CHAPTER 44

PHYSICS AND ASTROPHYSICS

Doctoral Theses

01. AMEER (Shaan)
Growth and Electronic Properties of Pure and Doped(C,Cr) Bifeo$_3$ Thin Films.
Supervisor: Prof. Vinay Gupta
Th24638

Abstract
(Not Verified)

BiFeO3 (BFO) being the only known multiferroic material at room temperature offers an exceptional potential for the development of futuristic multifunctional devices. There are good ferroelectric materials like PbZrTiO3, BaTiO3 etc but these materials exhibit wide bandgap which lie in the UV region, however, band gap of BFO (~2.5 eV) lies in the visible region of electromagnetic spectrum which makes it a suitable candidate for the development of visible light energy harvester. However, there as some issues associated with BFO: (1) quite higher leakage currents, (2) appearance of secondary phases, and (3) controversy regarding p-type or n-type conductivity in BFO. In the present work, efforts are made to address these issues theoretically as well as experimentally. In order to address the issue of high leakage current, B-site doping with Cr in BFO is considered and the films are grown using chemical deposition method. The results project the Au/BiFe1-xCrxO3/ITO/glass ferroelectric photovoltaic cell with photoresponse ~8.4×104 (for x=0.02) as useful for the development of cost-effective light-driven devices. First principle calculations are carried out on prominent secondary phase of BFO, Bi2Fe4O9 to study in detail the structural, electronic, and optical properties, and the effect of 3d transition metal doping on electronic properties. Thin films of orthorhombic (Pbam) Bi2Fe4O9 are grown using pulsed laser deposition (PLD) technique, where, the growth of rhombohedral (R3c) phase of BiFeO3 is optimized by varying laser fluence and oxygen partial pressure. Role of carbon in influencing the electronic structure and properties of BFO is studied in detail along with the energetics and kinetics of formation of carbon impurity related defects. The theoretical findings are corroborated with experimental results obtained on the grown carbon incorporated BFO thin films. Controversy regarding the conductivity type of BFO is resolved experimentally as well as theoretically.

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02. BANDAY (Azeem U Shan)
Investigation on Local Atomic Structure and Charge Transport Mechanism in Olivine Phosphate Crystal and Glass.
Supervisor: Prof.Sevi Murugavel
Th24637

Abstract
(Not Verified)

Lithium ion batteries (LIBs) are the most advanced rechargeable batteries available thus far because of their high power density, high energy density, light weight and are highly safe. Within the family of olivine phosphates, LiFePO4 is arguably one of the most potential candidates for cathode materials and has been under extensive study ever since its discovery. The main focus of the present thesis work is to improve the electronic conductivity of LiFePO4 which impacts the battery design to a great deal. We aim at studying the underlying mechanism of charge transport in LiFePO4 to improve its conductivity. In this regard we have prepared different nanosized LiFePO4 samples by a modified single step solid state reaction method. Similarly different crystallite sized FePO4 samples were also prepared by chemical delithiation method. The various analytical techniques have been employed to understand the structural, optical, morphological and electronic phenomena of different nanosized LiFePO4 and FePO4 samples. The polaronic conduction mechanism of LiFePO4 and FePO4 samples has been revealed by using Mott model of polaronic conduction and the influence of vacancies on the polaron transport has been established. Furthermore, a comparison between the olivine structured crystalline LiFePO4 and its amorphous analog glassy LiFePO4 has been drawn. The glassy LiFePO4 has been prepared by the standard melt quenching technique. The phase purity and structural properties of as-prepared samples has been characterized by various analytical techniques which attested that the obtained samples were without any parasitic impurity. The intrinsic electrical conductivity measurements were done using broadband impedance spectroscopy over wide temperature ranges. The physical parameters extracted from the Mott model of polaronic conduction firmly support the evidence of enhancement in the polaronic conductivity in case of glassy LiFePO4 samples. We believe that these revelations could instigate further insightful improvements in the electrochemical performance of next generation LIB's.

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03. BANERJEE (Akashrup)
Development of Peripheral Detector Assembly for Scanning Setup of a Gamma Tracking Array and Techniques for Decay Spectroscopy.
Supervisor: Prof. Samit Kumar Mandal
Th24625

Contents

04. BHAT (Mohammad Yasir)
Novel Compositions of Gel Polymer Electrolytes for Electrical Double Layer and Pseudo-Capacitor Applications.
Supervisor: Prof. S.A. Hashmi
Th24642

Contents

1. Introduction. 2. Experimental techniques 3. Studies of gel polymer electrolytes for supercapacitors 4. Pinecone derived porous activated carbon for high performance all solid state electrical double layer capacitors fabricated with flexible gel polymer electrolytes 5. Solid state pseudo capacitors based on MnO_2-nanorod electrodes and plastic crystal incorporated gel polymer electrolytes 6. Summary and conclusion.

05. HALDER (Krishna Kamal)
Development and Characterization of Polymer Composites for Electromagnetic Interference Shielding.
Supervisor: Prof. Vinay Gupta
Th24628

Abstract
(Verified)

In the last two decades, remarkable research has been performed on the development of EMI shielding materials. Despite enormous efforts, the development of a material with minimum thickness for wideband frequency range shielding applications still remains a challenge. In the present work PVDF and ABS have been used as polymer matrices and different fillers (metal powder, carbon based material and iron oxide nano particles) have been explored for the development of polymer composites for EMI shielding applications in the X-band frequency range.The copper incorporated polymer composites show dipole interaction, which improve the absorption ability of the composites and shows moderate EMI shielding values. Temperature treatment of charcoal crafts an increase in conductivity of ABS composites, primarily accountable for the enhancement of EMI shielding. Electromagnetic shielding effectiveness in X-band has been identified to increase significantly for composites with ascending temperature treated charcoals. Composite having 1100 °C temperature treated charcoal shows absorption dominated enhanced value of SE ~36.8 dB at 11.6 GHz. A comparative study of graphite and carbonized charcoal loaded PVDF polymer composites has also been done. Conductivity and dielectric constant (real and imaginary part of dielectric constant) play a crucial role in the improvement of shielding effectiveness.Free standing thin films of iron oxide and carbon based filler loaded PVDF polymer composites were successfully synthesized using simple solution mixing method as an excellent material for EMI shielding application. The high EMI shielding value for thin film is due to the incorporation of synergistic effect of both dielectric and magnetic loss of the composite. In addition to these losses, interfacial polarization induced by multiple interfaces developed due to heterogeneous filler structure also heighten in the absorption dominated high EMI shielding value for composite film (100 μm) of such a lower thickness.

