CHAPTER 39

PHYSICS AND ASTROPHYSICS

Doctoral Theses

01. ALNAJAR (Mohammed Hussain Mohammed Musa)
Synthesis and Characterization of rare Earth doped ZnO Nanostructures and GO/ZnO hybrids for Energy Harvesting application.
Supervisor: Prof Binay Kumar
Th 25738

Abstract

The present thesis includes synthesis and characterization of Er, Tm and Ce/Nd doped ZnO & GO/ZnO nanostructures. The synthesized Er and Tm doped ZnO & GO/ZnO nanostructures have been involved in the fabrication of piezoelectric nanogenerators whose electrical performance has been investigated. The thesis is divided into seven chapters. Brief details are described as follows begins with an introductory to the nanoscience and explains the uniqueness of physical properties of a material at nanoscale regime. A brief introduction to nanomaterials synthesis processes and growth mechanism along with their important applications are given. A general background and essential concepts of piezoelectricity and ferroelectricity are explained. Various properties of ZnO nanomaterial are addressed. The working principle and applications of piezoelectric nanogenerator are mentioned. presents a systematic review of various research groups results on dielectric, ferroelectric and piezoelectric properties of different doped ZnO nanostructures. The energy harvesting performance of diverse doped ZnO based piezoelectric nanogenerators studied by various researchers is comprehensively compared and discussed. Lastly, motivation and work plan of present thesis are summarized. in their subsequent characterizations. They include X-Ray Diffraction (XRD), Electron Scanning Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDAX), Fourier Transform Infrared Spectroscopy (FT-IR), Raman Spectroscopy, UV-Vis Spectroscopy, Photoluminescence Spectroscopy, Dielectric , Ferroelectric and Piezoelectric measurements. compares various properties of pristine and Ce/Nd co-doped ZnO nanoparticles synthesized by wet chemical co-precipitation and hydrothermal techniques with and without CTAB. The hexagonal wurtzite phase of ZnO in all prepared powders was confirmed using Powder X-ray diffraction. FT-IR and Raman spectroscopies were used to farther confirm the single-phase structure of ZnO of all samples. SEM technique was used to probe the morphologies of ZnO and Ce/Nd coiv doped ZnO nanoparticles which revealed collective nanostructure shapes of the synthesized nanoparticles. Cerium and neodymium concentrations in the doped ZnO composites were confirmed using Energy Dispersive X-ray (EDX) spectroscopy. The UV-Vis absorption spectra showed remarkable reduction in the optical band gap energies of the prepared samples. The photoluminescence study of pure and Ce/Nd codoped ZnO nanoparticles revealed less emissions of the defects where the green emission peaks were low intense and sharp. The dielectric phase transition was found at high Curie temperature (170 °C) in pure ZnO nanoparticles and it was enhanced up to 243°C upon doping. Ferroelectric loops of all pelletized samples were

studied. Due to the dual doping of cerium and neodymium elements into ZnO matrix the remnant polarization (Pr) was increased five times and coercive field (Ec) was decreased. The synthesized Ce/Nd co-doped ZnO composite is a promising optoelectronic lead-free high Tc ferroelectric material for designing photoelectric nanodevices, photodetectors and memory devices.

Contents

02. BATRA (Kriti)
Synthesis and Characterization of Lead-free Piezoelectric Materials for energy harvesting and Pressure Sensing Applications.
Supervisor: Prof. Binay Kumar
Th 25735

Abstract

This thesis presents the synthesis of three different lead-free piezoelectric materials, i.e., pure and (Nd-, Ba- and Tb-) doped ZnO nanoparticles, BNKT ceramic and KNNBNZ ceramic for piezoelectric energy harvesting and pressure sensing applications. The synthesized piezoelectric materials have been subjected to various characterizations for structural, morphological, dielectric, ferroelectric and piezoelectric properties, and further utilized for the fabrication of piezoelectric energy harvesting devices. The entire thesis has been organized into eight chapters and brief description of each chapter is given below: introduces the general background and basic concepts related to the present thesis work. It includes brief overview on nanostructured materials, ceramics, dielectrics, piezoelectricity, pyroelectricity and ferroelectricity. A discussion about the growing energy demands, need for green energy, various mechanical energy harvesting technologies, concept of piezoelectric energy harvesters and their working is also included. Further, literature review on various functional materials utilized for the fabrication of piezoelectric energy harvesters, important research works on zinc oxide (ZnO) and perovskite piezoelectric materials (in particular, BNKT and KNNBNZ ceramics) has been presented along with the motivation for this thesis work. describes the experimental techniques used in the process of material (nanoparticles and ceramics) synthesis, their characterization and application in the fabrication of piezoelectric energy harvesting devices. Wet chemical co-precipitation and solid-state reaction methods were employed for the synthesis of nanoparticles and ceramics, respectively. The structural and crystallographic characterization of synthesized nanoparticles and sintered ceramic pellets were studied using X-ray diffractometer (Rigaku Ultima IV) with Cu Kα radiation of wavelength 1.5405 Å. The microstructures and morphology of the samples were observed using scanning electron microscopy (JEOL JSM-6610 LV SEM and ZEISS GEMINISEM 500 FESEM). For electrical characterizations, the electrodes were prepared on both sides of the pellets using silver paste. Dielectric measurement were carried out using a LCR meter (Agilent E4980 A) as a function of temperature and frequency. The ferroelectric properties were examined using an automatic P-E loop tracer system (Marine India) and Radiant Precision LC

ferroelectric tester (Model: P-HVi210KSC). Pelletized samples were poled electrically in silicon oil using DC poling unit (Marine India). Piezoelectric charge coefficient (d33) of ceramic pellets was measured using Piezometer system (Piezotest PM300) at a tapping force of 0.25 N and a frequency of 110 Hz, while the piezoelectric properties of pelletized nanoparticles sample was measured using MTI-2100 Fotonic sensor coupled with ferroelectric tester. An electrodynamic vibration test system (Pacific dynamics, PDS-005/PDA-LK 'S') was used to apply periodic vertical compressive force to the piezoelectric energy harvester and the generated piezoelectric output voltage was recorded using digital storage oscilloscope (Rigol, DS6062).

Contents

03. DHULL (Nidhi)

Realization of NiO thin Film Based Electrochemical and Microfluidics Integrated Electrolyte Gated-FET Biosensors for Detection of Cortisol and E. Coli.

