Some Frontier Tools and Techniques for Materials Science

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Posterity bears evidence that Materials Science emerged as the first science which heralded the concepts of Interdisciplinary Sciences. We can take pride that one of the important initial proponents of Material Science happens to be an Indian: Prof. Rustam Roy of Pennsylvania State University of USA. In India the Scientists who brought Material Science at the Centre Stage are many. However, if we take in reference to BHU, relevant Scientists are Prof. C.N.R. Rao, Prof. A.R. Verma and Prof. T.R. Ananatraman.

Materials Science being dominantly an experimental science necessarily depends on a variety of special tools and techniques. These are far too many to be covered in this lecture. However, some of these will be elucidated. In this talk the main emphasis will be on electron and electron beam oriented microscopic techniques. The frontier technique of this type is Scanning Tunneling/Atomic force Microscopy. Although the STM/AFM are very recent techniques, their forerunner techniques: the transmission and scanning electron microscopy techniques are no less important. These techniques are applicable almost to all types of Materials including Bio-materials. These will be described and discussed in some details in the present talk.

Electrical Characterization of Fast ion Conducting Materials

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The material which exhibits high ion conductivity and negligible electronic conductivity at fairly low temperature below the melting points is called "Fast ion conductor". The present talk concerns the electrical characterization tools employed to characterize fast ion conductors. First of all, one should establish that the conductivity is due to motion of ions. For this the following transference number measurement techniques will be discussed:

i) Tubandt's electrolysis method

ii) Wagners's polarization technique

iii) Electrochemical potential measurement-EMF method

iv) AC-DC method used to characterize polymer electrolytes

Next, the electrical characterization by impedance spectroscopy will be discussed through the analysis of frequency dependent conduction characteristics in impedance, conductivity, permittivity and modulus formalisms. Finally the scaling approach of the above complex impedance data will be discussed.

X-ray Photoelectron Spectroscopy

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Knowledge of electronic configuration, band structure, oxidation states and chemical composition of any material is very essential for its technological applications. X-ray photoelectron spectroscopy is one of the state-of-art techniques widely used to get these information in a variety of samples ranging from bulk materials, thin films, nanomaterials and semiconductors. Though, photoelectron spectroscopy is based on simple photoelectric effect discovered more than a century ago, the development of this as a technique took very long time due to its requirement of ultrahigh vacuum and advanced electronics. Further this technique would give information only from a few atomic layers in the surface due to its very high surface sensitivity.

The basics of this spectroscopic technique will be introduced in this talk. Details of various information obtained by this technique will be given and the advantages of using synchrotron radiation for such measurement will be shown.

Techniques for Characterizing the Microstructure of Al-Si Alloys: Qualitative and Quantitative Aspects

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The unique combination of lightweight and high strength-to-weight ratio provided by aluminum alloys has been the reason for their extensive use in diverse applications, including automotive and aerospace components. Aluminum alloys usually contain several alloying elements in order to achieve the best combination of mechanical, physical and processing properties. Major alloying elements are Si, Cu, Mg and Zn. Silicon provides excellent castability, good wear resistance, and high thermal conductivity; Mg, Cu, and Zn provide strength through age-hardening. Iron is the most common impurity, and its presence is generally undesirable since it forms coarse Fe-intermetallic phases in combination with aluminum and other elements, which adversely affect the mechanical properties of the alloy.

Optical Spectroscopic Techniques for Characterization of Nanomaterials

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The optical properties of semiconductor nanoparticles have made them attractive materials in diverse fields of applications, such as optoelectronic devices, optical amplifier in telecom networks, biosensor, bioimaging, therapeutics and optical tracking. Quantum dots (QDs) have attracted considerable attention as novel luminescent probes in recent years. The widespread interest in these QDs is attributed to their high photostability and size tunability of luminescence. They also exhibit narrow emission and broad excitation spectra, allowing excitation of multiple QD with a single wavelength. These superior optical properties surmount the constraints of conventional fluorophores, thereby offering exciting new opportunities for sensing and bio-imaging. Semiconductor nanoparticles have been the focus of intensive research because of their size dependent optical properties and dimensional similarities with biological macromolecules. Luminescence of semiconductor QDs are known to be sensitive to surface states and binding of analytes onto the nanoparticle-surface affects these electronic states, which, in turn, influences the PL emission of QDs. The surface of the nanoparticles is modified with suitable molecules to make them biocompatible and amenable to several biological manipulations. The key issues in the synthesis of nanomaterial are particle size, distribution and luminescence quantum efficiency. In order to develop a new nanoparticle-based biosensor or to know any of its toxicological effects to the cells, it is essential to investigate the interactions of the nanoparticles with the biomolecules. Some important aspects of synthesis of good quality functionalized quantum dots will be presented. Here, how optical methods can be utilized to characterize these materials and to monitor the interactions with biomolecular systems will be discussed.

Irradiation as a Tool for Materials Modifications

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Irradiation in materials science has been very effectively used to modify the material properties in significance. Irradiation species like γ-ray, electrons, neutrons, protons and ions (of all kind) have been used with their energies ranging from keV to MeV and even of GeV. Low energy (keV) range irradiation has been used for implantation and creating isolated defects through displacement damage to enhance diffusion in materials. High energy irradiation has been used for causing melting, recrystallization, track formation and formation of nanostructures.

The swift heavy ion irradiation (~ MeV ions) and other radiations have been used effectively in electronic and magnetic materials to cause several interesting and significant features. Conductivity type change phenomenon like from n-type to p-type or otherwise in electronic materials, ferromagnetism in magnetic thin films, GMR (giant magnetoresistance) in magnetic interfaces with semiconductors and nanogranular phase have been formed from such application. The irradiation can be used to tailor the electronic and magnetic interfacial properties for magneto-electronics (Spintronics).

Overall, irradiation has been found as a versatile tool for materials modifications. usefulness of these techniques in materials characterization.

Micro and Nanostructured Epoxy Resin Based Polymer Blends

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Epoxy based blends have generated a lot interest recently due to their increasing commercial importance. Epoxy resin is often blended with rubbers and thermoplastics to generate micro morphologies for the better impact performance. Very recently, nanostructured blends based on epoxy resin/block copolymers systems have appeared in literature. These nanostructured blends have the potential to show super toughness. In the proposed talk, miscibility, phase separation, morphology, mechanical and viscoelastic properties of a series of epoxy based blends will be discussed. The phase separation, gelation and vitrifcation will be investigated detail. More attention will be given to the development of nanomorpholgies. Techniques such as SEM, TEM. OM , laser light scattering, rheology will be made use of for the characterization of the morphologies. Finally the role of the nano and micromorphologies on the mechanical and viscoelastic properties will be disused.

An Overview on The Application of A State-of Art Technique To Study Defects In Materials

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In today's fast paced research and development, the application of different techniques to characterize different types of defects in materials plays a pivotal role to make us very knowledgeable and this knowledge is irreversible

The existence of positron as predicted by Dirac was verified by Anderson in 1930's.Positrons are antiparticles of electrons, the annihilation of positron with electron in materials was first studied in 1940's. The emission of 2γ or 3γ depending on the relative orientation of their spins takes place during annihilation process The annihilation parameters were found to be sensitive to lattice imperfections and thus the positron electron annihilation has been widely used to investigate the presence of crystal defects in the material.The technique is a nondestructive and one of the most sensitive techniques for the detection of defects in the atomic scale.

In this talk an introduction to the Positron Annihilation Technique, a state of art technique and a brief review of its application in the field of defect studies in the materials will be presented.

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Novel materials via soft chemical routes and their characterization

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Metal complexes containing sulfur ligands have attracted a lot of attention during recent years as metal organic frameworks. Some of the simple compounds can easily be converted to metal sulfides by low energy soft chemical routes (Chimie Douce).

Our recent studies with a few compounds containing transition metals and some heavier main group metals revealed interesting structures and properties1-4. Characterization of the precursors and the materials were possible in most of the cases by X-ray crystallography where suitable single crystals could be developed. For a number of disordered crystals X-ray data collections were carried out at temperatures below 150 K while for twinned crystals careful data reduction permitted us to solve the structures.

In a few other cases various techniques such as DART MS, IR, 1H, 13C, 31P, 119Sn, NMR, (in solution or in solid state by magic angle spinning) UV/Vis spectroscopy powder X-ray diffraction, scanning electron microscopy have been used. Quantum chemical calculations using density functional theory have been found to be a powerful tool in identifying the lower energy pathways and structures, thus enabling us to study the reaction mechanisms in some cases.

Brief synthetic schemes and details of characterization techniques will be presented.

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Soft X-ray Spectroscopy- An effective probe to Characterise Nanostructured materials for Energy devices

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The ability to control the particle size and morphology of nanoparticles is of crucial importance nowadays both from a fundamental and industrial point for high tech applications. Controlling the crystallographic structure and the arrangement of atoms along the surface of nanostructured material will determine its physical and chemical properties. In general, electronic structure ultimately determines the properties of matter. Soft X-ray spectroscopy has some basic features that are important to consider. X-ray is originating from an electronic transition between a localized core state and a valence state. As a core state is involved, elemental selectivity is obtained because the core levels of different elements are well separated in energy, and the involvement of the inner level makes this probe localized to one specific atomic site around which the electronic structure is reflected as a partial density-of states contribution. The participation of valence electrons gives the method chemical state sensitivity and further, the dipole nature of the transitions gives particular symmetry information. In this paper, some recent findings regarding soft X-ray absorption, emission studies and microscopic investigation of various nanostructured systems will be presented for photovoltaic device applications

Status of solid state photoelectrochemical solar cell and dye sensitized solar cell using PEO-based polymer electrolytes

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Due to energy crisis in coming future many efforts are directed towards alternate sources. Solar energy is accepted as novel substitute to the conventional sources of energy. Out of the long list of various types of solar cells the solid state photoelectrochemical solar cell (SSPEC) and dye sensitized solar cells (DSSC) are now emerging area since it proposed as alternative for costly crystalline solar cell. In this talk we are going to discuss the current status of SSPEC and DSSC using polymer electrolyte particularly on PEO-based polymer electrolytes. Due to numerous advantageous properties of PEO it is frequently used as electrolyte in both SSPEC as well as DSSC [1-2]. In DSSC, so far high efficiency (more than 11%) could be obtained only using volatile liquid electrolyte which suffers many disadvantages like corrosion, leakage, evaporation. The PEO based solid polymer proves its importance and could be used to solve the problems stated above. The recent developments in solar cell using modified PEO electrolytes by adding nano size inorganic fillers, blending with low molecular weight polymers and ionic liquid (IL) are discussed in detail. The role of ionic liquids in modifying the electrical, structural and photoelectrochemical properties of PEO based polymer electrolytes are also suggested.

Keywords: Polymer electrolytes; photoelectrochemical solar cell, Ionic liquid; Ionic conductivity; SEM; TEM; Dye sensitized solar cell

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Polypyrrole coated neural electrodes with improved Electrochemical properties

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The efficacy of any neuroprosthetic device ultimately depends on the electrode material which is in intimate contact with the neural tissue. One of the major challenges in the field of neuroprosthetics is the creation of such a neural interface that is biocompatible, flexible, has low electrical impedance, good charge transfer characteristics and long-term electrochemical stability. Intrinsically conducting polymers like Polypyrrole (Ppy) and Poly (3, 4-ethylene dioxythiophene) (PEDOT) have recently emerged as a promising option to improve the mechanical, electrochemical properties and biocompatibility of neural microelectrodes. In this study, we aim to evaluate the enhanced electrochemical properties exhibited by Polypyrrole coated neural electrodes specifically targeting their utility in retinal prosthetic devices. We electrodeposited thin films of Polypyrrole doped with Poly Styrene Sulfonate (PSS) on tungsten neural electrodes and Indium-tin oxide (ITO) coated glass substrates and studied their charge storage capacities and impedances using the Cyclic Voltammetry (Scan rate – 20 mV/s) and Electrochemical Impedance Spectroscopy techniques respectively. To examine the employability of these polymer coated electrodes as retinal prosthetic electrodes, they were specifically characterized in Ames' medium since the in vitro studies with retinal tissues are usually performed in this medium and the results were compared with those obtained in standard 0.9 % saline solution. For uncoated ITO substrates, the charge storage capacity was found to be 1.048 mC/cm^2 in 0.9% saline solution and 0.64 mC/cm^2 in Ames' medium whereas the Ppy- PSS coated ITO substrate demonstrated much enhanced charge storage capacity values in both the solutions, 118.18 mC/cm^2 in saline solution and 127.27 mC/cm^2 in Ames' medium. Our preliminary studies on tungsten electrodes show approximately five fold increase in the charge storage capacities of PPy-PSS coated electrodes as compared to the uncoated ones. Thus, through this study we attempt to highlight the potential of Polypyrrole as a promising material for retinal prosthetic interfaces.

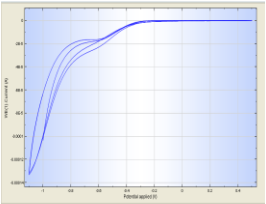

Fig.1: Cyclic Voltammogram of an ITO glass plate in 0.9 % saline solution prior to the PPy-PSS coating.

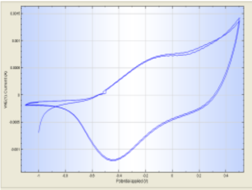

Fig.2: Cyclic Voltammogram of a PPy-PSS coated ITO glass plate in 0.9 % saline solution prior to the PPy-PSS coating.

Molecularly Imprinted Material Prepared by Surface Imprinting Technique for Trace Analysis of ‘Aspartame’

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Aspartame, the methyl ester of the dipeptide comprising of aspartic acid and phenylalanine is used widely as a low calorie sweetener. A molecularly imprinted polymer able to recognize selectively “aspartame” was prepared via photopolymerization on the surface of silica. The polymer N[2-ammonioethyl] piperazinium maleimido propane sulfonate copolymer was allowed to be grafted onto the surface of silica gel particles by the ‘grafting from’ technique. The molecular imprinting on the surface grafted polymer using “aspartame” as template was carried out following the non-covalent approach. Thus generated imprinted material has shown high selectivity and sensitivity in determination of aspartame in aqueous medium as well as in certain pharmaceutical samples without any pretreatment.

Thermodynamical Study of Solutions of PEG200 in Ethanolamine, m-Cresol and Aniline at 298.15 K

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To understand the intermolecular interactions in solutions of poly (ethylene glycol) 200 densities, absolute viscosities, ultrasonic velocities and refractive indices of binary mixtures of poly (ethylene glycol) 200 with ethanolamine, m-cresol and aniline have been measured at 298.15 K, under atmospheric pressure over entire composition range. This data of PEG mixtures are important because of the industrial interest. The experimentally evaluated data has been used to calculate deviation in viscosity, excess molar volume, deviation in ultrasonic velocity and deviation in refractive index as these are fundamentally important in understanding the intermolecular interactions and nature of molecular agitation in dissimilar molecules. These are sensitive towards difference in size and shape of the molecules. From the plots of excess parameters against mole fraction the interaction is found to be stronger in PEG+ethanolamine than in PEG+m-cresol and least in PEG+aniline. The results have been fitted to Redlich-Kister polynomial equation. The variation of these parameters with respect to the change in concentration of poly (ethylene glycol) 200 have been explained in terms of specific intermolecular and intramolecular interactions present in the mixture.

Isothermal compressibility for the binary mixtures were predicted by the equation based on Flory's statistical theory and three rigid sphere equations which are Thiele-Lebowitz model , Guggenhiem model and Carnahan-Starling model and the results have been explained in terms of average percentage deviations from experimental values.

Estimation of heavy metal ions using multi-imprinted polymer

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The method of molecular imprinting is carried out by polymerization of monomer in the presence of a template molecule, followed by removal of the template to leave a binding cavity with selectivity toward the template molecule. Now-a-days imprinting process does not have to be limited to a single template, and several compounds can be imprinted simultaneously. Advantages of multiple-template imprinting are that several different classes of compounds can be extracted, separated, assayed, detected, or otherwise analyzed at one time. Till date, multi imprinting has been done only in the case of organic biomolecules. Whereas, inorganic imprinting where the template used is an inorganic ion like Copper, Zinc, Iron etc. so far has not been reported. For the first time, we synthesized a new class of molecularly imprinted polymer which has recognition capability for two different heavy metal ions in a single format. For this, a new class of bi-functional monomer was also prepared which have phosphate group for the strong interaction between metal ion and monomer. The morphology of the polymer was characterized by IR, NMR, and SEM analysis. All the results indicated that the imprinted polymer exhibited better imprinting efficiency and higher rebinding capacity than the non-imprinted polymer. The multi-imprinted polymers could be used many times without decreasing their adsorption capacities significantly.

