MATERIALS SCIENCE:

A FIELD OF DIVERSE INDUSTRIAL APPLICATIONS

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Materials Science: A Field of Diverse Industrial Applications

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PREFACE

Material science comprises various classes of different materials and every class constitutes a separate field. New materials are developed through nanotechnology in various fields of material science that develop areas of research like biotechnology, environmental science, information technology and energy technologies. The present book attempts to cover recent developments of new materials and their application in various fields. This book consists of ten book chapters from well-reputed universities and institutes. Chapters of the book cover areas like nanomaterials in society, nanomaterials in medicine in health sectors, and nanomaterials as nano food. Some chapters of this book cover the application of materials/ nanomaterials for energy and their functionalization for particular applications like multifunctional advanced nanomaterials for energy applications, materials in dye-sensitized solar cells and for electrochemical sensing. The content of the book has three sections. A chapter-by-chapter brief description is as follows:

The first sections have five chapters related to the different modified materials and their versatility in different fields of science. In this respect, the authors of chapter 1 have discussed the silent characteristics of many inorganic materials and their medicinal significance. Chapter 2 highlights some basics of chalcogenide glasses, preparation techniques and a review of the latest technological developments along with structural properties, optical properties, and thermal and electrical properties of chalcogenide glasses. The author presents the method of fabrication of chalcogenides, in bulk and thin film forms in Chapter 3. Dr. Sunanda Das has provided a detailed study in chapter 4 about polymeric synthetic fibers and their commercial uses. She has also highlighted the points related to the environmental impact and health issues engendered by using a lot of synthetic polymeric fibres in different areas. Chapter 5 presents detailed surface morphological studies using AFM images of BaF_2 thin films deposited by the electron beam evaporation technique on three different substrates like glass, silicon (Si), and aluminum (Al) substrate and also estimates the fractal dimensions of the horizontal as well as vertical sections of the film surfaces.

The second section of the book content has three chapters on functionalized nanomaterials and also their applications. Chapter 6 deals with the synthesis and characterization of BFO and Sm-doped BFO nanoceramics. Chapter 7 presents a review of the development of nano-technology for the removal and safe disposal of radioactive ions from the environment using nanomaterials. Chapter 8 is the ephemeral study of nanocatalysts in organic synthesis.

The third section of the book contains chapters related to the role of modified materials in energy production and its utilization. In Chapter 9, *Pinki, Subhash* and *Ashu Chaudhary* have given an overview of the implications and applications of multifunctional advanced materials/gadgets for energy conversion and storage. They have explained different processes used for energy conversion and storage like lithium-ion batteries, supercapacitors, fuel cells, polyoxometalates, polyaniline-based two-dimensional dichalcogenides, chemical vapour deposition, thermal energy storage with phase change materials, *etc*. Chapter 10 describes the overall advancement in electrolytes used for producing low-cost and industrially stable dye-sensitized solar cells. For this purpose, Priyanka Chawla, *et al*. have explained the use of solid polymeric materials such as PEO, PVA, PVDF, and chitosan in place of liquid electrolytes.

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Part 1: Functional Materials and their Versatility

CHAPTER 1

Chalcogenides: Bulk and Thin Films

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Abstract: Chalcogens are the chemical elements of group 16 of the periodic table. Oxygen is treated separately from other chalcogens; it is even excluded from the term ‘chalcogen’ altogetherdue to its very different chemical behaviour from sulfur, selenium, tellurium and polonium. The heavier chalcogens have vacant d orbitals. A chalcogenide consists of at least one chalcogen element and one electropositive element. The term chalcogenide is more commonly reserved for sulfides, selenides and tellurides rather than oxides. The interest in these materials arises particularly due to their ease of fabrication in the form of bulk and thin films. Generally, chalcogenides have a large glass-forming region and thus, their physical properties can be tuned *via* chemical composition. These glasses have drawn great attention due to their striking electrical, optical and thermal properties, which ary with composition, heat treatment, irradiation, glass forming methods, *etc*. There is a high tendency for the atoms to link together to form link chains in chalcogenides. In general, the atomic bonding is more rigid than that of organic polymers and more flexible than that of oxide glasses. This chapter presents the method of fabrication of chalcogenides in bulk and thin film forms.

Keywords: Bulk form, Chemical methods, Chalcogenides, Physical deposition, Synthesis, Thin films.

CHALCOGENS

Chalcogens are the chemical elements of group 16 of the periodic table. The group consists of the elements oxygen (O), sulfur (S), selenium (Se), tellurium (Te) and polonium (Po) each having six valence electrons in the outermost shell.

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The term “chalcogens” was derived from the Greek word *chalcos* meaning 'copper or ore’ and *genes* meaning ‘formed or produced’ since they all are found in copper ores. The name became popular since it is analogous to the name of group 17 – halogens – meaning salt formers. Oxygen is a gas while the other group members are solids. Both oxygen and sulfur can be found in the pure form. Oxygen is generally extracted from air and sulfur is extracted from oil and natural gas. Selenium and tellurium are produced as byproducts of copper refining. Polonium – a radioactive element – is mostly available in particle accelerators. Oxygen is treated separately from other chalcogens; even excluded from the scope of the term “chalcogen” altogether, due to its very different chemical behaviour from sulfur, selenium, tellurium and polonium. One reason for this is that the heavier chalcogens have vacant d-orbitals. Oxygen's electro-negativity is also much higher than those of other chalcogens. This makes oxygen's electric polarizability several times lower than those of other chalcogens [1]. The metal character increases and the electro-negativity decreases, as the atomic number increases. The elements and their compounds vary in their toxicity. It is interesting that oxygen and sulfur are essential to all life, while the compounds of selenium, tellurium and polonium can be toxic. The chalcogens have varying crystal structures. Oxygen's crystal structure is monoclinic while sulfur's is orthorhombic. Selenium and tellurium have a hexagonal crystal structure while polonium has a cubic crystal structure.

CHALCOGENIDES

A chalcogenide is an inorganic chemical compound which consists of at least one chalcogen element and at least one more electropositive element. Although all group 16 elements of the periodic table are termed as chalcogens, chalcogenide is more commonly used for sulphides, selenides and tellurides only, rather than oxides. Oxides behave quite differently from chalcogenides. Their band gaps and optical and electrical properties are very different. Hence, chalcogenides may be defined as oxygen-free inorganic materials which contain one or more chalcogen elements along with at least one electropositive element. Chalcogenides possess large glass-forming region so their properties – physical, electrical, optical and thermal – can be tuned by altering the chemical composition, irradiation, heat treatment, glass forming method, *etc.* It is the chemical bonding in combination with the topology of glass network that determines their physical properties. Therefore, it is necessary that structure of these glasses is properly studied so as to form compositions with the best performance. Chalcogenides draw attention due to their properties which are found to vary with composition, Atoms have high tendency to link together to form link-chains in chalcogenides. Short-range inter-atomic forces are mainly covalent. These are highly directional and strong in magnitude. The weak van der waals forces contribute primarily to the medium-range order. By and large, the atomic bonding is comparatively more rigid than that of organic polymers whereas it is found to be more flexible than that of the oxide glasses. Due to the weak van der waals bonding between layers/chains, there is flexibility of structure which means changes in the structure can be done easily [2].

Since each atom needs two neighbours to fulfil the valence requirements, it can adjust its neighbouring environment. Amorphous selenium in its pure form consists of a mixture of two structural species – long helical chains and eight member rings (Se_8) – held to each other by weak van der waals forces. Additives such as Te, Sb, Cu, Pb, Cd, Bi, In, Ge, *etc.* are used with Se to form binary as well as ternary chalcogenide alloys for enhanced performance. Se-Te alloys are more advantageous than amorphous selenium (a-Se) due to their greater hardness, higher photosensitivity, higher crystallization temperature and smaller ageing effects [3]. The structure of a-Se consists of two-fold co-ordinations and has long polymeric Se_n chains. Addition of tellurium (Te) produces a catalytic effect on the crystallization of selenium. The presence of tellurium in Se chains favours their thermal dissociation, since the Se-Te bond is weaker than Se-Se bond. In Se-Te alloys, Te enters the structure by isoelectronic substitution and consequently changes the inter-chain van der waals bonding since the atomic size of Te is larger than that of Se. The addition of Te in Se also improves the corrosion resistance and reduces the band gap of Se [4]. Se-Te alloys can be used for fast change between amorphous and crystalline phases. But, these alloys have some significant setbacks during certain applications such as limited reversibility, low glass-transition (T_g) and crystallization (T_c) temperatures, *etc.* These difficulties can be removed by adding a third element in Se–Te binary alloys. An additive in Se-Te alloys behaves as a modifier and changes various properties *viz.* optical, thermal, electrical *etc.* of the host alloy. The cross-linkages between the chains strengthen the material. It can also create structural and configurational changes in the system. The conductivity type may switch from p to n [5]. A typical chalcogenide exhibits sharp optical absorption edge, single electrical activation energy, efficient photo-excited conductivity and luminescence. It has been found that elements, such as Cd, Sb, Sn, In, Pb, Bi, Ag, *etc.* when added in Se-Te alloy produce noticeable changes in the structural, optical, electronic and thermal properties [6 - 12]. However, reports about copper as metal additive are scarce in literature. Various examples of chalcogenides occurring in nature are PbS, PbSe, PbTe, HgS, ZnS, CdS, CdSe, Ag_2S, Ag_2Te, Cu_2S, Cu_2Se, As_2S_3, As_4S_4, $Sb_2 S_3$, Bi_2S_3, Bi_2Te_2S, $Pb_2Sb_2S_4$, $Pb_5Sb_4S_{11}$, Cu_3AsS_4, GeTe, MoS^2, *etc.* and those synthesised are crystals or thin films of CaS, PbS, PbSe, PbTe, HgTe, CdTe, Se, As_2Se_3, As_2Se_3, Ge-Sb-Se, Ge-Sb-S and Ge-La-S systems, Sb_2S_3, Sb_2Te_3, Sb_2Se_3, Bi_2S_3, Bi_2Se_3, Bi_2Te_3, Ge-Sb-Se, Ge-Bi-S, Ge-Bi-Se, $Ge_2Sb_2Te_5$, $Ge_8 Sb_2Te_{11}$, $Ge_8Bi_2Te_{11}$, *etc.*