Supervisor: Prof. Monika Tomar

Th 25745

Abstract

Since the existence of mankind, humans have always had a common goal: To lead a healthy and longer life! which has greatly motivated the advances in science. The people of modern century aim to accomplish longer and healthier living by scientific and technological developments through collaboration of medicine with basic and engineering sciences. The quality of life is seen to be improving with the analysis of simple analytes in blood, urine, saliva, and even sweat. A major factor that challenges a healthy living is the presence of toxic elements in food that requires monitoring too. The most recent challenge to the mankind, COVID-19, one of the worst global pandemics, has further challenged the existing diagnostic tools. Innovations in nanotechnology have laid the path for advancement of diagnostic techniques. However, currently employed analytical techniques require tedious sample preparation steps, extraction before analysis, sophisticated instruments, and trained technical staff. Nanomaterials offer unique properties of controllable chemical structures and large surface to volume ratios. Thin film based functional devices are captivating the interest of researchers owing to their exceptional performance and small sizes. Amid various functional devices, biosensors have gained the attention of researchers due to the growing demand for sensitive and portable devices for detection of various analytes. The requisite of continuous onsite monitoring with rapid, flexible, and reliable analysis has endorsed biosensors as suitable tools. Biosensors extend leads over traditional techniques in terms of high sensitivity, short analysis time, real-time analysis, low-cost instruments, and basic pretreatment steps. With various architectural modifications such as integrated microfluidics, apart from medical diagnostics,

biosensors find applications in the fields of security from bio-threats by air, water and food monitoring, chemical and agricultural industries. The present thesis aims towards development of an integrated biosensing platform which is versatile i.e. suitable for various analytes and can be implemented in point-of-care diagnostics. Among a variety of materials, metal oxides have been identified as the appropriate matrix materials. An extensive literature survey of metal oxide-based biosensors has led to the conclusion that NiO thin film holds remarkable properties such as excellent charge transfer and high isoelectric point for development of efficient biosensors. Further, physical deposition techniques, such as sputtering, provide a better control of structural stability and surface morphology in comparison to the largely exploited chemical route. Among different transduction techniques, electrochemical biosensors exhibit quick response, low cost, and simple apparatus. Additionally, microfluidics integrated biosensors are a step further towards POC devices. When coupled with a paper-based sensing platform, the diagnostic tool can be made cost-effective and disposable to cater to the needs of developing countries. Two different classes of analytes, pathogenic *Escherichia coli* (*E. coli*) O157:H7 and Cortisol hormone have been chosen as the targets for the present work. Pathogens such as *E. coli* need detection system with lowest possible limit for prevention of life-threatening diseases. Also, metallic and metal oxide nanoparticles have been identified as the new antimicrobials for such pathogens which have developed resistance to traditional antibiotics over time. There is an urgent need for the development of non-invasive diagnostic tools for cortisol that can be employed for stress monitoring in the fields of sports, space expeditions, and military operations. Most of the existing techniques are invasive and time consuming. RF magnetron sputtering has been employed for the development of nanostructured NiO thin film matrix with increased surface roughness and good charge transfer properties for application as an efficient bioelectrode. Structural, optical, and electrical studies have been performed on NiO thin films deposited by varying the sputtering pressure, deposition gas ambience, and substrate temperature. It is noteworthy to mention that even a slight variation in deposition parameters greatly influence the film properties. The thorough analysis has enabled to identify the deposition parameters for NiO thin film that can be used as a biosensing matrix for the detection of different analytes. The RF sputtered NiO thin film has been employed as the matrix for realization of a rapid sensor with high sensitivity for *E. coli* O157:H7. The sensor exhibits a wide linear range of detection from 101 to 107 cells/mL with a significantly low limit of detection i.e., 1 cell/mL. The NiO bioelectrode has also been successfully used in milk samples containing *E. coli* O157:H7. Additionally, paper based analytical devices (PADs) have been developed for the detection of the pathogenic *E. coli* as a low-cost alternative using commonly available tools such as paper, pencil, and glue. A detection limit as low as 5 cells/mL with a linear range of 102 to 1010 cells/mL has been exhibited using a 2D PAD design. Further, antimicrobial activities of metal and iii metal oxide nanoparticles such as silver (Ag), gold (Au), and zinc oxide (ZnO) have been qualitatively analyzed for growth inhibition of *E. coli* O157:H7. A non-invasive electrochemical immunosensor has been developed for detection of salivary cortisol using RF sputtered NiO thin film as the sensing platform and covalent binding as the immobilization technique for bioreceptor. A high sensitivity in a wide linear range of 1 pg/mL to 10 µg/mL and a low limit of detection of 0.32 pg/mL has been achieved by the NiO immunoelectrode. It has been further assessed to detect cortisol in actual saliva samples and the results exhibit a great scope to foster the development of portable, integrated, and efficient miniaturized non-invasive sensing devices for cortisol determination.

Contents

1. Introduction to Biosensors, Target Analytes, & thesis Outline 2. Development of NiO Thin Film Matrix by RF Sputtering Technique for the Realization of Efficient Bio electrode 3. *Escherichia Coli* O157:H7 Detection (Electrochemical and Paper based Analytical Devices (PADs) & Growth Inhibition (using Metal and Metal oxide Nanoparticles 4.Non- invasive Electrochemical Immunosensor for salivary cortisol Detection 5.Microfluidics Integrated Electrolyte Gated FET for Detection of Cortisol using NiO Channel. Conclusion of the Thesis and Scope and Suggestions for the Future Work.

04. ISSAR (Sheetal)
Electronic Conduction through Vertically Aligned Metal Oxide Nanostructures of Titanium Dioxide.
Supervisor: Dr. Ajit Kumar Mahapatro
Th 25744

Abstract

The shape and size dependent physical and chemical properties of nanostructure materials influence the electronic and optical properties, and enhance device performance with development of compact, fast, highly efficient and reliable devices in semiconductor industries. Titanium dioxide (TiO2) is a widely studied metal oxide semiconductor for its non-toxicity, abundance availability, rich crystal phases, and high chemical and thermal stabilities. The objective of the present thesis is to synthesize highly pure and extremely stable one-dimensional (1D) nanostructures of TiO2 in different morphologies over fluorine doped tin oxide (FTO) coated substrate using chemical process of hydrothermal method and study the electronic conduction through metal/TiO2-NSs/FTO vertical device structure (VDS). Optimally grown densely packed and uniformly distributed nanostructures of vertically aligned TiO2 nanorod arrays (NRAs) and nanoflowers (NFs) are synthesized over FTO substrate, and studied their morphological, optical, material, and electronic properties. A simple and novel, angle deposition technique (ADT) is developed to engineer a floating metal layer using the physical deposition technique over sparsely distributed TiO2-NRAs and TiO2-NFs. The newly developed technique is very effective to form a fault-free metal/TiO2-NSs/FTO vertical device structure (VDS) with a top metal layer isolated from the bottom electrode. The electronic conduction through TiO2-NSs (NRAs and NFs) are measured by recording the current voltage characteristics with application of voltage sweep cycle of $0 \rightarrow +Vmax \rightarrow 0 \rightarrow -Vmin \rightarrow 0$ to(Al,Cu,Au)/TiO2-NRAs/FTO and Al/TiO2-NFs/FTO structures in VDS configurations. The observed two distinctly captured events of resistance switching (RS) and negative differential resistance (NDR) are attributed to the presence of traps in TiO2-NSs originated from the oxygen vacancies in TiO2 nanorods and support the appearance of energy levels observed in optical spectra. Physical models are proposed and these electronic events are explained with potential landscape diagram. The experimental and theoretical understanding of this research work could be utilized to demonstrate for designing semiconductor switching devices.

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1. Introduction. 2. Experimental Detail 3.Chemical Recipe Optimization and Experiments Performed on Well-Defined TiO_2 Nanostructures 4. Engineering of Floating Metal Layer as Top Electrode over Vertically Aligned Nanorod Arrays Using Angle Deposition Technique 5. Electronic Conduction through Vertically

Aligned Titanium Dioxide Nanorod Arrays 6. Electronic Conduction through Layers of Titanium Dioxide Nanoflower over FTO Substrate 7. Summary and Future Work. Appendices and List of Publications.

