of small crystalline regions

Applications of XRD

- XRD is a nondestructive technique
- To identify crystalline phases and orientation
- To determine structural properties:
  Lattice parameters (10^{-4}Å), strain, grain size, expitaxy, phase composition, preferred orientation (Laue) order-disorder transformation, thermal expansion
- To measure thickness of thin films and multi-layers
- To determine atomic arrangement
- Detection limits: ~3% in a two phase mixture; can be ~0.1% with synchrotron radiation

  Spatial resolution: normally none

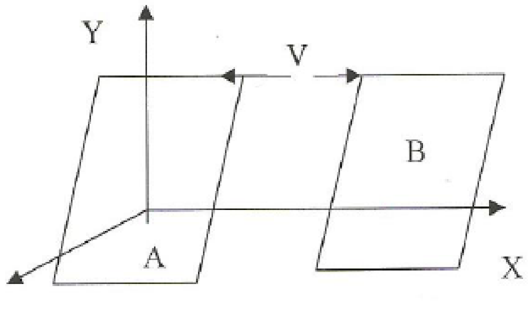
Electronic ballistic:-

The motion of a charged particle (usually an electron as electron beam) in the following type of electric and magnetic fields would be discussed:

1- Uniform electric field
2- Uniform magnetic field
3- Parallel electric and magnetic fields and perpendicular electric and magnetic fields.

1-uniform electric field:-

Let there be two large plane parallel (A & B) situated in vacuum at a distance of (d) meters from each other and having a potential difference (V) in volt between them, there will be a uniform electric field of strength (E=v/d) (volt /meter) between the two plates.
An electric placed at plate (A) will be attracted towards the positively –charged plate (B) .if free to move the electron will be accelerated towards plate belong (x-axis) as shown.
Since the negatively-charged electron is situated in an electron field it is acted upon by a force given by :-



$F= E\ e$…………..(1)

Also $F=ma$…………..(2)

eqn.1=eqn.2

$ma=eE$

$a=E\ e/m=(e/m) * (v/d)\ \ (m/sec^2)$

Velocity of the electron at any time (t) is given by:-

$v = a.t = (e/m).(v/d).t$ (volt/m) (use $v = v_0 + at$)

Example:-

Two parallel plates are situated (4cm) a particle vacuum and have a potential difference of (200v) between them. Calculate the force an electron situated between the two plates.

Solution:-

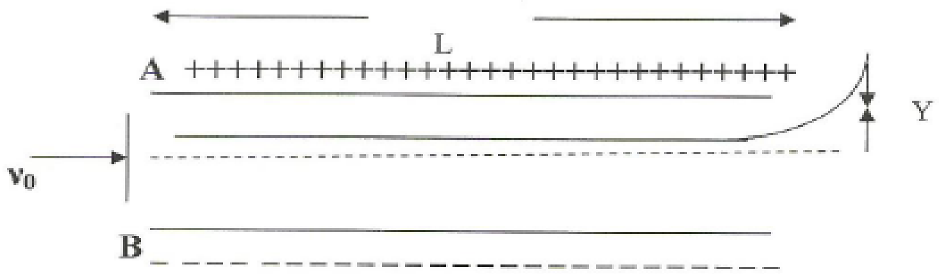
$F = e\ E = e .(v/d) = (1.6*10^{-19} *200) / 0.04 = 0.84 *10^{-16}$ N

Transverse electric field:-

Let an electron having an initial velocity of (v_0) along x-axis enter at point (0) the space between two planes parallel plates (A & B) where an electric field (E) exist along the y-axis as shown in figure while moving between the two plates the electron by vertical acceleration along y-axis but none along x-axis ,there is no force along x-axis.

The axial distance traveled by the electron during time (t) is: -

$$X = v_0 / t$$



There is no initial electron velocity along (y-axis) as the electron moves between the plates, its velocity along (y-axis) keeps on increasing

$$a_y = f/m = e.E/m = (e/m) .(v/d)$$

The velocity and displacement along (y-axis) after time (t) are given by :-

$$v_y = 0 + a_y t = a_y t \qquad (\text{use } v = v_0 + at)$$

And

$$S = \tfrac{1}{2} a_y t^2 \qquad (\text{ use } S = v_0 t + \tfrac{1}{2} a_y t^2)$$

Example:

A proton, with initial velocity of ($5* 10^6$m/s) passes through an electric field (transverse) of (200 v/cm). Calculate the transverse deflection in traveling a distance of (1 meter).

