3.2 Research Papers

3.3.3 Paper Published in National/International Conferences and Book Chapters

(*w.e.f. August 2021 - July 2022*)

S. No.	Name of Faculty	3.2 Research Papers with Date of Publication	3.3.3 Conferences and Book Chapters
1.	Dr. Davender Singh	1. Sugarcane bagasse: an important lignocellulosic substratefor production of enzymes and biofuels, P. Yadav, Anu, S.K. Tiwari, V. Kumar, **Davender Singh**, S. Kumar, Manisha, V. Malik, B. Singh, Biomass Conversion and Biorefinery, (2022). 28.05.2022 2. Cellulase Production by Myceliophthora thermophila in Solid State Fermentation and Its Utility in Saccharification of Rice Straw, Anu, **Davender Singh**, V. Kumar, V. Kumar, V. Malik, B. Singh, New Energy Exploitation and Application, 01 (02) (2022) 10-17. 10.05.2022	
2.	Dr. Kavita		1. Study of shell effects in fusion fission dynamics, A. Sen, Kavita, et.al. Proceedings of the DAE Symposium on Nuclear Physics, 65 (2021) 219-220. ISBN: 978-81-83720847 2. Study of mass angle correlations for the reaction $^{28}Si + ^{160}Gd$ populating ^{188}Pt compound system, Vikas, Kavita et. al., Proceedings of the DAE Symposium on Nuclear Physics, 65 (2021) 423-424. ISBN: 978-81-83720847
3.	Dr. Jitendra Gangwar	1. Probing into crystallography and morphology properties of MoS_2 nanoflowers synthesized via temperature dependent hydrothermal method, N. Kumar, P. Siroha, H. Shankar, D. Singh, Y. Sharma, R. Kumar, Ramovatar, N. Yadav, K.K. Dey, H. Borkar and Jitendra Gangwar, Nano Express 3, 035001 (2022) 06.07.2022. 2. Asymmetric resistive switching by anion out-diffusion mechanism in transparent Al/ZnO/ITO heterostructure for memristor applications, S. Gora, L. Thyda, G. Dasi, R. Muniramaiah, A. Thakre, Jitendra Gangwar, D.P. Joseph, M. Kovendhan, P.A. Azeem, D. Dinakar, K. Thangaraju, H. Borkar, Surfaces & Interfaces 30, 101950 (2022) 15.04.2022. 3. Electric field modulated photoluminescence in ferroelectric ceramics for photosensitive device applications, H. Borkar, S. Mishra, Jitendra Gangwar, D. Haranath and A. Kumar, Materials Research Bulletin 152, 111831 (2022) 24.03.2022. 4. Probing on crystallographic structural and surface morphology of hydrothermally synthesized MoS_2 nanoflowers consisting	1. P. Siroha, N. Kumar, R. Kumar, D. Singh and Jitendra Gangwar. 3D Visualization of Crystallography Information of Hydrothermally Synthesized 2H-MoS_2 Nanocrystalline Material. 65th *DAE SOLID STATE PHYSICS SYMPOSIUM*, 55 (2021) 212-213. ISBN No: 81-8372-085-4. (15-19.12.2021) 2. Book Chapter: Polymer-metal oxide heterostructures: formation, characteristics and applications Book Title: Metal Oxide-Based Heterostructures: Fabrication and Applications Y. Sharma, A.K. Sharma, N. Kumar, R. Kumar, P. Siroha and Jitendra Gangwar, ISBN: 978-0-323-85241-8, Publisher: Elsevier (Elsa), 141-190 (2022)

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		of nanosheets, N. Kumar, P. Siroha, Y. Sharma, D. Singh, K.K. Dey, R. Kumar, H. Borkar and J. Gangwar, Applied Surface Science Advances 6, 100167 (14.09.2021). 5. Effect of Annealing on Structural, Compositional and Optical Properties of Composite ZIO Thin Films, A. Khandelwal, R. Shukla, J. Gangwar, K.S. Sharma, The IIS University Journal of Science and Technology, 10(1), 65-70 (2021).	
4.	Dr. Jyoti Yadav		1. Poster entitled "Meissner effect in Superconductors" in 7th National Conference on Innovations in Science, Engineering & Technology (NCISET-2022) organized by Department of Chemistry, Arya Post Graduate College, Panipat, Haryana, on February 19, 2022. 2. Paper entitled "Location analysis of piezoelectric energy harvested in open channel hydrodynamic system" in 7th National Conference on Innovations in Science, Engineering & Technology (NCISET-2022) organized by Department of Chemistry, Arya Post Graduate College, Panipat, Haryana, on February 19, 2022.
5.	Mr. Sachin		1. Paper entitled "Nanostructured Metal Oxide for Photocatalytic Applications" in International Conference on Frontiers in Physics, Material Science & Nanotechnology (FPMSN-2022) held on 25-26th Mar, 2022 at Chaudhary Devi Lal University, Sirsa.
6.	Mr. Praveen Kumar		1. Paper entitled "Enhancement of Energy Storage in Supercapacitor" in International Conference on Frontiers in Physics, Material Science & Nanotechnology (FPMSN-2022) held on 25-26th Mar, 2022 at Chaudhary Devi Lal University, Sirsa.
7.	Mr. Somveer		1. Paper entitled "Comparative study on transition metal chalcogenides nanomaterials capability in energy storage devices" held in International Conference on Frontiers in Physics, Material Science & Nanotechnology (FPMSN-2022) held on 25-26th Mar, 2022 at Chaudhary Devi Lal University, Sirsa.
8.	Ms. Varsha	1. Impact of Artificial Intelligence in HR Practices in Service Sector in India. Varsha, International Journal of Creative Research Thoughts, 10 (1), 2022. ISSN: 2320-2882, Paper ID: IJCRT2201391. 15.01.2022	1. Book Chapter: The study of prospects of E-commerce in Rural areas (A case study of Bhiwani District in Haryana) Book Title: Strategic Advantage through Innovations Varsha, ISBN: 978-3-96492-396-1 Publisher: Weser Books (2022)