Synthesis, characterization and magnetic properties of cyanide bridged 1-D Metal coordination polymers based on $[Fe^{III}(s\text{-}bqdi)_2(CN)_2]^-$

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A successful strategy leading to heteropolymetalic systems consists of self assembly processes involving anionic, cationic or neutral building blocks. One of the building blocks contains a paramagnetic ion along with a potential bridging ligand and another contains a potential coordination site, which on association give rise to heteropolymetalic species. Cyanometallate complexes are efficient building blocks for constructing well defined materials because they stabilize the variety of transition metal centers, oxidation states and efficiently communicate spin information, M(µ-CN)M’ linkages also affects the physical properties of the metal cyanide derived materials (1-2). For instance, many cyanide bridged paramagnetic metal complexes of different dimensionalities ranging from 0-D to 3-D networks (3) have been characterized which are found to exhibit interesting spontaneous magnetization and photo magnetic properties (4). One dimensional assemblies were generally constructed by using two of the six cyanide groups of the hexacyanometallate, as bridging moiety and possess different kind of structural motifs: rope-ladder-like chain, zig-zag chain etc. A new series of transition metal complexes $K[M^{II}(s\text{-}bqdi)_2][Fe^{III}(s\text{-}bqdi)_2(CN)_2].10H_2O$ (M^{II}= Co, Ni and Cu) have been synthesized by the substitution of four out of six CN^- ligands of hexacyanoferrate by two bidentate ligands. All the coordination polymers display 1-D chain networks. Magnetic properties of $Co^{II}Fe^{III}$ complex were studied by SQUID magnetometer. Magnetic studies reveal low temperature antiferromagnetic interaction between the metal centers.

Keywords: 1-D Poly, Cyanometallate, heteropolymetallic, s-bqdi, SQUID, antiferromagnetic.

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An approach towards the designing of molecularly imprinted polymer via AGET-ATRP

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Molecular imprinting is a technique for preparing polymeric materials that are capable of recognizing and binding the desired molecular target with a high affinity and selectivity. The imprinting by free radical polymerization technique limits the degree of control over molecular-weight distribution, copolymer composition, and macromolecular architecture. However, the use controlled/living polymerization techniques within the field of imprinted polymers has the great potential to improve the structural homogeneity and drastically enhance the binding parameters. This work focuses on the synthesis of molecularly imprinted polymer (MIP) by the living radical polymerization process via activator generated-atom transfer radical polymerization (AGET-ATRP). It requires an alkyl halide (R-X) as an initiator, a transition metal complex as a catalyst, and a reducing agent. Herein, we used a chlorosilane as an initiator to make an inorganic-organic imprinted hybrid material. FTIR, NMR, and SEM analysis were performed to investigate the binding and morphological features of the imprinted polymer. The polymer testing showed that synthesized molecularly imprinted polymers have high affinity and selectivity for corresponding template in both the aqueous and real samples. Corresponding Blank polymers were unable to differentiate between analytes, suggesting that imprinting phenomenon was responsible for the recognition properties.

Variation in thermodynamic properties of Poly ethylene glycols methyl ether methacrylate 300 (PEGMA 300) with 2-ethoxyethanol and 2-methoxyethanol at varying temperatures

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Density (ρ), refractive index (n) and viscosity (η) data are required in many chemical engineering calculations involving fluid flow, heat and mass transfer etc. Poly ethylene glycols methyl ether methacrylates (PEGMA) have gained increasing attention as a class of chemical substances widely used in different industrial application. It is well known that alkoxyethanols have wide use as monomers in the production of polymers and emulsion formulations. They are also of considerable interest for studying the hetero proximity effects of the etheric oxygen on the –OH bond and, hence their influence on the associated nature of the species in these molecules. 2-methoxyethanol and 2-ethoxyethanol are versatile organic liquids used in chemical industries as a solvent for lacquers, oils and resins and as an antifreeze for explosives. The study of the excess thermodynamic functions provide useful information regarding the nature of intermolecular interaction and macroscopic behavior of fluid mixtures and can used to test and improve thermodynamical model for calculating and predicting the fluid phase equilibria. Studies on density, viscosity and refractive index along with other thermodynamic properties are being increasingly used as tools for the investigation of the properties of pure components and the nature of intermolecular interaction between the liquid mixtures constituents. Therefore, density, viscosity and refractive index measurements have been made on binary mixtures of PEGMA with 2- ethoxyethanol and 2-methoxyethnol respectively over entire composition range at varying temperatures. The estimation of various thermodynamic properties such as excess molar volume (V_m^E), excess viscosity ($\square^E$), molar refraction deviation (ΔR_m) and excess Gibbs's free energy of activation for viscous flow (ΔG^{*E}) have also been made to understand the molecular association between unlike molecules. Redlich- Kister polynomial equation has been used to correlate the experiment data. The observed values of various excess parameters indicate that 2- methoxyethanol interacts more readily than that of 2-ethoxyethanol.

AFM and SEM characterization of poly (2-methoxy-5-(2-ethylhexyloxy)-1, 4-phynylenevinylene) (MEH-PPV) blended poly (9, 9-dihexyl fluorenyl-2, 7-diyl) (PFO) thin films

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The phase-morphology inversion in blend systems of poly (2-methoxy-5-(2-ethylhexyloxy)-1, 4-phynylenevinylene) (MEH-PPV) and poly (9, 9-dihexyl fluorenyl-2, 7-diyl) (PFO) thin films has been studied after their thin films were prepared on glass substrates by spin-coating from a chlorobenzene. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to obtain information on the morphology of the thin films during heat treatment. It is clearly seen from the SEM micrograph that indeed an increased order is established at these grain boundaries on heat treatment. Grain boundaries may lie parallel to the direction of current flow, which facilitates the holes transport thus increases the carrier mobility. Grain boundaries act as surface states for charge carriers and can be accumulated .After heat treatment; the charges generated during the discharge are trapped in these surface states [1]. It was also found that the MEH-PPV riched PFO: MEH-PPV polymer blends are always phase separated after annealing in either of the blend thin films. To further support these observation of the pure and blended film morphology were characterized by atomic force microscopy (AFM) in tapping mode for films containing 0, 2wt%, and 25 wt % blend films [2]. Both the RMS and Ra roughness increase when MEH-PPV is blended in PFO. The root mean square (RMS) of pristine PFO was found to be 2.31 nm whereas the blend film of 2 wt % of MEH-PPV shows the RMS of 1.34 nm and the RMS of the blend film of 25 wt % of MEH-PPV shows the RMS of 14.33 nm. The average roughness (Ra) of pristine PFO was found to be 1.68 nm whereas the blend film of 2 wt % of MEH-PPV shows the Ra of 1.11 nm and the Ra of the blend film of 25 wt % of MEH-PPV has reached up to 8.44 nm.

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Conductivity and Discharge Characteristics of Solid Polymer Electrolyte Films

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Solid polymer films based on PEMA were prepared in different $NaClO_4$ salt concentrations by solution cast technique. The features of complexation of these electrolytes were studied by Fourier transform infrared (FTIR) spectroscopy. Transference number measurements using Wagner's polarization technique were carried out to investigate the nature of charge transport in this electrolyte system. The electrical conductivity of pure and $NaClO_4$ doped polymer films was studied in the temperature range 298 K – 398 K. The conductivity increased with increasing dopant concentration and exhibited Arrhenius type dependence with temperature. The increase in conductivity with dopant concentration may be attributed to the formation of charge transfer complexes. Transport number data showed that the charge transport in this electrolyte system is predominantly due to ions. Electrochemical cells of configuration $Na/(PEMA+NaClO_4)/(I_2+C+electrolyte)$ were fabricated .The discharge characteristics of these cells were studied under a constant load of 100 KΩ. The open circuit voltage, short circuit current was measured. Various other cell parameters were evaluated and are reported.

Structural Studies of Polymer Composite Electrolyte

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An attempt has been made in the present work to prepare polyvinyl alcohol (PVA) based proton conducting gel electrolytes in Lithium acetate (LiAc) solution and characterize them. Nano composite polymer electrolyte consisting of Poly vinyl alcohol (PVA), Lithium acetate with TiO_2 filler, is synthesized by the combination of solution cast technique and sol-gel process. The composite electrolyte films were characterized by different experimental technique. The average particle sizes of composite electrolytes were in between 25-30 nm. The XRD patterns of all the prepared polymer electrolyte reveal the amorphous nature of the film. The FTIR spectroscopic study indicates the detailed interaction of PVA with proton.

Ion transport property studies on hot-pressed solid polymer electrolytes: (1-x) PEO: x $KBrO_3$

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Ion transport property studies on hot-pressed solid polymer electrolytes (SPEs): (1-x) PEO: x $KBrO_3$, where x in wt. (%), are reported. The compositional (x) dependent conductivity (σ) studies revealed SPE film: (70 PEO: 30 $KBrO_3$) as the Optimum Conducting Composition (OCC) with room temperature conductivity $\sigma \sim 4.36 \times 10^{-7}$ Scm^{-1}, which is more than two orders of magnitude higher than that of pure PEO. To understand the ion transport behaviour in SPE films, the measurement on some basic ionic parameters viz. ionic conductivity (σ), ionic mobility (μ), mobile ion concentration (n), ionic transference number (t_{ion}) have been carried out using different experimental techniques. Material characterizations were done with the help of XRD, SEM & DSC techniques. The activation energies (E_a) values have been computed from 'log σ - 1/T' Arrhenius plots.

Effect of Plasticizer on Ionic behavior of PEO-Ammonium Adipate based electrolyte system

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Present work deals the effect of different plasticizer on ionic behavior of PEO based plasticized solid polymer electrolyte system. The solid polymer electrolyte is a novel material for electrochemical device applications like, fuel cell, solid state battery, super capacitor, ECD's etc. Solid polymer electrolyte films were synthesized by solution cast technique using polyethylene oxide (PEO) as polymer host, Ammonium adipate ($C_6H_{16}N_2O_4$) salt and ethylene carbonate (EC), polypropylene carbonate (PC), polyethylene glycol (PEG) plasticizers. These electrolyte system were characterized by XRD, IR and SEM measurement. Electrical characterization of the electrolyte was studied by impedance spectroscopy technique. The chemical structure of PEO [-(CH_2CH_2O)n-] explains most of the properties of polymer: a strong solvating character due to the high donating character of the numerous ether oxygen, a low dielectric constant arising from the high ratio of alkyl segments and a strong tendency for crystallization correlated with the high organization and rigidity of the segmental units. Moderate conductivity in amorphous materials is then a direct consequence of PEO features where high salvation is counter balanced by the energetic complexation of cations earlier, anion /cation mobility occurs in the amorphous phase and its diffusion occurs through a complex mechanism involving the PEO segmental mobility. The effect of plasticizers on the transport and electrochemical properties of polymer electrolytes has been examined. First, the mobility of cations and anions was increased by doping the ethylene carbonate and poly (ethylene glycol) in PEO-based electrolytes. However, the cation mobility in PEO-based electrolytes doped with propylene carbonate was suppressed resulting in a lower cation transference number. Nevertheless, all the plasticized electrolytes have higher bulk conductivity than the non-plasticized. The variations of a.c. conductivity with frequency of all samples were increasing with increasing temperature. The variation of dielectric constant with dielectric loss (cole-cole plot) are shows the Non-Debye relaxation process. The electrical conductivity with temperature of electrolyte system is shows VTF behavior.

Synthesis and characterization of electrodeposited polycrystalline Bi_2Se_3 thin film and its surface deformation study using holographic interferometry technique

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In the present work, we have successfully electrodeposited Bismuth Selenide (Bi_2Se_3) thin films onto stainless steel and fluorine doped tin oxide (FTO) substrate using bath containing Bismuth nitrate and Selenium dioxide. The structural, morphological and optical properties of the deposited films are studied using X-ray diffraction pattern (XRD), scanning electron microscope (SEM) and optical absorption techniques, respectively. Surface wettability tested by measuring contact angle. XRD pattern revealed that the Bi_2Se_3 films are polycrystalline in nature. Scanning electron micrograph of Bi_2Se_3 films clearly shows the formation bunch of cabbages at high magnification. The Bi_2Se_3 thin film shows direct band gap with energy 1.1 eV. Wettability test of Bi_2Se_3 thin films reveals hydrophobic nature with water contact angle 115^o. The determination of thickness, mass and stress of the Bi_2Se_3 thin film was carried out by Double Exposure Holographic Interferometry (DEHI) technique.

Keywords: Bismuth Selenide, Electrodeposition, bunch of cabbages, Double Exposure Holographic Interferometry (DEHI) technique, Contact angle.

Dielectric Studies of Polysulfobetaine zwitterionic polymer Poly (N-phenylene N'imino pentyl) imminiumpropane sulfonate based Electrolyte

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Molten salts, in which cationic unit is covalently tethered with anionic unit, are known as Zwitterionic Salts. Their polymers, known as Zwitterionic Polymers, are technologically very important. Ohno and coworkers first time introduced these materials in electrochemistry [1]. The advantage of zwitterionic polymer over IL/Molten salts is that they cannot migrate with potential gradient as both cation and anion are in intra molecular form. In Present paper we report dielectric property of a synthesized novel Polysulfobetaine based zwitterionic polymer. Synthesis of pure zwitterionic polymer and its characterization has been discussed elsewhere [2]. Synthesized polymer was crosslinked with Cellulose Acetate (CA) and doped with NaI. Complexation is confirmed by FTIR which showed a decrease of 30 cm^{-1} in iminium strech and $10cm^{-1}$ increase in sulfonate strech in doped polymer. Conductivity is found to be of the order ~ 10^{-4} S/cm. Dielectric behaviour, studied as a function of frequency, shows sharp rise at lower frequencies. This behaviour is more pronounced at higher salt concentrations. It is co-related to space charge polarization. In Modulus representation, peak due to interfacial polarization can be seen which is shifting toward higher side depending on salt variation. AC conductivity follow Jonscher power law $\sigma = \sigma_0 + A\omega^n$ and the power law exponent 'n' value comes to be nealy unity for all salt concentration. It seems that the morphology of prepared material has enough open space to assist the long range hopping (comparable to sample dimensions). In synthesised material humidity is plays an important role in transport behavior. Water intake was studied and discussed in the material. Material is also characterised for embient temperature changes.

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A Novel Tool for Synthesis of an Insulating Polymer

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Anodic Contact Glow Discharge Electrolysis(CGDE)in an aqueous solution is a novel electrochemical technique for generating radicals, mainly $H^{\cdot}$ and $OH^{\cdot}$ near the plasma |electrolyte interface at significantly high local concentration and its products are highly non-faradaic in nature(both product and yieldwise)[1,2].The present work is aimed to explore the radical generating capability of CGDE as a tool for radical polymerization.On the basis of a kinetic model for the reaction proposed,a determination of radical yield was made and it was found that the yield of $H^{\cdot}$ /$OH^{\cdot}$ is 9.8 mol(mol electron)$^{-1}$ of electricity[3].The significant yield of $H^{\cdot}$ point to generation of acrylamide radicals from acrylamide solution in aqueous K_2SO_4,which would further propagate the process of polymerization..

The results obtained for anodic CGDE of acrylamide at different monomer concentration and also in presence of iso-propyl alcohol as more powerful radical scavenger at different quantities of electricity are reported. It has been found that the molecular weight of the polymer is of the order 10^{5} g.mol $^{-1}$ and it increases with increase in monomer concentration.

The results calculated for percent monomer conversion (X%)also increases with increase in quantity of electricity passed(q)but the value correspondingly decreases in each case when iso-propyl alcohol, a powerful radical scavenger was added to 7% acrylamide.

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Study of electrical properties of novel PEO-based solid polymer electrolyte

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Polymer electrolytes are of technological interest. They have unique characteristics of high ionic conductivity similar to liquid electrolytes and mechanical stability comparable to solid electrolytes. PEO based polymer electrolytes are the most promising and extensively studied system with other polymers, and it dissolves high concentration of a wide variety of salt to form solid polymer electrolytes giving high ionic conductivity. In the present work we are reporting the characteristics of a novel polymer material synthesized in our laboratory using, triethylenetetramine, 1-3 propane sultone, methanol, NaI as a salt, GA (Glutaraldehyde). The sample preparation has been done by standard solution casting technique. Wagner polarization experiment confirms that the sample is ionic in nature and calculated transference number is 0.81. The electrical conductivity of the sample is 3.96×10^{-4}S/cm by applying an alternating field of 0.02V. Dielectric study shows that the dielectric constant of the material is very high. The frequency dependent dielectric study has been discussed. The temperature dependence conductivity has been done and the humidity dependence properties have also been discussed.

Effect of Divalent ion Substitution on Structural and Transport Properties of Lanthanum Manganites

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Studies on divalent ion substituted rare earth manganites $A_{1-x}B_xMnO_3$ (A = rare earth, B = alkaline earth), gained momentum in the recent past after the compounds were found to show colossal magnetoresistance. These materials have been of great interest due to their spectacular physical properties and their technological applications such as magnetic recording media, magnetic sensors, permanent magnets etc. In this paper we study the structural and transport properties of polycrystalline samples $La_{0.67}Ca_{0.33}MnO_3$ (LCMO), $La_{0.7}Ca_{0.2}Sr_{0.1}MnO_3$ (LCSMO) and $La_{0.67}Sr_{0.33}MnO_3$ (LSMO). These materials were prepared by standard solid state reaction method. The results of X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy indicate that all samples of the present investigation crystallize in single-phase with perovskite structure. From the rietveld refinement of XRD data by FullProf Suite program, we have been found that XRD data of LCMO and LCSMO can be fitted well to orthorhombic structure with Pbnm space group, whereas that of LSMO can be fitted to rhombohedral structure with $R\bar{3}c$ space group. Resistivity and magneto-resistivity of these samples have been measured with variation of temperature by standard four probe method. From these measurements we observe that the samples show two types of transitions: intrinsic and extrinsic. The intrinsic behaviour is indicative of the alignment of Mn spin within the grain, which is governed by double exchange mechanism. The extrinsic behaviour can be attributed to the interfacial tunneling due to difference in magnetic order between core and grain boundaries.