05. KUNDU (Richa)
Study of Extra-tidal Stars in the Galactic Globular Clusters Using the *Gata* Photometric and Astrometric data.
Supervisors: Prof. H.P.Singh and Prof. Dante Minniti
Th 25749

Abstract

A globular cluster is a group of stars having same age which were formed from the same cloud having same initial composition. As the cluster ages, stars with different masses evolve on different time scales making them perfect stellar laboratories for studying stellar evolution. Also, globular clusters are old stellar objects formed in the early stage of the host galaxy. Hence, they are also useful in studying chemical and physical properties of the host galaxy in its early history. All the stellar objects present in a galaxy are influenced by the gravitational forces of other stellar objects around them evolving under the influence of the galactic potential. Similarly, Galactic globular clusters also evolve under such potential. Owing to such forces the clusters may lose its loosely bound stars. The stars which were pulled out of the cluster radius, now residing outside it are know as the extra-tidal stars. These stars can have different distribution in the 2D phase space. They may be extended to several degrees in two opposite directions forming an 'S' shaped distribution known as tidal tails. They may form a spherical envelope around the cluster or they may form overdensities distributed around the cluster outside its tidal radius. The distribution of these stars around the cluster is dependent on the internal and external forces acting on the cluster. Hence, the distribution of the extra-tidal stars helps us in understanding the various forces that act on the cluster in its lifetime. In this work, we analysed the distribution of such stars around Galactic globular clusters (GCs). The extra-tidal stars reported in this work are selected on the basis of *Gaia* photometric and astrometric data. These stars are selected on the basis of their position in the 2D space, their proper motions (PMs) and cluster's color-magnitude diagrams (CMDs). All those stars which are at least one tidal radius away from the cluster center, whose PMs match with the proper motionof the cluster (within the sigma range) and lie on the color magnitude diagram of the cluster were considered as the extra-tidal stars. This approach is based on the fact that the stars which are lost from the cluster must have similar motion as the cluster itself (at least while they are in its vicinity) and should have similar metallicity. There is some probability of including contaminants, especially when dealing with the clusters present in the regions having high stellar density. We estimated these probabilities by taking dummy regions around the clusters and applying same criteria which were applied while selecting the extra-tidal stars. This provided us an estimate of the random stars which may fall under the similar range as the extra-tidal stars. In this thesis, firstly we analysed a sample of 56 Galactic globular clusters using *Gaia* DR2 catalogue for RR Lyrae stars. We searched the area between 2/3 tidal radius and 3 tidal radius around these clusters and found 30 extra-tidal RR Lyrae stars distributed around 11 of GCs. However, only 2 clusters, namely, NGC 3201 and NGC 5024 have more than 2 extra-tidal RR Lyrae stars. However, the presence of RR Lyrae stars around these 11 clusters indicated that more extra-tidal stars of differen population may be present. Next we used *Gaia* DR2 astrometric and photometric data to analyse the region around NGC 6362. Here, the area up-to 5 tidal radius away from the cluster center was considered. We found 259 extra-tidal stars distributed outside the cluster. We

estimated that the cluster loses ~4.1×10−6 M⊙ yr−1. We also used GravPot16 to extrapolate the orbit followed by the cluster in last 3 Gyrs. However, the extra-tidal debris detected is not aligned with the orbit. The distribution of the tidal debris and cluster's orbital parameters indicated that extra-tidal debris around the cluster may be due to the combined effect of both tidal forces and disc shocks. We also analysed NGC 2808, NGC 6266 and NGC 6397 using the same criteria stated above and found 126, 107 and 120 extra-tidal stars distributed around these clusters, respectively. Our analysis shows that the stars distributed around NGC 2808 and NGC 6397 are a result of the combined effect of both disc shocks and tidal disruptions. However, the stars around NGC 6266 are symmetrically distributed and most likely indicating that the cluster has an extended stellar envelope.

Contents

06. Munjal (Dipti)
Study of Confined atoms in external fields.
Supervisors: Prof. Vinod Prasad and Prof. Poonam Silotia
Th 26531

Contents

07. NEYAZ ALI
Dosimetry of High Energy Radiations Using Some Rare-Earth Doped TLD/OSLD Phosphors.
Supervisor: Prof. P. D. Sahare
Th 25743

Abstract

The thesis consists of seven chapters. First and second chapters the introduction and material characterization and techniques used are discussed, respectively. From third to fifth chapters include the research works on done on rare earth metal Ce and Tb doped and co-doped NaLi2PO4as well as on SrB4O7:Eu. The work is related to dosimetry of high-energy radiations (e.g., -rays) using TL and OSL techniques. NaLi2PO4 is a very interesting and versatile phosphor material. There are not many phosphors those could be used as TLD and OSLD phosphor but earlier work from our group shows that this this material has proved to be a good TLD and OSLD phosphor. Therefore, doping of other rare-earth impurities, such as, Ce, Tb and their cooping was tried. Other properties of the material that make it good phosphor material are easy method of preparation (solid state diffusion method), non-hygroscopic, non-toxic. This material has orthorhombic structure. In the present work it was found that the OSL sensitivity of NaLi2PO4:Ce is six times more sensitive than standard commercially available

OSLD phosphor Al2O3:C. This phosphor is so sensitive that after 500Gy it is unable to read the OSL as PMT gets saturated. The OSL could only be recorded using quite dark natural density filter. It was also found that dose range was linear from 3mGy to 500Gy. OSL study of NaLi2PO4:Ce was discussed in third chapter. TL and OSL of NaLi2PO4:Tb is discussed in chapter four. It was found that TL of the phosphor is 1.2 and 1.5 times more sensitive than TLD-900 and TLD-700H, respectively, whereas OSL intensity was five times more than Al2O3:C. The dose range was found to be 10 Gy-10kGy where the dose response was found to be almost linear. Fading of the phosphor was found 60% in two days. However, it does not fade much afterwards. TL and OSL studies of NaLi2PO4:Ce,Tb are discussed in Chapter five. It was seen that this co-doped phosphor has TL intensity was 4 and 4.6 times more sensitive than TLD-900 and TLD-700H. The OSL intensity is eleven times less than the standard phosphor Al2O3:C.The dose range where dose response is linear was found to be 10 Gy-10kGy. It is surprising to see that the phosphor is highly sensitive as well as it has very wide dose range and can be used for measuring very high doses that could otherwise be measured using nanophosphors only. The phosphor alsoshows very low fading, i.e., only 0.73% in 30 days. In chapter six deals with TL study of SrB4O7:Eu phosphor. SrB4O7 prepared again by solid state method. This phosphor is again non hygroscopic, non toxic and cost effective material. The TL intensity found 2 and 1.33 times than TLD-900 and TLD-700H, respectively. In the last 7th chapter is conclusion of whole thesis and future scope and plans are also discussed in this chapter.