CHAPTER 2

Recent Advances in Chalcogenide Glasses and their Applications

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Abstract: During the last two decades, by using a combination of both chalcogens (sulfur (S), selenium (Se), tellurium (Te), and polonium (Po)) and other elements like silicon (Si) and germanium (Ge), a huge number of chalcogenide glasses (ChGs) were prepared and studied. Compared to oxide-based glassy materials, ChGs have unique properties and functionalities which make them suitable for photonic applications. These materials are transparent in nature from the visible to the near-infrared region and can be used for the preparation of optical and electronic devices like ChG fibers, optical switches, sensors, and phase change memorizers. This chapter deals with some basics of ChGs, preparation techniques and a review of the latest technological development. The structural properties, optical properties, thermal and electrical properties of ChGs have been discussed. The physical aging effect has been explored. In the second part of this chapter, the applications of ChGs especially in dye sensitized solar cells (DSSCs), semiconductors, electrical memories and phase change memories have been discussed.

Keywords: Chalcogenide Glasses, Dielectric Properties, Electrical Conductivity, Melt-quench Technique, Optical Properties.

INTRODUCTION

Generally, materials are classified as solid, liquid, and gas. Solids have subcategories as crystalline and amorphous solids. Amorphous solids are considered distorted crystalline solids. X-ray scans of such solid comprise broad halos instead of characteristic sharp peaks as in the case of crystalline materials. A subclass of amorphous materials is Glass, which is the result of cooling from a normal cooling state to a rigid state without crystallization [1 - 3]. During the transition from a supercooled state to a glassy state, first-order thermo dynamical

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properties like volume(V), entropy(S) and heat content(H) remain continuous while second-order thermodynamical quantities like specific heat and thermal expansivity become discontinuous. Glasses have affected our life immensely as an optical material, insulating, and thermoelectric material. Depending upon the main constitutes of the glass, glasses are divided into three classes namely Fluoride-based glass, Heavy metal oxide (HMO) and Chalcogenide glasses. Chalcogenide glasses are inorganic glassy materials that contain as a key constituent one or more of the chalcogen elements (S, Se and Te except oxygen). These glasses are equipped with striking optical, thermal, electronic and electrical properties such as transmission extended into the infrared region, a higher refractive index, exhibit optical nonlinearities, optically and electrically induced memory effect and conductivity (photoconductivity). Obeying to these properties, they have applications in infrared devices, night-vision devices, solar cells/Dye-sensitized solar cells (DSSCs), waveguides, optical fibers sensors and lasers [4 - 6].

Structure of Chalcogenide Glasses (ChGs)

The glasses are non-crystalline (or amorphous) substances that lack a long-range order of arrangement of atoms in contrary to crystalline materials in which the structure can be described in terms of a periodically-continued, finite-sized unit cell. The structure of a glass consists of a bonding structure, called a normal bonding structure, which is topologically the same as the crystalline materials plus a defective structure [7]. The normal bonding structure is further divided into the short (≥0.5 nm) and the medium-range (0.5−3 nm) structures. The defective structure is similar to a defect in practical crystals like dangling and wrong bonds; however, defects such as dislocations and stacking faults do not exist in glassy materials. Short range order is determined by the atoms of the first coordination sphere and partially by the atoms of the second coordination sphere which are covalently bonded to the central atom [8]. Umbrella of short-range order encompasses the parameters like the number of nearest neighbors (first coordination number), their types, the distance between them and the central atom (radius of the first coordination sphere), their angle positions with respect to the central atom defined by bond angles (valency angles). The regular distribution of dihedral angles for a distance of about 10 atoms [9] determines the medium range order. In chalcogenide glasses, weak Van der Waals force between structural units determines medium-range order.

It is extremely difficult to determine the structure of glassy materials by a single technique (X-ray diffraction), static disorder in bond lengths and bond angles leads to a broader radial distribution function and hence the use of complementary techniques is unavoidable. Notable techniques are vibrational spectroscopic techniques such as IR absorption and Raman scattering, extended X-ray absorption fine-structure spectroscopy (EXAFS), magic-angle spinning nuclear magnetic resonance (MASNMR) and related NMR techniques, Scanning tunneling and atomic force microscopy (AFM). The structure of multi-component glasses has been explored using EXAFS. Direct images with diffraction patterns are facilitated by Transmission electron microscopy (TEM) [10]. Surface morphology is usually determined with the help of SEM (Scanning tunneling microscopy) and AFM [11]. X-ray photoelectron spectroscopy (XPS) is useful in determining the valences of constituent atoms [12].

Glassy selenium (g-Se) is the most prevalent form of non-crystalline selenium. There exist various forms (rings and chains) of selenium in the glassy state. These forms of selenium differ from each other in terms of ratio, size, form and mutual packing of structural units. The proportion of chains [Trans-coupling configuration, (Fig. **1b**)] and rings [*Cis*-coupling configuration, (Fig. **1a**)] in a particular sample depends on the method of preparation. Kaplow and Averbach [13] have studied the vitreous selenium and concluded that its structure consists of 95% selenium rings (8-membered) and 5% chain-like (strongly distorted) units. Some researchers [14] prepared films of g-Se, which consisted of only ring molecules Se_8 (amorphous analog of monoclinic selenium) or of only chain molecules Se_n (amorphous analog of trigonal selenium). Several models have been suggested for describing the structure of selenium. Richter and Breiting [15] put forward a model in which flat zigzag chains having a zero value of dihedral angle are proposed as structural units. Malaurent and Dixmier suggested a model in which any value of it permitted [16] is known as the 'free rotation chain model' (Fig. **2a**). Another model, known as the disordered chain model, was given by Lucovsky and Galeener [9] in which the changes in the sign of dihedral angle are allowed but changes in the value of dihedral angle are barred (Fig. **2b**).

Electronic Structure of Chalcogenide Glasses

We do not have Bloch-like wave functions for disordered solids. The disorder leads to the localization of electron wave function to a special extent Δr, which satisfies the uncertainty relation, $\Delta r.\Delta p \sim 1$ [17, 18]. Bonding and energy levels of atoms give rise to molecular orbitals. Overlapping of molecular orbitals leads to broadening of individual levels and hence, splitting into bands. DOS (Density of states) in glass is similar to the corresponding crystal DOS because both have short-range order. Therefore, band gap energies (E_g) and also optical absorptions at $h\omega > E_g$ are roughly the same. However, band edge structure is a modified medium-range structure (in crystalline materials, band edges are sharp) [19] and

CHAPTER 3

Al Doped ZnO Thin Films: Beginning to Developments Afoot

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Abstract: In the last three decades, Zinc oxide (ZnO) has been found to be one of the most resourceful materials having tremendous potential applications in manifolds covering a wide variety of areas. It is continuously explored in different forms and structures. ZnO-based layers have an established place in the industry that ranges from protecting degradable items to detecting toxic gases. A wide variety of ZnO-based advanced coatings and their surface treatments along with innovative functionalization technologies offer a multitude of options for making them useful in diverse industries. Multiple techniques ranging from exceedingly sophisticated ones like molecular beam epitaxy and atomic layer deposition to highly-cost effective ones like sol-gel spin coating and dip coating, *etc*. have been used for developing the ZnO based thin films. Doping suitable elements into ZnO matrix is the most promising strategy to alter its properties drastically. Out of numerous dopants, Aluminum (Al) offers some of the excellent and reproducible features in ZnO films which make Al doped ZnO (AZO) a reputable system in industries like thin film transistor manufacturing and solar cells. Specifically, its established and repeatable behavior in terms of transparency and conductivity becauseis finding huge applications as a transparent conducting oxide (TCO). Extensive research on AZO coatings derived from different methods day-b--day opens up a new gateway for interesting perspectives by optimizing surface nanostructures. Here a brief account of historical developments of ZnO to AZO films along with their applications in certain key areas like TCOs, solar cells, thin film transistors, flexible electronics and plasmonics, *etc*. is presented.