Keywords: Magnetoresistance; double exchange mechanism; M-I transition; Rietveld refinement.

Synthesis, Characterization and Mesomorphic properties of unsymmetrical N-[4'-(alkoxy)-2-hydoxybenzylidene]-N'-(4-alkoxybenzylidene)azine and their copper (II) complexes.

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Azine compounds have interesting chemical properties. They are attracting increased interest for their potential in medical and biological applications [1, 2], the design of metal complexes [3, 4] and other material applications [5]. Based on their versatile applicability a new series of mesogenic unsymmetrical azines, N-[4'-(alkoxy)-2-hydroxybenzylidene]-N-(4-n-alkoxybenzylidene)azines,$ROC_6H_4CH{=}N{-}N{=}CHC_6H_4O_2R$ where $R{=}C_mH_{2m+1}$ and (m = 6, 8, 10, 12 and 14) and their copper (II) complexes have been synthesized. They were characterized by elemental analyses, FT-IR, ^{1}H and ^{13}C NMR spectra, UV-visible and magnetic susceptibility measurements. The copper (II) complexes are square planar. The mesomorphic properties of these compounds were investigated by differential scanning calorimetry and polarizing optical microscopy. The unsymmetrical azines with m = 6, 12 and 14 exhibit monotropic nematic, enantiotropic smectic A and monotropic smectic A phases, respectively, whereas azines with m = 8 display enantiotropic nematic and m=10 exhibits both enantiotropic smectic A and nematic mesophases in heating and cooling cycles. The copper (II) complexes of the azines were non-mesomorphic in nature with high clearing temperatures and displayed polymorphism (crystal–crystal transitions) in both the heating and cooling cycles.

Keywords: Enantiotropic nematic mesophase; enantiotropic smectic A phase; monotropic nematic phase; differential scanning calorimetry; polarizing optical microscopy.

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Studies on Structural and Dielectrical behavior of Calcium doped Bismuth Titanate

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Bismuth Titanates are of great technological interest because of their applications as non-volatile ferroelectric memories (1) and high-temperature piezoelectric materials (2, 3). Bismuth titanate $Bi_4Ti_3O_{12}$ compound has good ferroelectric properties and relatively high Curie temperature, T_c. It shows a relatively high, anisotropic, electrical conductivity, which makes very difficult to polarize the ceramic bodies based on this composition. Calcium bismuth titanate, $CaBi_4Ti_4O_{15}$ is a compound belonging to the bismuth layer family and is a ferroelectric with the Curie point of around 790 ^{0}C which is an excellent candidate material for resonator applications with narrow frequency tolerances and high reliability at high temperatures. In the present work $CaBi_4Ti_4O_{15}$ ceramic sample is prepared through the solid state reaction by conventional mixed oxides by calcination at high temperature. The dielectric properties were measured using a HIOKI 3532 – 50 LCR meter at frequencies ranging from 100Hz to 100 KHz from room temperature to higher temperatures. Dielectric constant (ε_r) and Dielectric Loss (D) as a function of temperature measured are studied from frequencies 100Hz to 100 KHz. The dielectric constant increases gradually with an increase in temperature up to transition temperature (T_c, K) and then decreases. The ac conductivity is determined from the Arrhenius relation. At room temperature the a.c conductivity value for $CaBi_4Ti_4O_{15}$ is found to $5.8X10^{-7}\Omega^{-1}cm^{-1}$ at 100KHz. A.C conduction studies reveals that the conduction mechanism is electronic hoping. The activation energy is estimated from the slope of conductivity versus inverse absolute temperature plot and found to be 1.28eV. The crystallite size and lattice parameters for the sample are determined from X-ray diffraction (XRD) analysis. Bulk densities of the sintered ceramics were measured by the Archimedes method with xylene (density = 0.87 gcm^{-3}) as the liquid media and found to be 97~98% of X-ray density. Microstructural analysis using Scanning Electron Microscope (SEM) supplemented with EDAX were carried out to find the grain size as well as to find the chemical composition of the ceramic material.

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Dielectric relaxation, phase transition and Rietveld studies of perovskite $[Pb_{0.94}Sr_{.06}][(Mn_{1/3}Sb_{2/3})_{0.05}(Zr_{0.52}Ti_{0.48})_{0.95}]O_3$ ceramics

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The frequency-dependent dielectric relaxation of $[Pb_{0.94}Sr_{0.06}][(Mn_{1/3}Sb_{2/3})_{0.05}(Zr_{0.52}Ti0_{0.48})_{0.95}]$ O_3 ceramics, synthesized in pure perovskite phase by a solid-state reaction technique is investigated in the temperature range from 303 to773K by alternating-current impedance spectroscopy. Using Cole-Cole model, an analysis of the imaginary part of the dielectric permittivity with frequency is performed assuming a distribution of relaxation times. The scaling behavior of the imaginary part of the electric modulus (M") suggests that the relaxation describes the same mechanism at various temperatures. The variation of dielectric constant with temperature is explained considering the space-charge polarization. The SEM indicates that the sample has single phase with uniform grains of size ~14.2 µm. The material exhibits tetragonal structure. A detailed temperature dependent dielectric study at various frequencies has also been performed .

Keywords: A. Ceramics; B. Chemical synthesis; C. impedance spectroscopy; Rietveld analysis D. Dielectric properties

Design, Synthesis and Characterization of New Homologous Series of Aroylhydrazone based Mesogenic Ligands and their Nickel (II) Complexes

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Aroylhydrazone (RCONHN=CHR') based liquid crystals and their metal complexes are of special interest because aroylhydrazones may coordinate with divalent metal ion either in enolic or ketonic form (1-3). The chelate formation (enolic or ketonic form) of the aroylhydrazone is strongly dependent upon bonding ability of metal salt used (4). The tendency of ligand to react with divalent metal ion in enolic form becomes greater as conjugating ability of R group in hydrazine residue increases (5). A variety of mesogens and metallomesogens based on aroylhydrazones have been realized with a view to understanding structure-property correlations (6-7). Surprisingly, the effect of R group and anisotropic segments around the core group (hydrazine residue) on mesomorphism has not been reported hitherto, to the best of our knowledge. In order to investigate the effect of these segments on mesomorphism, a new homologous series of mesogenic ligands and their Ni(II) complexes have been synthesized. These compounds were characterized by elemental analyses, FT-IR and NMR (^{1}H & ^{13}C) spectra. The liquid crystalline (mesomorphic) properties of these compounds were studied by thermal polarizing optical microscopy (POM) and differential scanning calorimetry (DSC) techniques. All the members of the series are mesomorphic in nature and differ in alkoxy chain length around the core group. Therefore, it is of considerable interest to evaluate the effect of alkoxy chain length and also R group of hydrazine residue on mesomorphism.

Keywords: Aroylhydrazone derivatives, thermotropic liquid crystals, differential scanning calorimetry, polarizing optical microscopy, mesogenic properties, structure-property relationship.

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Designer Solids through Soft Interactions – A SCXRD Study

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Supramolecular/polymeric structures of coordination complexes formed by the operation of *soft forces* (coordinate bond, hydrogen bond, stacking interactions, atom-π, π-π, M…M (Au⋯Au, Ag⋯Ag, halide⋯halide) interactions and so on) find relevance in the field of material science as micro porous materials, molecular magnets, metallic and superconductors, ion-exchangers, optical materials and so on.[1-5] The interplay of soft forces in directing the structure is crucial in the context of exhibition of material characteristics. Such a knowledge of competing structure directing forces can be obtained by the single crystal xray diffraction technique (SCXRD), which gives the atom locations very precisely. Few Cu(II) supramolecular systems stabilized by soft forces and showing weak magnetic interactions will be presented.

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Structural and Dielectric Study of Some Heavy Rare-earth Zirconate

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The synthesis, characterization and dielectric properties of $R_2Zr_2O_7$, where R =Tb, Ho and Er have been studied. All the rare earth zirconate were prepared by solid state reaction technique and characterized by XRD, differential thermal analysis (DTA), thermogravimetric analysis (TGA) and derivative thermogravimetry (DTG). The XRD characterization shows the formation of single phase orthorhombic structure at room temperature. The dielectric constant (ε'), dielectric loss (ε'') and quality factor (Q) of the compounds have been measured at 1kHz in the temperature range 300 to 1125K. The dielectric constant of $Tb_2Zr_2O_7$, $Ho_2Zr_2O_7$ and $Er_2Zr_2O_7$ show rapid increase above 625K, 670K and 710K respectively. The dielectric loss shows similar behaviour as dielectric constant.

Keywords: Dielectric constant, Dielectric loss, XRD, DTA, TGA, DTG, $Tb_2Zr_2O_7$, $Ho_2Zr_2O_7$, $Er_2Zr_2O_7$

Effect of Calcium doping on Dielectric Properties of Double doped PZT

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Lead zirconium titanate [$Pb(Zr_{1-x}Ti_x)O_3$] system is a typical ferroelectric showing a ‘normal’ PE–FE phase transition and having perovskite type structure (ABO_3). Certain addition of lanthanum in PZT modifies its properties. Despite the fact that PZT is ferroelectric with structures such as tetragonal and/or rhombohedral the high optical transparency of PLZT is due to its paraelectric cubic structure. PLZT ferroelectric materials have many excellent functional properties, such as piezoelectricity, dielectricity and pyroelectricity. Several works have been focused on the effect of various additives on both dielectric and piezoelectric properties of PLZT ceramics. We have studied the effect of calcium doping on the properties of PLZT. Calcium doped PLZT with general formulae $Pb_{0.9}(La_{1-z}Ca_z)_{0.1}(Zr_{0.65}Ti_{0.35})_{0.975}O_3$ where z=0, 0.2, 0.04, 0.06 were synthesized by solid state reaction method. X-ray diffraction analysis indicates the formation of single phase rhombohedral structure. Crystallite size as calculated from Scherrer’s equation was found to be 128 nm. Measurement of dielectric constant as a function of temperature (35 - 450 ^{0}C) and frequency (100Hz-1MHz) indicate that the compound undergo diffuse type of phase transition. Dielectric constant and dielectric loss decreases with increase in frequency. Detailed will be discussed at the time of presentation.

Study of reaction kinetics and phase analysis of kaolinite and alumina in presence of hydroxyl-gel.

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In our study we mainly intend to trace the reaction kinetics and phase analysis of kaolinite and alumina in presence of hydroxy-gel and to detect the conversion of kaolinite (Al_2O_3, $2SiO_2$, $2H_2O$) to Mullite ($3Al_2O_3$, $2SiO_2$).Characterization of Rajmahal (white clay)was done by DTA, XRD and XRF analysis. The batches were prepared with varied proportions of Rajmahal (white) clay and alumina, further in some batches alumina was partly or wholly replaced by hydroxy gel. Aluminum nitrate was used in such cases the formation of reactive alumina phase which is incorporated in alumina–kaolinite mixture in the gel-like form by flash polycondensation method. Firing was done at different temperatures viz . 1200,1300,1400,1500° Celsius. Then nature of variation of percentage weight loss, percentage shrinkage and bulk density with varying composition was investigated.XRD pattern showed major phase was kaolinite and minor phases were muscovite and quartz and from DTA curve endothermic peak at 580°C and exothermic peak at 995°C were obtained. The endothermic peak at 580^0C corresponds to the dehydroxylation of the kaolinite mineral and the exothermic peak at 995^0C is an indicative of the crystallization of γ-alumina from the metakaolin. Moreover investigation reveals that different samples at varying temperatures follow similar nature of reaction kinetics, mainly first order kinetics. Further study reveals that with the increase of percentage of hydroxy- gel in the composition, shrinkage increases while bulk density decreases. This occurs due to the formation of open structure at high temperature which results in increase of porosity and water absorption.SEM and microstructure analysis of the samples reveal phase transformation to Mullite,

Keywords: Rajmahal (white) clay, Mullite, Flash Polycondensation.

Design of Gum Acacia Inspired-Silica Hybrid Xerogels for Enzyme Immobilization

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Dehydroxypolymerization of silica precursors tetraethylorthrosilicate (TEOS) and tetramethoxyorthosilicate (TMOS) in presence of gum acacia as mesoscopic porogen resulted into novel nanocomposites suitable for enzyme immobilization. The optimization of enzyme immobilization has been done on the basis of the ratios of the gum, silica precursors, solvent/co-solvent used. Enzyme impregnation was significantly enhanced on calcination of the composites. The immobilized enzyme reveals better stability and activity in a broad range of temperature and pH as compared to free enzyme. The activity of impregnated enzyme as a function of synthesis conditions as well as calcination temperature of the hybrid samples has been studied. The hybrids were structurally characterized using Infra red spectroscopy (FTIR), X-ray diffraction (XRD), SEM (Scanning Electron Microscope), Thermogravimetric analysis (TGA/DTA), Photoluminescence (PL) and BET analyses. Amylase has been used as representative enzyme for immobilization which has been monitored spectrophotometrically at 540 nm wavelength.

Keywords: Nano-composite, Sol-gel, Gum acacia, Silica, Enzyme immobilization.

Quasicrystalline phase in $Al_{70-x}Ga_xPd_{17}Mn_{13}$ alloy

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Quasicrystalline $Al_{65}Ga_5Pd_{17}Mn_{13}$ icosahedral phases have been synthesized by us [1]. It has been shown that the formation of pure icosahedral phase is possible up to 5 at % of Ga substitution in $Al_{70-x}Ga_xPd_{17}Mn_{13}$ alloy composition. In the present investigation, the effect of Ga substitution on the formation and stabilization of icosahedral phase in $Al_{70-x}Ga_xPd_{17}Mn_{13}$ and $Al_{70-x}Ga_xPd_{20}Mn_{10}$ alloys have been investigated by employing X-ray diffraction, transmission electron microscopy and differential thermal analysis. The as-cast and rapidly quenched alloys with x = 0, 2.5, 5, 7.5, 10 and 15 have been investigated. In both the cases, the alloys up to 5 at % Ga exhibit the formation of icosahedral phases and with higher concentration of Ga i-phase along with B2 type and ξ' crystalline (orthorhombic structure with unit cell a = 23.5Å, b= 16.6Å and c = 12.4 Å) and Al_3Pd_2 type hexagonal phase. The Energy dispersive X-ray analysis investigations suggest the presence of some quantities elemental Ga on the quasicrystalline surface of $Al_{55}Ga_{15}Pd_{17}Mn_{13}$ alloy. The quasicrystalline Al-Ga-Pd–Mn material provides a new opportunity to achieve quasicrystalline phases with low surface energy. The micromechanisms for the formation of layer like microstructural feature in the quasicrystalline alloy will be outlined.

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Observation of Multiferroic Behaviour of Quasi One Dimensional Oxide,Ca_3CoMnO_6 at room temperature

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Polycrystalline specimen of Ca_3CoMnO_6 was prepared by a conventional solid state reaction method. Proper proportions of high purity (99%) $CaCo_3$, Co_3O_4 and MnO_2 were thoroughly mixed in agate mortar and calcined in air at 1273 K for 24 h. Sample was characterized by X-ray diffraction (Cu K_α) and found to form single phase. Magnetic moment was measured by the VSM (vibrating sample magnetometer) at room temperature. Saturation magnetization was found ~ 0.010 emu/g at the field 10 kOe. Dielectric properties were measured by LCR-meter. Dielectric constant (ε) and dielectric loss (tan δ) was found constant with increase in frequency which may be due to inability of the electric dipoles to be in pace with frequency of applied electric field at high frequency. Variation of dielectric constant and dielectric loss both increase with increase in temperature. Ferroelectric behaviour was studied from polarization-electric field (P-E) plot. The saturated polarization (P_s), and remnant polarization (P_r) and coercive field (E_c) are $4.062\mu C/cm^2$, $1.235\ \mu C/cm^2$ and 0.569 kV/cm respectively. Grain size measured by scanning electron microscopy (SEM) was 695 nm. Chemical composition was verified by Energy Dispersive X-ray spectrometer (EDS). Magnetoelectric effect (ME) is an important property induced by coupling between electrical and magnetic dipole. We observed the variation of magnetocapacitance with magnetic field at room temperature. Magnetocapacitance was found to increase with increase in magnetic field. Therefore, our results show the multiferroic nature of quasi-one-dimensional oxide, Ca_3CoMnO_6 at room temperature.

