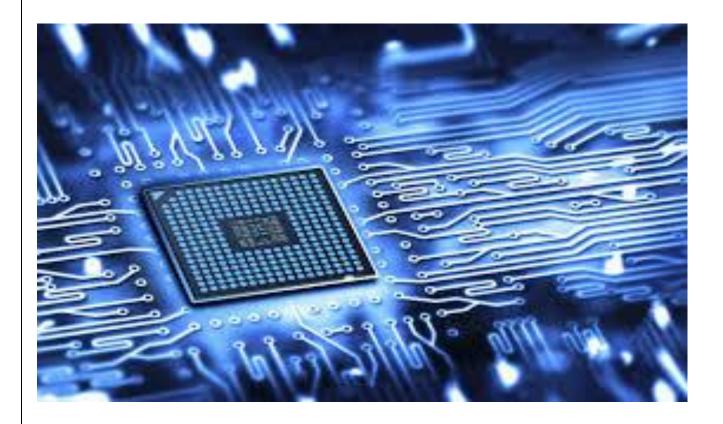
Summer of science-Mid-term report

Materials Related to Electronics and Photonics



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Introduction

Materials related to electronics and photonics is vast subject. It includes various materials as mentioned above. It also involves application of those materials in various devices like PV, transistor etc. The subject involves wide application Chemistry along with maths and physics. It has applications in energy technologies, optoelectronics and electronics technnogies. The basic of these subjects are semiconductors. Semiconductor is basically solid substance which has conductivity between metals and insulators and their conductiovity can be increased by the addition of some materials. Hence they have useful applications in modern electronics. The another topic involved in it is 'optics'. Optics is the scientific study light with their properties and materials required for it. Semiconductor has also wide applications in optics. The materials are needed for different aspects of subject. For e.g. to increase efficiency, to reduce cost etc. I learnt above topics with the help of Wikipedia and research paper from sites like ScienceDirect, springer etc. I mentioned references below each topic.

Materials Covered:

- 1|Inorganic Materials
- 2]Organic Materials
- 3]Nanostructured Materials
- 4]Ionic Crystals
- 5]Alloys
- 6]2D structured Materials
- 7]Conducting Polymers

1 INORGANIC MATERIALS:

Topics covered:

- 1] Zone refining process of purification of germanium with integrated analysis.
- 2]Writing a computer program for calculation of the zone refining process.
- 3]Germanium buffer layer on silicon. (factors affecting it.)
- 4]Growth of heavily doped Germanium single crystals for mid-infrared applications.

Brief theory:

1] Zone refining process of purification of germanium with integrated analysis.

Hyper pure Germanium is important for nuclear spectroscopy. This Hyper pure Germanium is obtained from the zone refining purification process. In this paper, there is a detailed discussion of computational analysis in the Zone refining process. This computational analysis is based on the velocity of heater, size and shape of heater and ingot, the quantity of impurity. In this topic, the heater is basically made up of reflectors on both sides and heat in the form of light radiation is coming from those lamps through reflectors. It is a powerful technique.

2] Writing a computer program for calculation of the zone refining process.

Calculations of the zone refining process is in the form of computer code. It is mainly based on K(equilibrium distribution coefficient of an impurity), Cs ,Co (both are impurity concentration in solid and liquid state resp.),no. of passes etc.

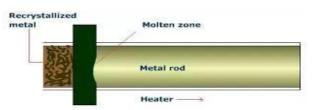


Fig 1: Zone Refining Process

3] Germanium buffer layer on silicon. (factors affecting it.)

Silicon is important in lasers and photonic integrated circuits which are low cost, low power and have high bandwidth. Ge buffer layer is preferred over GeAs layer on silicon due to its thinness and lower dislocation densities in crystals. This process is done by annealing (heating at high temperature and cooling it slowly). There are different factors affecting it such that,

i]annealing effect: mainly based on temperature

ii]effect of thickness: As thickness increases thread dislocation density decreases so we have to keep the thickness at a moderate level.

iii]Effect of doping: Doping affects the dislocation density and roughness (measured in RMS). for e.g. in case of Sb roughness is lesser than boron-doped silicon.

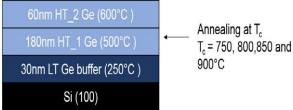


Fig.2: Annealing Tempretures

4] Growth of heavily doped Germanium single crystals for mid-infrared applications.

Heavily-doped germanium (Ge) represents a futuristic material which displays plasma frequencies in the mid-infrared (IR) range. This doping is done by PH3 and B2H6 as a dopant (n-type and p-type resp.) A high doping concentration of the order of 10^18 cm^3 could be obtained while retaining high crystalline quality.

2]ORGANIC MATERIALS

Topics covered:

i] PCBM - Uses of PCBM, organic solar cells, PCBM based n-type semiconductors.

ii] Synthesis of triphenylenes.

Theory:

PCBM - Uses of PCBM, organic solar cells, PCBM based n-type semiconductors.

- [6,6] phenyl C-61 butyric acid methyl ester. It is mainly used in organic solar cells. It is an electron acceptor. It is a more environmentally friendly and low-cost solar cell than a normal silicon solar cell, but it has low efficiency and strength. Some important terms

Organic solar cells –



Fig.3: Organic solar cell Model

1] Perovskite: A perovskite is any material with the same type of crystal structure as calcium titanium dioxide(CaTiO3). (It has mainly 8 atoms on corners.6 atoms at phase centres and 1 atom is at bodycentre)

2]PEDOT: PSS-(poly(3,4-ethylene dioxythiophene) polystyrene sulfonate). It is an organic thermoelectric material which can convert heat in electricity. Also, it is a very good antistatic agent to prevent electric discharges

Along with PCMB, in solar cells, methylamine lead halide (CH3NH3PbX3) is also used in organic solar cells.

For depositing a homogeneous layer on substrate various methods are used.

