

ASSIGNMENT.

UNIT - 1

1. Atomic Bonding can broadly be classified as Primary and Secondary bonds — While Primary bonds are those that involve sharing or donation of electrons to form stable configurations, secondary bonds arise as a result of subtle attraction due to uneven charge distributions.

They can be classified further —

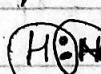
PRIMARY — Ionic, covalent and Metallic

SECONDARY — Van der Waals and hydrogen.

IONIC BONDING

- * It is a result of electrostatic attraction bet. +ve and -ve ions.
- * These ions are formed when metallic elements lose their outer \bar{e} s and electronegative elements gain \bar{e} s. \therefore These bonding happens between pairs of elements with a large EN difference. They result in complete shells.
- * When ions get closer, while inner \bar{e} s remain undisturbed, the outer shells causes overlap of wavefunctions — As no 2 \bar{e} s can have same state, a new set of energy states are created. This energy is experienced as repulsion, limiting the further closeness.
- * Ionic solids are generally hard, crystalline, with high MP & BP, Soluble in polar.
- * Few Examples — NaCl, NaF, KCl etc.

COVALENT BONDING

- * Here, the outer \bar{e} s are shared between atoms. Occurs bet. elements of low EN difference. Sharing in most cases results in noble gas configuration.
- * Covalent compounds are generally bad conductors of electricity, have low MP & BP, are insoluble in polar solvents, but soluble in non-polars.
- * Examples — Two H atoms with 1 \bar{e} each form a H₂ molecule 

METALLIC BONDING

- * Weaker than both ionic & covalent, occurs only in Metals/metal-like
- * In Metallic State, a common pool of \bar{e} s (cloud of free \bar{e} s) exists over an array of positive ions. MB is the attraction between the +ve ion and the delocalized ions.
- * They generally have high thermal & electrical conductivity, with low BP and mp, bright lustre and are also metals malleable & ductile
- * Ex — in Graphene.

SECONDARY

Van der Waals -

- * Temporary bond between neutral atoms/molecules, occurs due to uneven \bar{e} density. It is non-directional
- * Natural fluctuations cause temporary dipoles that in turn nipples the induction of dipoles to other atoms/molecules
- * Example - CH_3Cl and O_2

Hydrogen -

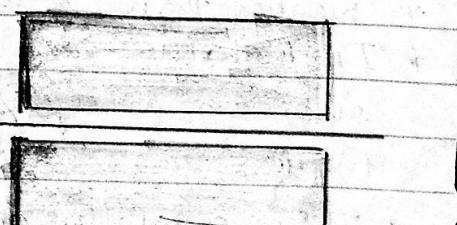
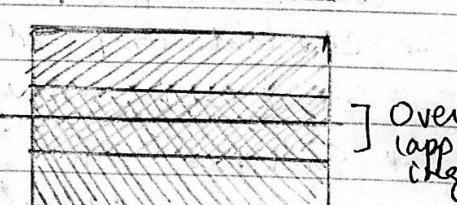
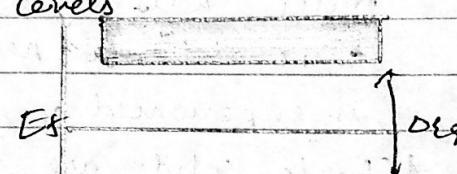
- * A covalently bonded H, when near, is attracted towards a more electro-negative atom/group. (Electrostatic in nature)
- * It results in changing the properties of the compounds
- * Example - among two H_2O 's,

Q3) In band theory of solids, the available energy states are in the form of bands, rather than discrete values.

Fermi level is the top of the available \bar{e} levels

- a) In Insulators - the energy gap bet. the valence & conduction band is so large that in ordinary temperatures, no \bar{e} can reach it.
- b) Semiconductors - the gap is small enough that thermal energy can bridge it.
- c) Conductors - there is no band gap, instead the conduction & valence band overlaps

- d) Superconductors - the band structure is similar to that of conductors in normal state but in superconducting state, there exists an energy gap, whose magnitude is the energy gain for the Cooper pairs. This gap is due to $\bar{e}-\bar{e}$ interaction and is typically very small



(in Superconducting State only)

Q2)

The free electron theory explains the structure and properties (electric, thermal, magnetic etc.) of solids through their electronic structure. It was developed in 3 stages -

1. The classical free e^- theory, developed by Debye & Lorentz postulated the handling of valence e^- similar to that of the ideal gas. The velocities obeyed the Maxwell-Boltzmann distribution.