Synthesis and Characterization of $BiFeO_3$-PZT Composite

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Lead zirconium titanate (PZT) has a high piezoelectric coefficient, a high dielectric constant and low tangent loss, and a high transition temperature. $BiFeO_3$ is a multiferroic compound (magnetoelectric coupling between ferroelectric and magnetic order) that have their magnetic transition and ferroelectric transition above room temperature so a good compound for memory devices, sensors etc. So it may be considered most suitable multiferroic material for making solid solutions with PZT. Therefore we have synthesized the composition of $xBiFeO_3$-$(1-x)Pb(Zr_{0.52}Ti_{0.48})O_3$ in different volume fraction, and studied their structural and electrical properties. The polycrystalline $xBiFeO_3$-$(1-x)Pb(Zr_{0.52}Ti_{0.48})O_3$ where x=0,0.02,0.04,0.06 ceramics were prepared by solid state reaction method. X-ray diffraction study indicated that the fully sintered materials were phase pure and close to the morphotropic phase boundary (MBP) between rhombohedrally distorted and tetragonally distorted perovskite type ABO_3 structure. Crystallite size was found to be ~ 20 nm, calculated by using the Scherrer’s equation. The transition from ferroelectric to paraelectric phase shifts towards lower temperature with increasing value of x i.e. x=0, 0.02, 0.04, 0.06. The dielectric constant and loss tangent measurement was done as a function of temperature (35^0C-500^0C) and frequency (100Hz-1MHz). The dielectric constant and loss tangent was found to decrease with increasing frequency by virtue of failure of the electric dipole to be in pace with frequency of applied electric field at high frequency. The maximum dielectric constant was found to be 7250 at frequency 1 kHz for 4% $BiFeO_3$ concentration.

Multiferroic Properties of 0.8BiFeO$_3$-0.2BaTiO$_3$ Ceramic

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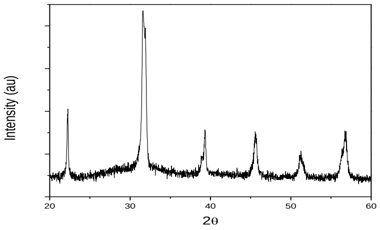
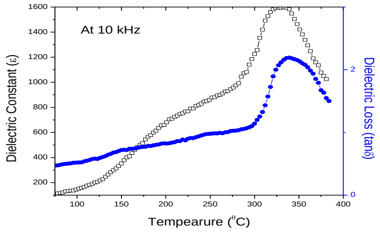
Multiferroics are the class of materials which exhibit co-existence of ferroelectric/antiferroelectric and ferromagnetic/antiferromagnetic orders.These materials have potential applications in devices. BiFeO$_3$ is one such material having antiferromagnetic Néel temperature (T_N) of 370^{0}C and ferroelectric transition temperature (T_C) of 810^{0}C[1-6]. Since cationic substitutions have led to enhanced magnetization in BiFeO$_3$, we have studied the multiferroic properties of 0.8BiFeO$_3$-0.2BaTiO$_3$ ceramics prepared by conventional solid state reaction method. The dielectric constant has been studied over a temperature regime of 75^{0}C to 400^{0}C for frequencies 10kHz so as to study the phase transitions in the sample. An anomaly in the dielectric constant (ε) in the vicinity of the antiferromagnetic Néel temperature (T_N) was observed. The variation of ε vs. frequency showed a relaxed behaviour. The high values of dielectric constant at low frequencies and low values at higher frequencies indicate large dispersion due to Maxwell – Wagner type interfacial polarization in agreement with Koops phenomenological theory. We have studied magnetization versus magnetic field (*M-H*) hysteresis curve at room temperature using VSM. The room temperature magnetic hysteresis loops was not saturated. Ferroelectric hysteresis loops were observed with maximum remnant polarization ($2P_r$) = 13.02 μC/cm^2. Ferroelectric and magnetic hysteresis loops measured at room temperature indicated the coexistence of ferroelectricity and magnetism





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Preparation, characterization and measurement of dielectric properties of ceramic samples of $AgNbO_3$

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Processing and sintering procedures have a marked effect on the characteristics of ceramics with and without additives. Ceramic pellets of silver niobate, $AgNbO_3$ system have been prepared by solid-state reaction and sintering method in two different sintering conditions. The prepared samples have been characterized by XRD and SEM technique. All samples prepared by both methods show orthorhombic structure at room temperature. Comparisons of lattice parameters, crystallite size and grain size of $AgNbO_3$ prepared by both methods have been reported. Frequency variations of dielectric constant, loss tangent and electrical conductivity have been investigated, at room temperature, in the frequency range 1 Hz – 10 MHz.

Preparation and characterization of ceramic samples of $Ag_{1-x}Li_xNbO_3$ mixed system

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Ceramic pellets of ceramic, $Ag_{1-x}Li_xNbO_3$ (x = 0, 0.3, 0.5 and 0.7), have been prepared by solid-state reaction method and sintering process. The prepared samples were characterized by XRD and SEM technique. Grain size has been calculated by SEM photographs and lattice parameters have been calculated by X-ray diffraction data for mixed $Ag_{1-x}Li_xNbO_3$ system, where x is varied from 0 to 70%. The variations of grain size & lattice parameters with composition at room temperature have been reported. All prepared samples show orthorhombic structure at room temperature.

Investigation of Testing Parameter Effects on Dry Sliding Wear Behaviour of Aluminium - Alumina Metal Matrix Composites Using Statistical Analysis

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The dry sliding wear behaviour of a cast aluminium alloy (Al-Si10Mg) and Al-Si10Mg - 5wt.% Al_2O_3 particle composite was studied at different loads and different sliding speeds. The dry sliding wear behaviour was predicted through statistical analysis of the measured wear rate at different operating conditions. The wear rate (*Y*) is expressed in terms of the coded values of the applied load (*A*), sliding speed (B) and interaction of applied load and sliding speed (C) by the following linear regression equation:

$$Y_{alloy} = 2.59 + 1.23\ A - 0.631\ B - 0.254\ C \qquad (1)$$

$$Y_{composite} = 2.30 + 1.15\ A - 0.549\ B - 0.203\ C \qquad (2)$$

where the multiplication factor is 10^{-3} mm^3/m. Equations 1 and 2 above suggests the following : the effect of applied load on the wear rate of both the alloy and composite is increases as compared to that of sliding speed. The effect of sliding speed on the wear rate of both the alloy and composite is decreases compared to that of applied load. The effect of load and sliding speed on the wear rate is relatively less in case of composite material than that of the alloy. The combinations of load and sliding speed, the wear rate of composite may be lower as compared to that of alloy. The above factors were explained on the basis of operating wear mechanisms.

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Structural and Electrical Properties of Double Doped PZT Ceramics

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$Pb(Zr_{1-x}Ti_x)O_3$ (PZT) is a perovskite type ABO_3 structured material with high piezoelectric, pyroelectric and dielectric characteristics. La modified PZT (referred as PLZT) solid solution emerged as a highly promising system due to its high optical transparency and relatively large electro-optic effect, relaxor-type ferro-paraelectric phase transition etc. In order to enhance ferroelectric and pyroelectric properties of PLZT, several researchers have studied double doped PZT. In this paper we have reported the systematic work on Nd doped PLZT. Double doped lead zirconium titanate (PZT) with general formula $Pb_{1-3x/2}La_x(Zr_{0.54}Ti_{0.46})_{1-5x/4}Nd_xO_3$; where x=0.00, 0.02, 0.04, 0.06 were synthesised by solid state reaction method. X-ray diffraction analysis indicated the formation of single phase orthorhombic structure. Crystallite size was calculated by Scherrer’s equation. The crystallite size was found to be ~ 50 nm. Dielectric constant measurement as a function of temperature (35 ^{0}C-400 ^{0}C) and frequency (100Hz-1MHz) indicated that the compound undergo diffuse type of phase transition. Maximum dielectric constant was found to be strongly dependent on doping and measuring frequencies having value 4000 for 2% Nd concentration at 10 kHz frequency. Well saturated ferroelectric hysteresis loops with better value of remnant polarisation (P_r) and coercive fields (E_c) were recorded on the samples. We have got the maximum value of remnant polarisation about 9.6 μc/cm^2 for 2% Nd concentration. Results will be discussed in details at the time of presentation.

Molecularly imprinted polymer-carbon composite fiber: A new format containing multiple recognition sites for ascorbic acid and dopamine

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Artificial molecular recognition elements prepared by imprinting techniques attract increasing attention due to their potential as selective sorbents in analytical sample pretreatment, chemical sensing, drug delivery, catalysis, dedicated separations, and finally screening elements in drug discovery. In most of the accounts of molecular imprinting, a single template molecule is used to create the specific binding site of the molecularly imprinted polymer. It may be possible to impart multiple recognition sites in MIPs, which could be used as elements capable of binding more than one component. Such systems could advantageously be used in the design of sensors having the ability to sense more than one compound at a time and could also be used as stationary phases in chromatography with broad separation potential as well as sorbents in micro-extractions. This paper discusses, for the first time, such a possibility by developing an molecularly imprinted polymer-carbon composite fiber for two model compounds, namely, ascorbic acid and dopamine in a single molecularly imprinted polymer format. Molecularly imprinted polymer-carbon composite fiber were obtained by a ‘reversible addition-fragmentation chain transfer polymerization’ technique involving a trifunctional monomer, 2,4,6-trisacrylamido-1,3,5-triazine and subsequent cross-linkage with ethylene glycol dimethacrylate, in the presence of carbon powder and template (ascorbic acid and dopamine) in a glass capillary. The binding characteristics of ascorbic acid and dopamine were evaluated with the help of spectral and surface characterizations.

Three Body Abrasive Wear Behavior Of Glass Fiber Reinforced Epoxy Composites With Alumina-Graphite Filler

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In this study, effect of alumina-graphite filler blending on glass fiber reinforced epoxy composites is evaluated.

Glass fiber epoxy composites without filler and with 2%, 4% and 6% filler additions are fabricated by 'Hand Lay Up' method. Each composite with filler additions has equal percentage of alumina and graphite by weight. Specimens from the fabricated plates are cut and Three Body Abrasive wear are conducted in accordance with ASTM G65. Tests were conducted for abrading distances of 150 m, 300 m, 450 m and 600 m. Specific wear rate of different composites is compared for different abrading distances.

Three body abrasive wear tests were conducted and results show increase in specific wear rate with increase in filler content for different abrading distances. A comparison between specific wear rates of different filler content is graphically represented.

Also surface morphology is done to study the nature of damage at the surface of the composites.

Key Words: Alumina, Graphite, Epoxy, Three Body Abrasive Wear, Surface Morphology.

Effect Of Alumina-Graphite Filler Blending On Tensile Behavior Of Glass Fiber Reinforced Epoxy Composites

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In this study, the effect of addition of alumina-graphite fillers on Tensile properties of glass fabric reinforced epoxy resin composites has been evaluated experimentally.

Glass Fiber/Epoxy composites without filler and with 2%, 4% and 6% filler content are fabricated using "Hand Lay Up" method. Each of the fabricated composite panel has equal percentage of alumina and graphite fillers by weight. Specimens from the fabricated plates are cut and testing is carried out in accordance with ASTM D-638. The properties like tensile strength, tensile modulus, elongation at break and deflection are studied. Modes of fracture and fiber-matrix adhesion are also studied.

Results revealed that composites with increase in filler content show a decrease in tensile strength, whereas lower elongation, and decrease in tensile modulus compared to composites without filler. Effect of incorporation of alumina-graphite fillers, does not show much improvement in the fiber-matrix interface in the composite. Elongation properties decreased with the presence of filler that indicates interference by the filler in the mobility or deformability of the matrix. This interference was created through the physical interaction and immobilization of the polymer matrix due to the filler particles imposing mechanical constraints. The tests showed brittle fracture of the tested samples.

Key Words: Alumina, Graphite, Epoxy, Tensile Properties, “Hand Lay Up” method.

Scanning electron microscope (SEM): An effective tool for microstructural analysis of composites

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The secondary electron imaging (SEI) and backscattered electron (BSE) modes in SEM were used to elucidate the different microstructural features present in ceramic reinforced ceramic and polymer reinforced ceramic composite material systems. The porosity present in the material systems was identified using SEI whereas phase identification was performed using BSE in conjunction with energy dispersive spectroscopy (EDS). Image analysis routines were employed to the SEM images for statistical quantification of the microstructural features. The challenges faced during metallographic sample preparation, image acquisition and analysis, and structural-property correlations would be outlined.

Accurate quantification of γ' precipitate statistics in nickel-based superalloys

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Nickel-based superalloys are widely used for manufacturing critical components that are exposed to high temperatures (0.5 - 0.7T_M) in land-based power generation and aircraft engines. They retain their strength at these temperatures primarily due to the presence of the γ' precipitate phase. Particularly the size, volume fraction, distribution and inter-particle spacing of the γ' phase influences the high temperature mechanical properties of superalloys. Quantitative analysis of γ' phase statistics (namely the size, the volume fraction, the distribution and the inter-particle spacing) is greatly affected by metallographic preparation, image acquisition and subsequent image analysis routines. This work highlights the importance of sample preparation to obtain high quality scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM) images that unambiguously reveal γ' morphology across different superalloys irrespective of initial processing conditions. These images obtained using SEM/TEM/AFM are subsequently post processed using image analysis routines to provide accurately the γ' phase statistics. The efficacy of the sample preparation and microscopic procedures has been illustrated through examples of coarsening and rafting studies.

Ultrasonic and Microstructural features of SiC_p/Al_2O_3 ceramic matrix composites prepared by directed metal oxidation of Aluminum alloy

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A composite of aluminum oxide with 35 to 43 vol.% of silicon carbide as reinforcement is fabricated by the directed oxidation of an aluminum alloy melt in oxygen atmosphere*. The process leaves a small amount of an interconnected aluminum alloy network which provides a certain amount of toughness and electrical conductivity to the composite. The resulting composite was subjected to various characterization techniques. These include preliminary phase analysis by X-ray powder diffraction and optical microscopy to reveal microstructural details like reinforcement particle size, its volume fraction, distribution and homogeneity. Particle-matrix interface was characterized with the help of electron probe micro analyzer coupled with wavelength dispersive analysis of X-rays. Bulk density and porosity of the composite were measured by Archimedes' liquid displacement method. The composites' Young's Modulus, Shear Modulus and Bulk Modulus are evaluated under sound wave velocity using ultrasonic pulse-echo technique.

The SiC_p/Al_2O_3 ceramic matrix composites with SiC volume fractions from 0.35 to 0.43 were found to possess average Young's Modulus was found to be 262 GPa, Shear Modulus of 89 GPa and Bulk Modulus of 190 GPa. Further the composites were found to possess lower levels of porosity, among those prepared by DIMOX process.

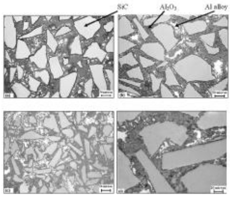

Figure 1: Microstructures of SiC_p/Al_2O_3 matrix composites (a) Al_2O_3 – 0.35SiC, (b) Al_2O_3 – 0.40SiC, (c) Al_2O_3 – 0.43SiC (d) metal content.

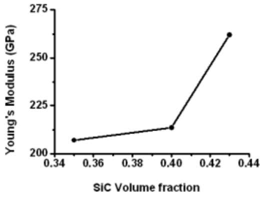

Figure 2: Variation of the elastic modulus of SiC_p/Al_2O_3 CMCs

Response of E-Glass/Epoxy Composite to Up and Down-Thermal shock after Hygrothermal Treatment for varying Time Periods

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Glass fiber/epoxy composite may use in the environment where these materials may susceptible to heat and moisture when operating in changing environment. The hygrothermally treated (2, 4, 6 and 8 days) eighteen layered glass fiber/epoxy laminates were exposed to up and down thermal shock under varying time periods. The inter laminar shear strength (ILSS) of shocked sample was measured for each sample and interpreted. The ILSS showed an increasing trend by exposing 2, 4 and 8 days hygrothermally treated sample to up-thermal shock for shorter duration, whereas it is decreasing for longer duration of shock. The ILSS increased for 6 days hygrothermally treated sample slowly up to very small extent from shorter to longer exposing time of up-thermal shock. The 2, 6 and 8 days hygrothermally treated sample showed the response towards down-thermal shock in a similar manner. The ILSS for 4 days hygrothermally treated sample decreased for shorter duration of down-thermal shock and then further increase is observed for longer duration. The glass transition temperature was measured for 8 days hygrothermally treated sample after up and down-thermal shock including no shock condition. The 8 days hygrothermally treated sample showed the enormous depression of T_g from no shock to up–thermal shock treatment. But the depression of T_g from no shock to down – thermal shock is negligible compared to that of up – thermal shock. The SEM micrographs give clear cut concepts of failure like delamination, debonding and fiber breakage after up and down-thermal shock treatment.

Key Words: Glass fiber/epoxy laminates, Thermal Shock, ILSS and Glass Transition Temperature.