Keywords: ZnO, TCO, AZO, TFTs, Plasmonics, Flexible Electronics.

INTRODUCTION

The ancient Indian medical text Charaka Samhita, dates of composition of which are uncertain, refers to the use of *pushpanjan*, most probably zinc oxide, as an

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ointment for eyes and open wounds. A book namely '2000 years of zinc and brass' by P. T. Craddock [1], which is supposed to be the first comprehensive review of the technical history of the production of zinc and brass, describes the inception and technical development of the processes by which zinc and brass were made at various centers around the world. Earlier zinc and zinc oxide (ZnO) were recognized and produced in India using a primitive form of the direct synthesis process. The main usage of zinc oxide also known as zinc white was in paints and as an additive to various ointments. Nowadays, a significant amount of ZnO (50% to 60% of its total applications) is finding numerous applications in the rubber industry [2]. Rest is being used in the ceramic industry [2], concrete manufacturing [3], skin ointments and sunblock creams, food (as a source of zinc), oil and pigments. An illustration shown in Fig. (**1**) depicts the applications of ZnO in several industries.

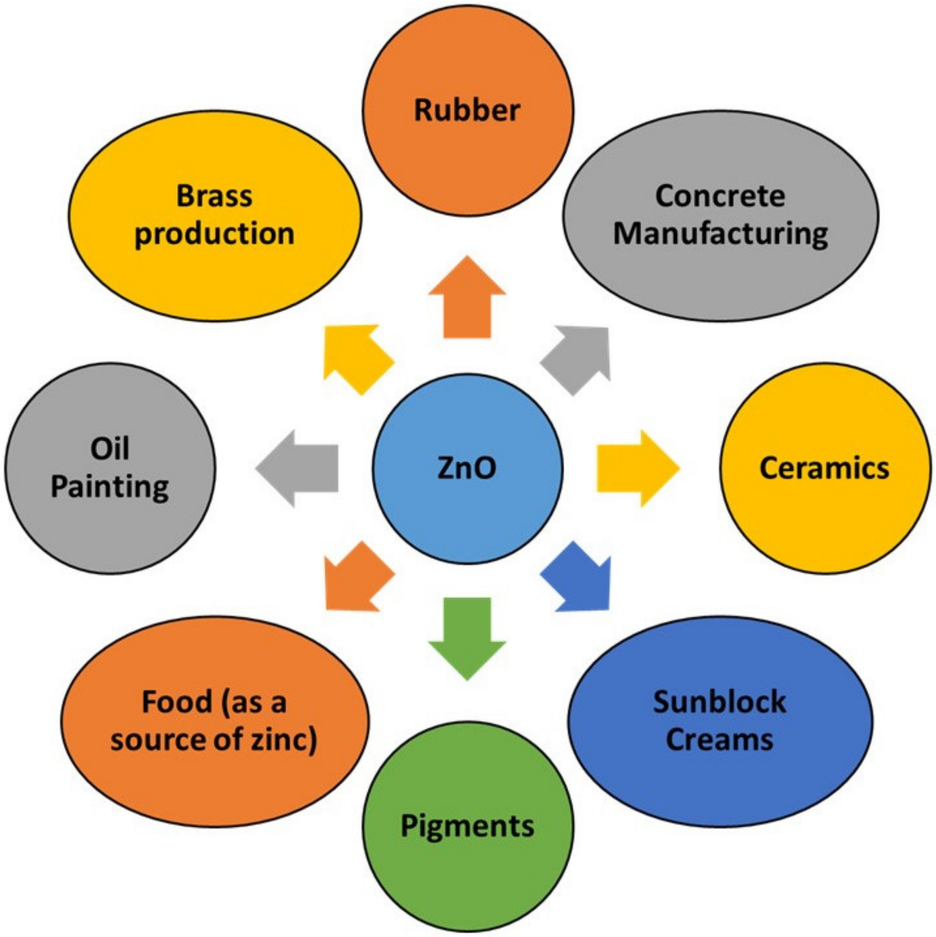

Fig. (1). Schematic illustration of use of ZnO in various industries.

A small portion of its total use is related to the study of its functional properties. Besides large-scale industries, it has been observed to be a promising candidate for thin film devices in the areas of optoelectronics [4, 5], piezoelectronics [6], transparent electronics [7], spintronics [8], sensing [9], and photovoltaics [10]. This is all possible due to its inherent characteristics and a wide range of achievable morphologies. The emergence of materials research has led to the modification of conventional compounds by alloying or doping. Currently, the traditional boundaries are being broken in forming solid solutions. ZnO has shown its potential to offer its matrix as a host, to a number of elements of the periodic table, which has opened tremendous opportunities for its applications as per the current needs. Despite greater achievements, two problems in the ZnO related technology are yet persistent: (1) the inability to achieve significant p-type conductivity which is reproducible and stable in time and (2) the development of almost incomprehensible diverse nanostructures with different properties under individual synthesis environment. Apart from these problems, the n-type conductivity of ZnO has a disputable origin, and p-type conductivity, if it is achieved, does not have a well-defined origin.

Several excellent features like higher transparency, tunable band gap and elevated conductivity *etc.* can be achieved by introducing a suitable dopant in the ZnO system or just from a non-stoichiometric configuration. Many metals such as Al, In, Ga, Ca, Mg, Sr and Ag have been found as an encouraging substitute of Zn in ZnO to achieve favorable properties. In the last two decades, a trivalent cation, Al has been highly popular as a dopant in ZnO because of the cheaper cost and ease of availability. Al-doped ZnO (AZO) has shown good thermal and chemical stability even under reducing ambient. It has emerged as a replacement of Indium Tin Oxide (ITO) on the commercial scale. Here, the importance and applications of AZO in various scientific fields along with the basic properties of ZnO are presented.

BASIC PROPERTIES OF ZnO

ZnO is probably the richest family of nanostructures among all one-dimensional nanostructures, including carbon nanotubes. In stoichiometric form ZnO, a wide-bandgap semiconductor belonging to the II-VI semiconductor group, is an insulator. Deviations from stoichiometry are, however, more the rule than the exception and this imparts semiconducting properties to metal oxides. As a best example, the oxygen vacancies or zinc interstitials in ZnO are found to make it an n-type semiconductor. A semiconductor material with a sufficiently wide band gap at room temperature makes it a candidate for optical sources in the visible region or UV region. It has several desirable properties like high transparency,

CHAPTER 4

Commercial Applications of Synthetic Fibres

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Abstract: Man-made fibres are produced from chemical substances known as synthetic fibres. Synthetic fibre or a synthetic polymer made from molecules of monomer joined together to form long chains, is also known as an artificial fibre. Besides polymer-based synthetic fibres, other types of fibres that have special commercial applications and importance. These include the fibers made of carbon, glass,metal and ceramics. Polymer-based synthetic fibres are produced by various processes such as melt spinning, dry spinning and wet spinning.

The melt spinning technique is used to produce polymers such as polyethene, polyetheneterephthalate, cellulose triacetate, polyvinyl chloride, nylon, *etc.* Cellulose acetate, cellulose triacetate, acrylic, modacrylic, polyvinyl chloride and aromatic nylon are artificial fibres manufactured by dry-spinning. In contrast, the wet spinning process is used for aromatic nylon, polyvinyl chloride fibres, acrylic, modacrylic and viscose rayon from regenerated cellulose.

The importance and usefulness of synthetic fibres are because they have enhanced properties compared to natural fibres, which come from plants or animals. Still, each type is valued for different reasons.

Keywords: Artificial fibres, Commercial applications, Polymers, Polyesters, Polyolefins, Polyamides, Polyurethane, Rayons, Synthetic fibres.

INTRODUCTION

Synthetic fibres, like natural fibres, are made up of small units known as monomers which join together and make extensive units called polymers. In comparison, natural fibres like cellulose are obtained from plants and animals. Synthetic fibres are obtained by processing petrochemicals chemically.

Synthetic fibres can be woven into fabrics like natural fibres and have wide-ranging commercial applications (Chart **1**).