- 1] Spin coating method
- 2]Dual thermal evaporation method (spin coating is better than this)
- 3]Vapour assassination method (a mixture of spin coating and dip coating methods)

Theory: In this paper, I learnt about the above terms and fabrication of organic solar cells. There are 6 layers in this solar cell. First in IOT layer, second is Pedot-Pss layer, third is perovskite, fourth is PCBM, a fifth is a calcium, and the 6th is an aluminium layer. Through electron microscopy and X-ray diffraction technique, we can detect total morphology of Organic solar cells.

2] Synthesis of triphenylenes:

This is a facile method for synthesis of substituted triphenylene and their heteroaryl analogues using ceric ammonium nitrate (CAN) via an oxidative biaryl coupling. Many Aromatic hydrocarbons, triphenylene has extremely great importance in organic electronics. The CAN oxidized Scholl reaction of various o-ter-phenyls with tolerance for a broad range of functional groups and the heteroaromatic system gave good to excellent yields.

Scholl Reaction: It is a coupling reaction between two arene compounds with the aid of lewis acid and a protic acid.

In this paper there are many more reactions similar to Scholl reaction.

3]NANOSTRUCTURED MATERIALS:

Topics covered:

1]Nanostructured materials - its properties, uses.

2] Types of nanostructured materials for e.g. nanotubes, box-shaped nanomaterials, nano fabrics, Nanofibers, nanoparticles, nanoflowers etc.-

Its definition, its applications and some interesting information (if any material have)

Theory: Nanostructured materials are the materials whose size is in the range of micrometre to nanometre. It includes nanotextured surfaces whose one dimension is only in nanoscale, Nanotubes whose two dimensions are in nanoscale and nanoparticles whose three dimensions are in nanoscale.

I will describe every nanomaterial in brief-

1]Nanotextured surfaces: A nanotextured surface (NTS) is a surface which is covered with nano-sized structures. Such surfaces have one dimension on the nanoscale, i.e., only the thickness of the surface of an object is between 0.1 and 100 nm. They are currently gaining popularity because of their special applications due to their unique physical properties



Fig 4: Nanotextured Surfaces

2]Nanotubes: Two dimensions are in nanoscale. Like diameter in nanoscale. Length can be any. Carbon nanotubes

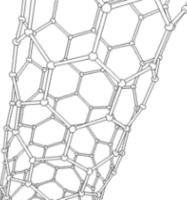


Fig.5 :Nanotubes

(CNTs) are tubes made of carbon with diameters typically measured in nanometres.

3]Spherical nanoparticles: All three dimensions are in nanoscale. The radius of a sphere in nanometres. Ultrafine particles (UFPs) are a particulate matter of nanoscale size (less than 0.1 micrometres or 100 nm in diameter).

4]Gradient multilayer nanofilm: Gradient multilayer (GML) nanofilm is an assembly of Quantum dots layers with a built-in gradient of nanoparticle size, composition or density.

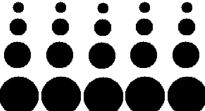


Fig.6: Quantum Dots

Properties of such nanostructures are finding its applications in the design of solar cells and energy storage devices.

5]Icosahedral Structures: An icosahedral is a nanostructure appearing for atomic clusters. These clusters are twenty-faced, made of ten interlinked dual-tetrahedron (bowtie) crystals, typic

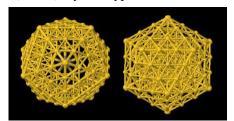


Fig 7 : Icosahedral Structures

having three-fold symmetry. It is like the self-assembly of material at the nanoscale.

6]Nanocages: Gold Nanocages are hollow, porous gold nanoparticles ranging in size from 10 to over 150 nm. They are mainly used as actuators. Actuators are mainly used for moving and controlling mechanisms of machinery.

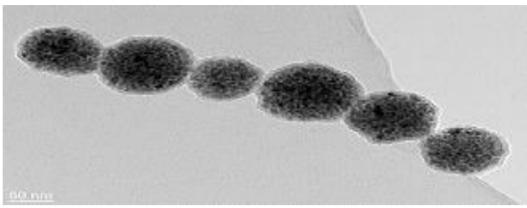


Fig. 8: Gold Nanocages

7]Nanocomposites: The nanocomposite is a multiphase solid material where one of the phases has one, two or three dimensions of less than 100 nm or structures having nano-scale repeat distances between the different phases that make up the material.

8]Nano fabrics: Nano fabrics are textiles engineered with small particles that give ordinary materials advantageous properties such as super hydrophobicity (extreme water resistance, also see "Lotus effect") They are useful for making Water-resistant materials.



Fig. 9 : Nano Fabrics

9]Nanofibers: A fibre that has a width of less than 1000 nanometres (1000 nm or 1 micrometre) is generally defined as a nanofiber. So, there is a difference between nano fabrics and nanofibers. Nanofibers is mainly known for biological fibres.

10]Nanoflowers:

A nanoflower, in chemistry, refers to a compound of certain elements that results in formations which in microscopic view resemble flowers or, in some cases, trees that are called nano bouquets or nano trees. Nanoflowers are composed of several layers of petals to encompass a larger surface area in a small structure for multiple applications in catalysis, biosensors and delivery of drugs

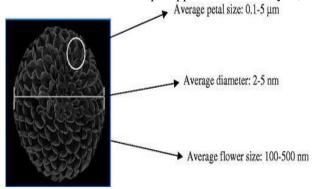


Fig 10 Nanoflowers

11]Nanofoams:

Nanofoams are a class of nanostructured, porous materials (foams) containing a significant population of pores with diameters less than 100 nm. Aerogels are one example of nanofoam. Nanofoams have surprisingly best magnetic properties.