Properties of SiC_p/Al_2O_3 ceramic matrix composites as a function of reinforcement content

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Silicon carbide particulate reinforced alumina matrix composites were fabricated using DIrected Metal OXidation (DIMOX) process. Continuous oxidation of an Al-Si-Mg-Zn alloy with suitable dopants along with a preform of silicon carbide has led to the formation of alumina matrix of surrounding silicon carbide particulates. SiC_p/Al_2O_3 ceramic matrix composites fabricated by the DIMOX process, possess enhanced properties such as flexural strength, fracture toughness and wear resistance, all at an affordable cost of fabrication. SiC_p/Al_2O_3 matrix composites were investigated for measurements of Density, Coefficient of Thermal Expansion, Thermal Conductivity, Flexural Strength, Fracture Toughness, Compressive Strength, Elastic Modulus and Hardness; the composite specimens were evaluated using standard procedures recommended by the ASTM[1]. The SiC_p/Al_2O_3 ceramic matrix composites with SiC volume fractions from 0.35 to 0.43 were used. The variations in the properties are compared further compared with experimental results available in the literature. The surface of a specimen fractured under a three-point loading was observed under scanning electron microscope and it was found that the nature of fracture is itself a composite of brittle and ductile modes. Further the composites were found to possess lower levels of porosity, among those prepared by DIMOX process. Attempts are made to relate their differences in properties to reinforcement content.

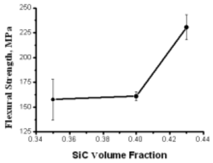

Fig. 1 A plot showing variation in Flexural strength of SiC_p/Al_2O_3 SiC_p/Al_2O_3 CMCs

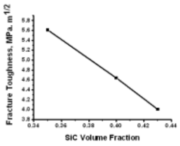

Fig. 2 A plot showing variation in fracture toughness of SiC_p/Al_2O_3 CMCs

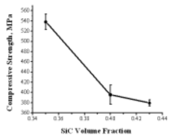

Fig. 3 A plot showing variation in Composites of SiC_p/Al_2O_3 CMCs

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Synthesis and Spectral Characterization of 4-alkyl-2H-1-benzopyran-2-ones

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Coumarins (2H-1-benzopyran-2-ones) are associated with enormous pharmacological, biochemical and therapeutic potentials and the substitutions in benzene and α-pyrone rings play major part in eliciting biological responses. Lots of coumarin derivatives have been synthesized and reported for their significant antihelminthic, antimicrobial, anticancer, anti-inflammatory, anticoagulant and other miscellaneous properties. Recently, several coumarin derivatives have been identified as inhibitors of glutathione metabolizing enzymes and DNA-topo II enzymes of the filarial parasite and reported as potent antifilarials. These observations prompted us to synthesize some simple coumarins and assess their effect on filarial parasites. The structures of synthesized compounds have been elucidated through elemental analysis, IR, ^{1}H and ^{13}C NMR spectra. The synthesis, characterization and activity data of these compounds will be highlighted in the poster.

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Phyto-technologies for Heavy metals removal

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Pollution of the biosphere with toxic metals has accelerated dramatically since the beginning of the Industrial Revolution. Further, due to discovery of mining and metal working techniques in ancient times, the close link between metals, metal pollution and human history was formed. Toxic metal contamination of aqueous water streams and ground water poses a major environmental and health problem which is still in need of an effective and affordable technological solution. The removal of heavy metals using living organisms attracted a lot of public attention and R&D spending. Present paper describes my work on phytoremediation in last six years and hand in hand addresses the various ecological issues, benefits and constraints pertaining to heavy metal pollution of aquatic ecosystems and its phytoremediation. I found wetland plants/macrophytes as ideal bio-system for heavy metals removal in terms of both ecology and economy, when compared with chemical treatments. However, there are several constraints or limitations in the use of aquatic plants for phytoremediation in microcosm as well as mesocosm conditions. On the basis of my past researches an eco-sustainable model has been proposed in order to resolve the certain constraints imposed. In relation to future prospect genetic engineering in macrophytes for enhanced heavy metal accumulation is still in embryonic stage and needs more attention in this area. Moreover, harvesting and recycling tools needs more extensive research. A multidisciplinary research effort that integrates the work of biotechnologists, plant biologists, soil chemists, microbiologists, and environmental engineers is essential for greater success of phytoremediation as a viable water cleanup technique.

Keywords: *phytoremediation; heavy metals; wetland plants; eco-sustainable technology*

Effect of photoconductive and dielectric constant of the photorefractive material on the oscillation behaviors of the semilinear photorefractive optical resonator with reflection gratings

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Photoconductive and dielectric properties dependence of four-beam coupling in a photorefractive crystal pumped with two counter-propagating waves for a semilinear coherent optical resonator on the oscillation conditions has been analyzed in the case of non-degenerate-wave mixing under the slowly varying amplitude approximation method. Self oscillation can be achieved when the gain arising from the four- beam coupling is large enough to overcome the cavity loss. The effects of frequency detuning (i.e., non-degeneracy), dielectric constant and photoconductivity of the photorefractive materials on the performance of the semilinear photorefractive coherent resonator with the reflection grating configuration have also been studied in detail. The phase-conjugate reflectivity of the pumped crystal and oscillation intensity are calculated numerically for different input pump beam intensity ratio, intensity reflectivity of the conventional mirrors, degenerate energy coupling strength of the interacting beams. It has been found that for the higher value of the photoconductivity $\sigma_p(> 2.0\ S/cm)$ of photorefractive crystal, the semilinear resonator can oscillate at almost any frequency detuning (Ω) of the oscillation beam with respect to the fixed frequency of the pump waves whereas for the lower value of photoconductivity $\sigma_p(< 0.1\ S/cm)$ oscillation occurs only when the frequency detuning is limited to small region around $\Omega = 0$. But reverse of the case is found for dielectric constant (ε), pump intensity ratio (p) and conventional mirror reflectivity (R).

Van der Waals Three Body Shell Model to Study Dynamical Behavior of Potassium Chloride

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A unified description of a series of phonon properties of Potassium Chloride by means of van der Waals three-body force shell model [VTBFSM]. This model includes van der Waals interactions (VWI) and three-body interactions (TBI) in the framework of both ion polarizable rigid shell model (RSM). In fact the present model [VTBFSM] has revealed much better descriptions of IR/Raman spectra and anhormonic properties and other dynamical properties of KCl. Excellent agreement is found between calculated values and measured data for phonon dispersion curve.

Substrate temperature influenced photoluminescence and optical properties of $Zn_{0.9}Mn_{0.1}Se$ films

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In this investigation thin films of $Zn_{0.9}Mn_{0.1}Se$ were deposited on glass substrates held at various temperatures in the range 303 – 523 K by employing vacuum evaporation method. The energy dispersive X-ray analysis revealed that the content of zinc and manganese increased while selenium decreased with the increase of substrate temperature due to the difference in the vapour pressures of the constituent species. The X-ray diffraction studies revealed that the films formed were polycrystalline in nature with zincblende structure with presence of (111) preferred orientation. The lattice parameter of the films increased from 5.681 to 5.695 nm with increasing substrate temperature from 303 to 523 K. Atomic force micrographs of the films formed at 303 K showed the pyramidal shape of grains with grain size of 70 nm. Further, the substrate temperature increased to 523 K the size of the grains increased to 180 nm with elongated pyramidal shape due to improvement in the crystallinity of the films. The photoluminescence emission spectrum shows two peaks at wavelengths of 440 and 445 nm. The peak intensities are increased with increase of substrate temperature. The emissions at 440 and 445 nm are assigned to donor-bound excitons and sub-band gap luminescence of ZnSe host lattice respectively. The optical band gap of the films increased from 2.60 to 2.67 eV with the increase of substrate temperature from 303 to 573 K. The refractive index of the films increased from 2.37 to 2.42 with the increase of substrate temperature from 303 to 523 K due to improvement in the cystallinity and packing density of the films.

Structural, electrical and optical properties of RF reactive magnetron sputtered Ag-Cu-O films: Effect of substrate temperature

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Thin films of Ag-Cu-O films were formed on glass substrates by reactive RF magnetron sputtering of $Ag_{80}Cu_{20}$ target at different oxygen partial pressures in the range $5x10^{-3}$ – $8x10^{-2}$ Pa and substrate temperatures in the range 303 - 523 K. The influence of oxygen partial pressure and substrate temperature on the crystallographic structure and surface morphology, chemical binding configuration, electrical and optical properties of the films was studied. The content of oxygen in the films was correlated with the oxygen partial pressure maintained in the sputter chamber during the growth of the films. X-ray diffraction studies on the films deposited at room temperature (303 K) and at low oxygen partial pressure of $5x10^{-3}$ Pa was mixed phase of $Ag_2Cu_2O_3$ and Ag. The films grown at oxygen partial pressure of $2x10^{-2}$ Pa showed the combination of $Ag_2Cu_2O_3$ and $Ag_2Cu_2O_4$ phases. The crystallinity of the films formed at a constant oxygen partial pressure of $2x10^{-2}$ Pa increased with the increase of substrate temperature from 303 to 473 K. The films formed at higher substrate temperature of 573 K were decomposed into Ag_2O and Ag. The grain size of the films increased from 85 to 345 nm with the increase of substrate temperature from 303 to 523 K. The electrical resistivity of the Ag-Cu-O films formed at oxygen partial pressure of $2x10^{-2}$ Pa decreased from 2.3 to 0.8 Ωcm with increase of substrate temperature from 303 to 473 K respectively due to improvement in the crystallinity of the films. The low electrical resistivity of $3.6x10^{-3}$ Ωcm was observed in the films formed at high substrate temperature of 523 K due to presence of Ag_2O and Ag which was mainly controlled by the metallic silver grains. The optical band gap of the Ag-Cu-O films increased from 1.47 to 1.83 eV with the increase of substrate temperature from 303 to 473 K. The films formed at higher substrate temperature of 523 K exhibited the band gap value of 2.20 eV related to Ag_2O phase.

Oxygen partial pressure influenced structure, dielectric and optical properties of DC reactive magnetron sputtered TiO_2 films

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Titanium dioxide (TiO_2) films find potential applications in multilayer optical coatings, dye-sensitised solar cells, microelectronic devices and gas sensors. In this investigation titanium dioxide thin films were deposited by DC magnetron sputtering technique and characterized the deposited films for structural and optical properties. Thin films of TiO_2 were deposited on (100) p- silicon and Corning glass substrates held at temperature of 673 K by sputtering of metallic titanium target under different oxygen partial pressures in the range $1x10^{-2}$ – $9x10^{-2}$ Pa. The films formed at an oxygen partial pressure of $4x10^{-2}$ Pa were single phase titanium dioxide as indicated the core level binding energies of Ti 2p and O 1s determined from the X-ray photoelectron spectroscopy. The X-ray diffraction profiles of the films were of amorphous with a weak (110) reflection of titanium dioxide in anatase phase embedded in amorphous matrix. This was also confirmed by Raman spectroscopy by the presence of an absorption band at 146 cm^{-1} related to the stretching vibration mode of Ti-O-Ti confirmed the growth of antase phase. The dielectric properties of TiO_2 films were studied on the MOS structure of $Al/TiO_2/Si$. The dielectric constant of the films formed at an oxygen partial pressure of $1x10^{-2}$ Pa was a high value of 6, while those formed at higher oxygen partial pressure of $9x10^{-2}$ Pa exhibited a low value of 3. The films were transparent in the visible region. Sharp absorption edge was observed below 400 nm and the absorption edge shifted towards lower wavelength side with the increase of oxygen partial pressure. The optical band gap of the films increased from 3.50 to 3.70 eV and the refractive index increased from 2.4 to 2.8 with the increase of oxygen partial pressure from $1x10^{-2}$ – $9x10^{-2}$ Pa respectively.

Molecular Structure, Vibrational Spectral Studies of 2-chloro-4-fluorobenzonitrile by FT-IR and FT-Raman Spectroscopy: Verification by Quantum Chemical Methods

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Computational chemistry is one of a useful way to investigate about the materials that are too difficult to find or too expensive to purchase and also helps us to make predictions before running the actual experiments. The Schrödinger's equation is the basis for most of the computational chemistry scientist's use. This is because the **Schrödinger's equation models the atoms and molecules with mathematics**. By means of solving Schrödinger's equation we can do electronic structure determinations ,geometry optimizations ,frequency calculations ,transition structures, electron and charge distributions, potential energy surfaces (PES) ,thermodynamic calculations,ete., .Computational chemistry is simply the application of chemical, mathematical and computing skills to the solution of interesting chemical problems such as solving Schrödinger's equation,ete.,. It uses computers to generate information such as properties of molecules or simulated experimental results. One of the most important computer software used by computational chemistry is **Gaussian 03 w**. By means of **Gaussian 03 w,** we carried out the ab initio Hartree-Fock (HF) method and Density Functional (DFT) Method (B3LYP), which is a hybrid method to solve Schrödinger's equation. **Since DFT methods considers electron correlation** it can capable of giving better result than ab initio HF methods. Since many derivatives of benzonitrile are widely used in industry and medicinal fields. We have choosen **2-chloro-4-fluorobenzonitrile (2Cl4FBN**) for the present investigation and carried out the Quantum mechanical calculations of energies, geometries and vibrational wavenumbers by using ab initio HF and Density functional theory (B3LYP) by using eh basis set 6-311++G(d,p) by means of Gaussian 03 view program package. It is observed that **The optimized geometrical parameters obtained by B3LYP method shows good agreement with available experimental X-ray data.** The difference between the observed and scaled wavenumber values of most of the fundamentals is very small. Also a **detailed interpretation of the infrared spectra of 2Cl4FBN was also done. The HOMO and LUMO energies are also calculated in order to show that the charge transfer occur in the molecule**. The **entropy of 2Cl4FBN** was also performed at HF/B3LYP/6-311++G(d,p) level of theory. The theoretical spectrogram for FTIR and FT-Raman spectra of **2Cl4FBN** molecule have also been constructed

Structural and optical characterization of MoO_3 thin films prepared by thermal oxidation

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Thin films of molybdenum oxide (MoO_3) find applications in electrochromic and gas sensors. By virtue of layered structure and electrochemical activity it is used as a cathode material in the development of high energy density solid state microbatteries. In this investigation, thin films of MoO_3 were grown on glass substrates by thermal oxidation of Mo films deposited by DC magnetron sputtering. The phase purity of MoO_3 films was confirmed by the X-ray photoelectron spectroscopy, chemical composition analyzed by the energy dispersive X-ray analysis and crystal structure with X-ray diffraction. The EDAX analysis of the films annealed in air at 673 K indicates the growth of nearly stoichiometric MoO_3. The XPS studies on the films annealed at 573 K showed the core level binding energy peaks related to the Mo^{6+} and Mo^{5+} oxidation states indicated the growth of mixed phase of α- and β-MoO_3. The films annealed at higher temperature of 673 K showed only the Mo^{6+} oxidation state revealed the growth of α-MoO_3. X-ray diffraction profiles of the films annealed at 573 K were polycrystalline with the presence of mixed phase of α- and β-MoO_3, while those annealed at 673 K were of single phase α-MoO_3. The Fourier transform infrared spectrum of the films annealed at 673 K showed the characteristic vibration of Mo - O of MoO_3. The optical band gap of the mixed phase MoO_3 films achieved at annealing temperature of 573 K was 3.15 eV. α- phase MoO_3 films showed the optical band gap of 3.31 eV.

Spectroscopic and electrical studies of some substituted thiourea ligands and their 3d-metal complexes

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Spectroscopic techniques such as ^{1}H and ^{13}C NMR, IR, UV-Vis are excellent experimental tools for structural assignment of a compound. We have synthesized two substituted thiourea ligands and their Cu(II) and Cu(I), Ni(II) and Co(II) complexes. These compounds have been characterized by the special techniques mentioned above. The bonding and stereochemistry of the complexes are discussed. The conducting and redox behavior of the complex are also discussed.

Theoretical study of diffraction efficiency of hologram recorded with weak external electric field in photorefractive media

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To record efficient holograms in the photorefractive media some innovative geometry have been proposed by various group of workers with and without externally applied electric field across the crystal in both the two and four-wave mixing geometries. We have also proposed a new geometry to record more efficient holograms in the photorefractive media using the phase conjugate beam of the signal beam itself act as other writing beam The diffraction efficiency has been calculated by solving numerically the beam coupling equations and the index of refraction used in calculation of diffraction efficiency is calculated directly from the material rate equations. The diffraction efficiency of the holograms recorded in photorefractive media is depend on the applied external electric field ,crystal thickness, diffusion field and absorption coefficient of the materials. The influences of these parameters on diffraction efficiency have been studied in details. In the presence of the applied electric field more efficient holograms can be recorded at much lower values of all the physical parameters appearing in case of no external field.

Keywords: Photorefractive materials; diffraction efficiency; diffusion field and reducedfringe contrast modulation ratio of the index grating

Modifications of structural, optical and surface wettability of bismuth sulphide thin films by using electron beam irradiation

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In the present investigation, the first effort is focused on the exploitation of electron beam irradiation as a tool to induce modifications in the optical, morphological, structural and wettability studies of Bi_2S_3 thin films. Bismuth sulphide (Bi_2S_3) films have been synthesized via an easy and simple electrodeposition process. The Bi_2S_3 thin films have been deposited on to stainless steel and fluorine doped tin oxide (FTO) coated glass substrates, in potentiostatic mode using bismuth nitrate ($Bi(NO_3)_3$) , sodium thiosulphate ($Na_2S_2O_3$) as a precursor sources and ethylene diamine tetra acetic acid (EDTA) was used as a complexing agent.