Contents

08. PANDEY (Rakesh Kumar)
Ion Implantation Induced Modification in the Structural, Morphological, and electrical Characteristics of GaSb films Grown By Molecular Beam Epitaxy.
Supervisors: Prof. Shyama Rath and Dr. Puspashree Mishra
Th 25737

Abstract

Semiconducting GaSb is suitable for various strategic and civilian applications such as IR detectors, transistors, lasers, superlattices, LED, etc. It is challenging to achieve a high crystalline quality of GaSb film due to its 7.8% lattice mismatch compared to the substrate, GaAs. There are reports to grow GaSb film on GaAs using different approaches yet low-temperature (LT) nucleation is a novel method, showing possibility for GaSb epitaxy on GaAs. This work aims to achieve a highly crystalline GaSb buffer layer on GaAs substrates using an approach of LT nucleation in molecular beam epitaxy system. As grown bulk or thin film GaSb is p-type. Ex-situ doping using ion implantation is an essential step in device fabrication. In this study implantation of natural donor S and amphoteric Si have been undertaken to act as n-type dopants in GaSb. Nanoporosity of semiconductors leads to sensing and alternate substrate applications. Various ion

species, e.g., Au, Ar, Kr, I, Ga, etc. are reported for porosity development in GaSb. Yet, there is no discussion on the doping characteristics of nanoporous GaS films using the implantation process. Porosity development using Si ion implantation in GaSb is studied and characterized with varying Si ion energies and fluences. Si ion implantation induced structural, topological, and chemical characteristics are studied using HRXRD, Raman spectroscopy, AFM, FESEM, XPS measurements. Doping characteristics of ion implanted GaSb is evaluated using Hall and variable temperature I-V measurements. Nanoporous GaSb with smooth topology and controlled electrical characteristics are obtained using Si ion implantation. The mechanism of porosity development and variation in electrical characteristics has been investigated using variable energies (50-150 keV) and Si ion fluences (1x1012-1x1015 ions/cm2. Finally, the dopant activation of both S and Si ions at room and low temperature has been studied.

Contents

09. PURI (Nidhi)
Electronic and Thermoelectric Properties of Hot-Pressed Ceramics of Calcium Cobalt Oxide.
Supervisor: Prof. Ajit Kumar Mahapatro
Th 25757

Abstract

The electronic charge conduction in bulk micro/nano-structured materials contributes significantly in understanding the inherent properties for development of emerging electronic, optoelectronic, and thermoelectric (TE) devices. The possible conversion of heat into electrical energy using the concept of TE power generation based on the principle of Seebeck effect, has been considered as one of the most promising approach to harvest electricity from waste heat sources. Potential TE materials require large Seebeck coefficient (S), low electrical resistivity (ρ), and low thermal conductivity (κ) to obtain enhanced figure of merit, ZT = S2/$\rho\kappa$. Oxide materials have gained attention due to non-toxic character, natural abundance, chemical/thermal stability, and potential to operate in high temperature TE applications. Among different oxides, calcium cobalt oxide (Ca3Co4O9) is a misfit-layered oxide structure showing characteristics with demonstration of an effective TE material with high thermal/chemical stabilities. The current thesis work is mainly focused on synthesizing perfectly composed and well-engineered micro and nanostructures of Ca3Co4O9 semiconductor material with tuned materials properties favorable for exhibiting enhanced TE behavior by following low cost processing techniques with mass-scale production capability. This work presents the preparation of Ca3Co4O9 micro- and nano-powders through ball milling and consolidation of resulting powders for achieving fully dense pellets using hot-pressing technique. Powder processing of Ca3Co4O9 through calcination of the mixed precursors and further consolidating into perfectly dense pellets, are the two essential steps followed sequentially to develop test materials for utilization in TE modules. Also, graphene oxide (GO) and

graphene oxide quantum dots (GOQD) are mixed in Ca3Co4O9 in various proportions to obtain optimized amount for achieving uniform and stable nanostructures of Ca3Co4O9 powders. Further, the temperature dependent (10-400 K and 300-770 K) electronic and TE transport properties are studied in newly developed hot-pressed pellets of pristine and GO/GOQD mixed Ca3Co4O9.

Contents

10. RAWAT (Bharti)
Model Independent Searches for Dark Matter at a Linear Collider.
Supervisor: Prof. Debajyoti Choudhury
Th 25746

Abstract

In 1933, Fritz Zwicky pointed out that the observed average velocity dispersion of galaxies in the Coma cluster was considerably higher than the expected values. By assuming only gravitational interaction and Newtonian gravity (F / 1=r2) for the galaxies in the Cluster and applying the virial theorem, Zwicky found that the vast majority of the mass of the Coma Cluster was for some reason non-luminous. In the 1970s, the independent studies by Vera Rubin and Albert Bosma on the measurement of the rotation curves of individual galaxies also indicated the presence of non-luminous matter. The astonishing 'flat' rotation curves obtained from various astrophysical observations are regarded as the beginning where the idea of dark matter (DM) which existed from the very early days started getting accepted. The fitting of the cosmological observables from the recent Planck data infers a value of DMh2 = 0.120 _0:001. The corresponding value deduced from the data collected from the 9-year WMAP measurements is DMh2 = 0.1138 _0:0045. These results imply that the total energy density of the universe receives a contribution of approximately 26% from cold DM, and the contribution of the baryonic matter is only about 4% of the total energy density. Further evidence comes from weak gravitational lensing and the matter distributions of colliding galaxies. Also, the requirement of DM in cosmology arises to generate the density perturbations that led to large-scale structure and to account for Big Bang nucleosynthesis.The quest to unravel the identity of DM is of central importance in studies focused on the understanding of the universe at both the largest and smallest observable length scales. Since the evidences are solely based on the gravitational influence of dark matter, it has piqued the interest of many particle physicists. The fact that a massive O(100GeV) stable particle _ with near–weak scale interactions can constitute an attractive candidate for the Dark Matter in the universe (while satisfying all of competing constraints from the relic density, large-scale structure formation as well as myriad other cosmological and astrophysical observations) is well-known. Astrophysical and cosmological observations allow us to infer the total density of dark matter in the universe. However, a precise determination of the dark matter properties and the parameters of the underlying theory requires other detection methods. The first class of experimental signatures

are the Direct detection ones where the key idea is to study the scattering of a DM particle off the detector material. The second possibility is the annihilation of DM particles resulting in the production of standard model particles which, in turn, could provide a possible way to detect these particles. This forms the basis of the Indirect detection methods where the focus lies in the observation of cosmic-rays created by WIMP annihilations in galactic halos and the signatures from WIMPs captured in massive bodies such as the sun or stars. The primary focus of the work presented in this thesis is the third category of dark matter detection experiments, i.e., particle accelerators. The collision of ordinary standard model particles at tremendous energies could lead to the emergence of undiscovered particles and, this fact forms the basis of collider experiments. We, therefore, look for the possibility of producing DM particles at a future linear collider (the ILC) via processes inverse to those that result in DM annihilation. The International Linear Collider is a proposed e+e collider

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1. Introduction. 2. A Brief Review of Relic Density Calculation 3. Fermionic Dark Matter 4. Dark Matter Detection Methods 5. Scalar Dark Matter 6. DM Production at ILC 7. Summary. Bibliography.