12]Nanoholes:

Nanoholes are a class of nanostructured material consisting of nanoscale voids in a surface of a material. Not to be confused with nanofoam or nano porous materials which support a network of voids permeating throughout the material. Nanohole structures have been used for a variety of applications, ranging from super lenses produced from a metal nanohole array, to structured photovoltaic devices used to improve carrier extraction] and light absorption

13]Nano mesh: The nanomesh is an inorganic nanostructured two-dimensional material, similar to graphene. It consists of a single layer of boron (B) and nitrogen (N) atoms, which forms by self-assembly

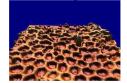


Fig.11:(honeycomb like structure)

Nanopillars: It is an emerging technology within the field of nanostructures. Nanopillars are pillar-shaped nanostructures approximately 10 nanometres in diameter that can be grouped together in lattice-like arrays. They have applications in solar panels, antimicrobial surfaces etc.

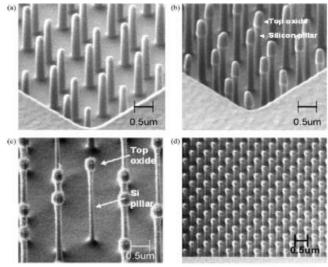


Fig. 12: Nanopillars

15] Nanopin films: Nanopin film is an experimental material in nanotechnology developed in 2005 with unusual superhydrophobic properties. It's a wide application in superhydrophobic material. (hydrophobic material is the material in which the contact angle is greater than 90 degrees)

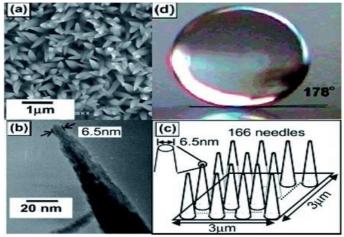


Fig 13: Nanopin Films

16] Nanoplatelets: Graphite nanoplatelets are new types of nanoparticles made from graphite.[1][2] These nanoparticles consist of small stacks of graphene that are 1 to 15 nanometres thick, with diameters ranging from sub-micrometre to 100 micrometres. These nanoparticles can change the fundamental properties of plastics, enabling them to perform more like metals with metallic properties. 17]Nanoribbons: Graphene nanoribbons (also called nano-graphene ribbons or nano-graphite ribbons) are strips of graphene with width less than 50 nm. These are used for bioimaging and in polymeric nanocomposites.

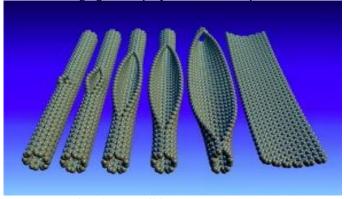


Fig 14: Nanoribbons

18]Nanorings: A nanoring is a cyclic nanostructure with a thickness small enough to be on the nanoscale. Uses: Optical and catalytic properties are useful.



Fig 15: Nanorings

19]Nanorods: In nanotechnology, nanorods are one morphology of nanoscale objects. Each of their dimensions ranges from 1–100 nm. They may be synthesized from metals or semiconducting materials. One potential application of nanorods is in display technologies, because the reflectivity of the rods can be changed by changing their orientation with an applied electric field. Another application is for microelectromechanical systems (MEMS).

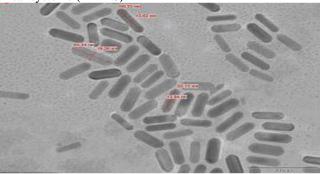


Fig 16:Nanorods

20]Nanosheets: nanosheet is a two-dimensional nanostructure with thickness in a scale ranging from 1 to 100 nm.

A typical example of a nanosheet is graphene, the thinnest two-dimensional material (0.34 nm) in the world. It consists of a single layer of carbon atoms with hexagonal lattices. 2017 Silicon nanosheets are being used to prototype future generations of small (5 nm) transistors. Carbon nanosheets (from hemp) may be an alternative to graphene as electrodes in supercapacitors.

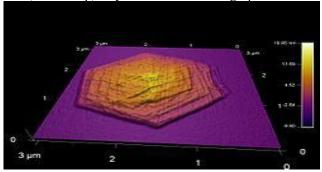


Fig 17: Graphene nanosheet.

21]Nano shells: A nano shell, or rather a nano shell plasmon, is a type of spherical nanoparticle consisting of a dielectric core which is covered by a thin metallic shell (usually gold)Their main usage is in treatment of cancer.

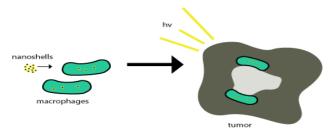


Fig 18: Nanoshells affecting tumour

22]Nanotips: Nanotips is a conductive liquid polyamide solution that will transform your favourite pair of gloves into touchscreen gloves. Formulated using nanotechnology, Nanotips mimics the touch of the human skin.

23] Nanowires: A **nanowire** is a nanostructure, with the diameter of the order of a nanometre (10–9 meters). It can also be defined as the ratio of the length to the width being greater than 1000. They are mostly used in electronic devices.



Fig. 19: Nanowires

24]Nanostructured film: A nanostructured film is a film resulting from engineering of nanoscale features, such as dislocations, grain boundaries, defects, or twinning. Nanostructured films with superior mechanical properties allow previously unusable materials to be utilized in new applications, enabling advances fields where coatings are heavily utilized, such as aerospace, energy, and other engineering fields.

25] Self-assembled nanomaterials: Self-assembly is a process in which a disordered system of pre-existing components forms an organized structure or pattern as a consequence of specific, local interactions among the components themselves, without external direction.

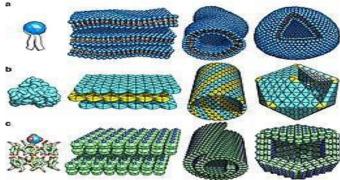


Fig. 20: Different Assemblies.

26]Quantum Heterostructures: Quantum heterostructure is a heterostructure in a substrate (usually a semiconductor material), where size restricts the movements of the charge carriers forcing them into a quantum confinement. This leads to the formation of a set of discrete energy levels at which the carriers can exist. Quantum heterostructures have sharper density of states than structures of more conventional sizes. In the below fig. It is given like a particle in an infinite well.