The irradiation experiments were carried out at 7 MeV linear electron accelerator (LINAC) set up at Bhabha Atomic Research Center (BARC), Mumbai, India. The samples were irradiated by these electron pulses at a repetition rate of 12 pulses per second for about 6.5 seconds, accounting for a cumulative dose of about 10 kGy. The Bi_2S_3 thin films were electrodeposited from a bath containing $Bi(NO_3)_3$, $Na_2S_2O_3$ and EDTA in the volumetric proportion as 4:6:1 respectively. The films were deposited from 0.05M bath concentration. The as-deposited and irradiated films were further characterized for their structural and morphological studies. The phase structure and morphology of the Bi_2S_3 products were characterized by XRD, SEM, optical absorption and surface wettability. It is observed that the band gap of the films gets red shifted and increase in crystallinity after irradiation. In addition, there is an increase in the grain size of the films due to irradiation, leading to the increase in contact angle.

Spectroscopic Characterization of halide ionic liquids

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Ionic liquids (ILs) have been attracting attention of large number of researchers because of its amazing possibilities both as solvents for green synthesis and as well as a whole new materials.[1, 2] A small variation in anion found to impart drastic changes in both physical and chemical properties of ILs. 1-butyl-3-methylimidazolium cation based ILs having Cl^-, Br^-, and I^- as anions have been synthesised following improved processes to get the pure form of ionic liquid suitable for spectroscopic investigations. It has been observed that while iodide IL is liquid at room temperature, corresponding chloride and bromide are solid. Interestingly, in addition, iodide IL is found to have pale yellow in colour even in pure form.[3]

We have employed various spectroscopic techniques to ascertain the reason for this difference in physical state as well as colour. DFT calculations have been employed to substantiate the experimental results [4]. Details will be discussed in the presentation.

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Reflection Bands in 1D Photonic Crystal Structure Containing Chalcogenide Glasses

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In this paper we study the reflection properties of one-dimensional chalcogenide photonic crystal structure with the first order reflection band in near infrared (NIR) region. For this we use bulk chalcogenide materials with the composition of $Sb_{40}Se_{60}$ and $Ge_{30}S_{70}$glasses as high and low refractive index layers because these materials have zero absorption in NIR region[1-2]. Also, these materials have very attractive properties such as high index of refraction, small absorption over a wide range of wavelength, large non-linearity and most importantly easier fabrication technique In order to calculate the reflectance spectra of the structure Transfer Matrix Method (TMM) has been employed. Reflection spectra of the proposed structure, calculated theoretically, for 4, 8, 12 and 15 layers and thicknesses 117 nm and 183 nm respectively, at normal incidence angle, are compared with the experimental results of Kohoutek *et al.* [3]. Theoretical results show nearly close agreement with the experimental values. Further, it has been found that by increasing the number of layers of $Sb_{40}Se_{60}$ and $Ge_{30}S_{70}$ the reflection bands can be enhanced over a wide range of spectrum for both polarizations at different angles. Thus the proposed structure can act as a broadband omni- directional reflector in NIR region of the wavelength.

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Fluorescence Enhancement of an optical Brightening Material Tinopal

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Tinopal is a fluorescent whitening agent and widely used to improve the appearance of various commercial products like washing powder, plastics, paper, paints, textile etc. In addition, tinopal is also used in the clinical biosciences to detect human fecal contamination in water[1-2], rapid recognition of pulmonary dirofilariasis[3], peroral infection of nuclear polyhedrosis virus[4]in bio-pesticides to understand the growth of crops[5], studying the behavior of pollinators in soil spray analysis[6] and cellulose fiber analysis[7], to name but just a few examples. Basically, Tinopal is a sulfonic sodium salt of 4,4'- distyrylbiphenyl which readily absorbs UV radiation and emits a strong blue fluorescence in the wavelength range from 400 to 550 nm. In the present work, the dramatic change observed in the fluorescence intensity and other parameters of Tinopal on silver islands deposited on both glass slides and adsorbed on cellulose filter paper. About 4.5 fold enhancements in far-field tinopal fluorescence is observed with near-field enhancement values about 50 fold grater, i.e. 225-fold as compared to a control sample containing no silver.These findings are helpful in the development of enhanced luminescence and prolonged photo-stability of optical brightener for potential applications on textiles and papers.

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Space Charge Field Dependence on the Applied Electric Field in Photorefractive Materials

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The photorefractive effect is an optical phenomenon observed in some photorefractive materials where the local index of refraction is changed by the spatial variation of the light intensity. This effect is generally believed to arise from the optically generated charge carriers which migrate when the material is exposed to a spatially varying pattern of illumination with photons having sufficient energy. Migration of the charge carriers due to drift, diffusion and photovoltaic effects produces a space charge separation which gives rise to a strong space charge field.

In the present paper, we have derived analytically the intensity dependent space charge field due to the two interfering beams by solving the material rate equations in the photorefractive medium under the influence of externally applied electric field. The space charge field has been studied with respect to variations in the concentration ratio and normalized diffusion field in the absence and presence of the externally applied electric field. It has been found that for the higher value of diffusion field, the space charge field appears to be independent of the externally applied electric field. It has also been found that for given value of intensity ratio the space charge field increases with the increasing applied electric field.

Two-wave mixing gain and phase conjugation in photorefractive materials show high amplification and reflectivities. These processes have been successfully demonstrated and utilized in various configurations, including ring resonators where an oscillating beam arising from scattered noise experiences large amplification.

Keywords: Space charge field, normalized diffusion field and externally applied electric field.

A Novel Design of Optical Filter Using Equivalent Layer of Magnetic Photonic Band Gap Materials

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Photonic crystals have drawn much attention due to its peculiar optical properties such as transmission, localization, reflection etc. Photonic crystals made of periodic modulation of dielectric materials in one, two or three spatial directions that exhibit electromagnetic stop bands or photonic band gaps. Photonic band gaps play an important role in controlling the propagation of light. As we know that the choice of materials with refractive indices intermediate to those of highest and lowest values is impossible in any spectral region. We can get rid of this limitation by using equivalent layered notion.

In this paper, we propose a novel design of optical filter using equivalent layer of 1-dimensional magnetic photonic band gap materials which is based on the two refractive index medium of high refractive index (nH) and low refractive index (nL). By using this structure we can control the photonic band gap width. As in simple two layered structure of high and low refractive indices we replace each of the low refractive index layer by a combination of symmetric three layers (equivalent layer).With equivalent layered structure we can adjust the photonic band gap width to corresponding values by setting the equivalent refractive index to any desired values between high refractive index and low refractive index of the medium.

In this paper we have described the characteristics of optical filter for TE mode, for different values of equivalent refractive indices between high and low refractive index value and also for different values of angle of incidence by taking take nH=4 and nL=2.We observe that the width of photonic band gap changes with the angle of incidence. Here the width of the photonic band gap increases and also shifted toward higher-frequency side with the increase of angle of incidence. It may be widely used in optoelectronic devices.

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A comparative study of the properties of M-doped Cerium nanoparticles (M= Yt,Fe,Cu,Ba,Au,Ag) and their analysis in microwave and sensor applications

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Nanocrystalline ceria is a unique multipurpose material widely used in industries. It is mainly used as protective coating for the absorption and redistribution of UV radiation, polishing compositions and as catalyst in gas sensors. With high conductivity doped ceria has been studied as an electrolyte for SOFC (solid oxide fuel cells).

in this paper we try to present a comparative study of the effect of doping several metals in the form of their nitrates and oxides into compounds containing ceria nano particles and we try to analyse their responses to the electric and magnetic fields and how their properties are getting varied by the different metals introduced.

We also shall try to answer some the reasons that is causing the behaviour of these ceria-metal composites to vary from each other.

Extraction of cellulose and preparation of nanocellulose from different plant fibers and its application

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There is an increasing commercial demand for nanocellulose due of their wide applicability in various areas such as medical science, paper, textile, food industries , biomaterial in cosmetics .In medical science nanocellulose used in formation of artificial blood vessels, cuffs of nerves surgery, animal wound dressing substances. In this work, we describe a cost effective and environment friendly technique for green synthesis of nanocellulose. In this work a study on the feasibility of extracting cellulose from different plant fibers like Ceiba pentandra(kapok), Cocos nucifera(coconut), Gossypium hirsutum(cotton) ,is carried out .These process included usual chemical procedures such as acid hydrolysis, chlorination, alkaline extraction, and bleaching. The final products can be characterized by means of UV-VIS Spectrometry, X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM),FTIR and Scanning Electron Microscopy (SEM). The cellulose can be transformed into nanocellulose for its future use as nanofiller for biodegradable matrices, and it is also characterized by means of microscopy analysis.

Keywords: Nanocellulose, green synthesis, nanofiller.

NIR excited UV-visible upconversion emissions in Ho:Gd_2O_3 nanocrystals

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The structural and spectroscopic properties of GdO nanosized spherical crystals doped with Ho^{3+} ions have been investigated. The DTA, XRD, TEM and SEM techniques have been used for thermal and structural characterizations. The phosphors formed porous agglomerates which consist of spherical nano-crystallites with a uniform size at about 30 nm. Enhanced IR to green and red photon avalanche upconversion is reported under 976 nm laser excitations. Further, annealing shows a significant improvement in emission intensity. Concentration dependence, temporal evolution and excitation power dependent upconversion intensity are measured, suggesting that a photon-avalanche mechanism is responsible for the upconversion process. The enhancement of emission explained and the photo-physics involved is correlated with the unique structural properties of the crystallites formed.

Effect of Quenching on Magnetic, Dielectric and Magnetocapacitance Properties of Ni Doped Bismuth Ferrite nanoceramics

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$BiFe_{1-x}Ni_xO_3$ (with $x= 0, 0.1$) nanoceramics were prepared by sol gel method. The effect of quenching (in liquid nitrogen) and normal sintering on dielectric, magnetic and structural properties was studied. Samples leached in diluted nitric acid were found to be of single phase. TEM analysis shows the particle size to be ~ 50 nm. Thermogravimetric analysis of as prepared powder indicates the formation of sample around 400 ^{0}C. Dielectric behaviour of the samples was as of normal ferroelectric materials. Both samples show conducting behaviour at higher temperature. We observed enhancement of Magnetic and dielectric properties in quenched sample. But low variation in magnetocapacitance with an applied magnetic field was found in the quenched sample. The splitting of zero field cooled (ZFC) and field cooled (FC) magnetizations at low temperature reveals spin- glass transition. Enhancement of blocking temperature in quenched sample sports to defect in gains size.

Thermal Decomposition Approach to Prepare Supported Nickel Oxide Nanoparticles

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Magnetic nanoparticles are desirable for many applications in the area of magnetism, sensing, electrochromics, catalysis, etc [1-4]. The support provides stabilization and high level of dispersion to magnetic nanoparticles, keeps them apart and reduce surface effects and magnetic dipolar interactions [5]. There are different methods, reported in the literature, for the preparation of supported magnetic nanoparticles such as deposition precipitation, spray pyrolysis, adsorption phase reaction and microwave synthesis. Thermal decomposition is a simple and an easy approach to prepare supported metal oxide nanoparticles. In the present study, we report the preparation of supported nickel oxide nanoparticles by the thermal decomposition of nickel acetylacetonate in the presence of two different MgO's (macro-crystalline and nanocrystalline) as supports in a high boiling solvent, diphenyl ether. The reactions were carried out at 225^{o}C for 70 minutes followed by calcination of the obtained powders at 350^{o}C for 3 hours. The supported magnetic nanoparticles were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDXA) and M-H magnetic measurements. The XRD and EDXA results indicated that the nickel oxide nanoparticles are well dispersed in the MgO matrix and the FE-SEM images showed agglomerated particles. The EDXA results also indicated a higher loading of NiO nanoparticles when nanocrystalline MgO was used as the support. The nickel oxide nanoparticles supported on two different MgO, after calcination, exhibit superparamagnetic behavior at room temperature indicating the presence of magnetic nanoparticles on the MgO support. The present method is one of the simplest and easiest methods for the preparation of supported magnetic nanoparticles and may be extended for the preparation of other supported magnetic nanoparticle systems, too.

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Structural And Dielectric Relaxation Studies On Magnisio Ferrite Based Nanocomposite Polymer Electrolyte System

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Nanocomposite polymer electrolyte (NCPE) materials are receiving special attention, particularly in the field of solid state ionics owing to their potential applications in advanced ionic devices such as high performance batteries, fuel cell, supercapacitor, sensors, smart window etc. NCPE have several distinct advantages over liquid electrolytes such as good mechanical properties, better thermal stability, corrosionlessness, light weight, flexibility and ease of fabrication / processibility as thin films etc. PEO is one of the most prominent polymer host which has been extremely investigated as polymer electrolyte using alkali salts, plasticizer and inorganic fillers in the recent past. The chemical structure of PEO i.e. $[(CH_2\text{-}CH_2\text{-}0)_n]$ explain most of the properties of this polymer, a strong solvating character due to high donating character of numerous either oxygen, strong tendency for crystallization correlated to high organization and rigidity of segmental units. Improvement in ion transport property of polyethelene oxide (PEO)-based polymer electrolytes have been investigated upon dispersal of Magnisio ferrite nanosize filler particles. The nanocomposite polymer electrolytes (NCPEs) system [93PEO-7NH_4SCN]: Mg-Zn ferrite (Magnisio ferrite) were prepared by solution cast technique while ferrite nano powder was synthesized through sol-gel process. The formation of nanocomposite has been ascertained by XRD pattern. This nanocomposite electrolyte system was subsequently characterized by XRD, IR and SEM measurements. Mossbauer investigations reveal the superparamagnetic nature of the Magnisio ferrite powder. XRD and SEM observations confirm formation of nano-composite system with crystallite size varying in between 25-60 nm. Variation of dielectric constant, dielectric loss, tangent loss and modulus spectra with frequency and temperature were studied with the aid of impedance spectroscopy data. Results show optimum d.c. conductivity for [93PEO-7NH_4SCN]: 1wt% Mg-Zn ferrite system is ($\sim 9.0\text{x}10^{-5}$ S/cm) and variation of a.c. conductivity of nanocomposite polymer electrolytes with frequency seems to follow the universal power law. Study of electrode polarization/interfacial polarization effect in the nanocomposite electrolyte system was investigated by scaling of complex modulus electric spectra.

Synthesis and Characterization of $NiFe_2O_4$ Nanoparticles

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Magnetic nanoparticles have been around for over a decade now. With the developments in the process of synthesis and control, these particles have found applications in diverse areas. Appropriately functionalized magnetic nanoparticles have found various in-vivo applications including therapeutic applications viz. treatment of cancers using hyperthermia. Hyperthermia is a mechanism wherein the tissue temperature is raised to around 41-46 degrees Celsius to kill cancerous cells while preserving the normal cells. Traditionally iron oxide nanoparticles have been used for such therapeutic application because of the control during the synthesis process (with regards to the size, size distribution, agglomeration behavior and surface modifications) and the ability to cap it with ligand of our choice. Here we report the synthesis of NiFe2O4 nanopowder was prepared using Microwave-Hydrothermal method. The Characterization of the magnetic nanoparticles was performed by X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM) and Fourier Transform Infrared Spectroscopy (FTIR). We measured Hysteries loop curve. We also measured dielectric constant and losses for the above powders and finally the nanoparticles developed we have made a study on self-heating of this magnetic nanoparticle at different temperatures on A.C Magnetic field. Finally it is found that the NiFe2O4 nanoparticle was required properties for the potential applications of Hyperthermia treatment of cancer.

Key words: Magnetic nanoparticles, Hyperthermia, NiFe2O4.

Synthesis and characterization of hot-pressed nano-composite polymer electrolytes: (75PEO:25 $NaPO_3$) : x SiO_2

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Synthesis and characterization of Na^+ ion conducting Nano- Composite Polymer Electrolyte (NCPE) membranes: (1-x) [75PEO: 25$NaPO_3$]: x SiO_2, where x = 0 - 15 wt. (%), has been reported. NCPE membranes have been casted using a novel hot-press technique in place of the traditional solution cast method. The conventional Solid Polymer Electrolyte (SPE) composition: (75PEO: 25$NaPO_3$), identified as the highest conducting film at room temperature, has been used as I^{st}- phase host matrix and nano- size (~ 8 nm) particles of SiO_2 as II^{nd}- phase dispersoid. As a consequence of dispersal of SiO_2 in SPE host, a conductivity enhancement of an order of magnitude resulted in NCPE film: [93 (75PEO: 25$NaPO_3$): 7 SiO_2]. This has been referred to as Optimum Conducting Composition (OCC). The ion transport behaviour in NCPE OCC has been discussed on the basis of experimental measurements on some basic ionic parameters viz. conductivity (σ), ionic mobility (μ), mobile ion concentration (n), ionic transference number (t_{ion}) etc. The conductivity as a function of temperature has also been studied to compute the activation energy (E_a) by least square linear fitting of ‘log σ – 1/T’ Arrhenius plot.