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9.	Dr. Yashpal Sharma		1. Chemistry: Lab Manual, Y.P. Sharma, R. Kumar, N. Chandel, Akash Publishing House (Code: CHEM 101 PR) ISBN: 978-93-91743-00-5 2. Chemistry: Lab Manual, Y.P. Sharma, R. Kumar, N. Chandel, Akash Publishing House (Code: CHEM 102 PR) ISBN: 978-93-91743-03-1
10.	Dr. Jitender Jindal		1. Chemistry: Lab Manual, R. Kumar, N. Chandel, Y.P. Sharma and J, Jindel, Akash Publishing House (Code: CHEM 202 PR) ISBN: 978-93-91743-71-4 2. Chemistry: Lab Manual, R. Kumar, N. Chandel, Y.P. Sharma and J, Jindel, Akash Publishing House (Code: CHEM 201 PR) ISBN: 978-93-91743-70-6 3. Book Chapter: Advanced Materials towards Environmental Protection Book Title: Advanced Materials for a Sustainable Environment N. Kumar, P.R. Makgwane, J. Jindal. ISBN: 9781003206385, Publisher: Taylor & Francis Group (2022)
11.	Dr. Hemant Kumar	1. Soil erosion assessment in a part of gully affected Chambal region, Uttar Pradesh (India), using Morgan–Morgan–Finney model, **Hemant Kumar**, P. Pani, Modeling Earth Systems and Environment, 8, 5279-5288 (2022). 26.03.2022	1. Paper entitled paper "Soil Erosion Risk Assessment in a Part of Lower Chambal Valley (India) using Morgan-Morgan-Finnèy Model"in Online **National Seminar** on "Geo-Spatial Technologies in Rural Development" organized by NIRDPR-NERC, Guwahati during 09th - 10th Feb, 2022. 2. **Workshop** on "Integrating Sustainable Development Goals into Rural Development Agenda: Water, Sanitation Services in Village Development Plans" held at National Institute of Rural Development and Panchayati Raj (NIRD&PR), Delhi Branch on 11th July, 2022.
12.	Mr. Rahul Sharma		1. Participated in Energy Conclave-2022 "Renewable Energy and Sustainable Development (RESD 2022)" the paper on "A Statistical Study of Social Waste Generation in India" held at Banaras Hindu University, Varanasi during 26th 27th March, 2022.
13.	Ms. Shardha	1. Human Resource Development and Skill Employment in present Era. Shardha, International Journal of Creative Research Thoughts, 10 (3), 2022. ISSN: 2320-2882 Paper ID: IJCRT2203267. 01.03.2022	

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REVIEW ARTICLE

Sugarcane bagasse: an important lignocellulosic substrate for production of enzymes and biofuels

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Abstract
Sugarcane bagasse (SCB), a by-product of sugarcane industry, is a rich source of cellulose (45%), hemicellulose (32%), and lignin (17%) with low ash content. Being produced in large quantities by sugar industries, it is a great challenge for environment because it is mostly burnt in-open or either disposed improperly causing environmental pollution. Due to rich source of fermentable sugars, it is used as a substrate for producing microbial enzymes and biofuels. Secondly, high fuel prices, limited fossil fuel reserves, and environment pollution due to burning of fossil fuels have also highlighted the need for renewable and sustainable sources of energy such as biofuels. Sugarcane bagasse is a renewable, easily available, and cost-effective alternative for synthesis of biofuels and various microbial enzymes in submerged (SmF) as well as solid-state fermentations (SSF). However, for biofuel production, the main hindrance in utilizing bagasse is the requirement of large amount of enzymes for conversion of lignocellulosic biomass into fermentable sugars. Therefore, there is an utmost need for the production of enzymes using cost-effective and easily accessible substrates such as sugarcane bagasse followed by utilizing these enzymes for saccharification of carbohydrate polymers into fermentable sugars for biofuels. However, the presence of lignin hampers the saccharification of cellulose and hemicellulose into easily fermentable sugars. Therefore, pretreatment reduces lignin content of sugarcane bagasse and makes cellulose and hemicellulose easily accessible for enzymatic hydrolysis. Enzymatic hydrolysate can be further fermented to biofuels using aerobic and anaerobic microorganisms.

Keywords Lignocellulosic biomass · Cellulolytic enzymes · Pretreatment · Fermentation · Value-added products

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Abbreviations

SCB	Sugarcane bagasse
SSF	Solid-state fermentation
ABE	Acetone-butanol-ethanol
U/ml	Unit per ml
U/g	Unit per gram
SmF	Submerged fermentation
STB	Stirred tank bioreactor
RSM	Response surface methodology

1 Introduction

Sugarcane is one of the major cultivated crops in tropical and sub-tropical parts of the world. India is the 2nd largest producer of sugarcane after Brazil with an estimated sugarcane production of 306 million tons per year [1]. Sugarcane bagasse (SCB) is the main by-product of sugar industry, which is produced in huge amount, i.e., 100 million tons per year in India. About 50% of SB is utilized in the generation

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ARTICLE

Cellulase Production by *Myceliophthora thermophila* in Solid State Fermentation and Its Utility in Saccharification of Rice Straw

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Abstract: Optimization of cellulase production by thermophilic mould *Myceliophthora thermophila* BJTLRMDU3 was studied in solid state fermentation. *Myceliophthora thermophila* produced maximum cellulase (45.81 U/g DMR) at substrate to moisture ratio of 1:3 with 5-d old inoculum at water activity 0.95, ammonium sulfate (0.5%) and PEG 20000 (0.5%) at 45 °C using "one variable at a time" approach. Further supplementation of Tween-20 (0.5%) and K_2HPO_4 (0.25%) enhanced the cellulase production (56.06 U/g DMR) by *M. thermophila* in SSF. Optimization of saccharification by partially purified cellulase of *M. thermophila* (20 U), liberated maximum reducing sugars at pH 5.0 (185.56 mg/g substrate) and 60 °C (190.83 mg/g substrate) after 24 h (203.91 mg/g substrate) from sodium carbonate pretreated rice straw as compared to untreated biomass. Liberated reducing sugars were higher in sodium carbonate pretreated rice straw than untreated rice straw.

Keywords: Rice straw, *M. thermophila* BJTLRMDU3, Optimization, Cellulase, Sodium carbonate, Saccharification

1. Introduction

Renewable biofuels have been emerged as an effective ecological and economical alternative in spite of conventional fossil fuels nowadays [1-3]. In this view, lignocellulosic substrates i.e., agro-residues are highly preferred as potential and renewable carbon sources for biofuels due to release of various fermentable sugars after their hydrolysis. Utilization of agro-residues for valuable products at industrial scale somewhat decreases the problem of environment pollution due to their improper practice of disposal and open burning [2]. Cellulolytic enzymes promote the breakdown of cellulosic

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Study of shell effects in fusion fission dynamics

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Introduction

The discovery of nuclear fission in 1938 coincided with the seminal developments of theories of quantum mechanics in the 1930s. To explain the newly discovered phenomena theoretical work based on classical and quantum physics was invoked, and the best minds of the time worked in the problem. It was evident that in order to explain the asymmetric mass split, quantum shell effects play the key role in the dynamics governing fusion fission. Various theories were proposed to explain the data from numerous experimental results with light/heavy ion induced fission as well as spontaneous fission.

As physics progressed experimentally as well as theoretically, the periodic table got extended (currently stretching upto 118 elements), and human kind was introduced to super heavy elements (SHE), which are elements with proton numbers more than 104. Classically, elements with more than 104 protons should not exist as the fission barrier would have been zero, and the element would undergo spontaneous fission. However, it is again the quantal shell effects which stabilizes these elements and the SHEs are formed with unique properties.