11. SARAN (Martina)
Thermoluminescence (TL) and Lyoluminescence (LL) in Some Luminescent Phosphors Effect of Particle Size.
Supervisor: Prof. P.D. Sahre
Th 25756

Abstract

In today's world where we are so much surrounded by electronic gadgets which constantly emit radiations, our lives are in the fear of radiation ill-effects. Radiation emission is a serious problem in the era of science and technology. Even if we travel in airplane flights our body is exposed to cosmic radiation from the universe which should be monitored. The world is brawling with nuclear wars and research work is going on nuclear power plants which again going to affect our well beings and can cause numerous health issues which can lead to even mutation. Some of the life-threatening diseases like cancer require radiation therapy in very low doses to cure by damaging only the malignant cells. Already Hiroshima, Nagasaki & Chernobyl are some examples of mishandling and misfortune. For measuring all those radiations some kind of accurate measuring dose detectors are required. For manufacturing such a sensitive tissue equivalent dosimeters we need TL/OSLD/LLD techniques to readout absorbed radiation in our body. However, the monitoring using TL/OSLD/LLD depends on the sensitivity of materials used. Till date, very few materials have find the commercial value and are very costly. So it becomes very necessary to get alternative to those materials. In this Thesis, we proposed a comparative study of some rare earth activated TL/LLD materials and evaluated them. However, the materials suggested in the report have sensitivity more than the commercial materials and we also investigated the nano form of such samples for TL also pH studies to enhance the intensity and check the characteristics of the decay curve with different solutions may found importance in personal as well as environmental radiation monitoring. On the basis of this review of the literature, we have found that none of the luminescent material has been followed the essential properties of ideal dosimetry material so far. Therefore in order to get started a systematic investigation for material synthesis and

characterization of luminescent properties for developing a new luminescent material.

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1. Introduction. 2. Characterization Techniques 3. Particle Size Effects on the dosimetry Characteristics of $K_3Na(SO_4)_2$:Eu TLD Micro-and Nanophosphors 4. Thermoluminescence in Eu Doped $NaLi_2PO_4$TLD Nanophosphor : Effect of Particle Size on TL 5. Effect of Particle Size and PH on Lyoluminescence of $K_3Na(SO_4)_2$:Eu^{3+} Phosphor for its Application in Dosimetry 6. Summary and Scope for Future. List of Publications.

12. SAURABH KUMAR
Laser-Plasma Proton Acceleration with Solid Targets.
Supervisor: Prof. D. N. Gupta
Th 25755

Abstract

With the advancement in pulsed laser technology, laser intensity reaches upto relativistic range with pulse duration in the picosecond or femtosecond range. These high intensity laser pulses give immense boost to the field of laser matter interaction. Over the past few decades, the generation of high energetic proton beams by relativistic intense laser pulses has attracted great attentions. Startin from the pioneering endeavors around 2000, several groups have demonstrated muliti-MeV proton beams along with low transverse emittance and ps-scale pulse duration emitted from solid targets. Due to these superior characteristics, laser driven proton beam can have many applications in various fields including medical, nuclear fusion etc. However, the different mechanisms that have been proposed to accelerate proton need to be further studied so that have a better understanding of the various physical aspects as well as getting control over the different laser and plasma parameters. The major aspect of this thesis is to understand the physics of laser solid interaction via particle-in-cell (PIC) simulation and theoretical analysis, and to explore new ways to increase energy and coupling from laser energy to the accelerated protons under current experimental conditions. Particle-in-Cell(PIC) simulation code has been used to study proton acceleration from solid targets to further extend our understanding about the acceleration process with the aim of creating improved proton beam quality. Simulation helps us to understand and interpret the experimental results and can also provide information which is difficult to measure experimentally. The works presented in this thesis are widely based on one acceleration mechanism namely "Target Normal Sheath Acceleration (TNSA)". It involves the interaction of solid target (thickness in the range of few microns) with ultraintense laser pulse (~ 1020 W/cm2) to accelerate protons at rear side of the target. Theproton beam quality in TNSA scheme depends on many laser-plasma parameters such as the target thickness, the target material, the lateral target confinement, the pulse polarization, the pulse length, the laser pulse shape and the presence of preplasmas. We have studied the acceleration process by modifying the target and considering preplasma in front of the main solid target and also employing asymmetric laser pulse. The combined effect of pulse asymmetry in the presence of preplasma enhances the peak energy of the protons. In our second task which is also based on TNSA method, we have employed dual laser pulse with an appropriate delay between them to modify the proton spectrum. We obtained the results for the optimized condition involving the laser intensity and pulse duration for the two laser pulse case. Continuing with target modification, we have proposed novel idea of groove target in one of our work. The presence of groove on the target surface greatly enhances the laser absorption and helps in increasing

the proton energy. This thesis also explore some other acceleration mechanisms such as radiation pressure acceleration (RPA) and shock wave acceleration. We have considered the case of mixed polarizatio consisting of linearly and circularly polarized for laser interaction with a near critical density target. The interaction shows the signature of hybrid acceleration mechanism involving RPA and shock wave acceleration with acceleration of protons at front as well as rear side of the target. All these studies suggest that there are various parameters that affect the acceleration mechanism and beam quality. Understanding their impact on the acceleration process is very important to get control over the generated beam. With continued research and new findings associated with laser-plasma interaction, there is a strong possibility to develop a table-top proton accelerator in near future.

Contents

13. SHANDILYA (Ankur)
Upconversion Luminescence and thermometry in lanthanide (Ln^{3+} = Er^{3+} , Yb^{3+}) doped $SrMoO_4$ Phosphor.
Supervisor: Prof. K. Sreenivas
Th 25734

Abstract

In recent years molybdates ($SrMoO_4$) with tetrahedrally coordinated $[Moo4]^{2-}$ clusters and rare earth dopants have proven to be stable host materials for light upconversion studies. The present thesis investigates structural distortion, luminescence quenching occurring at a specific dopant concentration, and the local disorder in Er^{3+}-Yb^{3+} co-doped $SrMoO_4$. The focus is towards a better understanding of the remarkable enhancement in the upconverted light intensity, and also examine the temperature sensing ability over a wide temperature range. The effects of interaction with Er^{3+} and Yb^{3+} ions in the $SrMoO_4$ lattice, cooperative luminescence from the Yb^{3+} ion pair, and the increased sensitization from Yb^{3+} - $(MoO4)^{2-}$ dimer complex have been analysed. Performance of the prepared phosphors in powder and ceramic form are compared and the influence of the dopants (Er^{3+}, Yb^{3+}) on the structural and thermometric properties has been studied. Single phase ceramic compositions of $Sr_{1-x-y}Er_xYb_yMoO_4$ were synthesized by solid state reaction with different combinations and concentrations of the dopants (Er^{3+}, Yb^{3+}). Structural changes in SrO_8 deltahedron and MoO_4 tetrahedral units due to Er^{3+} and Yb^{3+} ion substitution for Sr^{2+} show maximum tilt in the oxygen octahedra of the SrO_8 for an optimum Yb^{3+} content of y = 0.03. Concurrent changes in the Sr–O and Mo–O bond length for Yb^{3+} concentration (y = 0.03) lead to lattice distortion which correlates with the quenching observed in the UC emission intensity. Structural changes in SrO_8 and MoO_4 clusters, evolution of disorder and defect phase are evidenced through Raman spectroscopy. Distinct appearance of high-frequency Raman modes is attributed to the formation of a defect-induced phase which leads to a disorder in the $[MoO_4]^{2-}$ cluster due to Er^{3+} and

