Chem Unit5 - UNIT 5 NOTES

Unit: 5 : XRD, XPS, miller indices & Composites

No.

Date

① * XPS → Photoelectron Spectroscopy

⇒ used for analysing structure of atom & also gives info about I.E of particular e^- in atom. Now, provides info about Chemical nature of surface. Provide – qualitative & quantitative about chem. nature and comp. & layer of solids.

* Principle:

⇒ surface sensitive spectroscope technique – measuring elemental composition, empirical formulae, chemical & electronic state.

⇒ Obtained by radiating/ passing X-ray beams on the material, measuring KE of e^- simultaneously that escapes from 0 to 10nm. Penetration depth: in microscopes.

⇒ Thus, photons interact with atoms in surface, emitting of e^-s. From K.E, B.E calculated.

$$E_{Binding} = E_{photon} - (E_{K.E} + \varphi)$$

Binding energy

$$BE = h\nu - (E_{KE} + \varphi)$$

↳ work function (depends on spectrometer & material)

* Instrumentation:

1) Source
2) Sample holder
3) Energy analyser
4) Detector
5) Ultra-high vaccum.

Date

1) Source –

He single or doubly used – remaining valence e^- to produce ions

Yttrium (m) zeta rays – ejection of outer e^-

AlK_α / CrK_α / MgK_α – energetic rays to reach the inner shell causing radiation

Simplest sources are equipped with mg, Al targets. They are used because of high intensity, and narrow wavelength bands of $K\alpha$ light narrow bands are desirable, because they give rise to high resolution.

2) Sample holder – solid samples are mounted in fixed position one as close to photon/e^- source and the entrance of slit of spectrometer as possible.

3) Analyzer – Placed b/w sample & detector

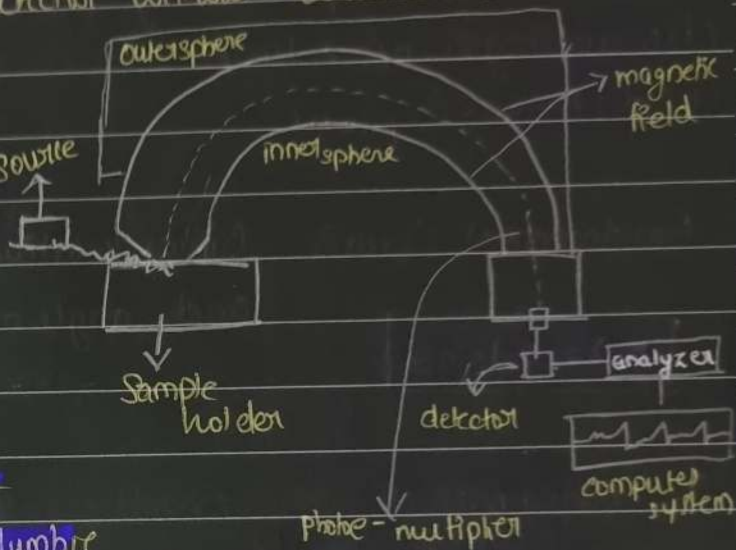
– must be sensitive enough to find the $e^\ominus$ beam. (coming out of curved path becomes quite tough for most of the e^- fail due to presence of magnetic field, only the $e^\ominus$ is expected travel along the curved path)

– 2 Cylinder (concentric) at diff Voltage, one +V and other 0V will create electric field b/w'em.

1) if eV is high, collide w outer
2) if eV is low, collide w inner cylinder
3) only $e^\ominus$ with right velocity will reach the detector

4) Detector- e^- multiplier usually employed as detector because of its sensitivity & convinience.

5) Ultra-high vaccum :- Provides contamination of surface for accurate analysis of sample allowing sample $e^{\ominus}$ to reach detector without disturbances.



* Working:

Sample-illuminated by photons($h\nu$) produces photo e^-, these leave atom with energy consumed. Thereby reducing by time. Done by overcoming coulumbic force of attraction.

XPS obtained by determining K.E and no. of $e^{\ominus}$ escaping from surface of sample under investigation.