For the formation of the SHEs, nuclear reactions using heavy ions are used. Two types of nuclear fusion reactions are used for the synthesis of SHEs: cold fusion and hot fusion. In cold fusion reactions doubly magic nucleus ^{208}Pb is used as a target along with the suitable choice of projectile, while in hot fusion reactions doubly magic projectile ^{48}Ca is used on actinide targets. The selection of magic nuclei i.e., the number of shell closures in the target projectile combination has been a subject of intense scrutiny, with multiple experiments being carried out at accelerator facilities all over the world. C. Siemenel, *et al.* [1] showed that for reactions involving heavy ions the competing quasi-fission process which hinders the formations of SHE, is comparatively lower for reactions involving magic target-projectile combinations. However, the change in the fusion fission dynamics due to the change in magicity in the target projectile combination is not clearly understood. In order to elucidate that, a set of experiments were carried out with target projectile combinations which would involve a change in magicity. However the relative contribution of quasi fission in the reactions is expected to be absent, as the chosen reactions had charge products $Z_P Z_T$ less than 800. The study was carried out on the actinide nucleus ^{224}Th, populated through three different channels, (i) ^{16}O+^{208}Pb , where both the target ^{208}Pb and projectile ^{16}O being dou-

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Study of mass angle correlations for the reaction ^{28}Si + ^{160}Gd populating ^{188}Pt compound system

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Introduction

The study of heavy ion induced fusion-fission reactions is a thrust area of nuclear science research for – the production of super heavy elements and to understand the mechanism of fusion fission reaction dynamics. A major hurdle in the super heavy elements formation is the Quasi-Fission (QF) or non compound nucleus fission. A large number of experimental studies were performed to understand the fusion fission dynamics of heavy ion induced reactions in A $\approx$ 200 mass region [1–4]. Fusion fission dynamics of interacting binaries depends on various entrance channel parameters, such as, product of projectile and target charge, Z_pZ_t, entrance channel mass asymmetry, N/Z ratio of reaction parteners, projectile – target deformation etc. These entrance channel parameters play a key role in deciding the path of a heavy ion induced fusion fission reaction starting from interaction phase till it scissions. Fission fragment mass distribution, angular distribution and mass angle correlation are considered as the sensitive tools to investigate the presence or absence of QF in a given reaction. In the present work, we have performed mass angle correlation study of fission fragments produced in the reaction ^{28}Si + ^{160}Gd populating ^{188}Pt compound system at various excitation energies.

Experimental Details

The experiment was performed using the General Purpose Scattering Chamber (GPSC) facility at Inter University Accelerator Centre, New Delhi. Pulsed beam of ^{28}Si from Pelletron accelerator, in the laboratory energy range of 120 – 140 MeV, was bombarded on ^{160}Gd target having thickness of 220 $\mu g/cm^2$. The target was fabricated on 20 $\mu g/cm^2$ carbon backing. Fission fragments were detected using two large area (16 cm x 11 cm) multiwire proportional counters (MWPCs), mounted on each arm of the chamber. Complete details of the experimental setup are given in ref. [1].

Analysis and Results

The calibrated position and time of flight (TOF) information from the two MWPCs were used to obtain the emission angles of the fission fragments. The time difference method was used to extract the masses of complementary fission fragments [5],

$$m_1 = \frac{(t_1 - t_2) + t_0 + m_{CN}(d_2/p_2)}{(d_1/p_1) + (d_2/p_2)}, \quad (1)$$

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Probing on crystallographic structural and surface morphology of hydrothermally synthesized MoS_2 nanoflowers consisting of nanosheets

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ABSTRACT

Hydrothermally synthesized MoS_2 were obtained and their morphological characteristics were ascertained via electron microscopy. Field emission scanning electron microscope (FESEM) micrographs revealed the formation of nano-flowers by accumulation of nanosheets. The Transmission electron microscopy (TEM) revealed the nanosheets to be of ~100 nm length and ~5 nm in edge width. X-ray diffraction pattern analysis showed the formation of 2H polymorph of MoS_2, having a long range stacking of about 14 (002) lattice planes in a single crystallite. The Fourier transform infrared (FT-IR) spectroscopic analysis revealed the presence of bridging S_2^{2-} ligands. Energy dispersive spectroscopy (EDS) analysis associated with the SEM indicates the presence of no other elements except Mo and S in the material. Visualization of atomic structural model and intense lattice plane has been carried out and correlated with crystallographic results. Such findings can be considered as important precursors in both experimental elementary aspects and theoretical approach towards the application-oriented research for crystallographic analysis of nanostructures.

Introduction

Nanostructured transition metal chalcogenides such as metal oxides (cobalt oxide (Co_3O_4), nickel oxide (NiO), vanadium oxides (VO_2, V_2O_5)) and metal sulfides (cobalt sulfides (CoS, Co_3S_4, Co_9S_8), copper sulfides (CuS, Cu_2S), iron disulfide (FeS_2), nickel sulfides (NiS, Ni_3S_4), tin sulfide (SnS_2), tungsten disulfide (WS_2)) have increasingly become an area of special interest in both fundamental research and applied disciplines [1–10]. Largely because of the promise shown by them for a broad range of applications; these materials for decades have captured the attention of the research community. An intriguing aspect of these transition metal chalcogenides is their well-known two-dimensional (2D) structure in which a plane (M) of transition metal element (e.g., Mo, Ta, Ti, V, W, Zr etc.) and two planes (X) of the chalcogenides (e.g., S, Se or Te) are arranged periodically in a hexagonal structure with a layered X-M-X sandwiched composition [11–16]. Similar to graphene these kinds of layers are held together by weak van der Waals's interaction between them and thus the distance between the layers are prone to easy manipulation by methods such as exfoliation [3,11–12]. Amongst various layered transition metal sulphides (LTMSs), nanostructured molybdenum (IV) sulfide (often referred to as molybdenum disulfide; MoS_2) materials have often received the most attention due to their unique physicochemical features such as simple 2D structure, ease of processing, inexpensiveness, and more importantly, close structural analogy to graphene nanosheets and a large number of potential applications [21–27]. The layered structure or 2D morphologies of MoS_2 have found potential for a varieties of applications such as electronic devices [1,5,8,36–39], sodium ion batteries [2,18,19], lithium ion batteries [25], hydrogen evolution reaction [12,22,27,30,34,35], solar cells [14], water filtration [15,24,46], electrochemical capacitors [17,20,23], lubricants [29], sensors [40,41] and in electromagnetic wave absorption [42,43].In fact, shielding from harmful electromagnetic waves is a potential application for such 2D nanostructures with high specific surface area and good carrier mobility [44–47].