Applications as low-permittivity barrier layers in electronic chips as well as solar cells have also been suggested. Biomedical applications such as tissue scaffolds, drug-delivery platforms, virus traps, and labs-on-a-chip are also in different stages of development

27]Sculptured Thin films: Sculptured thin films (STFs) are nanostructured materials with unidirectionally varying properties that can be designed and realized in a controllable manner using variants of physical vapour deposition. To date, the chief applications of STFs are in optics as polarization filters, Bragg filters, and spectral hole filters.

28] Nano water cubes: Plumbene graphene's latest cousin, realized on the 'nano water cube'.

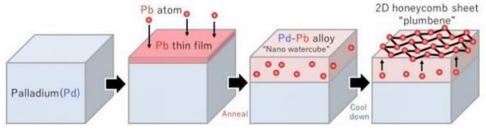


Fig. 21: Nano water cube

Research Papers:

1] Nanostructure material, basic concepts and microstructure

Categories of nanostructured materials

- 1]The *first category* comprises materials and/or devices with reduced dimensions and/or dimensionality in the form of (isolated, substrate-supported or embedded)
- 2] The *second category* comprises materials and/or devices in which the nanometre-sized microstructure is limited to a thin (nanometre-sized) surface region of bulk material.
- 3] The third category of bulk solids with a nanometre-scale microstructure. In fact, we shall focus on bulk solids in which the chemical composition, the atomic arrangement and/or the size of the building blocks.

Two classes of such solids may be distinguished.

- 1] In the first class, the atomic structure and/or the chemical composition varies in space continuously throughout the solid on an atomic scale.
- 2]. These materials are assembled of nanometre-sized building blocks—mostly crystallites Effects controlling the properties of nanostructured materials
- 11Size effects
- 2] Change of the dimensionality of the system
- 3]Changes in the atomic structure
- 4] Alloying of components (e.g. elements) that are immiscible in the solid and/or the molten state

2]Microwave-assisted synthesis of C-doped TiO2 and ZnO hybrid nanostructured materials as quantum-dots sensitized solar cells

- 1]Microwave-assisted solvothermal synthesis of C-doped TiO2 and ZnO hybrid materials.
- 2]C-doped TiO2 and ZnO showed a red-shift in the bandgap and electrochemical response to UV light irradiation.
- 3]Eco-friendly synthesis of nanostructured materials as photoelectrodes for quantum-dots sensitized solar cells.

3]Towards high thermal stability of optical sensing materials with bio-inspired nanostructure

The optical properties of iridescent nanostructures which were found in butterfly scales were investigated under varied temperature. An amazing hierarchical nanostructure with high thermal stability was revealed for the application of bio-inspired optical materials. Following are key points in the research paper: 1] The RSS and BLS models were constructed precisely.

- 2]Thermal dilation changes the reflection spectra of RSS and BLS.
- 3]The reflection spectra of RSS are sensitive to the thermal response.
- 4]The reflection spectra of BLS are stable under varied temperatures

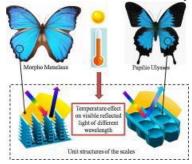


Fig 22: Optical sensing material.

4)Optical properties of nanostructured materials: a review

Depending on the size of the smallest feature, the interaction of light with structured materials can be very different. This fundamental problem is treated by different theories. From atoms and molecules to crystals and bulk components, optical materials are naturally structured at different scales. The interaction of materials with optical waves and photons is strongly dependent on the structure, which can then be used to control light field distribution and light propagation. This allows the development of a large range of key components for optical systems and it is now a major field of photonics. There are different types of surface structures:

- 1]Random surfaces
- 2]Controlled random surfaces.
- 3]Black silicon

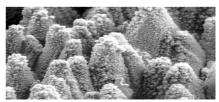


Fig 23: Black Silicon

Photonic crystals: For optical coatings, the light is reflected or transmitted through the sample. On the contrary, diffraction structures are generally used to distribute the light in a controlled way in different directions of the space. Photonic crystals can also be considered as metamaterials with optical properties impossible to achieve with nanostructured materials. As an example, the structure can behave like a material having a refractive index of zero or even negative.

4]IONIC CRYSTALS

Topics Covered:

- 1]Difference between crystalline and amorphous substances.
- 2] Various types of crystals.
- 3]14 Bravais lattices.
- 4] Types of Voids and radius ratios to determine structure of crystal.
- 5]Difference between structure of NaCl and CsCl.

6]Different properties of NaCl (Similar to another crystals)

71Defects in Solids

8]'Williams' book- write up on photonics and electronics related to semiconductors and ionic materials

Williams(writeup)

This write- up is all about how electronics and Photonics properties are seen in ionic crystals and semiconductors. There are two theories to explain this task. But later Mott (Scientist name) suggested that both theories are true and applied wherever its conditions hold true.

1]Band Theory

2] Hitler and London Theory.

1]Band theory: The band theory was originally investigated by Bloch, Brillouin and Wilson. It is essentially a molecular orbital method applied to the periodic lattice. The approximate one-electron wave functions involve the product of a periodic function and atomic wave functions

2]Hitlor and London theory: The Heider-London method is, of course, the familiar atomic orbital method and is applicable to systems in which the electrons are localized (on particular atoms. The approximate crystal wave functions are formed anti symmetrical linear combinations of permutations of products of atomic wave functions)

Mr. Mott suggested that Hitler and London theory is a good approximation for that crystal where electron and holes don't form easily that is substances having Frankl defect (like ZnS) and band theory is a good approximation for substances where Schottky defect is present (like NaCl).

IONIC CRYSTALS: In Ionic crystals, Lattice energy is defined by dipole and Quadrupole term with approximation and using electron wave Functions.