Contents

1. Introduction. 2. Development of copper metal particles loaded ABS,PVDF polymer composites 3. Development and characterization of charcoal as filler for polymer composites 4. A comparative study of carbonized charcoal and graphite loaded PVDF polymer composites 5. Study of magnetic nano particles (Iron oxide) and carbon based filler (Charcoal,MWCNTs) incorporated (PVDF) polymer composite thin film 6. Thesis summary 7. Scope and some suggestions and References.

06. GOEL (Sahil)

Effect of Rare Earth Doping on the Morphological, Dielectric, Piezoelectric and Ferroelectric Characteristics of Zno Nano-/Micro-Architectures Synthesized By Wet Chemical Route.

Supervisor: Prof. Binay Kumar

Th24632

Abstract
(Not Verified)

In this thesis, the synthesis of pure and Gd, Y, Ho, Sm & Dy-doped ZnO nanostructures has been presented. The synthesized nanostructures have been subjected to various characterizations for structural, morphological, dielectric, piezoelectricity, and ferroelectricity properties. The present thesis is divided into eight chapters. Chapter 1 begins with the introduction to the general background and necessary concepts which are relevant to the present thesis work. Also, motivation and work plan of present thesis is summarized, which is followed by the brief outline of the thesis. Chapter 2 narrates the synthesis of ZnO nanocrystals, and describes the working principle of various experimental techniques used for their subsequent characterizations. Chapter 3 describes the high temperature ferroelectricity and large piezoelectricity introduced in ZnO due to gadolinium doping (Pr = 0.29 µC/cm2, Ec = 16.41 kV/cm, Tc = 215 oC & d33 = 31 pm/V). Chapter 4 reports the yttrium (Y) doped ZnO nanosheets with high temperature ferroelectricity and large piezoelectricity (Tc ~138 °C, Ec ~5.87 kV/cm, Pr ~0.09 µC/cm2 & d33 ~420 pm/V) that have been developed here using wet chemical synthesis route. Chapter 5 presents a novel high temperature ferroelectric and giant piezoelectric (Tc ~205 °C, Ec ~4.72 kV/cm, Pr ~0.05 µC/cm2 & d33 ~230 pm/V) marigold-like holmium (Ho)-doped ZnO nanocrystals. Chapter 6 presents a novel hierarchical samarium (Sm)-doped ZnO nanorods-nanosheets architecture with high temperature ferroelectricity and large piezoelectricity (Tc ~110 °C, Ec ~3.64 kV/cm, Pr ~0.08 µC/cm2 & d33 ~106 pm/V). Chapter 7 discusses high temperature ferroelectricity and giant piezoelectricity (Tc ~435 °C, Ec ~6.15 kV/cm, Pr ~0.16 µC/cm2, d33 ~219 pm/V) observed in a novel 3D hierarchical dysprosium (Dy)-doped ZnO nanorods- nanosheets (NRs- NSs) architecture. Chapter 8 summarizes the general conclusions drawn from the present thesis work. The scope for future work has also been discussed in this chapter.

Contents

07. GUPTA (Surbhi)

Development of Strontium Barium Niobate (SBN) Thin Film Based Electro-Optic Modulator.

Supervisor: Dr. Monika Tomar `

Th24622

Abstract
(Verified)

The need of effective modulation of light waves over wide frequency range has become increasingly important in fiber–optic transmission systems where Electro-optic (EO) modulators find their potential application. A keen interest has been developed towards realization of EO devices utilizing Surface Plasmon Resonance (SPR). Strontium Barium Niobate (SBN) has been chosen as appropriate ferroelectric thin film grown using PLD technique for realization of EO modulator. Detailed study on growth of SBN60 and SBN75 films and their structural, optical, electrical and electro-optic properties are essentially required. UV-Visible spectroscopy and SPR technique are utilized to determine optical property of SBN films. Effect of different metal contacts such as Pt, Pd, Al and Cr has been studied on current-voltage characteristics, dielectric constant, dielectric losses and ferroelectric properties of SBN60 and SBN75 thin films. Linear Pockel's coefficient of about 0.0033cm/V and 0.0040cm/V has been estimated for SBN60 and SBN75 thin films respectively. Effective EO coefficient was about rc=-198pm/V and rc=-262pm/V respectively for SBN60 and SBN75 thin film over a wide frequency range (10 Hz to 25 MHz) of applied electric field. Resonance frequency for SBN60 (1 MHz) and SBN75 (3 MHz) thin films has been estimated using Modulated diffraction technique for WCSPR-EO modulators. The phase transition temperature was estimated for both SBN60 and SBN75 thin films and found to be 373 K and 338 K respectively. Thermo-optic coefficient of 88.3×10-4 K-1 and 89.9×10-4 K-1 at Tc was obtained for SBN60 and SBN75 thin film respectively without applied electric field. Percent modulation index increased from 16% to 55% and from 26% to 57.5 % for SBN60 and SBN75 thin film modulators at Tc with increasing electric field. Mach Zehnder Electro-optic modulator was fabricated using SBN60 and SBN75 thin film possessing half wave voltage of 1.6 V and 1.3 V respectively.

Contents

08. HUSSAIN (Abid)
Synthesis and di-/piezo-/pyro-/ferro-electric characterizations of pure and Sb-Ho-/Y- doped 0.64Pb ($Mg_{1/3}Nb_{2/3}$) O_3-0.36$PbTiO_3$ (PMN-PT) ceramics for piezoelectric application.
Supervisor: Prof. Binay Kumar
Th24630

Abstract
(Not Verified)