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Asymmetric resistive switching by anion out-diffusion mechanism in transparent Al/ZnO/ITO heterostructure for memristor applications

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ABSTRACT

In this report, the monovalent cations of sodium and potassium are doped into the ZnO matrix to explore for resistive switching. The structural analysis confirms that Na^+ and K^+ cations are incorporated into the interstitial sites of ZnO lattice. The Na^+ and K^+ doped ZnO thin films (NZO and KZO) have exhibited improved transparency slightly higher than 80 % for the wavelength range 400-1000 nm. Hall and impedance measurements confirms that resistance of the thin films increased after incorporation of Na^+ and K^+ cations into the ZnO lattice. The fabricated NZO and KZO thin films-based memory devices exhibited bipolar resistive switching phenomenon with excellent ON/OFF ratio of 10^4, endurance of ~ 100 cycles, and charge retention of 10^4 s in both the resistive states. These results imply that NZO and KZO films to have enormous potential to serve as an efficient resistive switching device.

1. Introduction

The present era of artificial intelligence (AI) and the internet of things (IoT) needs large data for various applications such as high-speed information transfer between the processor and the memory unit. However, the limited bandwidth of processor-memory in the present device architectures unavoidably results in deterioration of the performance of the system, which greatly hamper the positioning of AI algorithms on energy-limited IoT devices [1]. Complementary metal-oxide-semiconductor (CMOS) technology has been used for the fabrication of processor-memory systems and is dedicated to SRAM-based computing in-memory to perform various operations. Low memory density and high leakage power of CMOS-based SRAMs barely accommodate for data-intensive applications. Therefore, CMOS-based memory devices have poor energy efficiency for big data handling and the internet which requires fast memory scaling is now a central focus of the electronics industry. To overcome this issue, there is a necessity to search for a new generation of memory nanodevices. The resistance random access memories (ReRAMs) or Resistive switching (RS) memories can be alternative for next generation nonvolatile memories which may be equivalent to the CMOS technology and have capabilities of high switching speed and low-power consumption for operations [2–5]. The memristive phenomena is based on resistive switching initially predicted by Prof. Leon Chua [6] and experimentally verified by researchers at Hewlwtt Packard [7]. Memristive devices are based on resistive switching (RS) phenomena wherein memory conditions depend on resistive switching state and electrical biasing conditions. The RS phenomenon has several advantages in the field of memory devices such as very high-speed switching, higher endurance, high charge retention potentiality, higher scaling capability, and low power consumption [2, 4]. These aspects make RS devices have extraordinary application in the field of non-volatile random-access memory and memristors. Owing to these properties, the RS memories or ReRAMs have become complementary to the CMOS technology [2,4,5,8]. Although, RS has got considerable approach towards material exploration, still there are modifications of controlled parameters required at the electrode/oxide interface. To mention a few, the effect induced by Joule heating effect or by electroforming interaction of conductive filaments formed during the

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Electric field modulated photoluminescence in ferroelectric ceramics for photosensitive device applications

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ABSTRACT

The degree of freedom controlled by electronic excitations in ferroelectrics provides innovative opportunities for information processing and optoelectronics. In the current work, electrically modulated photoluminescence (PL) has been demonstrated in $Pb_{1-x}(Li_{0.5}Bi_{0.5})_x(Zr_{1-y}Ti_y)O_3$ (PLBZT) for $x = 0.3$–0.5 and $y = 0.80$, respectively. The primary approach was made directly to modulate the PL property by applying an external electric field in an *in-situ* way. However, the modulation of PL is possible in perovskite oxides when the distortion of structural symmetry arose under external electrical bias in particularly ferroelectrics, implying reversible and dynamic tuning of PL emission. Hence, there is emergence of new channels where radiative and/or forbidden transitions arise from the positional disorder of the system under the application of an external electric field. These studies establish the realization of tunable PL ferroelectric ceramics with high repeatability, flexibility, and faster response towards designing advanced light switching devices.

1. Introduction

Spectroscopic tuning of photoluminescence (PL) is a subject of interest because of its enormous applications in optical waveguides, lighting display, biomedicine, and medical imaging [1,2]. To understand the tuning of PL, energy transition is the most common phenomenon that needs to be explored. To date, the most common practice to get enhanced/decreased in PL response is by introducing luminescent centers into the host matrices by conventional chemical method *i.e. ex-situ* process. Therefore, crystallographic structure and its symmetry play a crucial role in influencing the PL emission [3,4]. Moreover, it is challenging to tune the PL under external stimuli such as pressure, temperature, electric and magnetic fields. This restricts the tuning of luminescence intrinsically and its related extended applications. The variation of PL in solids could be recognized by the energy transitions of materials and crystal field theory. Composition variation is one of the methods where the modified PL response can be achieved for particular materials. In general, phase transformations of inorganic materials are easily achievable by modifying stoichiometric calculations. From a device point of view, it's always desired to tune the property under any external stimulus that can alter the physical properties such as centrosymmetric, piezostriction, electrostriction including several other properties. Because of such a scenario, polar materials can efficiently respond to any external stimulus. In particular, centrosymmetric crystals react to external incitement, break the centrosymmetric, and show ferroelectric, ferromagnetic, and piezoelectric properties. Hence, there is a stringent need to find a pathway for variation of PL response by an external electric field which can modify the PL. Therefore, the PL property associated with photo-ferroelectrics is the center of attraction nowadays because of its giant multifunctional applications in the lighting industry, memory technology, and enormous bio-medical applications [5].

In ferroelectric materials, the electro-mechanical properties of the lattice are strongly correlated with polarization and crystal structure that makes it ready to transform under electric field [6]. Hence, is expected to break the crystal symmetry, and might affect the PL response. So, exclusive phenomena are correlated to the electric polarization and interaction with light that gives rise to the large photostriction [7] and the electrical control of the photovoltaic response [8]. The concurrence of photostriction in ferroelectric/magnetic materials has been used to change ferroics properties by light [9,10] and memory cells based on electrically can be controlled by polarization-dependent photoconductance [11–13]. Therefore, optically controlled polarization would be capable of fast switching the polar alignment in the direction

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PAPER

Probing into crystallography and morphology properties of MoS_2 nanoflowers synthesized via temperature dependent hydrothermal method

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Abstract

This paper reports the formation of flower-like hierarchical molybdenum disulfide (MoS_2) nanoparticles following a simple one-step hydrothermal process with varying temperatures (200 °C and 220 °C). The as-synthesized particles were examined crystallographically by X-ray diffraction (XRD) method which revealed the formation of hexagonal MoS_2 (2H-MoS_2) and that the crystallite size of the particles increased with increasing hydrothermal temperature. Surface morphological characteristics of the particles were investigated by a field emission scanning electron microscope (FESEM) and interesting details were revealed such as the rounded 3D flower-like microstructure of the MoS_2 particles and the petals of the flowers were composed of platelets built up by stacked-up MoS_2 nanosheets. With the increase in hydrothermal temperature, the interlayer spacing of stacked layers of intense (002) plane is slightly decreased although the crystallinity of the material is improved. Both diameter and thickness of the nanoflowers and the nanoplatelets increased twice with increasing the temperatures. A visual crystallographic perspective was presented through simulation of 3D wireframe unit cell associated with the individual lattice planes as observed in the XRD pattern of the samples. In addition, a plausible growth mechanism is proposed for the formation of the obtained MoS_2 nanoflowers on the basis of experimental observations and analysis.