Solid-state luminescence. -The alkali halide phosphors have been extensively investigated to determine the mechanism of solid-state luminescence. In ionic crystals, luminescence is generally by the presence of impurity (like Tl+ ion present in KCl ion at some places of K+). Johnson & Williams have formulated a general theory of the dependence of luminescent efficiency on activator concentration, based on the idea that activator ions are capable of efficient emission only if isolated from other activator ions. The presence of nearby activator ions reduces the activation energy for radiation less de-excitation, probably by overlap of wave functions; therefore, the efficiency-concentration interrelation is markedly temperature dependent

SEMICONDUCTORS: In semiconductors Band theory is very useful. It is assumed that at absolute zero temp there are no any electronics in conduction band. As temp. increases electron hole pairs increases but not significantly hence the concept of Doping is arrived and with this extrinsic semiconductor, the word 'electronics' takes a new path and now become of 'Heart' of every electronic material.

Germanium and silicon have been investigated as intrinsic and as N and P-type semiconductors. Both substances have the diamond structure with each atom making Sp3 tetrahedral covalent bonds with the four nearest neighbours. Thermal excitation of an intrinsic semiconductor to produce an electron in the conduction band and a positive hole in the valence band corresponds, as emphasized by Shockley (51), to removing an electron from a covalent bond.

5]ALLOYS

Topics covered:

- 1] Basics of alloys-properties, uses etc.
- 2] Gallium arsenide compound
- 3] Silicon germanium alloy

Theory:

1] An alloy is a combination of metals or metals combined with one or more other elements. For example, combining the metallic elements gold and copper produces red gold, gold and silver becomes white gold, and silver combined with copper produces sterling silver. Elemental iron, combined with non-metallic carbon or silicon, produces alloys called steel or silicon steel. The resulting mixture forms a substance with properties that often differ from those of the pure metals, such as increased strength or hardness. Some important alloys-

Pewter, Stainless Steel, Solder, Brass, Duralium etc



Fig 24: Duralium

2] Some important terms:

1] IR emitting diodes: An IR LED (infrared light-emitting diode) is a solid-state lighting (SSL) device that emits light in the infrared range of the electromagnetic radiation spectrum.IR LEDs allow for cheap, efficient production of infrared light, which is electromagnetic radiation in the 700 nm to 1mm range



Fig 25: IR emitting Diode

2]Laser Diodes: A laser diode, (LD), an injection laser diode (ILD), or diode laser is a semiconductor device similar to a light-emitting diode in which a diode-pumped directly with electrical current can create lasing conditions at the diode's junction. Ultraviolet Wavelength of laser diodes is between 180nm to 400 nm.



Fig 26: Lasor Diode

3]Integrated Circuits (IC's): An integrated circuit or monolithic integrated circuit (also referred to as an IC, a chip, or a microchip) is a set of electronic circuits on one small flat piece (or "chip") of semiconductor material that is normally silicon.



Fig 27: IC Chips

4]Tunnelling diodes: A tunnel diode or Esaki diode is a type of semiconductor diode that has effectively "negative resistance" due to the quantum mechanical effect called tunnelling. Tunnel diodes have a heavily doped positive-to-negative (P-N) junction that is about 10 nm (100 Å) wide. The heavy doping results in a broken bandgap.



Fig 28: Tunneling Diodes

5]Wafer: In electronics, a wafer is a thin slice of semiconductor, such as a crystalline silicon, used for the fabrication of integrated circuits and, in photovoltaics, to manufacture solar cells.



Fig 29: Wafer

6]MESFET transistors.: A MESFET (metal-semiconductor field-effect transistor) is a field-effect transistor semiconductor device similar to a JFET with a Schottky (metal-semiconductor) junction instead of a p-n junction for a gate.

JFET: normal transistor with 3 gates. The Schottky barrier is instead of the p-n junction, there is a metal-semiconductor junction. About Gallium Arsenide compound:

In the Gallium arsenide (GaAs) Wafer, each gallium atom is bordered by arsenic atoms. 5 valence electrons of arsenic atoms and 3 valence electrons of gallium atoms share each other. So, each of the gallium and arsenic atom gets 8 valence electrons in the outer shell. The main use of gallium arsenide (GaAs) is found in: Computers, Photovoltaic cells, Optoelectronic communications, Aerospace and defence, Integrated Circuits, High-Frequency Technology (because it cannot melt up to 450-degree Celsius temp.), Transistors .

Advantages of Gallium arsenide over silicon chips:

The advantage of gallium arsenide wafers over solar-grade silicon wafers is that it offers almost twice the efficiency. Another advantage of GaAs wafer refers to the increase in efficiency. In solar cells, we can give more than one layer of GaAs so surface area is increased and it acquires efficiency more than silicon solar cells.

Disadvantages of Gallium arsenide:

The big disadvantage, which explains its low utilization, is the price. To solve this dilemma, engineers and researchers say they have achieved new methods of manufacturing thin films of low-cost gallium arsenide, which would create devices that replace silicon and are as much as efficient like GaAs.

Silicon-Germanium Alloy

Siege or silicon-germanium is an alloy with any molar ratio of silicon and germanium, i.e. with a molecular formula of the form Si1-xGex. It is commonly used as a semiconductor material in integrated circuits (ICs) for heterojunction bipolar transistors or as a strain-inducing layer for CMOS transistors.

SiGe allows CMOS logic to be integrated with heterojunction bipolar transistors, making it suitable for mixed-signal circuits.[7] Heterojunction bipolar transistors have higher forward gain and lower reverse gain than traditional homojunction bipolar transistors. This translates into better low current and high frequency performance

6]2D STRUCTURES

Topics covered

- :1] Definition of 2D structures with some examples and their properties.
- 2]2D semiconductor materials and their properties.
- 3]Research paper:2D organic semiconductors, the future of green nanotechnology.
- 4]Research paper: GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures

Theory:

1] Definition of 2D structures with some examples and their properties.