In this thesis, the synthesis of pure and Sb, Ho, Y-doped PMN-PT ceramics has been presented. The synthesized ceramics have been subjected to various characterizations for structural, morphological, dielectric, piezoelectricity, pyroelectric, and ferroelectricity properties. In addition to above mentioned properties, the determination of true-remanent polarization and resistive leakage analysis of the ceramics have been carried out for the first time. Also, utilization of the synthesized pure and doped ceramics for generating piezoelectric voltage has been done. The present thesis is divided into eight chapters. Chapter 1 begins with introduction to the general background and necessary concepts which are relevant to the present thesis work. Chapter 2 discusses various literatures on dielectric, piezoelectric, pyroelectric, and ferroelectric properties of PMN-PT ceramics. The literature on various

past doped PMN-PT systems has also been presented in this chapter. Chapter 3 describes the experimental techniques used for ceramics synthesis and their characterizations. Chapter 4 presents the details of synthesis and characterizations of pure 0.64Pb(Mg1/3Nb2/3)O3-0.36PbTiO3 (PMN-PT) ceramic. Chapter 5 discusses synthesis of Sb-doped PMN-PT ceramic and effects of Sb-doping on microstructure and electrical properties of undoped PMN-PT. Chapter 6 and 7 present the effects of Ho3+ and Y3+, respectively on structural, morphological, dielectric, piezoelectric, pyroelectric, and ferroelectric properties of pure PMN-PT ceramic. Chapter 8 summarizes the conclusions obtained from thesis work and importance of synthesized ceramics in terms of their applications. In this thesis work, all the dopants resulted in increase in the values of dielectric constant, piezoelectric coefficients, remanent polarization (Pr), coercive field (Ec), and pyroelectric coefficient. The highest values of Pr, Ec, and p observed for Y-doped PMN-PT ceramic. In piezoelectric study, all the dopants caused to increase the value of piezoelectric coefficients and largest increment was observed for Sb-doped PMN-PT sample.

Contents

09. JAIN (Geetika)

Design and Characterization of the Silicon Strip Sensors For the Future Hadron Colliders .

Supervisor: Dr. Ashutosh Bhardwaj

Th24619

Abstract
(Verified)

Silicon sensors play a key role in High Energy Physics experiments due to their superior performance in terms of robust and reliable charged particle tracks and vertex reconstruction. Owing to the placement of these sensors in a harsh radiation environment imposed by current and future HEP experiments like Compact Muon Solenoid (CMS) in the Large Hadron Collider (LHC) phase and the high luminosity LHC (HL-LHC) phase, the radiation hardness study is inevitable. It is imperative to optimize the sensor design or develop new sensor configurations which can withstand such radiation scenario. This has generated an interest in the development and improvement of the radiation tolerance of the sensors which require better designs and better engineering technologies. The thesis primarily deals with the usage of silicon sensors in intense radiation environment, for example the environment faced by the Silicon Tracking System of the CMS experiment at the LHC.The results of the characterization studies performed on silicon strip sensors fabricated at BEL, Bangalore, development of silicon sensor hardware facility for sensor quality check and radiation hard study of novel sensor designs through Technological Computer Aided Design (TCAD) simulations are presented. The 2D TCAD device simulations were performed using the Silvaco simulator. The simulations were aimed at understanding and optimizing the designs of Low Gain Avalanche Detector (LGAD), pixel detectors, and low resistivity substrate silicon detectors. The parametrization of bulk and surface proton radiation damage model developed was used to simulate radiation damage. Silicon sensors play a key role in High Energy

Physics experiments due to their superior performance in terms of robust and reliable charged particle tracks and vertex reconstruction. Owing to the placement of these sensors in a harsh radiation environment imposed by current and future HEP experiments like Compact Muon Solenoid (CMS) in the Large Hadron Collider (LHC) phase and the high luminosity LHC (HL-LHC) phase, the radiation hardness study is inevitable. It is imperative to optimize the sensor design or develop new sensor configurations which can withstand such radiation scenario. This has generated an interest in the development and improvement of the radiation tolerance of the sensors which require better designs and better engineering technologies.The thesis primarily deals with the usage of silicon sensors in intense radiation environment, for example the environment faced by the Silicon Tracking System of the CMS experiment at the LHC. The results of the characterization studies performed on silicon strip sensors fabricated at BEL, Bangalore, development of silicon sensor hardware facility for sensor quality check and radiation hard study of novel sensor designs through Technological Computer Aided Design (TCAD) simulations are presented. The 2D TCAD device simulations were performed using the Silvaco simulator. The simulations were aimed at understanding and optimizing the designs of Low Gain Avalanche Detector (LGAD), pixel detectors, and low resistivity substrate silicon detectors. The parametrization of bulk and surface proton radiation damage model developed was used to simulate radiation damage.

Contents

10. JAMDEGNI (Monika)
Study of Charge Transport Mechanism in Electrochemically Synthesized Polyaniline Composites for Electrochromic Applications.
Supervisor: Prof. Amarjeet Kaur
Th24629

Abstract
(Not Verified)

Smart windows by controlling the optical transmittance level, can control the light and heat entering through a window and reduces the energy expenditure on air conditioning and lighting. In search of flexible, cost effective and easily processible materials, research in this field drifted towards conducting polymers. Their ample coloration, ease of synthesis, low cost fabrication and fast response makes them the most appropriate choice for electrochromic application. Among conducting polymers, polyaniline is one of the most exploited polymer for electrochromic applications. Its polychromic nature with transparent to green to blue and finally to black coloration is the prime reason for this special attention. Despite of PANI having huge potential to serve as multi electrochromic material for smart windows as well as display device applications, it has some major limitations which have to be overcome to take it upto commercial level. For example, its poor electrochemical cyclic stability at higher potential (>0.6 V) compels one to compromise with lower contrast. With this motivation, the prime objective of the present work is to improve the cyclic stability of PANI with parallel enhancement in other electrochromic parameters. For realising such improvements, different nanostructures of pristine polyaniline and composites of polyaniline have been prepared. For synthesizing nanostructures of pure PANI, surfactant assisted electrochemical route has been followed. Effect of different surface morphologies and the presence of surfactant molecules having

different polarities have been studied thoroughly. Furthermore, nanocomposites of PANI have been prepared using in-situ electrochemical polymerization method. Influence of incorporation of foreign materials like nickel oxide (NiO), zinc oxide (ZnO) in attached form via silane agent and graphene quantum dots (GQDs) attached via oxygen functional groups with PANI chains on the morphology, dc conductivity, electrochemical and electrochromic behaviour of PANI has been investigated in detail.