1. Introduction

Both the preparation and property studies of novel two-dimensional (2D) and/or three-dimensional (3D) nanostructured materials based on metal chalcogenides such as metal-oxides, -sulfides, -selenides, -nitrides with controlled morphology have attracted enormous interest that has steadily grown worldwide because of their exotic properties that are important for various innovative applications [1–12]. In recent years, intensive research has been devoted to producing high-quality 2D and 3D metal sulfide (CoS_2, FeS_2, MoS_2, NiS_2, SnS_2, and WS_2) nanostructures of various morphologies e.g. nanoparticles, nanoflowers, nanosheets, nanospheres and nanolamellar morphology [2, 6, 13–18]. Among the widely known metal sulfides, molybdenum disulfide (MoS_2) is a naturally occurring, well-defined two-dimensional (2D) layered material that has been reported to be an excellent material capable of various

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RESEARCH ARTICLE

Effect of Annealing on Structural, Compositional and Optical Properties of Composite ZIO Thin Films

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Abstract

In this work, the structural, compositional and optical properties of composite zinc indium oxide (ZIO), thin films grown on glass substrates using thermal vapor evaporation technique have been investigated for two different ratios of $ZnO:In_2O_3$=90:10 and 80:20 wt.% at room temperature. The films so obtained were annealed for 2 h at 500°C. The ZIO films are amorphous before annealing and become crystalline after annealing for both the ratios, as revealed by the X-ray diffraction patterns. The study of the composition of the surface and oxidation states present there in made by using X-ray photoelectron spectroscopy, also provides information about the binding energies of deposited materials. The effect of thermal annealing on these mixed oxide thin films has also been studied by using UV visible Spectroscopy. The optical band gap is found to increase on annealing the ZIO thin films.

Keywords: Composite ZIO thin films, Optical band gap, XPS, XRD.

Introduction

Thin films of Zinc oxide (ZnO) are superior choice for optical applications due to their excellent properties. It is non toxic and reasonably less rare. It has tunable electronic conductivity (Biswal *et al.*, 2014). It shows high degree of transparency for UV-vis electromagnetic radiation (Kumar *et al.*, 2004). ZnO has common uses in flat panel screen (Chae, 2001), in piezoelectric devices, as photo catalysts (Chang *et al.*, 2016), as antimicrobial agent (Lefatshe *et al.*, 2017), in photovoltaic devices (Sharma *et al.*, 2015), and in electrode applications such as in light emitting and absorbing devices (Liu *et al.*, 2010). For surface deposition it does not require very high substrate temperature (Muchuweni *et al.*, 2016). By doping of some materials the optical performance of these materials can be made more appropriate for application in several optoelectronic devices. This may happen due to change in their crystal structure on doping with impurities (Moditswe *et al.*, 2016). Several researchers have examined the properties of ZnO doped with different doping elements, including indium, aluminum (Bedia *et al.*, 2015), copper (Muiva *et al.*, 2011), fluorine (Ariyakkani *et al.*, 2017), cobalt (Dhruvashi and Shishodia, 2016), tin (Sanchez-Juarez *et al.*, 1998), iron (Chava and Kang, 2017) and a few doping elements.

In its pure form, Zinc oxide is very resistant and researchers are making efforts to enhance its optical properties with deliberate doping. Dopant selection should be based on the ionic size and electro negativity, since both factors determine the effectiveness of the dopant element higher valence (group III) elements are generally preferred to improve the properties of ZnO like optical properties. Thin films of optimized zinc oxide are doped with indium and investigated for its effect on the structural, optical and electronic properties of thin films of ZnO. On the other hand Indium Oxide (In_2O_3) is well- known transparent conducting oxide and prepared both in the form of powder and thin films. It finds application in solar cells, sensors, opto-electronic devices and as a useful electrode material (Hartnagel *et al.*, 1995) and (Lewis and Paine, 2000) and (Elliott, 2005). Recently it has been studied for its properties in different Nano structure shapes, such as spherical (Kim and Park, 2004), rods, wires (Yu *et al.*, 2004) and Nano tubes (Zhu *et al.*, 2004), where the focus has been mainly on preparation in different shapes and their applications.

Zinc indium Oxide (ZIO) is a useful binary oxide for research in view of its practical application. With change of doping percentage of indium oxide in Zinc oxide, a change in optical band gap of ZIO is observed, as reported in (Jain *et al.*, 2010). The goal of the present work is to synthesis high quality films of mixed oxides ($ZnO+In_2O_3$) and to examine their optical properties, the

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3D Visualization of Crystallography Information of Hydrothermally Synthesized 2H-MoS_2 Nanocrystalline Material

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Abstract

In this work, we demonstrate the visualization of atomic arrangement of crystal structures and lattice planes of 2H-phase of MoS_2 nanocystalline material prepared via inexpensive hydrothermal method. The phase identification and crystallography information are examined through powder X-ray diffraction technique and VESTA-3D theoretical tool. The associated crystal planes are created and displayed. This work is to be useful in modern structure-property relationships.

Introduction

Progress over the past decades has been made for understanding of manifold aspects of MoS_2 nanomaterials, including its processing, growth mechanism and structure-property relations. Based upon the coordination environments, MoS_2 crystal exhibits both stable phase (2H-MoS_2) and various metastable phases (1T, 1T', 1T'', 1T''', 1H, 3R and *etc.*), where the letters T, H and R correspond to trigonal, hexagonal and rhombohedral, respectively and the digits indicate the number of monolayers in unit cell. The tunable crystallographic structure of nano MoS_2 materials has aroused significant research interests among distinct scientists, engineers and researchers. Either experimental or theoretical works have extensively studied about the crystal structure information however they turn the attention to probably crystallographic, atomic and/or electronic structure analysis and synthetic approaches involve sophisticated instruments and chemical precursors. A simple and safe strategy to synthesize MoS_2 nanomaterial, therefore, is essential for technological applications and fundamental understandings about the visualization of distributions of atoms and lattice planes in unit cell at atomic level.

Herein, 2H-MoS_2 nanocrystalline material prepared by unique hydrothermal approach and theoretic predictions for crystallography properties such as phase identification, crystallinity, orientation factor and 3D-visualization of the crystal lattice plane is summarized.