* Application:

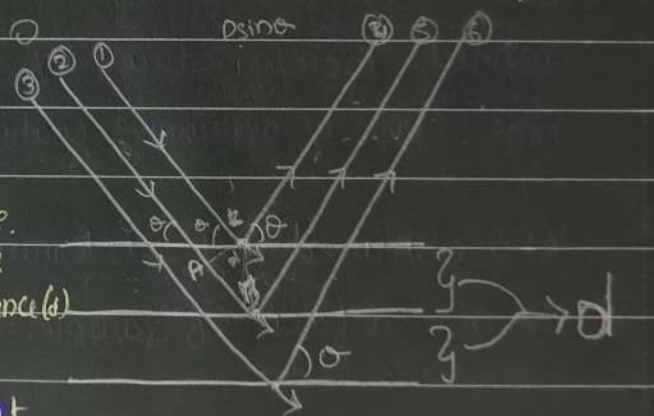
* identifying active sites
* determining surface contamination on semi-conductors
* study of oxide layer of metal
* Determination of oxide state
* elements of periodic table can be determined (Except H and He)
* Analyzing dust as sample.

② XRD → X-Ray Diffraction

Bragg pointed out that light scattering of x-Rays by crystal can be considered as reflection from successive planes of atoms in crystal. But unlike normal reflection here it takes place only particular angle determined by
(i) wavelength of X-Ray
(ii) distance of plane

Fundamental Equa: Gives relation b/w λ & θ b/w plane and angle of reflection ($\angle r$) → known as Bragg's equation.

$$\boxed{n\lambda = 2d\sin\theta}$$



In diagram,
horizontal lines → Parallel planes in crystal structure seperated from one another by a distance (d)
θ → angle at which X-Rays are incident

①, ②, ③ → incident ray
④, ⑤, ⑥ → scattered rays

(some are reflected while some absorbed)

~~let ABC & DEF~~ Reflected rays from layers will coincide with one another only if path length of ray = f no. of λ.
OL, OM ⊥ to incident, reflected beams the path length difference (Δ) of waves reflected in successive layers ($\angle r + \angle N$)

$$\Delta = AB + BC$$

$2AB = n\lambda$ ($AB = BC$) ($AB = d\sin\theta$)

$\boxed{n\lambda = 2d\sin\theta}$

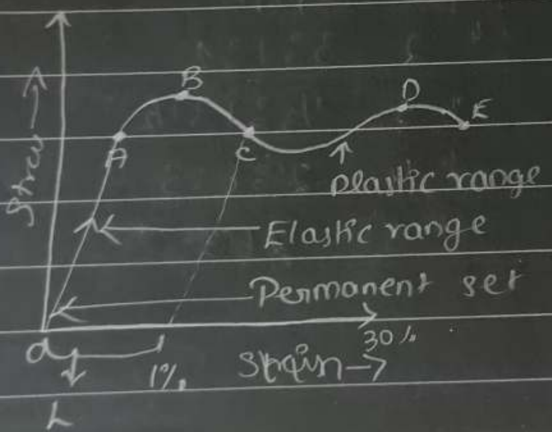
* Elastic limit: max stress upto which a body exhibits elastic property is called elastic limit.

* Hooke's law: states within elastic limit, stress ∝ strain

stress ∝ strain

$\boxed{E = \frac{\text{stress}}{\text{strain}}}$ E → coefficient of elasticity.

* stress-strain diagram & uses:



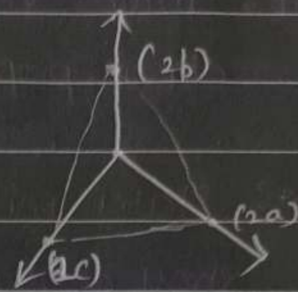
A → Proportional limit
B → Elastic limit
C → Yield point
D → Breaking point
E → Fracture point.