Yb^{3+} incorporation in $SrMoO_4$ lattice. The possible formation Yb-$[MoO_4]^{2-}$ dimer complex is envisaged to explain the observed enhancement in the green emission. Separate experiments have been designed with Mo^{6+} dopant in $SrWO_4$ to confirm the formation of Yb-$[MoO_4]^{2-}$ dimer. Selective enhancement in UC emission due to sensitization from $[Yb^{3+}$-$MoO_4]^{2-}$ dimer complex is further investigated by substituting Mo^{6+} for W^{6+} in $SrWO_4$ host lattice. Structuralchanges in SrO_8 deltahedron and WO_4 tetrahedral units due to Er^{3+}-Yb^{3+} ion substitution for Sr^{2+} and Mo^{6+} ion for W^{6+} are confirmed by Rietveld refinement of X-ray diffraction data. [Yb-$MoO_4]^{2-}$ dimer complex formation with Mo^{6+} ion substitution is confirmed, and its role in the enhancement of the green emission is ascertained and confirmed through excited state decay life time measurements. UC luminescence properties of the prepared phosphors are compared in powder and ceramic form. Enhanced grain growth in ceramics is shown to improve the emission intensity. Ceramics prepared with the optimized composition $Sr_{0.96}Er_{0.01}Yb_{0.03}MoO_4$ show a good temperature sensitivity over a wide temperature range (93-773 K), and maximum temperature sensitivity of (0.0139 K^{-1}) at 473 K. The linearity of the sensor is seen for a limited range 203 to 403 K, and measurement accuracy is found to be within ⍰0.2 K to +0.2 K.

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14. SHARMA (Mohit Kumar)
Cosmological Perturbations and Stability of Interacting Scenarios in Scalar-Tensor Equivalent Modified Gravity.
Supervisors: Dr. Sourav Sur and Prof. Amitabha Mukherjee
Th 25758

Abstract

In spite of a very long chain of success, the adequacy of General Relativity (GR) remains questionable till date, especially, when confronted with some of the stringent problems in cosmology, such as that circumventing the origin and nature of dark energy (DE), which is supposed to drive the late-time accelerated expansion of the universe. A considerable attention have therefore been drawn by the cosmological scenarios emerging from the so-called modi_ed gravity (MG) theories that go beyond the realm of GR. Although the observations grossly concord to its cosmological constant candidature of the DE component, some room is there to look for its dynamical evolution, at least to a substantial degree of mildness. Moreover, the cosmological studies involving e_ective DE interaction(s) with matter _eld(s) have gained importance in recent years, from the point of view of the potential aversion of the problem of coincidence, i.e. the same level of dominance of the DE and the (visible+dark) matter densities, right at the present epoch. Apart from the purely phenomenological suggestions for such DE-matter (DEM) interactions, there are instances of their natural perception in well-motivated cosmological scenarios, most notably, those emerging from the scalar-tensor equivalent MG formulations, under conformal transformations from the original

Jordan frame to the Einstein frame. As such, con- sidering the DE essentially as a dynamical geometric artefact, we focus on studying the consequences of its interaction with matter in this thesis, by resorting to a scalar-tensor formulation of a speci_c sort, having equivalence with that of a wide range of MG theories in the literature. While in the standard Friedmann-Robertson-Walker (FRW) framework, exact solutions of the cosmological equations exist for such a speci_c con_guration, we examine the mildness of the DE dynamics and the strength of the DEM interaction, by carrying out the statistical estimation of the relevant parameters, using the type Ia Supernovae and the Hubble observational data. One may nonetheless note that however mild the DE dynamics may be, at the background cosmological level, the e_ects of such dynamics on the spec- trum of the linear density perturbations may be signi_cant. Therefore, an analysis of the observational data on the growth of the matter density perturbation, or that of the large-scale structures (LSS), is crucial for constraining dynamical DE models, especially those in which the DE interacts with matter. Speci_cally, the matter density contrast, which is by and large scale-invariant I the deep sub-horizon limit, not only gets dragged as the interaction a_ects the background Hubble expansion rate, but also receives a contribution from the scalar _eld perturbation, which oscillates about a non-zero mean value. As such, the standard parametrization ansatz for the matter density growth factor becomesinadequate. So by modifying it suitably, and also _tting numerically the growth index in terms of the background level parameters, we make direct estimations of the latter, using a redshift space distortion (RSD) subsample and its combination with the observational Hubble data. On the whole, the para- metric estimates show consistency with that obtained separately by resorting only to the background cosmological solution, mentioned above. Finally, we carry out a detailed dynamical analysis for our DEM interacting system, up to the linear order of the density perturbations (i.e. inhomogeneities). While at the background level, the analysis shows a stable phase space trajectory representing a purely DE dominated (de-Sitter) phase of the universe asymptotically, a two-fold degeneracy in the spectrum of the critical points results at the inhomogeneous level, due to the possible growth and decay of the total matter density perturbation. Furthermore, the only physically relevant and stable phase space solution is the one that transpires to the exact analytical solution of the background level evolution equation for the scalar _eld.

Contents

15. SHARMA (Prerana)
Strong Coupling Effects on Different Instabilities in Non-ideal Plasma.
Supervisors: Prof. Avinash Khare and Debajyoti Choudhury
Th 26243

Abstract

This thesis investigates the effect of strongly or moderately coupled ions on various instabilities in the presence of weakly coupled classical or degenerate electrons, depending on plasma density. In the weak coupling regime (□□1), the plasma remains gaseous. At Γ ~ 1, viscosity enters the system profoundly, and as Γ increases, elastic property gradually becomes important as the plasma state

transitions from the gaseous to the liquid phase. At very high values of the coupling parameter □□□□□□□175 *c* the ion species in the plasma crystallizes. However, there is an intervening interesting regime of the coupling parameter, *c* 1□□□□□□□□□, where the ions are neither fixed at specific lattice locations like crystal nor can they freely move like gas. The particles are mobile but they tend to retain a certain memory of their past locations. This leads to the medium exhibiting certain elastic characteristics like solid and viscous fluid. It has, therefore, been felt that a visco-elastic fluid description may suitably be applied to the plasma medium. In our thesis, the dynamics of strongly coupled ion fluid are governed by the generalized hydrodynamic (GHD) model which was first proposed by Frenkel [Frenkel Y I, *Kinetic Theory of Liquids* (Clarendon, Oxford, 1946)] for viscoelastic liquids. GHD theory is a phenomenological model that extends the usual Navier-Stokes equation to higher frequencies and it is motivated by a model that combines the properties of both solid and liquid bodies by generalizing the transport coefficients in the Navier-Stokes equation, using a memory function *m* □ ,which is a function of □. For □ 0 *m* □ , there are no memory effects and the GHD equation reduces to the standard Navier Stokes equation for viscous medium. On the other hand, in the limit □□ *m* □ memory effects persist and the medium acquires solid-like elastic properties. The intermediate regime for which *m* □ is finite, the medium has viscous as well as solid-like elastic properties, i.e., visco-elastic fluid. The electrons are still considered in weakly coupling regime and they can bedegenerate or non-degenerate depending on the plasma density. Such plasmas are of interest both for technical applications such as inertial confined fusion (ICF), plasma heating, laser-driven ion accelerator and for basic scientific reasons (for example, astrophysical studies) etc.