Synthesis of Nanocrystalline MoS_2

MoS_2 nanocrystalline material was synthesized by a safe and facile hydrothermal method using $(NH_4)_6Mo_7O_{24}{\cdot}4H_2O$ and NH_2CSNH_2 as starting material. In a typical procedure, 1.2 and 2.2 gm of $(NH_4)_6Mo_7O_{24}{\cdot}4H_2O$ and NH_2CSNH_2, respectively were dissolved in 40 ml Millipore water under continuous stirring for 1 hour. After that, the formed solution was transferred into stainless steel Teflon-lined autoclave and further kept at 240 °C for 6 hours. After natural cooling, resultant black precipitate was washed four times with Millipore water and absolute ethanol and lastly dried in oven at 80 °C for 24 hours to produce black MoS_2 powder.

Characterization of Nanocrystalline MoS_2

Structural analysis was carried out using X-ray diffraction (XRD; PAN analytical X'pert pro, Netherlands) with Cu-$k_{\alpha 1}$ radiation (λ = 1.54 Å) in the 2θ range of 10-70°. 3D-visualization of crystal structure and lattice planes was created through Visualization for Electronic and STructural Analysis (VESTA) software.

Results and Discussions

Fig. 1 (a) shows the XRD pattern of the as-synthesized MoS_2 material. As shown in Fig. 1(a), XRD pattern demonstrate (002), (101), (103) and (110) crystal planes are observed which confirmed the crystalline structure of 2H phase of MoS_2 with hexagonal crystal system (S.G.: P63/mmc, $a = b =$ 3.14 and c = 12.54 Å, standard JCPDF No.: 01-075-1539). The prominent peak intensity corresponds to (002) plane reveals the maximum numbers of atoms are aligned in z-direction. Inset in Fig. 1 (a) shows the hexagonal crystal structure of MoS_2 indicating stacking layers of molybdenum (Mo) atoms lie in z-plane and sulfur (S) atoms situated in between these layers and form covalent bond with neighboring Mo atoms resulting crystalline 2H-MoS_2 structure. Fig. 1 (b) indicates the crystallite size (D), and orientation

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Polymer–metal oxide heterostructures: formation, characteristics and applications

5

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1. Highlights

- This book chapter covers the fundamental concepts of different conducting polymers-based metal oxides heterostructures.
- Formation mechanism is proposed to generate polymers (including PANi, PEDOT, PTh, and PPy)–metal oxides heterostructures (PMOHs) systems.
- Crystallographic characteristics and various nanoscaled morphologies are then briefly enclosed.
- The PMOH also explored their probable applications in gas sensors and supercapacitors.

2. Introduction

2.1 Trends of polymer–metal oxide heterostructures

Both energy and environmental issues, clean energy storage/conversion, and pollutant-free air and water are the persistent problems yet for the modern society in the 21st century that affected the ecosystem as well as significant damage to the human olfactory and respiratory system (Bairi et al., 2015; Chen et al., 2010; Fischer et al., 2007; Gangwar et al., 2013; Gong et al., 2010; Chmiola et al., 2006; Mallouki et al., 2007; Masarapu et al., 2009; Miller & Simon, 2008; Ram et al., 2020; Sassin et al., 2010; Sharma et al., 2008; Taccola et al., 2013). Owing to the preference and usage of highly combustible, explosive, irritating, and toxic gases such as liquefied petroleum gas (LPG), compressed natural gas, ammonia (NH_3), hydrogen sulfide (H_2S), and many other related gases, the frequency of accidental explosion has risen due to the increase in leakage of gases (Amita et al., 2020; Bai et al., 2014; Bandgar, Navale, Mane, et al., 2015a; Das and Sarkar, 2017; Dhawale et al., 2010; Gong et al., 2010;

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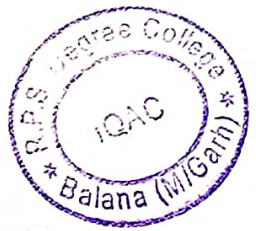

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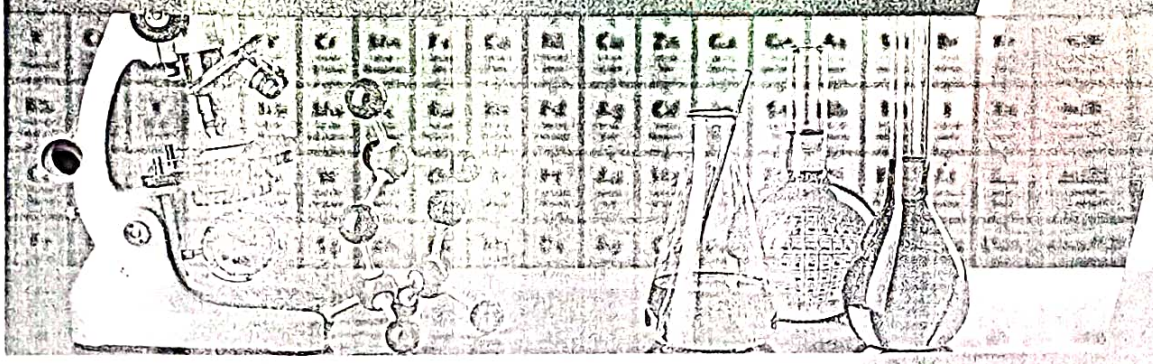

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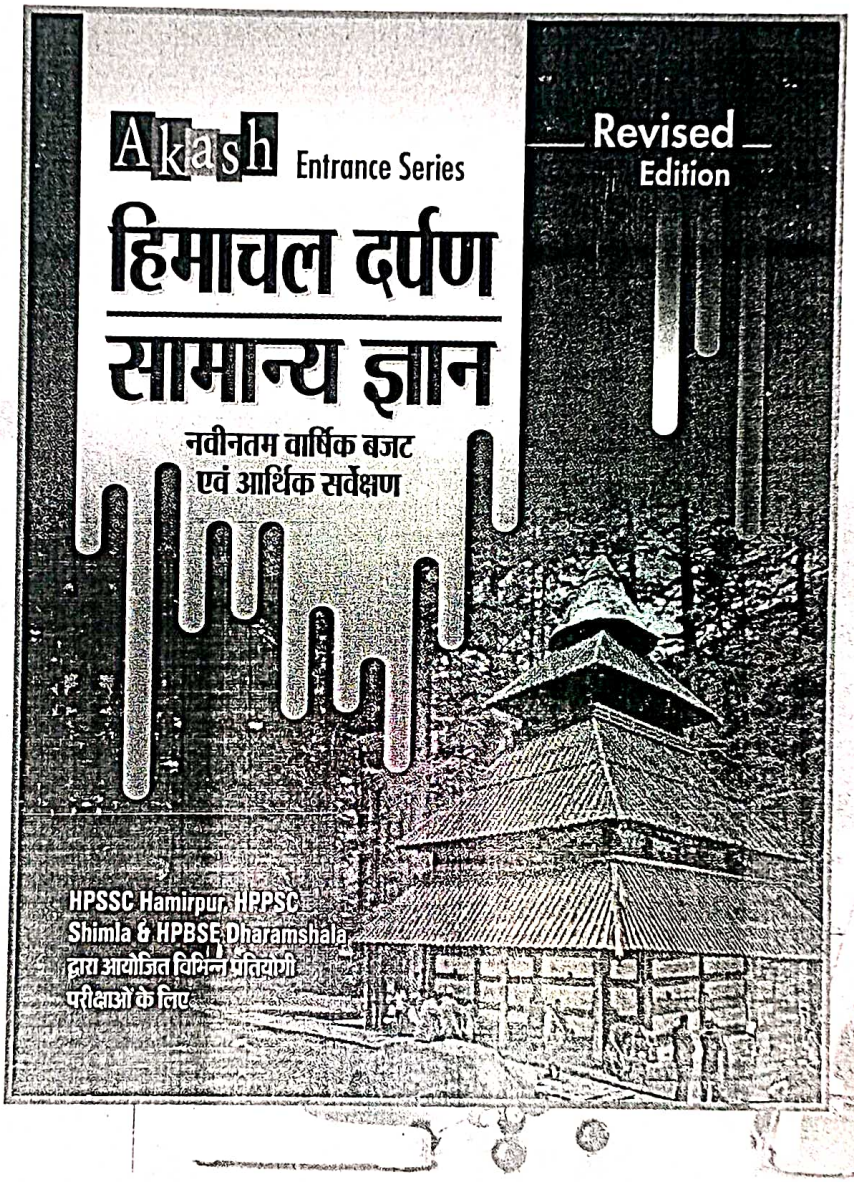