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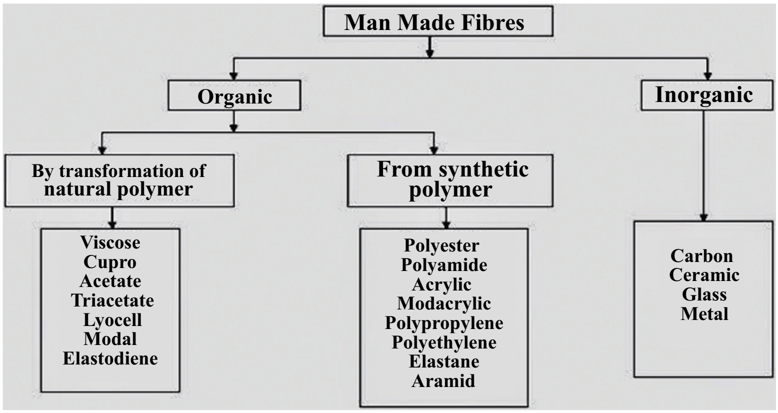

Chart. (1). Classification of synthetically made fibres.

In household articles, synthetic fibres find many uses ranging from ropes, furniture, buckets, and containers to many others. In addition, highly specialized uses are in ships, spacecraft, aircraft, healthcare, *etc.* The manufacturing of synthetic fibres depends upon the types of chemicals used. Fibres differ in their characteristics in their strength, water absorbing capacity, resistance to burning and heat, tensile strength, cost, durability, *etc.* In current scenarios, many synthetic fibres like nylon, rayon, polyester and acrylic are extensively used commercially.

The types, properties and uses of some synthetic fibers are explained in Table **1**.

Table 1. Synthetic fibres: Types, Properties and Uses.

Fiber Type	Flame Properties	Residue/Smell	Characteristic	Use
Synthetic	Melts and retreats from flame, flame burns with bright glow Catches fire easily Easy to melt Burns with dark and thick smoke	Hard, brittle or lumpy sticky beads Harsh acidic smell or blended smell	Raw materials-petroleum origin Do not bleed color and shrink when washed, easy to maintain, wash and dry, less expensive, easily available, more elastic in nature, resistant to insect attack, tough and durable	Warm and protective clothing for extreme climates, fabric for everyday wear, sportswear, fillers, hair wigs, ropes, parachutes, nets, tents, carpets, furnishing, upholstery, utensils,

(Table 1) cont.....

Fiber Type	Flame Properties	Residue/Smell	Characteristic	Use
Rayon	Burns with a steady flame with dark grey to black smoke	gritty and brittle, almost no ash paper or wood-like smell	Made up of chemically treating wood pulp, Known as artificial silk Absorbs moisture and comfortable to wear	Apparels like suits, slacks, jackets,etc Because of its strength used in making automobile tyre cords Mixed with wool to make carpets and blankets Mixed with cotton to make bedspreads, bed sheets, home furnishings
Acetate	Burns and melts sizzle, fiber continues to burn after the flame source is removed.	Hard and black bead. The acidic or vinegary smell.	Soft, smooth, natural feel, high flexibility, high gloss. Effected by acids and bleaches, resistant to alkalies. Effected by sunlight. Low moisture absorbance, high elongation, more sensitive to heat, thermoplastic	Dresses, foundation garments, lingerie, lining material, household furnishings, sportswear, garments where pleat retention is important, certain specialty fabrics, cigarette filter, diapers, surgical products, cellulose acetate ribbons,playing cards, photographic films
Polyester	Melts and burns at the same time, retreats from flame, Black smoke with melted or brown bead	Sweet or acidic smell. Drips while burning, drippings are sometimes with fire	Manufactured from petroleum. A polymer of ester. Extremely strong fiber, resistant to chemicals, less wrinkles, does not absorb water easily, easy to dry less fading, durable	Textiles-dress materials, sarees, upholstery, hosiery Blended with natural fibers(like wool and cotton) Sail of sailboats Water hoses(firefighting purposes) As Mylar for making film and magnetic recording tapes
Polyolefin	Shrinks quickly in flame, burns and melts, burns when flame is withdrawn.	Smell not defined Hard round bead maybe light brown.	Hard and opaque plastic, high thermal stability, heat-ageing resistance, stronger mechanical properties, good resistance to heat, flame, ozone, chemicals, solvents, low water absorption	Insulation of electrical wiring in high temp., lighting fixtures, heating cable for pipe, electrical insulators(radar, television), fuel hose products, air filters, pool filters, battery cover, tank linings, footwear, building products, shrink wrap films, containers, crates, lab equipment

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CHAPTER 5

Investigation of Substrate-effect on BaF_2 Thin Films: A Study of Fractal Nature

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Abstract: BaF_2 thin films of thickness 20 nm are prepared using the electron beam evaporation technique (at room temperature) on glass, silicon (Si) as well as aluminum (Al) substrate, respectively. These substrates play a crucial role in the evolution of thin film surface morphology. The thin films grown far from equilibrium have self-affine nature which is reminiscent of fractal behaviour. The surface morphology of films is recorded by atomic force microscopy (AFM). Scaling law analysis is performed on AFM images to confirm that the thin film surfaces under investigation have self-affine nature. The concept of fractal geometry is applied to explore-how different substrates affect the surface morphology of films. The fractal dimension of horizontal as well as vertical sections of AFM images are extracted by applying Higuchi's algorithm. Value of Hurst exponent (H) for each sample is estimated from fractal dimension. It is found to be greater than 0.5 for Al as well as glass substrates, indicating that the height fluctuations at neighboring pixels are correlated positively. However, for Si substrate, its value is less than 0.5 which suggests that the height fluctuations at neighboring pixels are not positively correlated.

Keywords: BaF_2 thin film, Atomic force microscopy (AFM), Self-affine, Hurst exponent, fractal dimension.

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INTRODUCTION

A famous quote about fractal by Benoit Mandelbrot *"Clouds are not spheres, mountains are not cones, coastlines are not circles, and bark is not smooth, nordoes lightning travel in a straight line"* [1]. There are many examples in nature such as mountains, rivers, coastline, leaves, air bubbles, cloud, *etc.*, which show the fractal characteristics. Modeling of such natural fractal behavior is impossible through a classical technique which is based on assumptions of smoothness. Over the time, many simple mathematical models were developed to deal with the fractal behavior. Some of them are Cantor set, Sierpinski Gasket, Sierpinski Carpet and Koch curve. Fractal can be defined as a set, for which Hausdorff Besicovitch dimension D (called fractal dimension) exceeds its topological dimension D_T [2]. In general, fractal objects remain invariant under certain transformations of scale.

Thin film exhibits unique physical and chemical properties as compared to its bulk counterparts [3]. The process of thin film deposition is highly crucial for fabrication of advance devices such as microprocessors, memory storage devices, photovoltaic devices, supercapacitors, *etc.* Surface morphology is also important in various biomedical applications namely biosensors, DNA/RNA sensing, biomedical engineering, *etc* [4 - 6]. Surface morphology plays an important role in optical [7], mechanical [8], magnetic [9], electrical [10], and tribological [11] based devices. This requires a deep understanding about the evolution of surface morphology. Interestingly, the surface morphology of the films exhibits a fractal nature. Therefore, the precise control over the growth of good quality thin films is necessary for its applications in highly efficient devices. The substrate plays a crucial role in governing the properties of thin films. It is found that the different growth mechanisms are governed by different morphologies.

Barium fluoride (BaF_2) is a wide band gap material with a fluorite cubic phase structure and shows insulating properties [12 - 14]. BaF_2 can be used in various applications like CO_2 laser, low index optical coating, high stopping power and very fast scintillators, *etc.* It has also been employed in fabrication of single-layer antireflection coatings for NaCl optical components [14 - 16]. It was also used as a molten bath component in aluminium raffination and welding rod coatings and welding powders [16].

Classically the surface morphology of films is measured through average roughness and interface width [17]. It is worthy to mention that it cannot characterize the local roughness behavior which depends on the resolution of the measuring devices. The precise information about local roughness can be obtained through a parameter known as roughness exponent. This parameter governs the scaling of local surface height fluctuations with measurement of resolution. It is important to emphasize here that the growth of thin film surface is not a smooth process rather it is a well stochastic process. It means this behaviour is not linear at small scale and it shows fractal nature. There is a global need to characterize the complex or irregular structure of a surface using a scale invariant technique. The fractal analysis is the one which fits to provide such alternative by measuring fractal dimensions of the samples [18]. Fractal dimension can be determined indirectly by different techniques such as power spectral density (PSD) method, detrended fluctuation analysis (DFA), height-height correlation, *etc* [19 - 24].