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Band Structure of Carbon Nanotubes: A Tight Binding Approximation

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We investigate the tight-binding approximation for the dispersion of the valence and conduction electronic bands in carbon nanotubes. The geometry-dependent nature of their electronic structure has been explained using the tight-binding energy model .The nearest-neighbor tight-binding approximation applies only to a very limited range of wave vectors. Band structure is calculated using an improved tight-binding electronic dispersion by including up to third-nearest-neighbor interaction and overlap, which gives realistic results, even though it fails to account for small band gap induced by the coupling between s and p bonds. This effect is due to the curvature of the tube in semi-metallic tubes, that is, tubes where (n-m) is an integral multiple of three.

Effect of Oxygen Vacancy in Phase Transformation and Magnetic Properties of $Ti_{1-x}Co_xO_2$ (x=0 to 0.05) nanoparticles3

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TiO_2 is a widely studied material due to its wide application in sensors, photocatalysis, smart technology and electronics etc. It exhibits three major crystalline structures: rutile (tetragonal), anatase (tetragonal), and brookite (rhombohedral) with decreasing order of stability. With heat treatment both brookite and anatase irreversibly transforms to rutile. This phase transformation temperature mostly depends on particle size, particle packing and grain boundary concentration. In addition to it, we observed that anatase to rutile phase transformation (ART) temperature depends on pH of precipitation. Nanoparticles synthesized at pH 6.5 shows ART temperature at 650^{o}C while samples prepared at pH 4.5 transforms from anatase to rutile at 850^{o}C. We realized that instead of particle size oxygen vacancy plays a crucial role in driving the ART temperature to lower value. Oxygen concentration in the former sample is found to be higher than the later case which is confirmed from x-ray photoelectron spectroscopy. Further, we showed that oxygen vacancy also decides the magnetic properties in Cobalt doped TiO_2 nanoparticles. To realize this we synthesized $Ti_{1-x}Co_xO_2$ (x=0.01, 0.03, 0.05). Surprisingly, we observed higher magnetic moment in undoped TiO_2 than Co doped sample. X-ray photoelectron spectroscopic analysis reveals higher oxygen concentration in undoped TiO_2 than Co doped samples.

Structural and Optical Properties of Co doped ZnO Nanoparticles Synthesized by co-Precipitation Technique

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In the past decade, there have been many studies on the fabrication and optical properties of semiconductor nanoparticles, because they will become new functional materials for future optoelectronic devices. In particular, the semiconductor nanocrystals doped with luminescence centers exhibit efficient luminescence even at room temperature. Many different techniques have been developed for the fabrication of high-quality semiconductor Nanocrystals. The wurtzite semiconductor ZnO is a wide-band-gap materials (Eg ~3.37 eV at room temperature) with an exciton binding energy of 60 meV. Therefore, it is interesting to study the Co doped ZnO nanparticles. In the present study Pure and Co-doped ZnO nanoparticles have been synthesized by an aqueous precipitation technique with polyvinylepyrrolidone as capping agent. These as-prepared samples have been studied using X-ray diffraction (XRD), energy dispersive spectroscopy (EDS), UV-visible spectroscopy and photoluminescence (PL) spectrometer. The XRD studies revealed that the ZnO crystallinity was slightly impede by Co doping. The amount of Co doping contents is about 3.0 at% in ZnO nanoparticles and dopant Co^{2+} ions substitute Zn^{2+} ions sites in ZnO nanocrystal without forming any secondary phase. The optical measurements show that the Co doping can enrich surface states in both UV and Visible regions and, effectively tune energy band structure.

Synthesis of Cobalt Aluminate Nanoparticles by Simple Sol-Gel Method

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$CoAl_2O_4$ nanoparticles are widely used as a blue pigment in glass, ceramics and paint industries [1, 2]. They are also used in the field of heterogeneous catalysis [3]. $CoAl_2O_4$ nanoparticles are conventionally prepared by high temperature methods, which require temperature as high as ~1300^{o}C that influences particle size and morphology. Recently, many wet-chemical techniques have been used for the synthesis of $CoAl_2O_4$ like hydrothermal, co-precipitation and polymeric precursor method. Most of these methods are complex and time consuming. In the present study, a simple sol-gel synthesis of cobalt aluminate nanoparticles is reported. In the sol-gel method, the chemical elements become uniformly distributed during the gel formation step and good stoichiometric control and production of ultrafine particles with narrow size distribution in relatively short processing time at lower temperature can be achieved [5, 6]. For the synthesis of $CoAl_2O_4$ nanoparticles, Co-(acac)$_2$ and Al-(O^{i}Pr)$_3$ were taken in 1:2 molar ratio and then a mixture of ethanol and toluene was added followed by the addition of distilled water. The hydrolysis of the alkoxide led to a gel which was dried and finally calcined at 700^{o}C in air. The XRD pattern of the blue powder obtained after calcination at 700^{o}C matches with that of $CoAl_2O_4$ nanoparticles. The FT-IR and DRS spectra of the calcined sample showed the characteristic bands for $CoAl_2O_4$. The FE-SEM images of the $CoAl_2O_4$ nanoparticles showed irregular morphology and agglomeration of nanoparticles and the EDXA analysis indicated an Al/Co ratio of 2 which also supports the stoichiometry of $CoAl_2O_4$. The present method is an easy method to synthesis cobalt nanoparticles at low temperature.

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Effect on electrical and magnetotransport properties of Fe nanoparticle admixed $La_{0.7}Ca_{0.3}MnO_3$

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The electrical and magnetic transport properties of composite samples of $La_{0.7}Ca_{0.3}MnO_3$ + x wt% Fe nanoparticles (Fe-NP) with x = 0, 1, 3, 5, 10, 20 and 30 were studied in a temperature range 20-300K. LCMO were synthesized by sol-gel route and Fe-NP was obtained after ball milling Iron for 50 hours. All these samples were annealed at 700°C in oxygen atmosphere. XRD observation reveals the single phasic nature of LCMO and also the presence of Fe_2O_3 as a secondary phase. That suggests that Fe-NP oxidizes to Fe_2O_3 when annealed under O_2 ambient. Resistance of the samples increases with increasing percentage of Fe-NP while AC susceptibility values decreases. Fe_2O_3 present at grain boundaries act as a barrier for charge carriers thereby increasing the resistance and also lowering the insulator-metal transition temperature (T_{IM}). Fe_2O_3 being paramagnetic in nature affects paramagnetic-ferromagnetic transition (T_C) temperature also. Magnetoresistance (MR) vs. temperature shows almost similar behavior for all the samples. It exhibit two different slopes from 270K to 200K increasing rather quickly and below 200K almost constant up to the lowest measured temperature. To correlate these properties with microstructure HRTEM is done. HRTEM images shows LCMO and Fe_2O_3 grains in contact and hence confirming the presence of Fe_2O_3 as a barrier layer for charge carriers. An almost constant ~ 20% MR ranging 120K from 200K to 80K may be important from application point of view.

Viscosity Coefficient Of Liquid Alkali Metals

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The statistical mechanical theory of atomic transport process in liquids deals, with a knowledge of the molecular properties. Rice and Allnatt developed the theory of transport phenomena for a model monatomic dense fluid in which the intermolecular pair potential has the form of a rigid core repulsion, superimposed on an arbitrary soft potential. The effective pair potential has strong repulsive core which implies that the ions may be treated as hard –spheres, which interact, when they are not actually in contact through a weak and long range potential. An attempt is made to study the transport properties of liquid alkali metals. The shear and bulk viscosity coefficients of alkali metals are computed using, the Ashcroft's local model potential and the non-local Shaw's model potential, and are compared with the available data over a wide range of temperature. The results of the shear and bulk viscosity coefficients are in agreement with each other.

Historical building stones in Varanasi district: role of petrography, mineralogy and geochemistry in provenance and durability assessment

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Ferruginous red sandstone from Kaimur Group, Vindhyan Supergroup from Mirzapur district has been extensively used in the historical buildings and various ghats of Varanasi district. Petrography, mineralogy and geochemistry of over 20 different rock species which have been studied in historical monuments of district Varanasi, are described in detail. The resulting petrographic description provides a powerful identification and decision tool in restoration. The study deals with macroscopic and microscopic features of the natural stones. The geographical distribution of these sandstones in the monuments reflects local geology. Petrography is very helpful, especially in discriminating different varieties of ferruginous, quartz arenitic, litharenitic and subarkosic sandstones. Moreover, thin-section analysis helps in assessing provenance, weathering and bioreceptivity potential. Electron microprobe data of these red sandstones shows the presence of ferruginous and siliceous cement between the detrital grains .Finally, geochemical data greatly helps in characterization of these sandstones. Petrographical together with geochemical analysis is also a strong tool for assessing the durability of historical building materials because it largely depends on intrinsic parameters such as mineralogy, texture and composition of building materials. The chemical composition shows that SiO_2 wt% of these sandstones varies between 85-95 wt% apart from 1-2 wt% of Iron oxide. Silica oxide is the composition of mineral quartz. X-ray diffraction data corroborates that quartz is the dominant mineral in these sandstones. Quartz is the most resistant mineral to weathering. The study also helps us to understand their weathering potential and the reasons for withstanding erosion inspite of the prolonged exposure to adverse climatic conditions.

Temperature-dependent current-voltage (I-V) characteristics of the nickel Schottky contacts to n-type InP

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The temperature-dependent of current-voltage (I-V) characteristics of the Ni Schottky contacts on n-InP (100) has been measured in the temperature range of 200-400K. Based on thermionic emission (TE) theory, the forward and reverse bias current-voltage (I-V) characteristics are analyzed to estimate the Schottky barrier parameters. It is observed that the decrease in ideality factor and increase in barrier heights (BHs) with increasing temperature. The estimated values of barrier height and ideality factors are varied from 0.48 eV and 3.01 at 200 K to 0.83 eV and 1.89 at 400 K respectively. An abnormal decrease in the experimental barrier height and an increase in the ideality factor n with decrease in temperature have been explained by the barrier inhomogeneties at the metal-semiconductor (MS) interface. This behavior has been interpreted by the assumption of the Gaussian distribution of the barrier height. The zero-bias barrier height Φ_{bo} versus 1/2kT plot has been drawn to obtain the evidence of a Gaussian distribution of the barrier height. The obtained mean value of Φ_{bo} is 0.99 eV with standard deviation σ_o = 135 meV. The modified Richardson plot, according to inhomogeneity of the BHs, has a good linearity over the temperature range. The values of Richardson constant (A**) has been found to be 5.57 $Acm^{-2}K^{-2}$, which is close to the theoretical value of 9.4 $Acm^{-2}K^{-2}$ for n-type InP. The series resistance is also estimated from the current-voltage characteristics of Ni/n-InP Schottky contacts using Cheung’s method and found that it is strongly dependent on temperature.

Ancillary Component Method: Using in the Research and Synthesis of Pure Inorganic Compounds

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It is well known that the type and concentration of the point defects specify the properties of inorganic solids. In turn, concentration of the point defects depends on pressure (as well as – on temperature and composition). Usually in case of volatile compounds the appreciable values of equilibrium vapor pressure can be easily reached. As a result the *P-T-x* phase diagrams and homogeneity regions of these compounds can be directly and precisely investigated. Besides, the desired properties of these compounds can be easily obtained in the course of annealing in the presence of vapor. However what can we do in case of low-volatile solids? The obstacle of practically absence of vapor can be avoided by the ancillary component introduction. Instead of the equilibrium

$$A^{\text{in the solid}} = A^{\text{vapour}} \tag{1}$$

one can attain the other equilibrium – type as

$$A^{\text{in the solid}} + nC^{\text{vapour}} = AC_n^{\text{vapor}}. \tag{2}$$

Investigating the equilibrium (2) one can evaluate the chemical potential of the component *A* (*A* is one of the components of the scrutinized solid phase – $A_{x\pm\delta}B_y$ for example):

$$\mu_A = RT\ln\kappa_P + F(T) \tag{3}$$

where μ_A – the chemical potential of the component A, $\kappa_P = p_{ACn}/(p_C)^n$

and the term $F(T)$ is the difference in *standard* chemical potentials of spices in vapor: $F(T) = \mu^\circ_{ACn} - n\cdot\mu^\circ_C$. It should be stressed that the information on the chemical potentials is a pass key to the manifold properties of solids.

In the present work we show the results of the ancillary component using for

- the investigation of Ga-Se, Ga-S and In-S phase diagrams;
- the synthesis of gallium and indium chalcogenides having specified properties;
- the preparation of metastable structures type as skeletal nickel or copper as the catalysts;
- the modification of structure and properties of indium and copper-indium sulfide (selenide) thin films.

Single Crystals of NaCl Doped with Divalent Cations as new material for dosimetric purposes

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In this work, is analyzed the interactions of the gamma-radiation with two homemade alkali halide single crystals: NaCl doped with Ca^{2+} (0.3 %) or Mn^{2+} (0.3 %), at two irradiation temperatures (298 K and 77 K), and different doses at a fix dose rate, for their possible use as dosimeters. The irradiated crystals were analyzed using their thermoluminescence properties. The application of the thermoluminescence (TL) phenomenon has been proved to be a very efficient method to evaluate energy deposited by gamma radiation on irradiated samples. Fig. 1 shows the glow curve for NaCl:Mn (0.3%), irradiated at 77 K

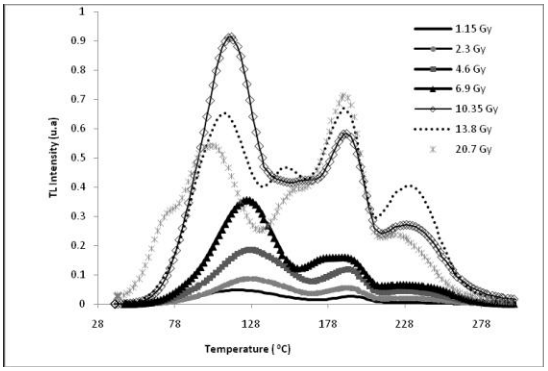

Fig. 1 glow curve for NaCl:Mn (0.3%)

The productions of irradiation defects in the solid were correlated with the glow curve. F-centers were measured as function of the dose. The bleaching of the F-centers produced a decrease of the peak of the glow curve. We have measure the color centers using UV and visible spectroscopes. The bleaching of the color centers associated with the reduction of the glow curve suggests that F centers are intimately involved in the production of the thermoluminescence phenomenon. Their exact role can not be centered and much discussion has still to be done. Nevertheless, these behaviors suggest that the glow peaks very probable are result from the thermal release of holes from different kinds of traps, recombining at F centers. The preliminary results show that the linear response obtained was fairly good for the system NaCl: Cd, at low irradiation doses.

The Corelation Between Reduced Glass Transition Temperature And Glass Forming Ability Of Undercooled Polymeric Glasses

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The glass transition temperature (T_g) of six polymeric glass forming materials [O-terphenyl, Tri-α-naphthyl benzene, Glycerol, Ethanol, 2-methylpentane and Phenyl salicylate (salol) have been correlated with reduced glass transition temperature, between the liquid and the corresponding equilibrium solids. The expression obtained by expanding free energies of the undercooled liquid and solid phases in the form of Taylor's series expansion. The procedure for the estimation of the ideal glass transition temperature has been reviewed together its importance in the glass forming ability of materials. The glass forming ability of undercooled materials is also explained in terms of ratio of reduced glass transition temperature and ideal glass transition temperature. It has also reported that Glycerol has the largest melting interval with the poorest glass forming ability among these six polymers. It has also been found that the best polymeric glass forming materials are at near eutectic composition. There is a strong correlation between glass forming ability of these polymeric materials and their reduced glass transition temperature (T_{rg}) while a less correlation between T_{rg} based on T_g/T_m and glass forming ability is observed.

Key words: glass transition temperature, undercooled , Taylor's series expansion, ideal glass transition temperature.

Observation of Conductivity Type Change in Swift Heavy Ion Irradiated Metal/Semiconductor Devices

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Metal/Semiconductor (n-type & p-type) devices were irradiated with Au(7^+) and Si(8^+) ions of energy ~100MeV with different fluencies (10^{10} – 10^{13} ions/cm^2). Electronic properties have been studied from I-V and C-V characteristics of the devices before and after the irradiation. Hydrogenation of the irradiated devices has also been performed to investigate the hydrogen passivation effect of the irradiation induced defects. The devices were annealed upto 400°C and Infrared spectroscopic studies have been carried out at each annealing temperatures to study the nature of irradiation induced defects. The result has been discussed in the realm of radiation hardness and the conductivity type change of the irradiated electronic devices.

Keywords**:** Swift Heavy Ions, Irradiation, Radiation Induced Defects, Hydrogenation

Some comments on the new approaches to experimental techniques for creation and investigation of nanoscale confined system

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The creation of nanoscale confined system and investigation of structural evolution in thin films growth and instability phenomena is presently an off the edge process in present status of experimental development for attending such problems at frontier area of science on micro and nano scale with a desired accuracy below the range of the observed values. I look for the possibility and scope of such a new instrument or modification(s) in experimental tool. Such a proposal would require atomic scale plane very thin conduction sheet which can form a confined geometry when placed over a thin micro or nano film fabricated on plane silicon or some other highly planar sophisticated surface. Atomic scale thin conducting sheet can be moved in XYZ 3D space using the electromechanical motion of the piezo-electronically controlled laser-interferometer device or by using a touch sensor atomic scale pin tip as used in conventional STM on a high quality sophisticated balance stage. The problems which are likely to be posed for meeting such objectives are mainly those as making atomistically smooth conducting or non-conducting surfaces, high quality balancing stage and high cost of developing piezo-electronically controlled laser- interferometer. Though there have been significant developments in nano thin film fabrication by accurate correction using proximity-effects, thickness control on the quality of the crystallinity of thin films, stress characterization of metal films, measurement of surface roughness by AFM and STM etc., theoretical development of nucleation, spinodal dewetting and growth processes of thin films including elecrtomigration damage, better growth control of thin films using ab-initio total energy calculation of epitaxial effects and availability of high quality and commercially cheaper touch sensor devices etc. In this paper I shall discuss some nano scale problems and present a theoretical model/sketch of the proposed device/instrument and will argue for its feasibility on theoretical grounds with relevant analytical calculations.