While it explained some properties, it did not explain many others including the photoelectric effect, Blackbody radiation, ferromagnetism among others.

2. The quantum free e^- theory, by Sommerfeld said that the free e^- s moving with constant potential, obeyed quantum laws and abided by the Fermi-Dirac statistics. This however, could not explain crystal structures.

3. The zone theory, by Bloch theorized that free e^- moving in a constant potential, moved in a periodic field provided by the lattice. This eventually resulted as the Band theory of solids.

- 5) Incomplete filling up of energy bands causes conductivity. In ordinary conductors (non-magnetic), the conduction band is identical for both spin-up and spin-down e^- s.

Diamagnetism -

These substances are weakly repelled by a magnetic field and is shown by substances which have no unpaired electrons. The equal no. of spin up and spin down electrons cancels each others' magnetic moments. The band structure is similar to that of normal conductors.

Paramagnetism -

- Paramagnetic substances are weakly attracted by magnetic field. They are magnetized in the same direction as the external magnetic field.

It is due to the presence of up unpaired $\bar{e}s$.

When a magnetic field is applied, the conduction band splits apart into spin-up and spin-down ~~bands~~ bands. ~~when a mag~~ due to the difference in the magnetic potential energy for spin-up & spin-down $\bar{e}s$.

* Since the fermi level must be identical for both bands, this means that there will be a small surplus of the type of spin in the band that moved downwards, known as Pauli Paramagnetism.

4) Semiconductors can be classified wrt many parameters -

- On the basis of purity.

A. INTRINSIC SEMICONDUCTORS — A semiconductor in which properties are controlled by the element or compound itself and not by dopants / impurities.

B. EXTRINSIC SEMICONDUCTORS — A semiconductor prepared by adding dopants, which determine the no. and type of charge carriers. The presence of donor/acceptor atoms also changes the fermi energy level in the forbidden band. Two types - N-type and P-type exist depending on the type of impurity.

- On basis of bandgap

A. Direct Bandgap — An \bar{e} can be promoted from conduction band to valence band w/o changing its momentum. When it falls back, the combination of hole- \bar{e} produce light known as radiative recombination.

B. Indirect Bandgap — \bar{e} s cannot be promoted w/o change in momentum. The combination of holes & \bar{e} s produce heat known as non-radiative recombination.

UNIT-2

(i) The grains in nanomaterials are in the order of 10^{-9} m , resulting in a large surface to volume ratio - a high % of atoms/molecules are on the surface. Hence, the surface forces become much more important than bulk.

- In nano-scale, since the \bar{e} s become confined, some materials that were conductors in bulk form behave as semiconductors/poor conductors at ∞ in nanostructure.
- Since \bar{e} s cannot move as freely as in bulk form, they react to lights differently. Example - Gold nanoparticles may appear ~~green~~, Quantum dots change in their optical appearance.
- Unlike in bulk where the magnetization is stable (multi-domain structure), nano sized structures ^{are} single domain.

Some magnetic materials can exhibit superparamagnetism in nano scale.

Q2) Top-down method starts with a large scale object and gradually reduces its dimension(s). En - by lithography.

Advantages -

- * It is beneficial in the production of structures in a far-reached order.
- * It provides better control, and simple process.

Disadvantages

- * It is not cost-effective and scalable.

Bottom-up method collects, consolidates and arranges individual atoms/molecules into the structure. En - by chemical reactions

Advantages -

- * Beneficial in production of structures in a short-range order.
- * Better precision, with less defects and homogenous composition.

Disadvantage -

- * Highly complex process prone to failure.

Q4) Carbon Nanotubes (CNTs) are of two types - Single walled (SWCNTs) and Multivalled (MWCNTs)

- Single walled have a diameter < 1nm & MWCNTs have many concentrically interlinked nanotubes with diameters > 100nm.

(i) Conductivity - MWCNTs are always conducting and at least similar to metals, SWCNTs' conductivity depends on their chiral vector. It is conducting in armchair structure.

(ii) Strength - MWCNTs are much stronger than SWCNTs

(iii) Reactivity - MWCNTs are more resistant to corrosive environments than SWCNTs.

(iv) Purity - MWCNTs have greater purity than SWCNTs

(v) SWCNTs can twist easily than MWCNTs.

(vi) Structure - SWCNTs are held by sp^2 hybridization, come in three types - zig-zag, armchair, chiral.