Contents

16. SHARMA (Yashika)
Investigations on Structural, Thermal and Charge Transport Properties of Binary and Ternary Chalcogenide Glasses.
Supervisor: Prof. Sevi Murugavel
Th 25736

Abstract

In this modern technology world, the necessity of collecting data through a safe and reliable media is of much concern and remarkably in demand. Starting from the music player to store email and important information in mobile phones and the data that we store in our pen drives are the basic requirements of our daily routine. Commercially, the information storage market has grown tremendously in the last two decades to reach 20 $ billion /year of turnover in the research industry of semiconductors. The concept behind this success story is related with providing the higher density chip in a short pack with reduced cost and fast handling speed. Thus, the memory based applications tends to increase with increasing research and developments. However, this concept is not fully served because of various limitations in the existing flash memories and hence, there is still a need for next generation non-volatile memory (NVM) that will show the path towards bringing a multilevel storage concept with better endurance and input/output performance. Fortunately, the next in-line candidate for the flash replacement are phase change

random access memories (PCRAM). Currently, PCRAM are progressing towards the real time integration. In the past few decades, they have achieved tremendous success in many issues like programming current reduction, large cycle endurance and increased data retention and fast switching speed. This memory is based on the switching between its two phases that can exist at the same temperature and pressure conditions. The state of the material can be switched between these two phases rapidly and reversibly with large number of cycles. The performance of NVM- PCM devices is based on the properties of these two phases thus it is very important to understand the material's properties at atomic scale level. The material that are suitable for phase change memory applications are chalcogenide materials which are the special class of amorphous semiconductors (can be binary, ternary and quaternary compositions) of chalcogen atoms Te, Se or S alloyed with group IV or group VI elements. Among the chalcogen atoms, telluride gasses are of much importance because of its large optical and electrical contrast between their two phases. It has been already proved that the material of pseudo binary tie line between Ge-Te and Sb2Te3 are very much suitable for PCRAM applications and has already been commercialised in blue-ray discs

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1. Introduction. 2. Experimental and Characterization techniques 3. Role of quenching rate on the Structural Thermal and Electrical Properties of $Ge_{20}Te_{80}$ Glasses and Crystals 4. Effect of aging on thermal and Electrical Properties of $Ge_{20}Te_{80}$ Chalcogenide Glass 5. Effect of Te Addition on the Structural, Thermal and Electrical Transport Behaviour in $Ge_{20}Se_{80}$ Glass 6. Structure, Thermal and Electrical Transport Behaviour in Te Incorporated $Ge_{20}S_{80}$ Glass 7. Summary and Future Perspective.

17. SINGH (Gaurav)
Multi-Wavelength Study of Hot Stellar Population in Galactic Globular Clusters.
Supervisors: Prof. Patrick Das Gupta and Ramakant Singh Yadav
TH 25747

Contents

1. Introduction. 2. Observations, Data Reduction and its Calibration 3.Feild Star Decontamination of Structural Parameters 4. Dynamical Status of Galactic Globular Clusters 5. Study of Peculiarities in the Horizontal Branch stars and Second Parameter 6. Highlights, Conclusion and Future Prospects.

18. SINGH (Gurvinder)
Aspects of Primordial Nucleosynthesis in a Linearly Coasting Universe.
Supervisor: Prof Brajesh Chandra Choudhary
Th 25739

Abstract

Big Bang Nucleosynthesis (BBN), the theory of chemical element formation in the early universe, offers a probe to the universe when it was young, hot and dense. BBN in the standard model of cosmology known as Standard Big Bang Nucleosynthesis (SBBN), accounts roughly well for the primordial abundances of light elements spanning a range over 9 orders of magnitude. The primary cocordance of SBBN is believed to be the abundances of deuterium and helium. However, a closer examination of the theoretical predictions contrasted with the

observations unveils a few challenges to the theory. Examples are: (i) deuterium dispersion in high-redshifted QSOALS (quasi-stellar objects absorption line systems), (ii) inconsistency in the theoretical predictions and observational values of lithium-6 and lithium-7, and (iii) extremely low level of metallicity produced primordially. In view of these challenges to SBBN, we report our study of primordial nucleosynthesis in an alternative class of cosmologies known as "Power Law Cosmologies". Such cosmologies are characterized by a scale factor, a(t), having a power law variation: $a(t) \propto t^{\alpha}$. We confine ourself to a particular class having $\alpha = 1$. Such a linearly coasting cosmological model provides a good account for the high red-shift objects, resolves the age problem of universe and is free from the fine-tuning problems. In such a universe, however, the baryonic mass density required to produce the correct amount of helium is more than twice the dynamical mass estimates of the universe. In this thesis, we attempt to resolve this mass discrepancy in the linearly coasting cosmology by proposing that the baryon density was inhomogeneous at the epoch of primordial nucleosynthesis in the early universe. Such inhomogeneities arise as a consequence of a first-order phase transition from quark-gluon plasma to hadronic matter in the early universe. The observed metallicity at high red-shifts and in low-mass stars can be hopefully accounted for in such a model. We study a simple minded two zone model and demonstrate how a possible parameter space can be obtained in a high baryonic-density versus low baryonicdensity plane from the observational constraints on helium abundance. In this allowed region the amount of metallicity produced is sufficient for the fragmentation of protostellar clouds, leading to star formation. This amount of metallicity is consistent with the lowest metallicitycontent observed in galactic halo stars. The resulting mass density would allow a closure of the mass density of the universe by baryons alone, with no need for any exotic dark matter. The estimates of these elemental abundances depend on the thermonuclear reaction rates. These reaction rates could be the key to alter nucleosynthesis yield in a way so as to be in agreement with the observations and simultaneously, the required baryonic mass density could be consistent with the mass density estimates of the universe. The challenge is to identify, quantify and rectify the possible uncertainties in these rates. One such aspect of these rates is the screening of Coulomb potential between charged nuclei due to the presence of a large number of charged particles surrounding each nucleus in the early universe. In his thesis, we also investigate the screening of Coulomb potential between the charged nuclei at high temperatures when all the nuclei were in ionized form in a plasma consisting of a dense cloud of electron - positron pairs. We have numerically evaluated the screened Coulomb potential between the two charged nuclei for a few reactions that are important for the primordial nucleosynthesis in the linearly evolving universe. The potential is evaluated at different temperatures as a function of distance between the nuclei. We find significant differences between the Coulomb and screened Coulomb potentials for the heavier nuclei. The probability of a nucleus to tunnel through this potential barrier is also numerically evaluated.