Contents

11. KESHRI (Sumit)
Search For A New Scalar Resonance $X \rightarrow ZZ \rightarrow 2\ell 2\nu$ In P-P Collisions at $\sqrt{s}$ =13 TeV By The CMS Experiment.
Supervisor:Prof. Kirti Ranjan
Th24634

Abstract
(Verified)

After the discovery of the SM Higgs boson by the Compact Muon Solenoid (CMS) and A Toroidal LHC Apparatus (ATLAS) experiments at the Large Hadron Collider (LHC), CERN, the SM is complete. Even though SM successfully explains several phenomena, still it can't explain many observed facts, for e.g. dark matter, dark energy, matter-antimatter asymmetry, etc. that require a theory beyond the SM (BSM). Several extensions of the SM include a new scalar resonance of high mass. For example, the two Higgs Doublet Model (2HDM) in supersymmetry (SUSY) considers two Higgs complex doublet and the electroweak singlet model, which includes a hidden Higgs sector with heavy Higgs field. The search is performed using p-p collision data collected by the CMS experiment at √s=13 TeV corresponds to an integrated luminosity of 2.3 fb-1 and 35.9 fb-1 in the year 2015 and 2016 respectively. During 2015, search is performed for the heavy scalar resonance with the SM like widths and production cross-section in the mass range of 200 GeV to 1500 GeV and then interpreted for the electroweak singlet model and Type-II 2HDM model. during 2016, the same search is performed in a model-independent way, while varying both width of the resonance and fraction of the vector boson fusion (VBF) production mode in the mass range of 300 GeV to 3000 GeV. The Matrix Element Likelihood Approach is used to model the interference as well as different width (ΓX) for each mass of X (mX). No significant excess of events with respect to the SM expectation is observed, and hence an upper limit at 95% confidence level (CL) is set on the product of cross-section for X and the branching fraction for its decay to ZZ.

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12. NEERAJ KUMAR

Study of Fission Dynamics Using Neutron Multiplicity & Mass Distribution Measurements and Through Dynamical Model Calculations.

Supervisor:Dr. Shsahi Verma

Th24626

Abstract
(Not Verified)

Study of the nuclear fission process and the associated phenomenon is unique approach to understand the fundamental properties of nuclear matter. The theoretical and experimental efforts carried out in the last decades established the dynamical aspects of formation and decay of Compound Nucleus (CN). Pre-scission neutron multiplicity and fission fragment mass distribution measurement has emerged as one of the most effective probes to address various features of nuclear fusion-fission processes. In the present work, the main aim of the theoretical work is to investigate the role of dynamical deformation of the CN on pre-scission neutron multiplicity. The experimental part of the thesis addresses the entrance channel effect and the influence of Quasi Fission on fusion-fission dynamics. In the theoretical work, one dimensional Langevin dynamical model is used to calculate the pre-scission neutron multiplicity for both spherical and evolving deformed shapes of CN. The neutron multiplicity contribution from saddle to scission phase is also calculated for various systems. In addition to the above theoretical investigations, the dissipation strength is extracted. In the experimental aspect, experiments have been performed with the National Array of Neutron Detectors (NAND) facility at Inter University Accelerator Centre (IUAC), New Delhi. Pre-scission neutron multiplicities and fission fragment mass distributions have been measured for a CN 208Rn populated by two different entrance channels 30Si + 178Hf and 48Ti +160Gd at similar excitation energies. The measured pre-scission neutron multiplicities are analysed within the framework of Langevin dynamical model calculations. The Langevin dynamical model calculations to estimate the capture cross-section and effective fusion time are also performed. The fission fragment mass distribution measurements for the CN 208Rn is also performed in the present work. The widths of the normalised mass ratio distributions are compared with existing data for 16O +194Pt system. Study of the nuclear fission process and the associated phenomenon is unique approach to understand the fundamental properties of nuclear matter. The theoretical and experimental efforts carried out in the last decades established the dynamical aspects of formation and decay of Compound Nucleus (CN). Pre-scission neutron multiplicity and fission fragment mass distribution measurement has emerged as one of the most effective probes to address various features of nuclear fusion-fission processes. In the present work, the main aim of the theoretical work is to investigate the role of dynamical deformation of the CN on pre-scission neutron multiplicity. The experimental part of the thesis addresses the entrance channel effect and the influence of Quasi Fission on fusion-fission dynamics. In the theoretical work, one dimensional Langevin dynamical model is used to calculate the pre-scission neutron multiplicity for both spherical and evolving deformed shapes of CN. The neutron multiplicity contribution from saddle to scission phase is also calculated for various systems. In addition to the above theoretical investigations, the dissipation strength is extracted. In the experimental aspect, experiments have been performed with the National Array of Neutron Detectors (NAND) facility at Inter University Accelerator Centre (IUAC), New Delhi. Pre-scission neutron multiplicities and fission fragment mass distributions have been measured for a CN 208Rn populated by two different entrance channels 30Si + 178Hf and 48Ti +160Gd at similar excitation energies. The measured pre-scission neutron multiplicities are analysed within the framework of Langevin dynamical model calculations. The Langevin dynamical model calculations to estimate the capture cross-section and effective fusion time are also performed. The fission fragment mass distribution measurements for the CN 208Rn is also performed in the present work. The widths of the normalised mass ratio distributions are compared with existing data for 16O +194Pt system.

Contents

13. NEWMAI (M. Boazbou)
Investigation on the Growth Of Vinylpyrrolidone Mediated Plasmonic Metal Nanostructures .
Supervisor:Dr. P. Senthil Kumar
Th24631

Abstract
(Not Verified)

Noble Metal Nanoparticles (MNPs) has received widespread research interest owing to many important applications such as photothermal therapy, nanocatalysis, Surface Enhanced Raman Spectroscopy (SERS), photonic devices etc. In this thesis, the monomer, N-Vinylpyrrolidone (NVP), was extensively used to fabricate the anisotropic plasmonic metal (Ag and Au) nanostructures under ambient conditions, owing to its intriguing oligomerizing property in acidic medium, via the simultaneous reduction of metal precursors. This process of oligomerization of NVP, initiated by the dissociated H+ ions from HAuCl4, consecutively forms the intermediate metal complexes, which in turn, reduces to zerovalent Au atoms, leading to the nucleation of tiny Au seeds. The excessively oligomerized NVP immediately stabilizes these Au seeds through its carbonyl group, ensuring their controlled growth/stabilization, thereby enabling a unique synthesis protocol for the synergistic process of oligomerization as well as the reduction and stabilization of ultrasmall metal nanoparticles even at room temperature in the absence of any other external energy resources. Such a distinctive synergistic process has been effectively extended to the synthesis of Ag-Au nanoalloys in presence of solvent, dimethyl formamide (DMF). In the catalytic reduction of 4-Nitroaniline (4-NA) to p-Phenylene diamine (p-PDA) in presence of excess sodium borohydride (NaBH4), the reduction rate increases drastically in the presence of Ag-Au nanoalloys. Furthermore, deposition of anisotropic plasmonic silver nanoparticles onto the surface of NVP-functionalized silica nanospheres (synthesized using modified Stober's method) was achieved in a meticulous manner. Sequentially increasing the deposition cycle of Ag nanoparticles leads to decrease in inter-particle distance of the Ag nanoislands, thereby facilitating the inter-particle plasmonic interactions, which results in intense EM field enhancement. The plasmonic Ag nanoislands on the silica surface were utilized for highly sensitive molecular detection using SERS with enhancement factors as high as 108, enabling us to detect bio-chemical molecules in as low as picomolar concentration.