An efficient algorithm was developed by Higuchi to compute the fractal dimension of a time series. This algorithm has been employed in various fields of science and technology. The fractal analysis can be used to study the brain dynamics through electroencephalographic (EEG) signals. The Earth's geomagnetic activity was also studied. Yadav *et al.* calculated the grain size, fractal dimension (D_f) and Hurst exponent (H) for different films of varying thickness as well as deposition angle [25]. Their study suggests that with increase of thickness of the film, there is a decrease in fractal dimension while Hurst exponent increases. This reveals that complexity decreases when the thickness increases. Talu *et al.* used the similar technique to establish a strong correlation between electrical resistivity and fractal dimension for Ag/Cu thin film [26]. Their finding suggests that the electrical resistance decreases sharply as the fractal dimension decreases [26].

In this chapter, we present detailed surface morphological studies using AFM images of BaF_2 thin films deposited by the electron beam evaporation technique on three different substrates. The Higuchi algorithm was applied to the digitized AFM data for estimating fractal dimensions of the horizontal as well as vertical sections of the film surfaces.

EXPERIMENTAL DETAILS

The evaporation technique was used for the deposition of BaF_2 thin films on glass, silicon (Si) and aluminum (Al) substrates at room temperature in vacuum [12]. The vacuum of the chamber was kept at $\sim 10^{-6}$ mbar. Standard cleaning process was performed for the cleaning of the substrates [12]. During this process, the rate of deposition was constant at $\sim 0.5\times10^{-9}$ meter/sec. The thicknesses of the films were measured *in-situ* using a quartz crystal monitor. The thickness of each sample was estimated to be 10^{-9} meter. The surface morphologies were recorded using atomic force microscopy (AFM). Further, the AFM images of size 2.0 μm×2.0 μm were digitized into 512×512 pixels [12].

Part 2: Nano Functional Materials and Their Application

CHAPTER 6

A Detailed Study of Structural, Dielectric and Luminescence Properties of Sm^{3+} Doped $BiFeO_3$ Nanoceramics

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Abstract: Observation of at least two coexisting switchable ferroic states viz., ferromagnetic, ferroelectric, and/or ferroelastic at room temperature with promising coupling among order parameters, has made $BiFeO_3$ a highly explored material in the field of multiferroics and/or magnetoelectric multiferroics, which creates the possibility for its application in various technological devices such as spintronics, spin-valve, DRAM, actuators, sensors, solar-cells photovoltaic, *etc.* Intrinsically, its low coupling coefficients, difficulty to prepare in pure phase in bulk, high leakage current, *etc.* have restricted $BiFeO_3$ from technological reliability. However, the effect of doping with iso- and alio-valent ions, nanostructure, thin-film-form and nanoparticles, *etc.*, has been carried out to improve its physical properties by several research groups over the decades. In this chapter, the structural, luminescence, and dielectric properties of samarium (Sm^{3+}) doped $BiFeO_3$ nanoceramics synthesized using a modified gel-combustion route are discussed in detail. The effect of Sm^{3+} doping in $BiFeO_3$ is explored using the X-ray diffraction (XRD) technique. The XRD studies exhibit a possible structural phase transition above Sm^{3+} doping of 15% from rhombohedral (R3c) space group to the orthorhombic (Pbnm) space group. The dielectric study shows interesting behavior accompanied by structural transition. Our study suggests that Sm^{3+}

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doping plays an important role in governing the structural, luminescence, and dielectric properties of $BiFeO_3$ samples.

Keywords: Bismuth Ferrite (BFO), Multiferroic, Dielectric Properties.

INTRODUCTION

In the last few decades, the world has been witnessing a quantum leap in the digitalization of data in day to day routine and storage devices [1 - 3]. As a result, rapid advancement has also been seen in the field of memory storage electronics devices and their allied area of technologies. The current global demand is a storage device which is fast, and robust with low power consumption. In general, the memory devices fundamentally use ferroelectric and ferromagnetic materials for data writing and operations [1, 3, 4]. The ferroelectric (FE) or ferromagnetic (FM) materials have been extensively used in memory devices due to their switchable polarization (magnetization) states [1, 4, 5]. In commercial magnetic memory device (MRAM), the data is stored (or write operation) by switching the magnetic states from $-M$ to $+M$ or vice versa while, the information can be read by changing the magneto resistance. Currently, the memory devices fabricated using ferromagnetic materials with high coercivity consume a lot of energy for switching from one state to the other. In ferroelectric random access memory (FeRAM) devices, the switching from one state to another state can be done by simply changing the state of polarization. FeRAM devices show a faster writing speed and consume a comparatively smaller amount of energy [1, 4, 5]. But, these devices show some limitations like slow reading operation [3].

Therefore, it is necessary to find a cost-effective suitable material in which the above properties simultaneously coexist and reduce the processing steps with better. Interestingly, the multiferroic materials are the materials in which two and/or more switchable ferroic order parameters such as Ferroelectricity, ferromagnetism and /or Ferroelastic exist simultaneously [6, 7]. Sometimes, multiferroics showing magnetoelectric properties through direct and /or indirect coupling coefficients prove to be quite useful for storage applications [8]. In such magneto-electric (ME) multiferroic materials, the spontaneous magnetization (M_s) and /or spontaneous polarization (P_s) can be switched by controlling external electric and /or magnetic fields [3]. In both cases, the spontaneous deformation can also be switched /reoriented by applying stress (σ) [9, 10]. These materials show many technological prospects in the field of switching devices, novel memory media, transducers, new functional sensors *etc.*, [2, 11]. Hitherto, functional devices made of multiferroic materials are yet to be realized [12, 13]. There are only few materials like $BiFeO_3$ [14], $TbMnO_3$ [15], $BiMnO_3$ [16] and

$YMnO_3$ [17] *etc.*, that exhibit multiferroic properties and, therefore the current demand is to synthesize and explore the new materials for their application in multifunctional devices. Among these materials, $BiFeO_3$ (BFO) is the only material showing prominent multiferroism at room temperature [2, 6]. BFO has a distorted rhombohedral crystal structure with R3c space group symmetry which permits anti-phase octahedral distortion and ionic displacement from the centro-symmetric position. The BFO shows ferroelectric property at room temperature with very high Curie temperature $[(T_C)\sim 1103K]$ and G-type anti-ferromagnetism up to Neel temperature $((T_N)\sim 640K)$ [18, 19]. Moreover, in BFO, the neighboring magnetic spins are oriented antiparallel to each other. In addition, it makes a spiral spin structure with a large cycloidal period of ~620 Å precise throughout the crystal [20].

In order to obtain intriguing properties of the BFO, several direct and indirect methods can be employed. The multiferroic properties can be improved by substitution of rare earth (lanthanide series) elements at A-site (*i.e.* Bi site) and transition metals at B-site (*i.e.*, Fe site), respectively [21, 22]. BFO has been explored for their application in photo-catalytic activity for the degradation of organic pollutants [23]. There are reports that Sm and Mn doping enhances the photocatalytic activity of $BiFeO_3$ nanoparticles [24]. Lou *et al.* reported that $SrTiO_3$-coated BFO core-shell nanostructures can be employed as a water splitter under visible-light illumination [23, 25].

Here, we have discussed the synthesis and characterization of BFO and Sm doped BFO nano ceramics. All the samples are prepared using the modified gel-combustion route. The effects of Sm doping in BFO on structural, luminescence and dielectric properties are systematically investigated. The structural analysis of the samples suggests that the suitable doping of Sm in BFO plays an important role in governing structural, luminescence and dielectric properties.

EXPERIMENTAL PROCEDURE

Ceramics samples of $Bi_{1-x}Sm_xFeO_3$ $(0.0 \le x \le 0.40)$ were synthesized using a modified gel-combustion route. The details can be found elsewhere [26]. To start, a stoichiometric ratio of $Bi(NO_3)_3{\cdot}5H_2O$ (99.0% purity, MERCK, India), $Sm(NO_3)_3$ (96%, purity, MERCK, India) and $Fe(NO_3)_3{\cdot}5H_2O$ (99% purity, MERCK, India) was dissolved in distilled water. Citric acid (99% purity, MERCK, India) was used for complexation as well as a fuel agent. The molar ratio of bismuth to citric acid was maintained at 1:1.5. Due to the different pH of individual solutions, it was difficult to obtain a clear solution on mixing. Therefore, dilute HNO_3 was added drop wise for precipitate dilution until the murky solution transformed into a clear solution. The obtained solution was then

CHAPTER 7

Application of Nanotechnology in Wastewater Cleaning Process

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Abstract: With the advancement in research, new techniques are growing very fast these days. The environmental contamination by many hazardous elements is seen in today's world. The radioactive materials and their byproducts or the leakage of nuclear reactors is a potential serious health threat. The ground water and drinking water get contaminated and it is a big challenge to remove these radioactive ions from the environment. The radioactive ions leach into groundwater and contaminate drinking water supplies for large population areas. The key issue in developing technologies for the removal of radioactive ions from the environment mainly from wastewater and their subsequent safe disposal is to devise materials which are able to absorb radioactive ions irreversibly, selectively, efficiently, and in large quantities from contaminated water. Hence, nanotechnology proved to be a great success in this area. Nanotechnology is the science and technology working at the molecular level *i.e.* in nanometre and embraces many different fields and specialties, including engineering, chemistry, electronics, medicine, pharmaceuticals, agriculture and waste management. The present chapter deals with the development of nano-technology for the removal and safe disposal of radioactive ions from the environment using nanomaterials.