Shi Irradiation Effect on Makrofol-Kg Polymer

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Polymeric foils such as Makrofol are very important in modern industry as a new substitute of traditional films and electronic equipments. In the present study, the effects of Swift heavy ion beams irradiation on the structural, chemical and optical properties of Makrofol solid state nuclear track detector (SSNTD) were investigated. Makrofol-KG films of thickness of 40 microns were irradiated with two different beams (Li and Ni) with fluences ranging between10^{10} ion/cm^2 and 10^{12} ion/cm^2. Structural, chemical and optical properties were investigated using X-ray diffraction, FTIR spectroscopy and UV-Visible spectroscopy methods. It is observed that the direct and indirect band gaps of pristine Makrofol-KG are 4.1 eV and 3.9 eV, respectively, which decreases sharply after irradiation. The XRD study shows that the crystalline size in the films decreases at higher fluences. The intensity plots of FTIR measurements indicate the degradation of Makrofol at higher fluences of the Ni beam.

Theoretical Study of the Nematogenic Behaviour of para-hexyl-p’-cyanobiphenyl

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Para-hexyl-p’-cyanobiphenyl (6CB) is a nematic liquid crystal which passes from crystalline to nematic phase at 14.3°C and nematic to isotropic phase at 30.1°C. Intermolecular interactions between a pair of 6CB molecules have been evaluated using modified second order perturbation theory along with multicentred- multipole expansion method. Stacking, in-plane and terminal interaction energy studies have been carried out. Using Maxwell- Boltzmann formula, probability calculations for various intermolecular complexes formed due to a pair of 6CB molecules have been performed. Results have been used to understand the nematic behaviour of the system.

Keyword: Intermolecular interactions, Liquid crystals, ab initio, Molecular ordering.

Augmentation of Graft Compatibility through Electric control

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Grafting is an important tool for getting good yields in plants because it does not implicate soma clone variations in products. The augmentation of graft compatibility contributes significantly in horticulture, floriculture and forestry production. The graft compatibility and its augmentation depend upon various natural factors like environment, weather, soil conditions and protective measures etc. The present study examines the role of external electric field on augmentation of graft compatibility. For this purpose, the external forward and reverse DC electric currents of 5, 10, 20 and 30 microampere were passed across the scion and stock in more than two hundred specimens of the Rosa indica graft for 24 hours after grafting and their percentage growths were recorded. The electric control of graft compatibility, its dependency on direction of the current and its pattern of variation have been envisaged in the findings.

Key words: Electrical control, graft compatibility augmentation, directionality, electric field effect

Ionic Conduction in Sodium Silicate: An Experimental Study

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The electrical conductivity (σ) and thermoelectric power (S) of solidified melt sample of Sodium Silicate (Na_2SiO_3) have been studied. It has been observed that this compound undergoes phase transition from lower temperature low conducting phase to higher temperature high conducting phase. Above phase transition temperature (T_p), the compound is typical superionic solid with Na^+ ion as the entity of charge carrier. The activation energy, heats of transport and enthalpy for the formation of defects have also been calculated. The extended lattice gas model provides a better explanation of the electrical transport mechanism in superionic phase of solid. Below T_p the compound behaves as normal ionic solid with relatively high conductivity.

Keywords: Phase transition, electrical conductivity, thermoelectric power, activation energy

Experimental studies on the Transport Properties and Phase Transition of Lithium Borate

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The paper reports the results of the measurement of electrical conductivity (σ), thermoelectric power (S), dielectric constant (K) and magnetic susceptibility (χ) of the Lithium Borate ($LiBO_2$) in the temperature range from 440K to nearly the melting point of the solid. The ionic (σ_i) and electronic (σ_e) contributions to the total conductivity (σ) have been evaluated using time dependence study of dc electrical conductivity at different fixed temperatures. The phase transition temperature (T_p) of this compound has been observed at around 825 K. Contribution of σ_i to total σ is found to be more than 99.89% for $T>T_p$ and values of σ are more than 3.20 $\Omega^{-1}m^{-1}$, indicating the existence of superionic phase of the material for $T>T_p$. Activation energy (E_a) and heat of transport (Q) have also been evaluated. The observed superionic phase has been suitably explained using extended lattice gas model.

Keywords: Phase Transition, Ionic conductivity, thermoelectric power, critical temperature, dielectric constant, magnetic susceptibility

Theoretical Study of Molecular Ordering in Nematogens: 4-(4-propoxybenzilideneamino) benzoic acid

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The peculiar changes-characteristics of mesomorphic behaviour, which occur at phase transitions, are primarily governed by intermolecular interactions acting between sides, planes and terminals of a pair of liquid crystalline molecules. In view of this fact, intermolecular interactions between a pair of 4-(4-propoxybenzilideneamino) benzoic acid (3BABA) molecules have been evaluated using modified second order perturbation treatment along with multicentred- multipole expansion method. Using the results of stacking, in-plane and terminal interaction energy studies, probability calculations at varied angular and positional configurations in a molecular pair of 3BABA have been carried out employing Maxwell-Boltzman formula. An attempt has been made to elucidate the nematic behaviour of 3BABA molecules in terms of translational freedom, orientational flexibility etc.

Keywords: Intermolecular interactions, Liquid crystals, ab initio, Molecular ordering.

Raman Spectroscopic Investigation of Protonated And Deprotonated Form Of Warfarin

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Warfarin is a widespread anticoagulant used as medicine to prevent strokes. Racemic warfarin [3-α-(acetonylbenzyl)-4-hydroxycoumarin], a synthetic 4-hydroxycoumarin derivative and vitamin K antagonist [1], has been utilized for more than two decades as an oral anticoagulant (OA) and as a rodenticide. Its two enantiomers (chiral center at C-9) do not exhibit equivalent anticoagulant activity due to complex factors, including different intrinsic activities as well as differences in pharmacokinetics, pharmacodynamics and metabolism.

Theoretical prediction of molecular interaction at molecular level helps a lot to understand the interaction mechanism. In quantum chemistry, density functional theory (DFT) has become an efficient tool for the prediction of molecular structure, conjugation, hydrogen bonding, vibrational frequencies, and IR and Raman activities of the bioactive molecule [2]. The present work deals with the Raman and IR spectral investigations of warfarin supported by DFT calculation. We have studied the structure and frequency of neat, protonated and deprotonated warfarin in aqueous medium.

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Surface morpholgy of ZnO based films derived by screen printing and sol-gel method

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Zinc oxide(ZnO), a versatile n-type semiconductor material, has got tremendous applications in various areas of materials science and nanotechnology. ZnO thin films show several kinds of surface structures depending upon the method of deposition. Methods like pulsed laser deposition, thermal evaporation, spray pyrolysis, sol-gel spin coating etc. are commonly used for the deposition of thin films of ZnO. Dopants like Mg, Cd, Na etc have been used to enhance the physical and chemical properties of ZnO thin films. Here films of undoped ZnO and Ca doped ZnO are deposited using two methods, screen printing and sol-gel spin coating. Screen printing is a dry method and sol-gel spin coating is a wet chemical method. The films obtained from both the methods show different morphlogies when their scanning electron micrographs (SEM) are recorded. Figures 1 (a) and (b) are SEM of undoped and 5at%Ca doped ZnO fims deposited by screen printing and figures 2 (a) and (b) are the SEM of undoped and 5at%Ca doped ZnO fims derived from sol-gel spin coating. Films from screen printing contain granular structure and the grain density seems to decrease with doping of Ca. Sol-gel derived ZnO film has some point-like structures formed over the uniform background, which after doping change to irregular structures higher in density.

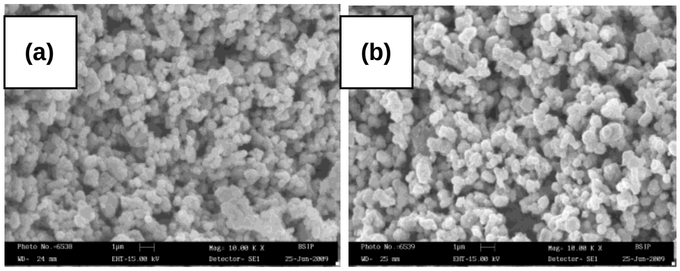

Figure 1: SEM of (a) undoped and (b) 5at%Ca doped ZnO films deposited by screen printing.

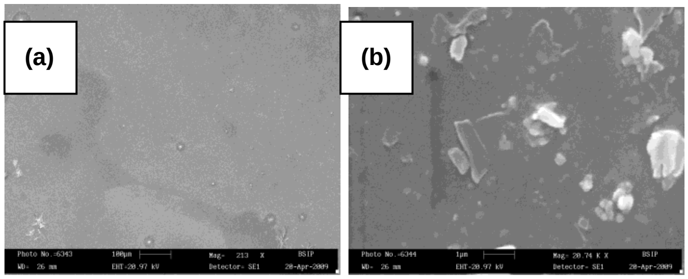

Figure 2: SEM of (a) undoped and (b) 5at%Ca doped, ZnO films deposited by sol-gel spin coating.

Synthesis, Structure, Electric Transport and Magnetic Properties of Layered Perovskite Manganites $La_{1-x}Sr_{1+x}Mn_{0.5}A_{0.5}O_4$ (A=Transition metal ion)

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The layered perovskite manganites are known to exhibit interesting structure and physical properties. In the present investigation, the layered perovskite manganites with composition $La_{1-x}Sr_{1+x}Mn_{0.5}A_{0.5}O_4$ (A=Transition metal ion) have been prepared by traditional ceramic method. The oxygen content in the phases has been determined by iodometric titrations.Their crystal structure has been established by the powder X-ray diffractometry. The electrical resistivity of the phases has been studied as a function of temperature in the temperature range 150-300 K. The results suggest that the phases are electrical insulators and the electrical conduction occurs by a 3D variable hopping mechanism. The magnetic susceptibility has been studied as a function of temperature in the temperature range 100-300 K in the Faraday magnetic balance. The magnetic studies suggest that the phases are antiferromagnetic.

Observation of Multiferroic Properties in Ti-doped $CoFe_2O_4$

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Existence of ferroelectricity have been observed for the first time in magnetically ordered (ferrimagnetic) $Co(Fe_{1-x}Ti_x)_2O_4$. The magnetization of $Co(Fe_{1-x}Ti_x)_2O_4$ (x=0-0.1) was found to increase with doping concentration of Ti. The XPS study indicates a significant migration from octahedral to tetrahedral sites for Co on doping with Ti.

Structural and Dielectric Properties of 0.90(bafe$_{0.5}$nb$_{0.5}$)o$_3$-0.10srtio$_3$ Ceramics

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We have synthesized 0.90(BaFe$_{0.5}$Nb$_{0.5}$)O$_3$-0.10SrTiO$_3$, (BFN-ST) ceramics by a solid state reaction technique and performed preliminary X-ray diffraction (XRD) analysis and the temperature and frequency dependence dielectric measurements on them. It is investigated by Impedance spectroscopy in a temperature range from 30° to 270°C and in the frequency range from 100 Hz to 5 MHz. Impedance spectroscopy is an effective method to study (a) the properties of the intragranular and interfacial regions and their interrelations, (b) their temperature and frequency dependent phenomena in order to separate the individual contributions from the total impedance and (c) their interfaces with electronically conducting electrodes. In view of the important applications, complexity in structure and wide variation in the properties on suitable substitution have attracted us to examine the titled compounds. All the observations indicate the polydispersive relaxation of BFN-ST. Study of electrical properties, such as dielectric constant, loss tangent, AC conductivity, etc. in this oxide over wide range of frequency and temperature will help us in assessing its insulating character for potential application.

Synthesis and Characterization of $Pr_{1-x}Sr_xFeO_3$ ($0 \leq x \leq 0.6$) Perovskites

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Sr doped rare earth perovskite materials are useful as cathode materials in Solid Oxide Fuel Cells (SOFC). $Pr_{1-x}Sr_xFeO_3$ ($0 \leq x \leq 0.6$) perovskite oxides are prepared using sol-gel process. The crystal structure, and thermal expansion of of these oxides are studied by X-ray diffraction and dilatometry respectively. The lattice parameters are calculated using Xutil software. It is found that all the materials in this composition are crystallized in the orthorhombic perovskite structure. The thermal expansion coefficients (TEC) are determined from the dilatometric measurements and it is found that the value of the TEC increases upto 0.4 concentrations of Sr then it decreases. Thermal expansion coefficients of these materials are in the range of 10 to $14 \times 10^{-6} / {}^{0}K$ which are compatible with the coefficient of thermal expansion of electrolyte materials of solid oxide fuel cells. The detailed analysis of these results will be discussed.

Moisture Sensing Properties of Polyaniline Pellets of Varying Thickness

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This paper presents humidity sensing properties of polyaniline. Humidity plays a major role in different processes in industries ranging from food to electronic goods besides human comfort and therefore its monitoring is an essential requirement. Polyaniline has a wide use for making sensors as it can be easily synthesized and has long stability. Polyaniline is synthesized here by chemical route and is found to sense humidity. The results were supported by FTIR, and Scanning electron microscope (SEM). The variation of resistance with variation in relative humidity is recorded for the three polyaniline pellets of 0.55mm,0.62mm and 0.89mm thickness respectively. The results are presented here for a range of 25 to 90 RH%.

Nature of Bonding of In_2S_3 and In_2Se_3 Using Compton Spectroscopy

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Momentum density measurements of semiconductor In_2X_3 (X=S, Se) was made using 59.54 keV γ-rays emitted by 100mCi ^{241}Am Compton spectrometer [**1**]. In_2S_3 and In_2Se_3 used as solar cells and photovoltaic devices have been studied by experimental and theoretical methods. However momentum density measurements have not been made earlier.

In this paper we have reported energy bands, density of states and Compton profiles using linear combination of atomic orbitals within Density Functional Theories [2]. The equal-valence-electron-density (EVED) profiles are derived from the measured and calculated CPs [Fig.1]. EVED gives information about nature of bonding in materials. To compare the bonding character of In_2S_3 and In_2Se_3, we have scaled the convoluted theoretical (LCAO-DFT-GGA) Compton profile and the experimental profiles on p_z/p_F scale. This method has been very useful in determining the nature of bonding of isoelectronic compounds, which shows that In_2Se_3 is more covalent than In_2S_3 which is in agreement with the Mullikan's population analysis.

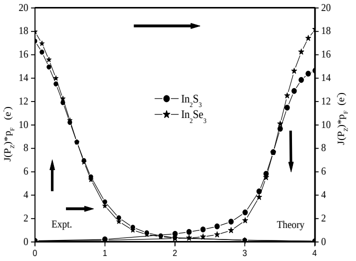

Fig 1: Experimental and theoretical (DFT-GGA) EVED profiles (on p_Z/p_F scale) of isoelectronic In_2X_3 (X=S, Se)

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Efficiency of hologram recorded with weak external electric field in photorefractive media

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To record much efficient holograms in the photorefractive media much innovative geometry have been proposed by various group of workers with and without externally applied electric field across the crystal in both the two and four-wave mixing geometries. We have also proposed a new geometry to record more efficient holograms in the photorefractive media using the phase conjugate beam of the signal beam itself act as other writing beam The Diffraction efficiency has been calculated by solving numerically the beam coupling equations and the index of refraction used in calculation of diffraction efficiency is calculated directly from the material rate equations. The diffraction efficiency of the holograms recorded in photorefractive media is depend on the applied external electric field ,crystal thickness, diffusion field and absorption coefficient of the materials. The influences of these parameters on diffraction efficiency have been studied in details. In the presence of the applied electric field more efficient holograms can be recorded at much lower values of all the physical parameters appearing in case of no external field.

Keywords: Photorefractive materials; diffraction efficiency; diffusion field and reduced fringe contrast modulation ratio of the index grating

Spectroscopic study of Ce ions co-doped in barium fluoroborate glass

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The spectroscopic properties of Ce doped in barium fluoroborate glasses are reported and discussed. Under 266 nm and 355 nm excitations, Ce^{3+} ion emit broad blue emission due to 5d–4f transition Luminescence spectrum. The intensity of cerium doped fluoroborate glass is maximum at 0.1 mole% concentration of cerium ion for both the excitation. It is found that for same doping concentration of cerium the peak position in emission spectrum of 355 nm excitation is shifted towards higher wavelength as compared to 266 nm excitation i.e. Peak shifted from uv to visible. Uv absorber properties of cerium doped fluoroborate glass have also been studies.