Contents

14. PRIYANKA
Measurement of the Production Cross Section for Single Top Quarks In Association With W Bosons At √s = 13 Tev With the CMS Experiment.
Supervisors:Prof. Kirti Ranjan and Ashutosh Bhardwaj .
Th24624

Abstract
(Not Verified)

Ever since the discovery of top quark in pair production mode by CDF and D0 collaborations at Tevatron in 1995, the study of top quark has assumed great interest. Top quark can also be produced singly through electroweak production known as single-top production. The cross-section of single-top quark production provides a direct probe for Vtb matrix element of CKM matrix. Single-top quark production acts as background for many SM and BSM searches. Single-top quark production occurs mainly through three processes: t-channel production, s-channel production, and associated production of top quark with W boson (tW-channel). Evidence and observation of tW production was given by ATLAS and CMS experiment at centre-of-mass energy of 7TeV and 8TeV respectively. In this work, first measurement of inclusive cross-section of tW production at √s=13TeV is performed using full 2016 data corresponding to integrated luminosity of 35.9 fb−1 collected by CMS experiment at LHC, CERN. This study is conducted in cross-lepton (electron and muon) decay channel. Events with two well identified leptons of opposite charge with leading lepton pT > 25GeV having invariant mass of lepton pair greater than 20 GeV are selected. A multivariate boosted decision trees (BDT) analysis is used to separate tW signal from dominant t\bar{t} background. The estimation of reducible backgrounds like Z/γ+jets and non-W/Z, are performed using data-driven approach. Various sources of systematic uncertainty that affect the analysis are also presented. A likelihood fit to the BDT discriminants of 1j1b, 2j1b regions and sub-leading jet pT distribution of 2j2b region, is used to extract signal strength parameter μ. The measured value of μ is 0.88±0.02 (stat)±0.09 (syst)±0.03 (lumi), corresponding to cross section of tW=63.1±1.8 (stat)±6.4 (syst)±2.1 (lumi) pb which is consistent with SM prediction.

Contents

15. RANA (Akshay)
Some Applications of Statistical Tools in Cosmology.
Supervisor: Prof. Shobhit Mahajan and Dr. Deepak Jain
Th24937

Abstract
(Not Verified)

This thesis revolves around three fundamental pillars of cosmology i.e. theory, observations, and statistical tools. We explore different observational datasets and use non-parametric statistical tools to investigate the theoretical assumptions and outcomes of various cosmological models.Once equipped with cosmological data and statistical tools, we mainly probed two cosmological assumptions in this thesis:(a) First, we investigated a fundamental relation in the framework of General Theory of Relativity, Cosmic Distance Duality Relation (CDDR). It is a relation between the luminosity distance and angular diameter distance of an object in an expanding

universe. (b) The second assumption, we investigated is the validity of the FLRW metric which is derived under the purview of the cosmological principle namely the assumption that the universe is homogeneous and isotropic at cosmological scales. Once the validity of FLRW is established, we extended our analysis to probe the spatial cosmic curvature using statistical properties of the strong gravitational lensing. Chapter 2 of the thesis provides a brief overview of cosmology followed by details of some prominent observational probes used in this thesis like Type Ia supernova (SNe Ia), Hubble parameter, Baryon Acoustic Oscillations (BAO), Cosmic Microwave Background Radiation (CMBR) and Gravitational Lensing in Chapter 3. In Chapter 4, we discuss the basic statistical tools required in cosmology and give a detailed discussion of two non-parametric statistical methods namely Gaussian Process and LOESS and SIMEX. Consistency tests of CDDR are explored in Chapter 5 and Chapter 6. In Chapter 7 we investigate the validity of the FLRW metric and the spatial curvature of the universe. Finally, in Chapter 8, we highlight the main results of the thesis.

Contents

16. SACHDEVA (Divya)
Phenomenology of Light and Heavy Dark Matter.
Supervisor:Prof. Debajyoti Choudhury
Th24621

Abstract
(Verified)

Recent results from several direct detection experiments have imposed severe constraints on the multi-GeV dark matter (DM) models. However, many of these experiments are not sensitive to MeV scale DM as the corresponding recoil energies are lower than the detector thresholds. We reexamine the light scalar DM in a model-independent approach, beginning by developing an appropriate methodology to determine the effective coupling of such a DM to hadrons, thereby allowing for the determination of the corresponding annihilation rates. We find that while the parameter space can be constrained using cosmological and astrophysical observations, a significantly large fraction is still viable. The sensitivity reaches pertaining to the available parameter space is then determined for Belle-II. We also examine the prospects of Direct Detection experiments and juxtapose the results. TeV scale DM is another well motivated candidate that can evade bounds from direct detection experiments owing to its smaller number density and Extra-dimensional models represent one such category that admit TeV scale DM naturally. We offer two set-ups defined in a six-dimensional spacetime. For first, a 5-dimensional Universal Extra Dimension (UED) model emerging from a six dimensional space-time with nested warping is considered. The AdS_6 bulk protects both the Higgs mass as well as the UED scale without invoking unnatural parameter values. The graviton excitations in the sixth direction open up new (co-)annihilation channels for the DM particle, allowing for phenomenological consistency to the minimal UED scenario. In the second, a six-dimensional alternative with the SM quarks and leptons being localized on 4-branes extended in orthogonal directions but with the electroweak gauge bosons traversing the entire bulk is proposed. These models

are consistent with all the current constraints opposing the minimal UED scenario and also allow for a multi-TeV dark matter particle without the need for any fine-tuning.