Two-dimensional (2D) materials, sometimes referred to as single-layer materials, are crystalline materials consisting of a single layer of atoms. These materials have found use in applications such as photovoltaics, semiconductors, electrodes and water purification.

Some definitions and terms:

1]Graphene: First 2D structure which is a single layer of Graphite isolated in 2004. Graphene is a crystalline allotrope of carbon in the form of a nearly transparent (to visible light) one atom thick sheet. It is hundreds of times stronger than most steels by weight Uses: Graphene has a lot of other promising applications: anti-corrosion coatings and paints, efficient and precise sensors, faster and efficient electronics, flexible displays, efficient solar panels, faster DNA sequencing, drug delivery.

2]Maxine: In materials science, MXenes are a class of two-dimensional inorganic compounds. These materials consist of few-atoms-thick layers of transition metal carbides, nitrides, or carbonitrides.

Uses: It has supper biological properties, water purification properties. It is mainly used in lithium-ion batteries and sodium-ion batteries, Supercapacitors, Optoelectronic devices, Antennas, Porous Mxenes etc.

3]Silicene:

Silicene is a two-dimensional allotrope of silicon, with a hexagonal honeycomb structure similar to that of graphene. Contrary to graphene, silicene is not flat, but has a periodically buckled topology; the coupling between layers in silicene is much stronger than in multi-layered graphene

4]Graphyne:

another 2-dimensional carbon allotrope whose structure is similar to graphene. It can be seen as a lattice of benzene rings connected by acetylene bonds. Depending on the content of the acetylene groups, graphyne can be considered a mixed hybridization, spn, where 1 < n < 2. Recently it has been claimed to be a competitor for graphene, due to the potential of direction-dependent Dirac cones.

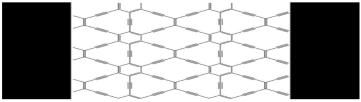


Fig 30: Graphyne

5]Borophene: Borophene is a crystalline atomic monolayer of boron and also known as boron sheet.

Uses - The alkali metal ion batteries, Li-S batteries, hydrogen storage, supercapacitor, sensor and catalytic in hydrogen evolution, oxygen reduction, oxygen evolution, and CO2 electroreduction reaction.

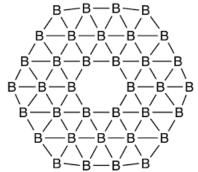


Fig.31: Borophene

6]Germanene: Germanene is a two-dimensional allotrope of germanium, with a buckled honeycomb structure. Uses: It is mainly used in field-effect transistors and electronic devices.

7]Si2BN: In 2016 researchers predicted a 2d hexagonal, metallic allotrope of Si2BN with only sp2 bonds.

A graphene-like 2D material Si2BN, is computationally explored for the anode of Li/Na ion batteries, The host 2D material exhibits exceptionally high stability., The material undergoes a phase transition from planar to buckled structure due to ion-adsorption, This phase transition facilitates superior specific capacity higher than several other 2D analogues, Computed ionic diffusion barriers suggest very fast ion diffusion especially for Na ion.

8]Stanene: It is composed of tin atoms arranged in a single layer, in a manner similar to graphene. Its buckled structure leads to high reactivity against common air pollutants such as NOx and COx and is able to trap and dissociate them at low temperature Applications:

excellent quantum effects, superconductivity, and thermoelectric properties. Focusing on the promising 2D elemental material stanene, the fundamental electronic properties

9]Plumben: It is a two-dimensional allotrope of lead, with a hexagonal honeycomb structure similar to that of graphene.

Uses: It is a topological insulator, plumbene in batteries, machine manufacturing, Shipbuilding .

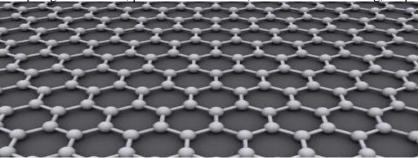


Fig.32:Plumben

10]Phosphorene:Phosphorene is a 2-dimensional, crystalline allotrope of phosphorus(It is a black phosphorus, the most stable allotrope of P). Its mono-atomic hexagonal structure makes it conceptually similar to graphene. However, phosphorene has substantially different electronic properties; in particular, it possesses a nonzero band gap while displaying high electron mobility. It is better semiconductor than graphene.



Fig 33: Phophorine

Uses: solar cell material donor material(optoelectronics), transistor, inverter, flexible circuits.

11]Antimonene: It is a two-dimensional allotrope of antimony, with its atoms arranged in a buckled honeycomb lattice. Theoretical calculations predicted that antimonene would be a stable semiconductor in ambient conditions with a suitable performance for (Opto)electronics. It has good super capacitive properties.

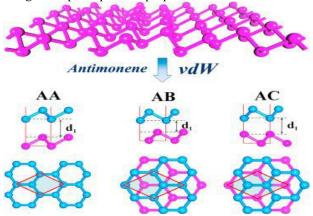


Fig 34 Antimonene

12]Bismuthene: Bismuthene, the two-dimensional allotrope of bismuth, was predicted to be a topological insulator. It was predicted that bismuthene retains its topological phase when grown on silicon carbide in 2015.

13 Metals: Single and double atom layers of platinum in a two-dimensional film geometry has been demonstrated.

14]2D alloys: Two-dimensional alloys are a single atomic layer of alloy that are incommensurate with the underlying substrates. The 2D ordered alloy of Pb and Sn has been synthesized and characterized with scanning tunnelling microscopy and low-energy electron diffraction in 2003.

15]graphane: Graphane is a polymer of carbon and hydrogen with the formula unit (CH)n where n is large. Graphane is a form of fully hydrogenated (on both sides) graphene. Graphane's carbon bonds are in sp3 configuration, as opposed to graphene's sp2 bond configuration. Thus, graphane is a two-dimensional analogue of a cubic diamond.