- Hooke's law: OA - straight line stress ∝ strain thus perfectly elastic. A is called point of proportionality.
- Elastic limit: On further ↑es in stress till B.
  B → elastic limit (max point at which wire can regain length) (beyond that not possible)
- Yield point: ↑ing further till C. slight ↑ in stress causes large strain.
  C → Yield point

③ **Miller's indices** : → smallest possible 3 ratio integer (x, y, z)

Steps to find -

1) Find integer along axis
2) Take ratio $P : Q : R$
3) reciprocals of ratio $\frac{1}{p} : \frac{1}{q} : \frac{1}{r}$
4) Reduce to lowest whole number.
5) write integer w. parameter, without commas



2 : 2 : 1

$\boxed{\text{Ans: } 221}$

Prob 1 - (4, 4, 2)

Step 1 (4, 4, 2)

" 2 4 : 4 : 2

" 3 1/4 : 1/4 : 1/2

" 4 1 : 1 : 2

" 5 112

Prob 2 - (3, 1, 2)

Step 1 (3, 1, 2)

" 2 3 : 1 : 2

" 3 1/3 : 1 : 1/2

" 4 2 : 6 : 3

" 5 263

Prob 3 - (1/4, 1, 1/2)

Step 1 (1/4, 1, 1/2)

" 2 $\frac{1}{4} : 1 : \frac{1}{2}$

" 3 4 : 1 : 2

" 4 4 : 1 : 2

" 5 412

1) Explain mechanical properties of solids:

(i) Stress (ii) Strain (iii) Relationship (iv) Tension Strength

(v) Hardness (vi) Fatigue.

Ans: (i) Stress:

It is the force applied on a material divided by the material's cross-sectional area.

(ii) Strain:

It is the deformation or displacement of material that results from an applied stress.

(iii) Relationship:

Hooke's law expresses the relation between the two solids stress and strain. It states that within an object elastic range, the strain within an object is proportionate to the stress appled on it.

(iv) Tension Strength:

It is the maximum stress that a material can withstand while being stretched or pulled breaking.

(v) Hardness:

Measure of the resistance to plastic deformation.

(vi) Fatigue:

It is an important aspects of mechanical response of materia and sufficient fatigue resistance is crucial.

Unit-5: Composites & types (Continue).

No.

Date

Composites → natural /artificial materials composed of two or more macro/micro/nano materials such as a metal, ceramic and polymer, with interface seperating them that differ in form & chem. composition.

→ Minimize weakness of materials to enhance the prop. of Composites.

→ In simple words,
Composites are materials formed by combining 2 or more chemically distinct materials that are insoluble in each other and retain their own individual identities.

There are 2 types:

* Natural composites (Ex: wood - Combination of cellulose fiber & lignin)
* Synthetic composites (Ex: concrete - cement + gravel.

Components

1. Primary phase: forms matrix within which secondary phase is embedded.

2. Secondary phase: imbedded phase sometimes called as ~~ref~~ reinforcing agent because it usually serves to strengthen the composite.

Plastic (matrix) + glass (made into thin threads) (reinforcement) → sort of plastic based glass.

No.

Date

(R) is added to M to enhance prop., becoming a composites.

Matrix : (M)	Reinforcements (R)
* one of the component of the composite.	* one of components of the composite.
* maintains the reinforcement	* Nes entire mechanical characteristics of matrix
* to create the req shape.	* Strengthens by extra support thro. & enhances properties of composite.
* Provides the bulk form.	
* Polymer, metal, ceramic	* fiber, plastic, carbon fibre.

Composite materials

- Reinforcement
  - ⇒ Glass
  - ⇒ Carbon
  - ⇒ organic
  - ⇒ Boron
  - ⇒ Ceramic
  - ⇒ metallic
- matrix
  - ⇒ polymer
  - ⇒ metal
  - ⇒ plastics
  - ⇒ ceramics
- interface.
  - ⇒ bonding
  - ⇒ surface.

Metal matrix composite (MMC)
Ceramic matrix composite (CMC)
Organic matrix composite (OMC)

Classification of Composite materials

- matrix
  - (OMC) Polymer
    - thermo plastic
    - thermo setting
  - (MMC) metal
    - Eg: Cu, Al, Ni, Ti
  - (CMC) Ceramic
    - (i) Glass
    - (ii) SPC
    - (iii) alumina
- Reinforcement
  - particle
  - Fiber
    - Continous (aligned)
    - discontinous. (short)
  - Laminates

Date

Continous fibers → very long, offers continous path by which a load can be carried by composite part.
→ prop. doesn't vary w fibre length

dis continous fibres → chopped sections of continous fibres
→ prop varies from length.

Nanocomposite → matrix reinforced by added nanoparticles.
→ reinforcing material can be particles, sheets or fibres.
→ Types:
* Metal matrix nanocomposites
* Ceramic matrix "
* polymer matrix ".