Keywords: Nanotechnology, Nanomaterials, Radio Wastes, Radionuclides.

INTRODUCTION

Nanotechnology is one of the fastest and widest fields of science in this decade. New inventions using nanomaterials as a tool prove to be a boon to society, *i.e.* research and technology development at the atomic, molecular or macromolecular levels, approximately 1-100 nanometers in length. All nanomaterials of this size

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can control and manipulate the atomic scale since the properties are different from the bulk materials. We know many radioactive materials that help our society, and improve the quality of life, ranging from power generation to industrial uses, medical, diagnostic, therapeutic, and research purposes.

In medicine, a number of unsealed sources are used for diagnosis while sometimes they need to be diluted before use. Also, a number of biomedical researchers use radionuclides which may increase the volume of wastes requiring further management. Radioactive waste is mainly a byproduct of all such nuclear power generation and is strictly regulated as a highly hazardous material to human beings as well as the environment. Radioactive materials create ions, which initiate free radical formation. These free radicals can damage protein membrane and nucleic acids by “oxidizing” them generally known as “OXIDATIVE STRESS”. Many forms of cancer are thought to be the result of reactions between free radicals and DNA, causing mutations that can adversely affect the cell cycle and potentially lead to malignancy. Leaching of such radiowastages and byproducts into groundwater can contaminate drinking water supplies is a serious health threat.

Today, newer generation nanomaterials as functionalized nanomaterials proved to be very effective for radioactive wastewater decontamination, such as carbon-based nanomaterials, metal nanoparticles, nano-sized metal oxides, metal sulfides, nano-sized natural materials, layered double hydroxides, hydroxyapatite nanoparticles, metal-organic frameworks, cellulose nanomaterials, and biogenic nanocomposites. Functionalized materials can effectively remove specific ions of interest, in chemical separation methods. Recent progress in the synthesis of nano-structured materials helps to remediate radioactive contamination at the source, by removing radioactive ions from the different source of contamination. There are several methods that can use nanotechnology as a reactive media for separation and filtration, bioremediation and disinfection [1 - 3]. Some of them are discussed below:

INORGANIC CATION EXCHANGE MATERIALS- MATERIAL FOR WATER CLEAN UP

“Natural inorganic cation-exchanger materials, such as clay and zeolite, have been extensively studied and used in the removal of radioactive ions from water *via* ion exchange and are subsequently disposed of in a safe way”, Dr. Huai Yong Zhu [4] explains to “Nanowerk”. According to Dr. Zhu, the Queensland University of Technology in Brisbane, Australia, “Synthetic inorganic cation exchange materials - such as synthetic micas, g-zirconium phosphate, niobate molecular sieves, and titanate - have been found to be far superior to natural materials in terms of selectivity for the removal of radioactive cations from water. Generally, ion exchange materials exhibiting a layered structure are less stable than those with 3D crystal structures and the collapse of the layers can take place under moderate conditions" says Zhu. "Then again, it has also been found that nanoparticles of inorganic solids readily react with other species or are quickly converted to other crystal phases under moderate conditions, and thus are substantially less stable than the corresponding bulk material". The uptake of large, radioactive cations eventually triggers the trapping of the cations - by itself represents a desirable property for any material to be used in the decontamination of water having radioactive cations (Fig. **1**).

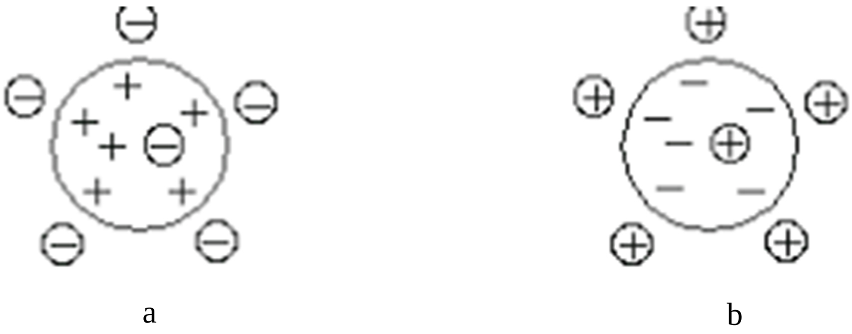

Fig. (1). a) Anion exchanger - attracts negatively charged particles and collects them and **b)** Cation exchanger - attracts positively charged particles and collects them.

Zeolites have properties such as high cation exchange capacities, high specific surface areas (due to porous crystalline structure) and high hydrothermal stability [5]. Zeolites have the ability to remediate water containing cationic species, such as ammonium and heavy metal ions also. Radioactive species drained out from the nuclear plants as wastewater and polluted groundwater such as ^{137}Cs and ^{90}Sr can be treated using these zeolites. For synthesizing zeolites, conventionally on the scale of 1,000 to 10,000 nm or 1 to 10 μm but since the pores size range between 0.4 to 1 nm and hence, zeolites are considered nanomaterials. Recently, nanocrystalline zeolites are being synthesized for discrete, uniform crystals with dimensions of less than 100 nm [6].

IRON NANOMATERIALS

Iron nanomaterials are prominently used for cleaning radiowaste-water. 'Pump and Treat' system [7] and Permeable Reactive Barrier (PRB) are the two techniques used. 'Pump and Treat' is the most widely used method since 1998 for

CHAPTER 8

Nanomaterials in Organic Synthesis

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Abstract: Multidisciplinary research in chemistry, physics and other engineering sciences often addresses nanotechnology. In almost all branches of science and technology, nanotechnology is commonly used. Nanomaterials are not just something developed in the laboratory but nanotechnology has made it possible for humans to manufacture nanoform-containing materials. Metal nanoparticles have been used in different areas such as catalysis, sensor, and medicine. Nanoparticles have good efficiency, selectivity and yield of catalytic processes. Nanoparticles have higher selectivity in the reactions because the reactions continue with fewer impurities and less waste. Hence this technique is safer and more environmental-friendly. The specific emphasis of this chapter is on the applications of nanoparticles in organic synthesis.

Keywords: Green Synthetic Method, Dichroism, Surface Effect, Nanotechnology, Nanoparticles, Mizoroki-Heck Reactions.

INTRODUCTION

In scientific literature, the term nano derived from the Greek “nanos” which means “dwarf”, is becoming increasingly popular. Nanoparticles are materials ranging in size between 1 to 100 nm in a single unit. There are many examples of nanomaterials such as titanium dioxide, silver, synthetic amorphous silica, iron oxide, azo pigments and Phthalocyanine pigments. One of the most fascinating examples of nanotechnology from the ancient world is the Roman Lycurgus cup. Its dichroic glass changes hue, which means that the cup has two different colors. When in light, the dichroic glass appears red-purple in color.

The scientists studied the cup in 1990 using transmission electron microscopy (TEM) that was used to clarify the dichroism phenomenon. The dichroism phenomenon is attributable to the existence of nanoparticles with a diameter of 50-100 nm. These nanoparticles have been found to be silver-gold alloys, which

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have a 7:3 ratio and contain around 10 percent copper (Cu) in a glass matrix which is dispersed. Au nanoparticles absorb light (~520 nm), and produce red color. The red-purple color is due to absorption by the bigger particles while the green color is attributable to the dispersion light by colloidal dispersion of Ag nanoparticles > 40nm in size. Nanotechnology, now has become a more academic focus. This technology is being used to treat several illnesses. Nanotechnology can be described as "The nanoscale."

NANOMATERIALS VS BULK MATERIALS

There are mainly two primary factors which distinguish nanomaterials from bulk materials; one is surface effects (causing smooth scaling properties due to surface fraction atoms) and quantum effects (showing discontinuous behavior due to quantum confinement effect in materials with delocalization of electrons). Such variables influence their magnetic, optical, electrical and mechanical properties.

IMPORTANCE OF NANOMATERIALS

Nanomaterials are widely distributed and are very valuable for all kinds of practical uses as shown in Fig. (**1**). These materials are not just something made in the laboratory but nanotechnology has made it possible for humans to create materials that include nano form.