Solution:-

Let the proton direction as (x) and that of the electron field as (y). time taken to travel a distance (L) along the (x-axis)

$$t = L/v = 1/5*10^6 = 2 *10^{-7} \text{ sec}$$

Force acting on the proton due to electric field = $eE_y = m\, a_y$

Proton acceleration $a_y = eE_y /m$

Note:_the transverse deflection $Y = = \tfrac{1}{2}\ a_y t^2$

$$Y = \tfrac{1}{2} * (q E_y /m) * t^2 = \tfrac{1}{2} *1.6\ 10^{-19} * 2*10^4 *(2 *10^{-7})^2 / 1.6 *10^{-27} = 0.04 \text{ m}$$

2-Moving charges in magnetic field:-

If a particle of charge (q) is introduced with its initial velocity (v_0) in the plane normal to (B) , then the force F = q (V*B) will act on it in this plane in the direction (⊥) to (V & B).since the force (F) due to magnetic field is always (⊥) to the direction of motion and (V & B) are constant in magnetic ,hence force (F) will also be constant and the particle will move along (α) circular path of radius (R) given by centerfugal force.

$$m V^2 /r = \text{Force} = e .V.B$$

$$r= m v/ q B$$

and angular velocity = V / r = eB/m

Example:

A proton is shot with a speed of ($1*10^6$ m/sec) along a line at an angle of (30^0) to the x-axis parallel of which a uniform field of (0.02 wb/m^2) exist .describe the motion of the proton .

Solution:-

$F_x = ev_x$ B sin θ (and hence v_x in un effected by the field)

Thus the proton moves in the x-direction with constant velocity ($v_x =1*10^6\cos\theta$) as B is (⊥) to v_y ,the y-component of v, the proton travels in a circle which is in (y-z plane) the force is:

$$m V_y^2 /r = e.V_y.B \Longrightarrow r= m.v / B.e$$

$$r = \frac{1.67* 10^{-27} * 1*10^{-6}*0.5}{0.20 * 1.6* 10^{-19}} =2.6 *10^{-2} \text{ m}$$

Hence time period $T = 2\pi r/ v_y = 2 \pi\, 2.6\, 10^{-2}/ 1*10^6 *0.5 = 3.26 *10^{-7}$ sec

The proton will have traveled a distance $v_x t$, the distance

$$v_x t =0.866 *3.26 *10^{-7}= 0.282 \text{ m}$$

3-Charged particles in electric magnetic fields:-

consider a particle of charge (q) and mass (m) emitted at the origin with zero initial velocity into a region of uniform electric and magnetic fields, the field (E) is acting along x-axis and field (B) IS along y-axis . the force (q E) due electric field will act along (z-axis) .as the charged particle is placed in a magnetic (B) it will experience force (q V*B) acting in the direction perpendicular (B) and (V) . Hence the particle will bent. The resultant force also known as Lorenz forceis this given by :

$$F = e(E_i + (V_j * B_j))$$

Our particular case $E = E_i$, $V = V_X i + V_y j + V_z k$
And $B = B_j$

$$F= e[E_i + V_x * B_k - V_z * B_i] = q[E- V_z * B]_I + q V_x * B_k$$

Example:

An electron is moving with a velocity (2i +3j) m/sec in an electric field of intensity (3i+6j+2k) and α-magnetic field of (2j+3k) tesla find the magnitude and direction of the Lorenz force acting on the electron?

Solution:-

Lorenz force = F= q [E + V* B]

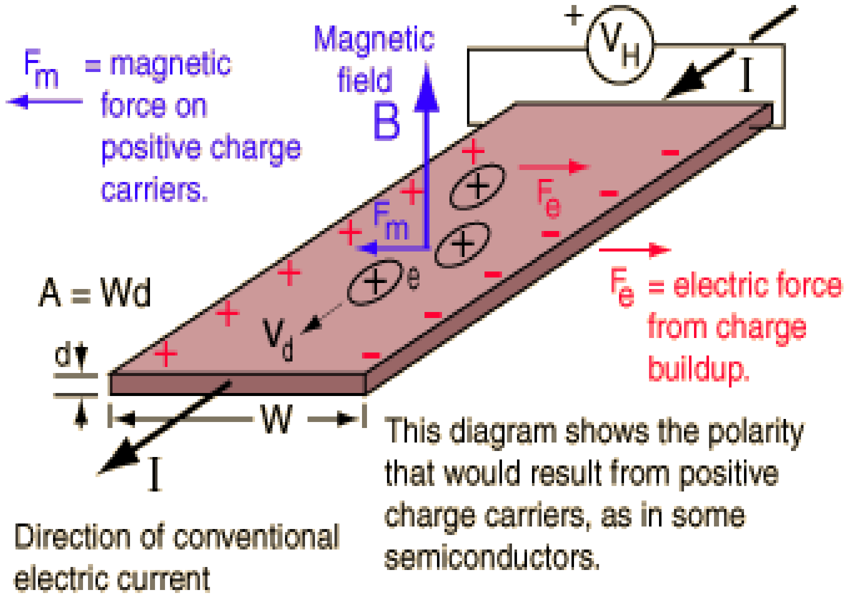
$$F = 1.6*10^{-19} [3i+6j+2k+(2i+3j) * (2j+3k)]$$