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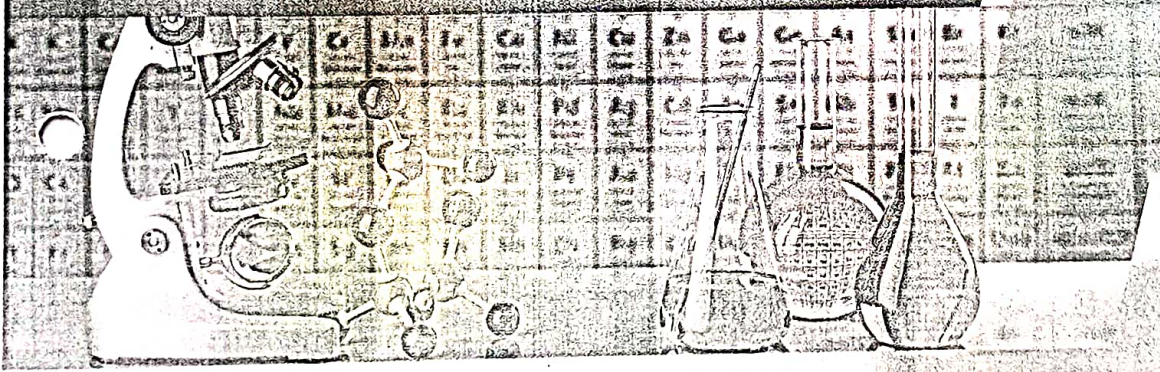

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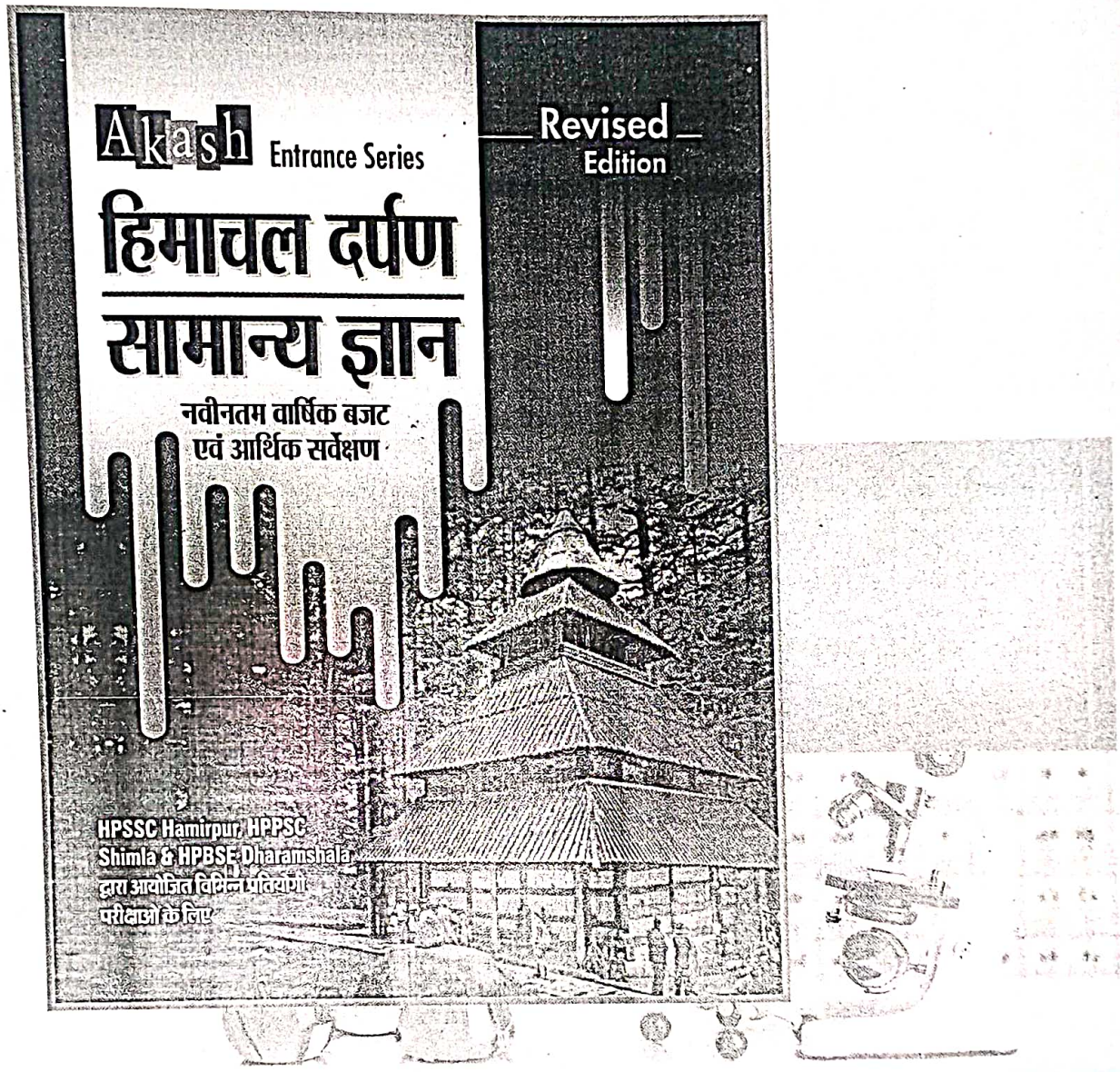