Contents

1. Background 2. Cosmological constraints on MeV scale DM 3. Collider signature detection of light DM 4. Heavy Dark Matter candidate and Extra dimensional models 5. Model I: Gravity rescue UED 6. Model II: living orthogonally- Quasi-universal extra dimensions 7. Conclusion and outlook.

17. SAINI (Pooja)
Electronic Properties of Annealed Grapheme Oxide Thin Films.
Supervisor: Dr.Ajit Kumar Mahapatro
Th24635

Abstract
(Not Verified)

The new discoveries on nanostructured materials (NSMs) with physical properties sensitive to size are expecting to play an important role in addressing the on going and future challenges in field of electronics, optoelectronics, medical, and communication technologies. Recently, Graphene and its derivatives, graphene oxide (GO) and reduced graphene oxide (rGO) have shown potential for developing future high-speed electronics for diverse applications. The objective of thesis is to prepare thin films of GO on various metal substrates and fabricate device structures for studying the electronic properties through these thin films. Thin films of GO on various metal substrates M1(ITO,Al,Au) were prepared by spin coating technique. These thin films were annealed at 100, 200, 300, and 400 °C in a furnace and nomenclatured as GO(T)/M1. GO thin film based device structures are fabricated by depositing top metal contact (Al Au) using thermal deposition technique. The bipolar resistive switching (BRS) is observed only in M2/GO(T)/M1 structures with Al as one of the electrodes (M1 or M2=Al). The BRS mechanism is proposed to be due to breaking and formation of the initial metal filaments formed due to atom diffusion from the electrode metal through the thin film of GO.The observed temperature coefficient of resistance (α) of aluminium in Al/GO/Al, and gold in Au/GO/(ITO,Au) devices, are estimated from the temperature dependent agree well with the expectable values. The material content in GO thin films of different structures GO(T)/M1(ITO,Al,Au) and M2(Al,Au)/GO(T)/M1(ITO,Al,Au) identified from the depth profile XPS. The functionalization of GO surfaces with organic polymers of PAA and PVP, and GNC, are characterized using various spectroscopic, electrical, and optical tools. The observed spectroscopic and electronic properties of GO(T) and functionalized GO provide understanding of various electronic events and could be translated to fabricate components of future electronic devices.

Contents

1. Introduction 2. Experimental details 3. Morphogical and spectroscopic study of annealed thin films of Graphene Oxide 4. Bistable resistive switching in annealed grapheme oxide thin films based Al/GO(T)ITO device structures 5. Effect of metal contacts in the electrical resistive switching and material content through GO thin film devices 6. Functionalization of organic polymers and gold nanoclusters with Graphene oxide 7.Conclusion and future implications and List of publications.

18. SATISH KUMAR
Materials Characterization of Ion Beam Induced Mesoporous and Self Assembled Nanodots Structures on Gallium Antimonide Epilayers .
Supervisor:Dr. Ajit Kumar Mahapatro
Th24636

Abstract
(Not Verified)

This thesis explores the formation of different shapes of nanostructures (mesoporous with interconnected nanofibers (MSINs), nanodots and ripple structures) on GaSb epilayers grown on semi-insulating (001) gallium arsenide (GaAs) substrate using molecular beam epitaxy (MBE) with ion irradiation. The effect of ion irradiation parameters (ion species, energy, fluence, incidence angle, and substrate temperature during irradiation) on evolution of nanostructures have direct impact on thickness of mesoporous layer, diameter of nanofibers, diameter of pore size, nanodots size and density. No impact on GaSb surface is observed after irradiation with Ar+-ion at low ion-fluences (11012 to 11015 ions/cm2). The field emission scanning electron microscopy, transmission electron microscopy, atomic force microscopy (AFM), high resolution x-ray diffraction (HRXRD), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy, have been used for analysis. The materials and spectroscopic analysis indicated that the Ar+-ion irradiated at higher ion-fluences onto GaSb epilayers transforms to amorphous structures with presence of elemental antimony (Sb). Swift heavy silver ion (Ag+7) irradiated GaSb surfaces prepared at substrate temperature of 300 and 77 K shows crystalline nature of the nanostructures with additional elemental Sb is due to dynamic self-annealing process during irradiation. The formation mechanism of dots is attributed to the surface instability introduced by combination of sputtering, Ehrlich-Schwoebel barrier effect, and surface diffusion of mobile ad-atoms.The surface passivation on GaSb epilayer is carried out using different wet chemical passivating agents of 20% aqueous ammonium sulphide ((NH4)2S), aqueous sodium sulphide nonahydrate (Na2S.9H2O), and base-thioacetamide (base-TAM). Topography, recorded using AFM shows the formation of smooth surface for base-TAM treated GaSb. XPS results reveal presence of lowest concentration of Ga2O3 and hall measurement shows improvement in electrical properties for TAM passivated GaSb samples.The above Ion beam induced nanostructures could have potential applications in photo-detectors, laser diodes, photovoltaic cells, high electron mobility transistors, and tunnel diodes.

Contents

19. SHUKLA (Manish Kumar)
Thermodynamics of Dusty Plasmas Theory and Simulation.
Supervisor:Dr. Avinash Khare
Th24620

Abstract
(Not Verified)

In this thesis, the thermodynamics aspects of dusty plasma is explored using Particle within Plasma (PWP) model and molecular dynamics (MD) simulation. To verify the predictions of PWP model, an an

OpenMp parallel two dimensional and three dimensional molecular dynamics (2DMD/3DMD) code is developed and benchmarked it against the previous known results.In the first problem, an isothermal equation of state (EOS) for weakly coupled dusty plasmas is obtained using MD simulations. Our result reveals that the EOS for Yukawa gas in weak coupling limit contains not only the usual kinetic pressure term but also a term proportional to the square of dust density. This term is attributed to ES pressure which provides a significant contribution to dust pressure, even in the weak coupling regime. In the second problem, free expansion phenomena for weakly coupled dusty plasmas is studied in the constant plasma background. The evolution of temperature with volume reveals that Yukawa gas becomes warmer in the process of free expansion and change in dust temperature is directly proportional to change in number density of gas. In the third problem, we demonstrate an application of EOS for Yukawa gas in the context of "structure formation" for self-gravitating dusty plasmas in the astrophysical conditions. The interaction among the dust grains is modeled as superposition of Yukawa repulsion and gravitational attraction. In equilibrium, a spherically symmetric structure is formed. These equilibrium structures could be a possible candidate for the small scale structures observed in the HII region and interstellar medium. Finally, we use the equation of state of dusty plasma in the moderately coupled regime and seek the effect of finite dust correlations on the marginal stability of dust acoustic waves driven by ion stream instability. Our results show that the dust-dust correlation effect stabilizes the dust acoustic waves.