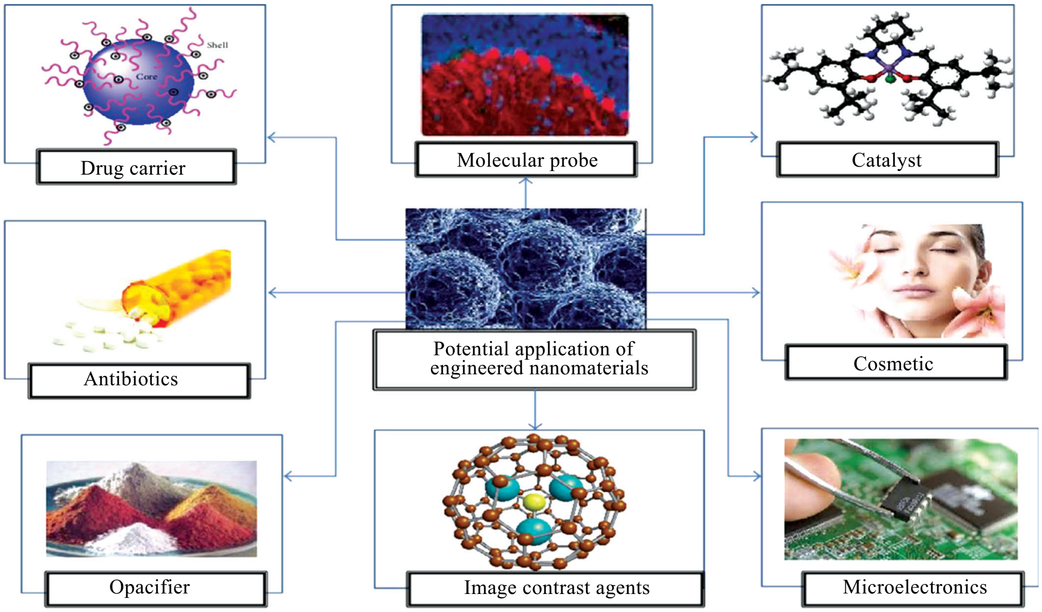


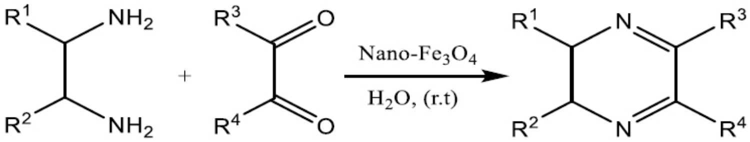
Fig. (1). Applications of Nanomateriales.

APPLICATIONS OF NANOPARTICLES IN ORGANIC SYNTHESIS

Nanomaterials have often been used in textiles, nanofibers, nanowires, coatings and plastics. Nanomaterials in reactions have higher selectivity. There are less waste and less impurity in these reactions, hence this is a safer technique and more environmental-friendly.

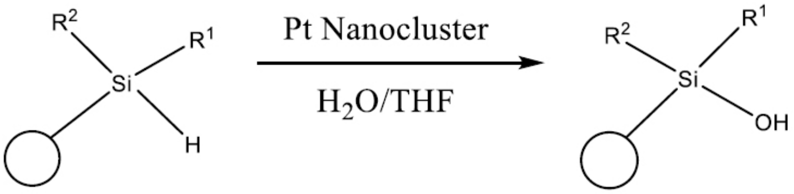
Iron nanoparticles are used in different organic synthesis reactions. These nanoparticles are synthesized as green solvent using polymers taken as a capping agent in water. The value of iron nanoparticles is that hydrogen peroxide is catalyzed for the treatment of organic pollution and also used as environmentally benign catalysts for alkenes and alkynes hydrogenation.

Zhang Z-H *et al.* described the formation of tetraalkylpyrazine with the presence of Fe_3O_4 and various solvent like acetonitrile, toluene, dichloromethane, ethyl acetate, ethanol and water (Scheme **1**). The solvent has been shown to play an important role in product yield. Generally non-polar solvent such as ethyl acetate, toluene and dichloromethane afforded low yield of product. In the presence of water, the best conversion takes place. The product yield was found to be influenced by the amount of Fe_3O_4 and the best result was obtained when 10 mol-percent Fe_3O_4 was used during the reaction in water at room temperature [1].



Scheme 1. Synthesis of tetraalkylpyrazine.

In the presence of Pt-metal complexes, silane was hydrolytically oxidized. In the above mentioned reaction, Pt-nanoparticles provide a selective route to the formation of silanols (Schemes **2** & **3**) [2 - 4].



Scheme 2. Formation of Silanols.

Part 3: Functional Materials for Energy Conservation

CHAPTER 9

Implications and Applications of Multifunctional Advanced Materials/Gadgets for Energy Conversion and Storage

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Abstract: The expanded interest in vitality assets, extraordinary endeavors, advocacy of convenient hardware and electric vehicles globally animates the improvement of energy storage gadgets, *e.g.,* lithium-ion batteries and supercapacitors, toward higher energy density, which essentially relies on new materials utilized in these gadgets. Besides, energy storage materials assume a key part in productive, clean, and adaptable utilization of energy, and are vital for exploiting sustainable power systems. The usage of the thermal energy storage (TES) framework with phase change material (PCM) is a viable route for energy preservation and green-house gas emission reduction. Ongoing advances in atomically thin two-dimensional transition metal dichalcogenides (2D-TMDs) have prompted an assortment of promising innovations for nanoelectronics, photonics, energy storage, and so on. Graphene and graphene-based materials have attracted extraordinary consideration due to their interesting properties of high mechanical adaptability, huge surface zone, chemical stability, prevalent electric and thermal conductivities that render them incredible as alternative electrode materials for electrochemical energy storage frameworks. The straightforward Chemical Vapour Deposition (CVD) and Atomic Layer Deposition (ALD) approaches offer another route for the creation of permeable materials for energy storage. Alteration of organic substrates with inorganic polyoxometalate (POM) clusters can be utilized to build nanocomposite materials with improved properties and various functionalities. Nanotechnology offers up new frontiers in materials research and construction to address the energy challenge by forming novel materials, particularly carbon nanoparticles, for efficient energy transformation and capacity, Polyaniline (PANi) as an auspicious material for energy storage/transformation, is merited for serious investigation and further progress. This book chapter discusses the various methods in materials for energy, their storage, and applications in numerous fields.

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Keywords: Energy Conversion & Storage, 2D-TMDs, Polyoxometalates, Polyaniline, Supercapacitors, Fuel Cells.

INTRODUCTION

The prerequisite for elective and sustainable sources of power turns out to be more critical as we move further into the 21st century [1]. Spotless, modest, and safe high energy and power density resources are needed to empower the generation, stockpiling, and transformation of energy through non-contaminating methods. Energy storage is cultivated by gadgets or physical media that store energy to perform valuable activities. The energy present at the underlying development of the universe has been put away in stars, for example, the sun, and is currently being utilized by humans legitimately (for example through sun-oriented warming), or in a roundabout way (for example by growing yields or transformation into power in solar-based cells). Researchers have never given up trying to improve the electrochemical presentation of existing energy storage device measures in order to satisfy the need of individuals who yearn for a reliable and clean power source that can keep up with advancements in daily life and invention [2].

Among the innovations for not-so-distant future energy stockpiling are battery-powered lithium-ion batteries, fuel cells, and supercapacitors (SCs) [3]. In the previous twenty years, lithium-ion batteries (LIBs) have accomplished extraordinary triumphs because of their superior exhaustive battery execution, contrasted with lead-acid, Ni-Cd and Ni-MH batteries. In any case, similar to the past battery procedures, its advancement has likewise met a bottleneck in the present time [4]. Supercapacitors (SCs) overcome any barrier between ordinary capacitors and battery-operated types of equipments. Fuel cells (FCs) are a gadget that renovates over the chemical energy from a fuel into power through a chemical reaction with oxygen or another oxidizing agent.

Around the world, there is an expanding research enthusiasm on solar-powered thermal energy as plentiful, modest, viable, and clean energy. However, a never-ending energy source using solar thermal energy is being searched due to the absence of daylight at night or its rarity on a gloomy day. In that unique circumstances, researchers are searching for an approach to store this huge energy to use it without daylight/sunlight. It could be the arrangement of the two present issues, for example, the investigated consumption of petroleum derivatives at a high rate and the natural impacts of global warming [5].

Thermal energy storage (TES) framework with phase change material (PCM) could be a decent alternative to decrease these issues. It is likewise required to control the present hazardous global warming rate. Over the most recent 150 years, extremist advancement of industrialization and related human exercises have collected tremendous measures of GHGs to the environment [6]. Alexiadis (2007) arranged a model to measure the impact of the CO_2 outflow because of anthropogenic exercises. He indicated that the anthropogenic CO_2 discharge has become the principal driving force in an unnatural weather change [7]. Ozone-depleting substances from the burning of petroleum derivatives, production, transportation, and energy transformation bring about atmosphere changes by influencing the environment artificially in the long term [8].