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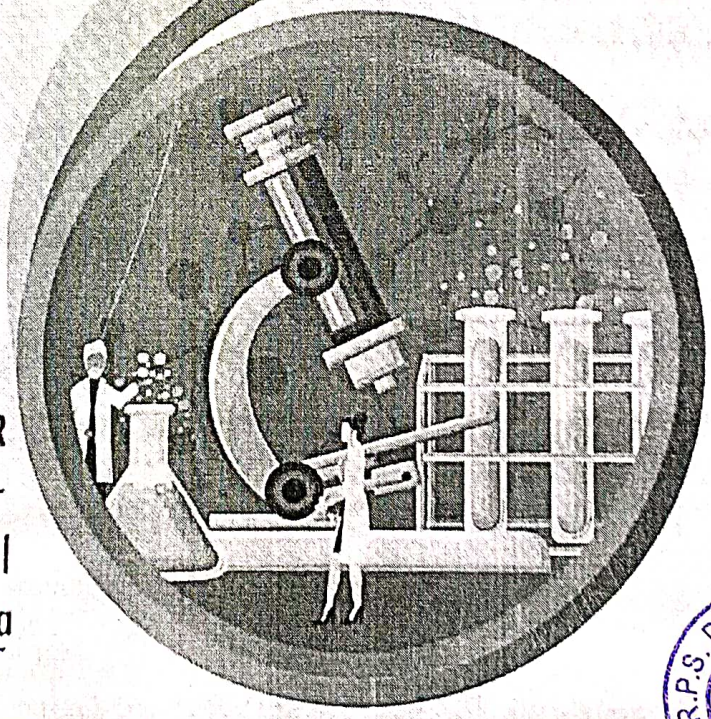

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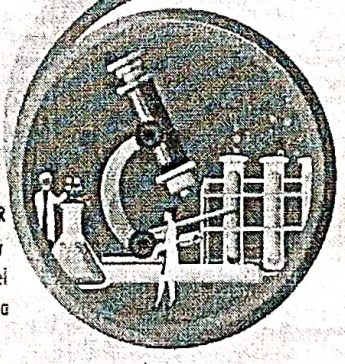

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Chapter

Advanced Materials towards Environmental Protection

Attributes and Progress

By Naveen Kumar, Peter R. Makgwane, Jitender Jindal

Book Advanced Materials for a Sustainable Environment

Edition	1st Edition
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Imprint	CRC Press
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eBook ISBN	9781003206385

ABSTRACT

This chapter highlights the progress in advanced materials with respect to their applications in environmental detection, remediation, and monitoring. Emerging pollutants in the atmosphere (air) and water contaminations demand for the innovations in advanced materials, which can decontaminate these environmental pollutants efficiently and sustainably. First, the emerging pollutants from different sectors are discussed, which is followed by the design and engineering strategies of the various advanced materials. The prominent materials exhibited advanced superior performance and structural characteristics ranging from doped compounds, mixed metal oxides' heterostructures, hybrid materials such as carbon nitride-based materials, polymer-assisted materials, metal organic framework hybrids, Mxene-based materials, ionic liquid-assisted materials, clay-based materials, and zeolite-based materials. This chapter further emphasizes on highlighting developments in material application-integrated technology approaches towards environmental protection, like photocatalysis, hydrogen production and storage, chemical sensing, adsorption, and lithium-ion batteries. Finally, conclusions with respect to the future opportunities for further developments are

Modeling Earth Systems and Environment
https://doi.org/10.1007/s40808-022-01375-w

ORIGINAL ARTICLE

Soil erosion assessment in a part of gully affected Chambal region, Uttar Pradesh (India), using Morgan–Morgan–Finney model

Hemant Kumar[1] · Padmini Pani[2]

Received: 28 November 2020 / Accepted: 3 March 2022

Abstract

Soil erosion of fluvial landscape is a worldwide problem, which affects the agrarian society the most. The tectonically uplifted fluvial deposits of Yamuna-Chambal are facing the worst form of soil erosion in India. About half of the study area comes under the gully and ravine affected area. The encroachment of cultivable land by gully and ravine network is posing serious socio-economic challenges to the society of the region. To assess the magnitude and intensity of soil loss, the region needs better methods for soil erosion. GIS based soil erosion modelling have this potential. In present study, an attempt has been made to estimate the soil loss rate by using Morgan-Morgan-Finney Model and GIS. It has been found that the average annual soil loss rate is 18.20 t ha^{-1} year^{-1} in the study area. The highest rate of soil loss (above 70 t ha−1 year^{-1}) have been estimated in unconsolidated flood deposits & steep slop part of gullies. The lowest soil loss rate (4.0 t ha^{-1} year^{-1}) have been identified in densely forested land followed by intensify cropped area of the region. Due to the undulating surface and high intensity of rainfall in a short period of time, the transport capacity of running water in this region is very high. Although seasonal vegetation cover is a major protection against erosion, the weathering nature of the soil and steep slopes provide significant amounts of erosive material here. Land management and degree of slope favouring low erosion in intense cropped field in the study area. The Morgan-Morgan-Finney model and Geographic Information System is used to identify potential soil erosion risk zones, that can be used to prepare a land management plan for the region.

Keywords Lower Chambal region · Soil erosion modelling · Morgan–Morgan–Finney model · Geographic information system

Introduction

Removal of soil material commonly by wind and water is known as soil erosion. It is a type of soil degradation in which the physical, chemical and biological qualities of the soil are sacrificed. Soil removal has substantially affected one third to half of the world's agricultural land. (Pimentel et al. 1995; Lal 2000, 2006 and Morgan 2005), that directly have an effect on livelihood of rural society (Lal 1985; Kerr 1997). Due to onsite effects of land degradation, about 2% of gross domestic production or 7% of value of agricultural outputs are losing annually by South Asian nations like India, Pakistan, Bangladesh, Nepal, Bhutan Sri Lanka, Iran, and Afghanistan (World Soil Resources Reports 1994). Soil erosion is encroaching new land, hence posing serious threat to human food security, environment and sustainable development (Pimentel 2000).

In India, soil erosion is widespread over half (53%) of its total geographical area (NCA 1976). The annual loss of soil in India is about 16.4 t ha^{-1} year^{-1} (Jain et al. 2001; Srinivas et al. 2002a; Pandey et al. 2009). Major regions of soil erosion in form of gully and ravine are spread along banks of Yamuna, Chambal, Mahi and in Shiwalik Himalayan belt (Kothyari 1996). There are 3.67 million hectares area under effect of gully erosion in India (Mircea 1999). Formation of ravines are worst form of land degradation in semi-arid region of India whose foremost effects are on land quality and economic scenario of the people of the region (Pani 2012). Loss of top fertile soil resultant in to loss of soil

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