Contents

20. SWETA GAURAV
Gravitationally Bound Equilibrium and Instabilities in Dusty Plasmas.
Supervisors:Prof. Avinash Khare and D.N. Gupta
Th24633

Abstract
(Verified)

This thesis presents the study of gravitational bound instability and wave phenomena in dusty plasma. Main objective of the thesis is to understand the physics of different forces that act on a charged dust grain and mechanisms that are responsible for wave and structure formation. I begin in chapter 1, which contain introduction about dusty plasma. Dusty plasmas support a rich diversity of physical states ranging from solids to liquids to gas. In chapter 2, we present an exactly solvable model of equilibrium and stability of a gravitationally bound low dust density cloud embedded in background plasma.This model serves to give qualitative view of stability and structure of dust cloud in HII region through the complete set of radial eigenmodes and corresponding frequencies. Chapter 3 focuses on the impact of ion drag force and ionization on the stability of self-gravitating dusty plasma. It is shown that ion drag force aids gravitational collapse and threshold ion drag coefficient is defined. The resulting dispersion relation is utilized to obtain the explicit expression of growth rate. The work in chapter 4 details the Jeans instability in spherically symmetric dusty cloud, where self gravity of dust is balanced by the force shielded electric field on the charged dust. It is shown that dust correlation effect stabilizes the cloud while the increasing flux of incident photoelectrons reduces the mass limit. Chapter 5 presents the nonlinear features of dust acoustic waves in weakly and moderately coupled dusty plasma by using the reductive perturbation method. Augmented Debye Huckel approximation is used to define correlation. The measured parameters such as amplitude, width and propagation

velocity of solitary wave in both cases are compared. The thesis is finally concluded in chapter 6. The future scope of the thesis and application is also discussed briefly.

Contents

1. Introduction 2. Equilibrium and stability of a gravitationally bound uniformly charged dust cloud 3. Ion drag effect on jeans instability 4. Gravitational collapse of dust cloud 5. Nonlinear wave equations in weak and moderate coupling regime 6. Summary and conclusion.

21. SHAH (Aashaq Hussain)
Search For a New Light Boson in Exotic Higgs Boson Decays and the CMS Muon Spectrometer Upgrade Using GEM Technology.
Supervisor:Dr. Ashok Kumar
Th24643

Abstract
(Not Verified)

The present thesis is based upon extensive work on three aspects: R\&D on Gas Electron Multiplier (GEM) detectors, Phase-2 upgrade of the Compact Muon Solenoid (CMS) experiment at the Large Hadron Collider (LHC) and physics data analysis. The R\&D on GEM detectors includes important study in the context of the CMS muon upgrade using GEM technology. The part of the R\&D work on GEM foils has been performed in collaboration with Indian industry for their possible usage in scientific and other industrial applications. The Phase-2 work includes the development of large area GEM detectors for the forward muon endcap of the CMS experiment and the physics analysis includes a search for a new light boson in the exotic decays of Higgs boson in the $b\bar{b}\mu^{-}\mu^{+}$ final state.

Contents

1. Prologue 2. Theoretical background and overview of the LHC 3. The CMS muon endcap upgrade using GEM technology 4. R & D on GEM foils 5.Search for exotic higgs boson decay in h→Za→bbμ-μ+ 6. Search for exotic higgs boson decayin h→aa→ bbμ−-μ+ 7. Epilogue.

22. SHARMA (Monika)
Unravelling Structural Implications on Polaronic Transport Mechanism Nanostructured Electrode Materials for Energy Storage Devices.
Supervisor:Prof. S. Murugavel
Th24641

Abstract
(Not Verified)

One of the most interesting class of cathode materials for rechargeable Li-ion batteries are olivine-structured LiMPO4 (M = Fe, Mn, Ni) which is the topic of intense research by different research groups in world wide. The olivine structured LiMnPO4 (LMP) has very high electrochemical potential and gravimetric capacity as compared to the other members of the olivine family. With many advantages, the main limitation in LMP as a cathode material is its very sluggish kinetics. In this regard, we attempted to improve the structural and charge transport properties of the olivine LMP by tuning the crystallite size as external variable quantity. This conversion reaction based anode material is under development due to large volumetric changes in the structure during cycling process. The most beneficial aspect for improving the electrochemical properties of anode material is the reduction of particle/crystallite size. In this regard, we investigate the crystallite size dependent structural and

charge transport properties of the α-Fe2O3. In the present thesis work, we have reported for the first time the lattice contraction in addition to lattice expansion in the unit cell parameters with decrease in the crystallite size and explained the origin of structural change in terms of variations in the bonding characteristics. Additionally, we have investigated NaFePO4 (NFP) which exists in two different phases, namely Olivine and Maricite structure. The thermodynamically stable form of NFP, Maricite phase is limited due to its electrochemical performance, whereas the olivine structure can only be produced with the electrochemical route. In order to improve the polaronic and ionic diffusion, we have reduced the crystallite size of the m-NFP and observed favorable structural and transport the properties. Further, we also investigated the theoretical calculation for the structural and electronic properties of m-NFP with different sodium ion vacancy concentration using the density functional theory (DFT).

Contents

23. SHARMA (Ramkishor)
Viable Scenarios of Magnetogenesis in the Early Universe.
Supervisor: Prof. T.R. Sheshadri
Th24623

Abstract
(Not Verified)

Inflationary generation mechanisms offer a natural way to generate magnetic fields that are coherent over large scales in the Universe. Within the framework of standard electromagentic theory, this is not possible due to the conformal invariance of the electromagnetic field and the conformal flatness of the background spacetime. One of the models to generate significant magnetic field is where conformal invariance is broken by introducing A coupling between the inflaton field and the electromagnetic field such that the modified Lagarangian density of the electromagnetic field takes the form $f^2 F^{\mu \nu} F_{\mu \nu}$. Although the strength of the generated magnetic field in this model is sufficient to satisfy the observational constraints, it potentially suffers from strong coupling and backreaction problems. To address this in our model, the coupling function grows from unity, during inflation and decrease back unity post inflation. To ensure back-reaction, we find that the reheating temperature is restricted to be below $ \sim 1.7 \times 10^4$ GeV resulting in a magnetic field that is non-helical, has a blue spectrum and satisfies the gamma-ray bound below a certain reheating temperature.Further, we study the possibility of generating helical magnetic fields in the above mentioned model by adding an $f^2 \tilde{F}^{\mu\nu} F_{\mu\nu}$ term to the Lagrangian. The scale of reheating in our model is found to be lower than 3500 GeV to avoid back-reaction post inflation and the generated magnetic field spectrum is found to satisfy the γ-ray bound for all the reheating scales considered in our model.We also investigate the energy spectrum of the resulting stochastic background of Gravitational Waves from these generated electromagentic fields, and compare their strength with the sensitivity of the upcoming LISA mission for GWs detection.