An energy stockpiling measure takes a shot at three principal exercises, for example, charging (stacking), putting away, and releasing (delivering) [9]. In addition, one of the flourishing methods to store thermal energy is the phase change material execution. Thermal energy storage frameworks can assist with upgrading energy productivity and relieve energy-related ecological impacts particularly in building heating, cooling, and power generation. Subsequently, thermal energy storage frameworks could assume an essential part for climate by moderating emissions of CO_2, SO_2, NO_x, and CFCs [10]. The incredible accomplishment of graphene has been trailed by an equally impressive surge in the advancement of other 2D materials that can frame nuclear sheets with exceptional properties. These incorporate 2D transition metal dichalcogenides (for example molybdenum disulfide (MoS_2), molybdenum diselenide ($MoSe_2$), tungsten disulfide (WS_2), and tungsten diselenide (WSe_2)), hexagonal boron nitride (h-BN), borophene (2D boron), silicene (2D silicon), germanene (2D germanium), and MXenes (2D carbides/nitrides) [11 - 18].

As a building block for carbon constituents of every other dimensionality, the two-dimensional (2D) single nuclear carbon sheet of graphene has immediately developed as an alluring contender for energy applications because of its interesting structure and properties, including a huge explicit surface territory, fantastic electrical conductivity, great warm conductivity, and high charge versatility, extraordinary mechanical quality, low optical absorbance (2.3%), and density and eccentric adaptability [19, 20]. Like every other material, however, it is extremely uncommon for a graphene-based material with desirable bulk properties to likewise have the surface qualities required for certain particular applications. Consequently, surface functionalization is fundamental in making graphene materials of good bulk and surface properties as requested for effective energy transformation and capacity.

Polyoxometalates (POMs), at class of metal-oxygen groups of the early transition elements, are the absolute most important structural blocks for nanocomposite materials. Polyoxometalates have an unequaled scope of physical and chemical properties which emerge from their interminable assortment of atomic structures

CHAPTER 10

Investigation on Various Polymer Electrolytes for Development of Dye Sensitized Solar Cell

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Abstract: Dye sensitized solar cells (DSSCs) based on TiO2 nanoparticles film have attracted extensive attention from both industry and academia. Generally, the liquid electrolyte is used in dye sensitized solar cells, but the vaporization of liquid electrolyte hinders its commercialization as its affects its stability. And also the reduction in performance of dye sensitized solar cells was observed due to electron recombination in semiconductor liquid electrolyte interfaces. The situation worsens when the photoanode is in contact with the vaporization of electrolyte solution that affects the charge distribution at the semi conductor electrolyte interface and initiates photo corrosion on the photoanode. With the finding of ionic conductivity in polymer, electrolytes complexed with salt give a breakthrough to the development of DSSC devices. Various types of electrolytes have been developed and tested in different DSSCs configurations to overcome this problem. Among all polymer electrolytes, PEO (Polyethylene oxide) based polymer electrolyte has shown excellent performance in different electrochemical application areas. In DSSCs, it is also considered a novel candidate due to its excellent ability to form complexes with ionic salts. Poly(vinyl alcohol) (PVA) is also a promising candidate acting as a host polymer due to its inherent characteristics like high mechanical strength, good tensile strength, high temperature resistance, non toxicity, good optical properties and high hydrophilicity. PVA have a large extent of poly hydroxyl group, which makes PVA highly hydrophile. It also offers other advantages like excellent chemical stability, ease of preparation, and flexibility. In the present paper, we review different types of polymer electrolytes which have been used for improving the performance and stability of DSSCs.

Keywords: Dye Sensitized Solar Cell, Polymer Electrolyte, Polyethylene Oxide, Polyvinyl Alcohol, Chitosan.

INTRODUCTION

Solar cells are the devices that convert solar energy into electricity. The conventional solar cell device is silicon based solar cells with high conversion eff-

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iciency. But the high cost of developing these silicon-based solar cells limits their widespread application. Therefore in last few years, new concepts of solar cells have been considered. These technologies mainly focussed on concentrating photovoltaic technology, organic solar cells, dye sensitized solar cells and novel emerging solar cell concepts, and together these are known as third generation solar cells. Because of their low cost materials and easy fabrication, these technologies are expected to take a significant share in the fast growing photovoltaic area.

Since the breakthrough work by Gratzel in 1991, Dye sensitized solar cells (DSSCs) have attracted the interest of both industry and academia for future clean energy. The four major components of DSSCs are sensitizers, nanocrystalline porous semiconductor based photoanode, electrolytes and counter electrode [1 - 3]. The performance of a DSSC is affected by the properties of metal oxide, as well as the choice of electrolyte and dye. Therefore the researchers working in the field of DSSCs are focusing their attention on improving one or the other component of DSSCs so that efficiency comparable to silicon based solar cell can be achieved.

The liquid electrolyte, which is the most important component of DSSCs, hinderers its stability as the electrolyte leaks and vaporizes with time. Thus scientists are focusing their attention on the solidification of an electrolyte such as inorganic or organic hole conductors, ionic liquids, polymer electrolytes [4 - 6]. Polymer electrolyte is the most important ionic conductor that is used in electrochemical devices. Polymer electrolytes are solid ionic conductors that are prepared by the dissolution of salts in a suitable high molar mass polymer containing polyether units. For obtaining good performance from electrochemical devices, the polymer electrolyte used must have excellent properties such as good ionic conductivity, and thermal, mechanical and electrochemical stabilities. Among all these properties, we have focused our attention on enhancing ionic conductivity of the polymer electrolyte. The ionic conductivity of a polymer electrolyte is given by the equation:

$$\sigma=\eta\mu e$$

Where η is number density $\mu$is the mobility of charge carriers, and e is the elementary charge. From the equation, it can be seen that η and$\mu$are two important parameters that control the ionic conductivity of polymer electrolytes. Thus, it is essential that η and μ be determined quantitatively.

Polymeric electrolytes are materials of special interest because they show many advantageous properties when used in devices such as low cost, easy film formation *etc.* The studies on polymer electrolytes are relatively motivating to physicists, chemists and engineers for their fundamental physical properties and potential applications in many electrochemical devices such as batteries, fuel cells, super capacitors, sensors and display devices. They are in crystalline and amorphous phases. The existence of an amorphous phase and lower values of glass transition temperature are accountable for ion conduction in such systems. These materials have various advantages over liquid electrolytes, such as; corrosion, self-discharge, bulky design, miniaturization *etc.* Various approaches have been adopted for the synthesis of new polymer electrolytes exhibiting higher ionic conductivity at ambient temperature such as polymer blends, copolymers, comb branch polymer, cross-linked networks, addition of plasticizers, addition of ceramic filler, and use of a larger anion of dopant salt (acid) [7 - 10]. Though the highest reported efficient DSSC contains a volatile organic solvent which suffers from the major drawback of leakage and vaporization of organic solvent which hinders its long-term practical operation. Moreover, the corrosion of iodine on platinum electrolytes is also an additional barrier. Therefore, by using polymer electrolytes, one can overcome these problems [11 - 14].

BASIC PRINCIPLE OF DYE-SENSITIZED SOLAR CELLS

The disparity between DSSCs and p-n junction solar cells is about their components and working. In p-n junction solar cells, the semiconductor performs both the tasks of light harvesting and charge carrier transport, while in DSSCs these two functions are performed separately. Moreover, the solar energy conversion mechanisms in DSSCs are the interfacial processes while in p-n junction cells these bulk processes. Hence most studies on DSSC are made to understand the prevailing role of electron transfer dynamics and kinetics at nanocrystalline metal oxide/sensitizer/electrolyte interfaces. Though researchers are performing studies on this subject, still not much understanding of the kinetics of the interfacial processes has been made. If we properly understand the kinetics of interfacial processes, we can improve the efficiency of DSSC and scale up their manufacturing.

Dye sensitized solar cells (DSSCs) are nanostructured photoelectrochemical device in which photons are absorbed by the sensitizers attached to the large band gap semiconductor oxide. The conversion of photonic energy into electricity takes place by the transfer of electrons from the excited dye molecule to the conduction band of the semiconductor oxide. The electron moves from the semiconductor oxide to the current collector and the external circuit. In the pores, there is a redox mediator which ensures that the oxidized dye species are continuously regenerated over and over again and the cycle is not stopped as shown in Fig. (**1**).

SUBJECT INDEX

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Currently, she is working as Senior Assistant Professor in Department of Chemistry, Central University, Bilaspur, India. She has also worked as Examiner of Patents and Design, Government of India, New Delhi. She did her D Phil from University of Allahabad, India. She has been awarded with the DST Fast Track Young Scientist award from DST, and Research Associateship from CSIR, India. She has published more than 35 papers, four books and one Indian patent. She worked as Adaptor in Modification of 3rd Edition of Popular Text Book on Polymer Science by F W Bilmeyer. She has published more than 16 Book chapters in national and international publication house.

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Kalpana Awasthi

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