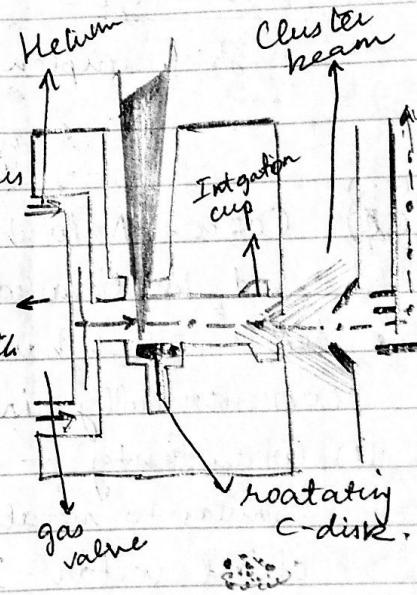
(vii) CNTs are efficient thermal conductors. However, they insulate laterally (along axis) from moving heat.

- Q5) Nano particles are engineered so that they are attracted only to the diseased cells, allowing direct treatment of these cells & and reducing damage to the healthy cells.
- These particles are in the same scale of many other biological structures too.
- Nano particles can directly carry cancer drugs to the tumors. Bi nanoparticles are radioactive and can attach to tumor cells.
 - gold nano rods attached to tumor cells can absorb infrared light and the heat releases drug to kill cancer cells.
 - Nano-diamonds embedded in contact lenses can deliver drug to treat glaucoma.
 - Nanovesicles attached to stem cells are attracted to injury sites in damaged heart tissues.

Q3) Bottom-up technique—

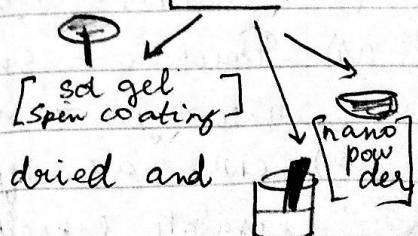
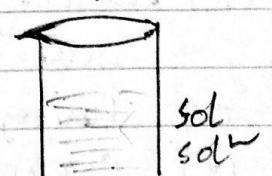
1. CLUSTER BEAM EVAPORATION —

- Solid metal is heated by \bar{e} bombardment.
- During deposition, temperature of the crucible is kept as high as the MP of the solid.
- The chamber is evacuated with high vacuum to minimize impurities and increase mean free path.
- The temp. of the substrate is either at room or liquid nitrogen temperature. The size of the nano particles are much smaller.



2. SOL-GEL METHOD —

- The Sol-gel process is a wet chemical technique a.k.a. chemical Sol° deposition
- The liquid colloidal soln to a solid 3D network.
- After polycondensation, semi-rigid mass obtain in a gel. During process, ions in the sol, arranged in a 3D network gel.
- First it is hydrolyzed, next condensed, then dried and calcinated and finally nano particles.
- pH, solvent, temperature & catalysts affect the process.



[sol gel dip coating]

Top-down techniques

1) BALL MILLING —

- A simple, low cost and high yield method of synthesis
- In high energy ball milling, plastic deformation, cold-welding and fracture are predominant factors.

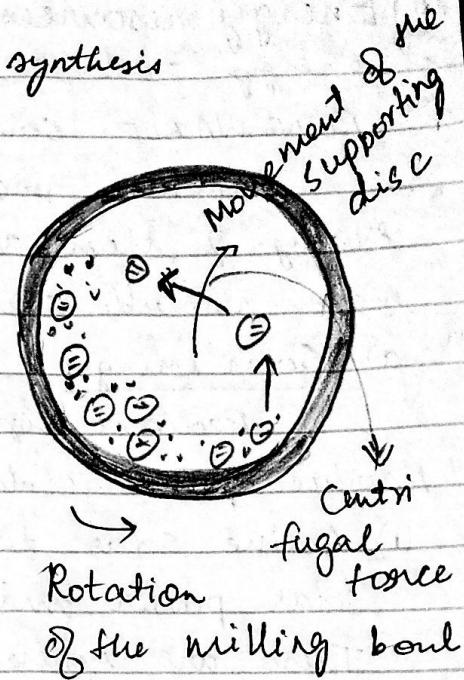
⇒ Deformation leads to change in particle shape.

⇒ Cold welding leads to increase in size.