$$V * B = \begin{vmatrix} I & j & k \\ 2 & 3 & 0 \\ 0 & 2 & 3 \end{vmatrix} = i(9-0) - j (6-0) + k(4-0) = 9i - 6j + 4k$$

$$F = 1.6 *10^{-19} [3i+6j+2k+9i -6j+4k] = 1.6 *10^{-19} [12i +6k]$$

The Hall Effect

the Hall effect is used to experimentally determine the charge carrier density n or p of a n- or p-doped semiconductor sample as a function of temperature in the range 80–300 K. We can use the *Hall effect* to determine whether the mobile charges in a given conductor are positively or negatively charged.



The Hall effect occurs because a charged particle moving in a magnetic field is subject to the Lorentz force given by:

$$\boldsymbol{F_{Lorentz} = q\, v \times B} \text{ ....(1).}$$

$|F_{Lorentz}| = q\, v\, B \sin(\theta)$ (1b) (θ is the angle between ***B***-field and velocity vector ***v***).
Where *q* is a signed quantity representing carrier charge**,** ***v*** is the particle velocity vector, and ***B*** is the vector magnetic field. The basic Hall measurement is performed on a semiconductor bar with an electric field applied along its long axis, and magnetic field applied perpendicular to it.
If the sample is n-type, the majority carrier electrons will move opposite the applied electric field, right to left (-***x***) . The ***v*** *x* ***B*** cross product is in the positive ***y*** direction for a ***B*** field directed upward in the page. The carrier charge in this case is negative so the force is actually in the **–*y*** direction. This force causes the majority carrier electrons to be pushed towards the front edge of the sample.
The system reaches equilibrium when the force applied on carriers by the second electric field ***Ey*** equals and opposes the forced due to the **B** field.

$$q\,|E_y| = q\,|v_x \cdot B_z| \text{ ....(2)}$$

Ey gives rise to a voltage which can be measured from the front to the back face of the sample.

$$E_y = v_x B_z$$

The Hall voltage ***VH*** **=** ***Ey w*** (see the above Figure for the definition of *w*).

Now consider a p-type sample. Here the majority carrier holes move with the applied electric field, as shown in below figure. The force due to the magnetic field, $q\,\mathbf{v} \times \mathbf{B}$ is in the *–y-* direction and once more carriers are crowded to the front face of the sample resulting in an electric field. This time, however, because the carriers are positive, the Hall voltage measured from front to back on the sample will be positive. Thus, the majority carrier type determines the sign of the Hall Voltage.
The velocity we have been discussing is the carrier drift velocity and is related to the current by:

$$J = \sigma E,\ or\ J_x = nqv_x = nq\mu E_x = I_x/A \text{........(3)}$$

$$v_x = E_x\,\sigma/nq \text{ ....(4)}$$

where n or *p* is the carrier concentration per cm^3, and *A* is the cross sectional area of the sample in cm^2 (width times thickness: *w.t*). The quantity *v* can easily be solved for and the result substituted in Equation 2, resulting in:

$$E_y = J\,B/q\,n = B_z E_x\,\sigma/nq \quad \text{(n-type)}$$
$$E_y = J\,B/q\,p = BE_x\,\sigma/pq \quad \text{(p-type) .... (4)}$$

If we substitute the product *wt* for *A* in Equation 4, where *w* is the sample width and *t* the sample thickness, we can multiply Equation 4 by the width to get the Hall voltage:

$$V_H = w\,E_y = w\,B_z\,E_x\,\sigma/nq \quad \text{(n-type)}$$
$$V_H = w\,E_y = w\,B_z E_x\,\sigma/pq \quad \text{(p-type) ....(5)}$$

Since V_H, B_Z, and q are all known (by measurement), it is possible to solve for the carrier concentration *n* or *p*, and determine whether the sample is n-type or p-type.

$$V_H = \frac{IB}{ned}$$

$$n = -B_z J_x / E_y\,q = -\,w\,B_z\,J_x / V_H\,q \text{...............(6)}$$

$$n = -\,w\,B_z\,J_x / A\,V_H\,q$$

where A is the cross-section area of the specimen. Since A = wxd then we can write eqn.(6).

$$\boxed{n = -\,I_x\,B_z / d\,V_H\,q}$$