16]BN: 2D boron nitride is a sp2-conjugated compound that forms a honeycomb structure of alternating boron and nitrogen atoms with a lattice spacing of 1.45Å. Due to several similar structural similarities with graphene, boron nitride nanosheets are considered graphene analogues, often called "white graphene"

Applications:

Electrical: Boron nitride nanosheets have a wide bandgap that ranges from 5 to 6 eV and can be changed by the presence of Stone-Wales defects within the structure, by doping or functionalization or by changing the number of layers, it acts as an excellent insulator

Thermal: It is an excellent thermal conductor.

17]Boron carbonitride: Borocarbonitrides are two-dimensional compounds that are synthesized such that they contain boron, nitrogen, and carbon atoms in a ratio Bx Nz. Boro Carbonitrides are distinct from B, N co-doped graphene in that the former contains separate boron nitride and graphene domains as well as rings with B-C, B-N, C-N, and C-C bonds.

Electrical properties: It has significant band gaps like semiconductors. The wide range of composition of boron nitrides allows for the tuning of the bandgap, which when coupled with its high surface area and Stone-Wales defects may make boron nitrides a promising material in electrical devices.

18]Germanane:

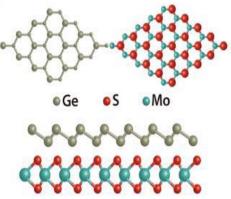


Fig 35: Germanene and MoS2

Germanane is a single-layer crystal composed of germanium with one hydrogen bonded in the z-direction for each atom. Germanane's structure is similar to graphene.

19]Molybdenum disulphide: Molybdenum disulphide monolayers consist of a unit of one layer of molybdenum atoms covalently bonded to two layers of sulphur atoms.

Electrical: The electrical properties of molybdenum sulphide in electrical devices depend on factors such as the number of layers, the synthesis method, the nature of the substrate on which the monolayers are placed, and mechanical strain.

Thermal: It has very low thermal conductivity compared to graphene.

20]Organic 2D structures: Ni3(HITP)2 is an organic, crystalline, structurally tenable electrical conductor with a high surface area. Multiple layers naturally form perfectly aligned stacks, with identical 2-nm openings at the centres of the hexagons. Those are suitable for advanced composites, paints and coatings, lubricants, oils and functional fluids, capacitors and batteries, thermal management applications, display materials and packaging, inks and 3D-printers' materials, and barriers and films They have biological applications too.

2] 2D semiconductors:

i]Graphene

ii]Hexagonal Boron Nitride

iii]Transition metal Dichalcogenides(like MoS2)

Applications

il Electronic Devices: 2D Semiconductors can be used as transistors for digital electronics.

ii] Energy and Harvesting Devices: 2D semiconductors have the potential for application in the harvesting of solar energy. The atomically thin structure allows for lower surface recombination velocity, which leads to better photocurrent conduction. An improvement in solar cell performance has been shown while stacking 2D semiconductors with multilayers of graphene.

iii] Flexible and Transparent Substrates: The thin layer of 2D materials can be used for flexible electronics. In particular, 2D MoS2 can be used to create thin displays and wearable electronics due to its out of plane flexibility, strong covalent bonds, and diverse electronic properties.

iv]Magnetic NEMS: 2D layered magnetic materials are attractive building blocks for nanoelectromechanical systems (NEMS): while they share high stiffness and strength and low mass with other 2D materials, they are magnetically active.

Research paper:

2D organic semiconductors, the future of green nanotechnology.

Some important terms:

Ballistic transportation: In mesoscopic physics, ballistic conduction (ballistic transport) is the transport of charge carriers (usually electrons) in a medium, having negligible electrical resistivity caused by scattering. Without scattering, electrons simply obey Newton's second law of motion at non-relativistic speeds.

Coffee ring effect: In physics, a "coffee ring" is a pattern left by a puddle of particle-laden liquid after it evaporates. The phenomenon is named for the characteristic ring-like deposit along the perimeter of a spill of coffee. It is also commonly seen after spilling red wine. The mechanism behind the formation of these and similar rings is known as the coffee ring effect or in some instances, the coffee stain effect, or simply ring stain.

Introduction:

This paper mainly focuses on organic 2D crystals and their electronic, optical, mechatronics properties etc and also different synthesis methods for this material.

Also, organic 2D crystals have great advantages on inorganic 2D materials because it is economic and ecological benefits. The properties like depending on no.of layers, how they are arranged so we can vary properties according to our need. There are two types of organic 2D materials 1]Small molecules like pentacene, rubrene and 2] large polymers.

Different synthesis methods of organic 2D crystals:

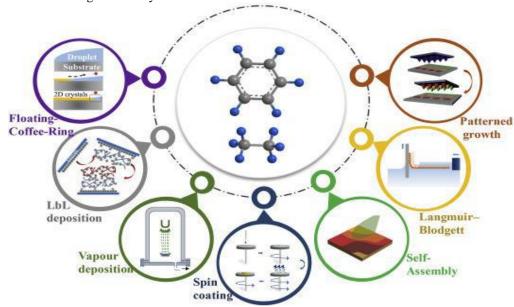


Fig 36: Synthesis Methods Of 2D Crystals

Advantages of 2D Organic semiconductors:

- 1] Eco-friendly materials
- 2[Flexible devices
- 3]Bio molecular integration electronics
- 4]Property tuning: surface functionalization, doping, heterostructures.

Applications:

- 1]Organic thin film transistor.
- 2]Organic light-emitting diode.
- 3]Photo diodes
- 4]Some mechatronics devices
- 5]Solar cell
- 6]Optical waveguide

GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures

Some important points:

- 1]The structure and electronic properties of GeAs and SiAs monolayers by first-principles calculations.
- 2] Their monoclinic structures are dynamically stable. The interlayer cohesive energies are of moderate strength.
- 3]The bandgap of GeAs and SiAs monolayers are 1.66 eV (2.06 eV by HSE06) and 1.84 eV (2.50 eV by HSE06), respectively.
- 4] Their carrier effective masses are relatively small. SiAs monolayer is a suitable photocatalyst for water splitting.