⇒ Fracture leads to decrease in particle size

- Results in formation of fine dispersed alloy particles

- The type of mill, powder, speed, size, temperature and duration of milling govern the energy that is transferred from the balls to the powder



2) LITHOGRAPHY —

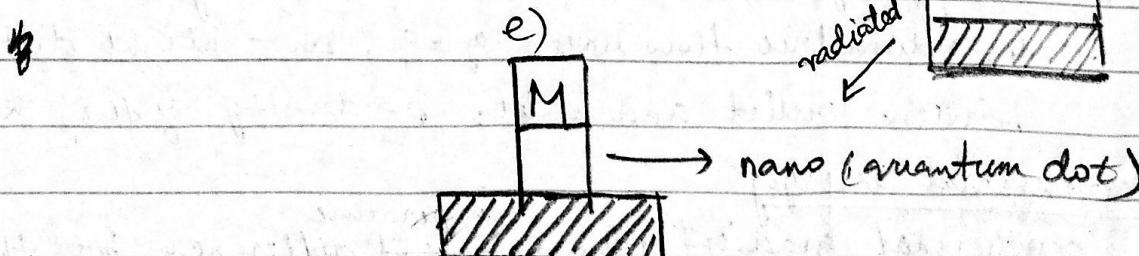
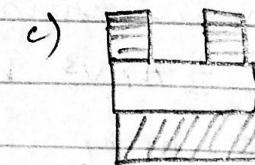
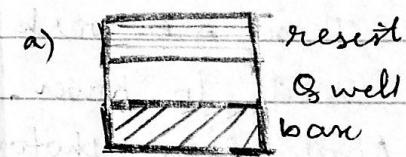
- We start with a quantum well located on a substrate and covered by a resist.

(A typical resist is $[C_{50}O_2H_8]_n$)

- This sample is then irradiated, shielded by a template.

- A mask is then inserted in the irradiated portion, the remaining resist and Q well are irradiated as well.

- The final nanostructure on substrate after removal of the etching mask.



UNIT-3

(i) Energy resources can broadly be classified as Renewable energy and non-renewable energy sources.

RENEWABLE SOURCES -

These sources are naturally replenished (on a human timescale). Many of them are sustainable and carbon neutral. The main renewable sources are -

a) Solar energy

Radiant light and heat from the sun is harnessed to produce power. Solar power does not emit harmful residues.

(i) Active solar techniques use photovoltaic systems, concentrated solar power and solar water heating to harness energy.

They are generally used to generate power on a large scale.

(ii) Passive solar techniques try to orient the building to the sun, select appropriate materials and design the space suitably.

They work to reduce the amount of energy traditionally used to power.

Applications - photovoltaic solar cells, solar cookers, solar water heaters

b) Wind energy

The power harnessed via winds is intermittent and variable.

It helps generate power in off-grid locations.

The power generated can be approximated as -

$$P = \frac{1}{2} \rho v^3 A \eta$$
 where A = cross-sectional area, ρ = density of air, v = velocity

c) Hydro energy

It uses falling / fast - running water to produce electricity.

$$P = -\eta \rho V g \Delta h$$
, where, η = efficiency of the turbine,

V = volumetric flow rate, $g = 9.8$, Δh = height difference

between outlet and inlet, ρ = density of the water

d) Geothermal energy

The geothermal gradient, the temperature difference bet the planet core and the surface, drives a continuous conduction of thermal energy.

e) Bioenergy

Derived from biological material, it can be used directly via combustion to produce heat, or indirectly after converting to various forms of biofuel.

NON RENEWABLE SOURCES -

a) Fossil fuels -

Class of hydrocarbon-containing materials of biological origin, occurring within earth's crust. All fossil fuels are burned in air to provide heat which can be used directly or to produce steam to drive generators.

CO_2 is a main by-product which behaves as a green house gas.

CH_4 , also is a green house gas, is main constituent of natural gas.

Fossil fuels include coal, petroleum, natural gas, heavy oils etc.

b) Nuclear fuel -

Nuclear fuels contain include ~~cont~~ heavy actinide elements that are capable of fission. Sn. ^{233}U , ^{235}U , ^{239}Pu .

When the unstable nuclei of these atoms are hit by slow-moving neutrons, they split, creating 2 daughter nuclei and extra neutrons.

These neutrons then create a chain reaction which produces heat

Q2)



The operation ^{requires} has 3 main attributes - The absorption of light, generating e^- -hole pairs or excitons, the separation of charge carriers of opp types and the separate extraction of those carriers to an external circuits.