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19. SRIVASTAVA (Priyanka)
Study on Carbonaceous Aerosols over the Central Himalayas.
Supervisors: Prof. T. R. Seshadri and Dr. Manish K. Naja
Th 25748

Abstract

In this era of rapid urbanization and industrialization, large dependence on carbon-based fuel has led to a substantial increase in the concentrations of carbonaceous aerosols (organic carbon-OC and black carbon-BC), which are emitted from their incomplete combustion. These aerosols are important because of their direct adverse impacts on health and radiation budget in addition to their indirect effect in altering the properties of clouds. However, assessing their overall impact is challenging due to the large spatial and temporal variations in their emissions, types of mixing states and the dynamic atmospheric processes. Despite the scientific attention on this, continuous and high-resolution observations of carbonaceous aerosols are still very limited in South Asia and almost nonexistent in the serene yet fragile Himalayan region, which has a complex topography with largest ice mass outside the poles and lies near polluted regions like the Indo-Gangetic Plain. Addressing the aforesaid issues, this thesis work presents results from the comprehensive analysis of the rigorous long-term online observations of OC, elemental carbon (EC), BC, CO and absorption cross-section along with results from satellite observations and model simulations over a high-altitude location in the Central Himalayas (ARIES, Nainital, 29.4oN, 79.5oE, 1958 a.m.s.l.). It starts with a thorough introduction of aerosols, particularly focusing on carbonaceous aerosols, the significance and challenges in their study over this region and the importance of this work to overcome these challenges. Later, it explains the *in-situ* instruments, satellite products and models used in the work for their characterization. Then it chapter-wise details the obtained results. In Chapter 3, the first year-round diurnal variations of OC and EC over a Himalayan site are presented. Analysis of continuous high-resolution measurements from 2014 to 2017 reveals a unimodal diurnal variation in both OC and EC, in contrast to the bimodal pattern observed at any continental polluted site. Using concentration weighted trajectory (CWT) and coinciding rise in OC/EC ratio from 4.6 to 7.9 during fire events it is shown that the biomass burning in northern India is one of the major sources for the springtime maximum even at this high-altitude. Correlation between OC-EC and the boundary-layer height suggests the influence of local sources during autumn and winter. Towards the end, radiative forcing estimates at diurnal scale are derived and it is shown that the atmospheric radiative forcing due to EC during the afternoon is about 70% higher than the forenoon one. Several studies have shown large variability in Mass Absorption Cross-section (MAC) values over distinct geographic locations and seasons. Therefore, in Chapter 4, we examine the accuracy and consistency of MAC in Aethalometer (AE-42) by deriving the foremost multispectral site-specific MAC values over the site. The results reveal that the annual mean value of MAC (5.03 ± 0.03 m2 g-1 at 880 nm) is significantly lower than the constant value used in the Aethalometer (16.6 m2 g-1 at 880 nm). The estimated MAC values do not show a clear diurnal variation but significant seasonal variation (e.g., 3.7 to 6.6 m2 g-1 at 880 nm) owing to variation in air mass, meteorology and contribution of absorption by species other than EC. It is shown that not using the site-specific MAC, leads to an underestimation of BC by a factor of upto 3.58 and lower radiative forcing (upto ~24%). Chapter 5 elucidates the diurnal scale phenomena with respect to emission sources, quantification of transported pollutants, the influence of biomass burning and radiative forcing. The deconvolution of OC to primary and secondary OC (POC and SOC) is performed using four methods, all of which consistently show that POC (>64%) with a prominent unimodal diurnal variation dominates over SOC (< 44%) at an annual time scale. The contribution of fossil fuel combustion (eBCff) in BC is found to be 3.5 times greater than that of biomass burning (eBCbb). Radiative forcing estimates are made at diurnal scale,

and it is shown that noon time eBCff contributes to more atmospheric forcing than eBCbb in the same duration. In view of the discrepancies associated with CO emissions (co-emitted with BC) and its increasing levels over the South Asian region, Chapter 6 utilizes BC measurements to provide crucial *in-situ* information to robustly constrain the relative source fractions of CO. As a novel approach, multiple linear regression based (MLR) framework is used to serve this purpose. MLR does quite well in replicating the diurnal and monthly variation of CO with a r2 of > 0.8 over the training period of 2014-2017, performing much better than the CO from MOPITT satellite and MERRA-2 reanalysis data. Predicted CO values for the year 2018 lie in the range of -16.1% to 16.8% of the observed average CO values in any given month. The source segregation results show that fossil fuel combustion (COff) fractions of CO is the major contributor (27%) in CO after background CO (58%). Biomass burning (CObb) CO shows a large increase and reaches up to 28% during April as a result of increased agricultural and forest fires in the Northern Indian region. Against the MLR derived CO fractions, WRF-Chem tracer runs for source segregation are foundto underestimate the biomass burning CO emissions (-38% to -98%) while they largely overestimate the fossil fuel CO mixing ratios especially during monsoon

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20. SUDHANSHU KUMAR

Investigations on Structural, Electrical, and Magnetic Properties of Magnesium Ferrite ($MgFe_2O_4$.) Powders and Ceramics.

Supervisor: Prof. K. Sreenivas

Th 25750

Abstract

Ferrite nano-particles and sintered ceramics of high phase purity are of immense interest for biomedical and electronic applications. Single step processing at low temperatures is becoming important for mass production of ferrite powders to meet the ever-increasing demand. The present thesis investigates the usefulness of DL-alanine as a fuel in the combustion method to synthesize magnesium ferrite (MgFe2O4) powders, and examines the structural and electrical properties of ceramics prepared from powders developed in this work. Preparation of nano-particles by sol-gel auto-combustion technique, and sintering conditions for the preparation of dense ceramics have been optimized. Annealing the as-prepared powders at 900 °C is found necessary to eliminate the residual carbon (C), hydrogen (H) and nitrogen (N) content. Crystallographic and magnetic structure determined by X-ray, Electron and Neutron diffraction studies reveals the formation of phase pure cubic structure of MgFe2O4. Variations in the magnetic properties due to annealing temperatures are correlated with changes in the cation distribution at the octahedral and tetrahedral sites estimated from both structural and magnetic measurements. The nano-particles are largely agglomerated, and

shifts in the Raman and farinfrared absorption spectra show changes in the cation distribution. Inversion parameters calculated from X-ray diffraction and magnetization measurements show good agreement. Differences in the magnetic properties of powders and ceramics are observed when annealed/sintered at different temperatures, and have explained in terms of the changing crystallite size and domain size which are influenced by the post heat treatment. Dielectric properties over a wide frequency (10-1 – 106 Hz) and temperature range (153 -393 K) have been analysed to understand the charge carrier transport in MgFe2O4 ceramics. The temperature dependent dc conductivity, and the relaxation data from dielectric, impedance and electrical modulus show a transition at 313 K in the conduction mechanism varying from variable range hopping type conduction to a thermally activated conduction. Impedance Cole-Cole analysis reveals the individual contributions arising from the grain, grain-boundary and electrode effects. The non-polar nature of MgFe2O4 with low dielectric constant ~14 is confirmed from the insignificant variation seen in the grain capacitance (*C*g) and the relaxation distribution parameter (*n*g) with temperature. Frequency and temperature dependent AC conductivity obey Jonscher's universal dielectric response closely. The exponent *s* is found to depend on both frequency and temperature and shows a minimum around 313 K indicating Overlapping Large Polaron Tunnelling (OLPT) type conduction. Thus, a mixed VRH+OLPT conduction for T□313 K, and Arrhenius + OLPT type conduction for T≥313 K are inferred from the dc and ac measurements. Influence of Gd3+ doping on the structural, electrical, dielectric and magnetic properties in MgFe2-*x*Gd*x*O4 has been analysed. A limited solubility is observed up to $x = 0.08$ with effectual Gd3+ substitution for Fe3+ at the octahedral sites. In comparison to pure MgFe2O4 improvement is seen for an optimum Gd3+ concentration ($x = 0.02$) i.e., Mg2Fe1.98Gd0.02O4 ceramics which exhibit a high electrical resistivity and a low dielectric loss factor and a low porosity in the microstructure 5.38 %. Whereas an increasing Gd3+ doping concentration lowered the densification in ceramics and increased the porosity up to 18% although the resistivity continued to increase.

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