7] CONDUCTING POLYMERS:

Topics covered:

- 1] Definition of conducting polymers, History, Types, Synthesis and applications
- 2] Preparation of elastic polymer slices have the semiconductors properties for use in solar cells as a source of new and renewable energy.

Theory:

1] Conductive polymers or, more precisely, intrinsically conducting polymers (ICPs) are organic polymers that conduct electricity.[1][2] Such compounds may have metallic conductivity or can be semiconductors. The biggest advantage of conductive polymers is their processability, mainly by dispersion. Conductive polymers are generally not thermoplastics, *i.e.*, they are not thermoformable.

Applications: Due to their poor processability, conductive polymers have few large-scale applications. They have promise in antistatic materials[3] and they have been incorporated into commercial displays and batteries, but there have been limitations due to the manufacturing costs, material inconsistencies, toxicity, poor solubility in solvents, and inability to directly melt process. Literature suggests they are also promising in organic solar cells, printing electronic circuits, organic light emitting diodes, actuators, supercapacitors, chemical sensors, biosensors etc.

Research paper:

Preparation of elastic polymer slices have the semiconductors properties for use in solar cells as a source of new and renewable energy

To prepare elastic polymer slices that have semiconductors properties for use in solar cells based on charge transfer (CT) complexation. For this purposefirst six derivatives of 1,8–naphthalimide fluorescent dyes were synthesized. Secondly, the synthesized fluorescent dyes were complexed with p–chloranil acceptor via CT interaction in methanol solvent. The obtained CT complexes were dispersed in poly (methyl methacrylate) (PMMA) matrixes using methylene chloride solvent at room temperature. The obtained polymer sheets were characterized by several spectroscopic and physicochemical techniques, such as IR and UV–vis spectroscopies; and SEM technique. The microstructural and morphological changes occurred in the sheets of the PMMA matrix blended with the CT products were observed using the positron annihilation Doppler broadening (PADB) and the positron annihilation lifetime (PAL) techniques. Finally, the photostability and the direct current (DC) electrical characteristics as a function of the temperature for the CT products dispersed in PMMA matrixes have been studied.

Some terms:

1]CT: charge transfer complexes.

2]1,8-naphthalimide fluorescent dyes:

Dye is used for generating CT.

3SEM technique: Ascanning electron microscope(SEM) is a type of electron microscope that produces images of a sample by scanning the surface with a focused beam of electrons. The electrons interact with atoms in the sample, producing various signals that contain information about the surface topography and composition of the sample.

4]positron annihilation Doppler broadening-Doppler broadening positron annihilationspectroscopy is used to measure the concentration, spatial distribution, and size of open-volume defects in low dielectric constant (low-k) hydrogen-and methyl-silsesquioxane thin films.

Updated Plan Of Action:

Dates	Subjects
0.5.84	Onlaw David
3-5 M ay	Solar Panel
6-8 May	Diode
9-11 May	Transistor
12-14 M ay	LED
15-17 M ay	Lasor
18-20 May	Radio trnascivers
21-22 May	Polycrystalline materials
23-28 May	correlate materials with devices,
	mechanism of construction
29 -30 may	Revision
31 may onwards	Preaparing final report

Ref:

1]Inorganic materials:

Journal homepage: www.elsevier.com/locate/jcrysgro

- 1]Integrated analysis and design optimization of germanium purification process using zone-refining technique
- 2]Simulation for purification process of high pure germanium by zone refining method
- 3] Thin Ge buffer layer on silicon for integration of III-V on silicon
- 4] Growth of heavily-doped Germanium single crystals for mid-Infrared applications

2]Organic materials:

- 1] https://en.m.wikipedia.org/wiki/Phenyl-C61-butyric acid methyl ester
- 2] https://nanoscalereslett.springeropen.com/articles/10.1186/s11671-015-1020-2
- 3|https://en.m.wikipedia.org/wiki/Triphenylene
- 4]https://www.researchgate.net/publication/327649977_Facile_synthesis_of_Triphenylenes_and_Triphenylene_Phenanthrene_fus ed_heteroaromatics

3]Nanomaterials:

- 1] https://en.wikipedia.org/wiki/Nanostructure
- 2]https://en.wikipedia.org/wiki/Nanomaterials
- 3] https://www.sciencedirect.com/science/article/pii/S1359645499002852
- 4] https://www.sciencedirect.com/science/article/pii/S0169433217332142
- $5]\ https://www.spiedigitallibrary.org/journals/journal-of-nanophotonics/volume-5/issue-01/052502/Optical-properties-of-nanostructured-materials-a-review/10.1117/1.3609266.full?SSO=19$
- 6] https://www.sciencedirect.com/science/article/pii/S0167577X1830435X

4]Ionic Crystals:

- 1] https://en.wikipedia.org/wiki/Ionic crystal
- 2]https://www.annualreviews.org/doi/pdf/10.1146/annurev.pc.03.100152.002011

5]Alloys:

- 1] https://link.springer.com/chapter/10.1007%2F978-0-387-68650-9 6
- 2] https://en.wikipedia.org/wiki/Alloy
- 3]https://nanografi.com/blog/gallium-arsenide-gaas-wafer-structure-properties-uses- advantages/
- 4] https://en.m.wikipedia.org/wiki/Silicon-germanium

6]2D structures:

- 1]Ref: https://en.wikipedia.org/wiki/Two-dimensional_materials
- 2]https://en.wikipedia.org/wiki/Two-dimensional_semiconductor
- 3]https://www.sciencedirect.com/scienc/article/pii/S2589965119300674
- 4]https://www.sciencedirect.com/science/article/pii/S1386947717311736

7]Conducting Polymers:

- 1] https://en.m.wikipedia.org/wiki/Conductive polymer
- 2]https://www.sciencedirect.com/science/article/pii/S101060301731852X