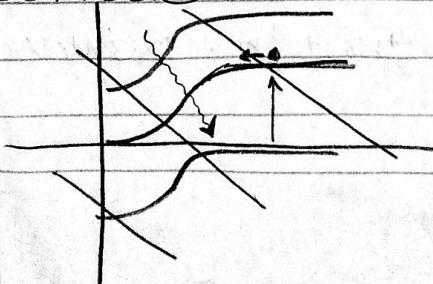
PRINCIPLE -

When the photons of the light hit the cell and eject e^- s from the semiconductor producing e^- -hole pairs. The e^- s move to the cathode and holes move to the anode due to the E field.

CONSTRUCTION -

A PN Junction diode which is generally semiconducting, has its ^{and bottom} top layer of metallic grid, forms electric contact and allows light to fall on the junction. The anti-reflective layer coated in the ~~bottom~~ intermediate helps to absorb max light.

MECHANISM -



Mechanism -

When light enters into the junction created by p-n type semiconductors, the energy ejects electrons and creates hole. The electrons drift towards n-type and are collected. Holes drift to p-type and are collected at p-type end.

When the two ends are electrically connected through a conductor, there is a flow of electrons. Thus photoelectric current is produced.

Q3)

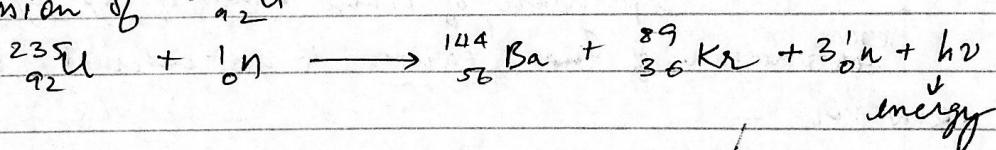
Fission & fusion

Nuclear fission -

Nuclear fission is that the reaction in which the nucleus of an atom splits up into two or more smaller nuclei. The nucleus is radioactive and generally a heavy actinide element.

When it is bombarded with \bar{n} neutron, a huge energy is produced and smaller nucleus and neutrons and the process results in a chain reaction.

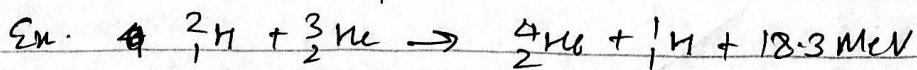
Example of fission of $^{235}_{92}\text{U}$



Nuclear fusion -

Nuclear fusion is a rxn in which 2 or more atomic nuclei combine to form one or more diff. atomic nuclei and subatomic particles. There is a difference bet. the mass of reactants and products which manifests as energy ($E = mc^2$). Fusion occurs in stars naturally.

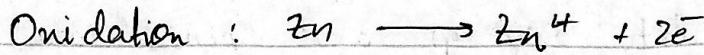
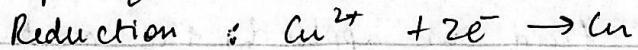
Elements having smaller mass/nucleon & large binding energy per nucleon, like lighter elements - H, He etc. are more suitable for fusion.



(Deuterium-Helium-3 fusion)

- (Q4) Electrochemical energy is a field of energy concerned with electrochemical methods
- (Q4) Electrochemical energy is obtained via electrochemical methods, e.g. like e^- transfer, reduction & oxidation (REDOX reactions).

Example of a classic basic cell run -

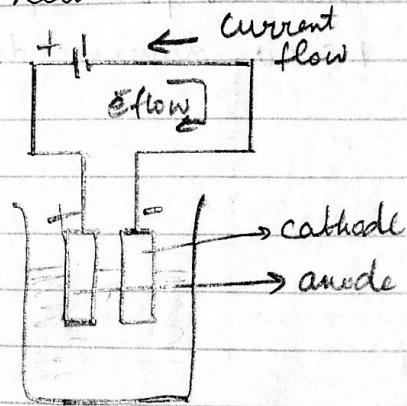


We can either use EC cells to generate electrical energy from chemical energy or ~~electrical~~^{chemical} energy from electrical energy.

GALVANIC CELLS

* converts CE to EE, a.k.a, voltaic cell.

* Zinc from the zinc anode dissolves into the soln as Zn^{2+} ions, releasing e^- which consequently enters the external conductors. This triggers the ions that travel through the salt bridge to the cathode trigger e^- from the copper cathode accept the incoming Cu^{2+} ions.



ELECTROLYTIC CELLS

- * Converts EE to CE, by a process aka electrolysis.
- * There are three main components - electrolyte, cathode & anode.
- * Atoms & ions are removed or added due to the applied current. Electrode attracts ions of opposite charges.
- * This can also be used for electroplating, & electrorefining.
- * The amount of EE to be added equals the change in Gibbs free energy of the reaction.