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mangetogensis: helical magnetic field 5. Generation of gravitational waves during magnetogenesis 6. Conclusion. Appendix and References.

24. SINGH (Prabhjot)
Extraction of Neutrino Oscillation Parameters Using a Simultaneous fit of νμ Disappearance and ν_e Appearance Data with the NOvA Experiment.
Supervisor:Prof. Brajesh C. Choudhary
Th24627

Abstract
(Not Verified)

This thesis presents the analyses and results of the νμ → νμ disappearance and νμ → νe appearance due to neutrino oscillations using 8.85 × 10E20 protons on target (POT) equivalent of data collected by the NOvA experiment. The data analyzed in this thesis was collected from February 06, 2014 to February 20, 2017. NOvA is an accelerator-based, long-baseline neutrino oscillation experiment and uses the two detector set-up to study the phenomenon of neutrino oscillation using a beam of muon neutrinos produced at Fermilab. One NOvA detector is placed within the Fermilab campus, 100 m underground, at a distance of 1 km from the neutrino source and is called the Near Detector (ND). The ND is 300 ton in mass and smaller in size than the Far Detector (FD) which is 14 kton in mass and is placed 810 km away from the neutrino source in Ash River, Minnesota (MN). Both ND and FD are made of the same material and are functionally identical. The ND being closer to the neutrino source, analyzes the neutrino beam before the neutrinos oscillate and the FD analyzes the neutrinos after oscillations. The ND is used to predict the signal and background expectations in the FD. The similarity in the ND and FD help to reduce the systematic uncertainties in the FD prediction. The combined oscillation fit to the νμ → νμ disappearance and νμ → νe appearance gives the best fit values of the Δm232, sin2θ32 and δCP oscillation parameters and are presented in this thesis.

Contents

25. VYAS (Manoj Kumar)
Polymer Composites for Electromagnetic Shielding.
Supervisor:Prof. Amita Chandra
Th24639

Abstract
(Not Verified)

The objective of the thesis is to synthesize ion and mixed conducting polymer electrolyte/composite films for electromagnetic shielding application. The work is divided into six different chapters. Chapter one has addressed the effects of electromagnetic radiation on living cells and electronic devices' performance along with EMI shielding mechanism. A brief review of various kinds of shielding materials and the significance of ion conducting polymers using various fillers have also been given. In the end, a brief write-up about the objectives/motivation of the work presented in this thesis is given. Chapter two describes the synthesis of magnetic and dielectric filler particles. The synthesis of polymer composites with the help of PVdF-HFP, EMIMBF4, LiBF4 and the fillers has also been discussed. The various kinds of materials' characterization techniques used have also been given.Chapter three describes the synthesis of transition metal oxide nanoparticles and preparation of polymer electrolyte

composites. The main constituents of the polymer electrolyte composites are; PVdF-HFP, EMIMBF4, LiBF4, MWCNTs and Fe3O4. Shielding effectiveness of the polymer composites has been measured in the Ku-band. Chapter four is focused on the synthesis and characterization of polymer electrolyte composites prepared by the dispersion of BaTiO3 in the mixed (ion+electron) conducting polymer composite. Various types of BaTiO3 particles have been obtained by the solid-state reaction method at different calcination temperatures using (i) mixed phase of TiO2 and BaCO3 and (ii) rutile phase of TiO2 and BaCO3. Shielding properties of the polymer composites have been measured in the X-band. Chapter five consists of studies on the synthesis and characterization of BaTiO3-Fe3O4 and f-MWCNTs-Fe3O4 dispersed mixed (ion+electron) polymer composites and the shielding effectiveness of these composites has been measured in the X-band.

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26. YADAV (Nitish)
Development of Porous Polymer Electrolytes for Supercapacitor Applications.
Supervisor:Prof. S.K. Hashmi
Th24640

Abstract
(Not Verified)

The objective of the thesis is to synthesize ion and mixed conducting polymer electrolyte/composite films for electromagnetic shielding application. The work is divided into six different chapters. Chapter one has addressed the effects of electromagnetic radiation on living cells and electronic devices' performance along with EMI shielding mechanism. A brief review of various kinds of shielding materials and the significance of ion conducting polymers using various fillers have also been given. In the end, a brief write-up about the objectives/motivation of the work presented in this thesis is given.chapter two describes the synthesis of magnetic and dielectric filler particles. The synthesis of polymer composites with the help of PVdF-HFP, EMIMBF4, LiBF4 and the fillers has also been discussed. The various kinds of materials' characterization techniques used have also been given.Capter three describes the synthesis of transition metal oxide nanoparticles and preparation of polymer electrolyte composites. The main constituents of the polymer electrolyte composites are; PVdF-HFP, EMIMBF4, LiBF4, MWCNTs and Fe3O4. Shielding effectiveness of the polymer composites has been measured in the Ku-band.Chapter four is focused on the synthesis and characterization of polymer electrolyte composites prepared by the dispersion of BaTiO3 in the mixed (ion+electron) conducting polymer composite. Various types of BaTiO3 particles have been obtained by the solid-state reaction method at different calcination temperatures using (i) mixed phase of TiO2 and BaCO3 and (ii) rutile phase of TiO2 and BaCO3. Shielding properties of the polymer composites have been measured in the X-band.Chapter five consists of studies on the synthesis and characterization of BaTiO3-Fe3O4 and f-MWCNTs-Fe3O4 dispersed mixed (ion+electron) polymer composites and the shielding effectiveness of these composites has been measured in the X-band. chapter six presents the conclusion drawn from the work carried out in the thesis along with the scope of future work.

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