

A.2: Utilization activities of Indus beamlines

Indus-1 and Indus-2 synchrotron radiation sources are national facilities, which have been attracting a large number of researchers from all over the country. In the period July 2019 to June 2020, the total number of user experiments that were carried out at the Indus-1 and Indus-2 beamlines were 518. These include users from the industry who have used the EXAFS and XRD beamlines for their R&D programmes. As a consequence of the COVID-19 pandemic, no user experiments could be carried out from April to June 2020.

As a part of our continued efforts towards beamline upgradation, the monochromator mirrors of the soft x-ray reflectivity beamline BL-03, Indus-2, were cleaned and reinstalled inside the monochromator of the beamline. This was necessary, as it is a well-known phenomenon that with exposure to synchrotron radiation, x-ray mirrors get coated by carbon, thereby reducing their efficiency. The contamination also introduces carbon absorption features in the reflectivity spectra. The mirror cleaning was carried out using an in-house developed RF plasma based cleaning setup. This indigenous development of both the system and the process parameters for cleaning and carbon contaminated mirrors, has resulted in significant cost and time saving. Figure A.2.1 shows the pictures of the gold coated x-ray mirrors before and after cleaning.

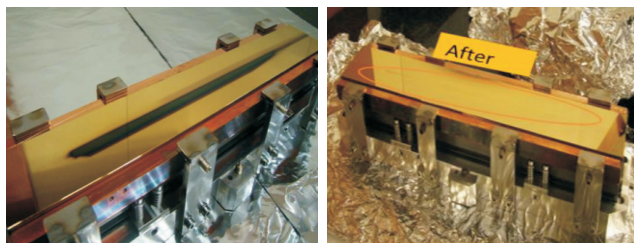


Fig. A.2.1: The picture of the gold coated x-ray mirror before cleaning (left) and after cleaning (right).

During this period, about 175 papers were published in different peer reviewed international journals. The topics in these publications cover diverse range of disciplines that include: materials science, biology, chemistry, nanoparticles, industrial applications, etc. Some of the interesting research results that have been published in the last one year are summarized below.

Different groups have carried out experiments on novel energy materials. These include studies on nanostructured NiTi films and its role for providing 'stress buffering' during electrochemical Li-alloying/de-alloying in supercapacitors (Ref: Manoj K. Jangid et al, ACS Applied Energy Materials, Vol. 2, p 8181 (2019)). In order to improve the performance of supercapacitors, 3D hierarchical boron-doped diamond-multilayered graphene nanowalls as an efficient supercapacitor electrode were studied. (Ref: Debosmita

Banerjee et al, J. Phys. Chem. C, Vol. 123, p15458 (2019)). An understanding of the role of oxygen and cerium defects in determining the structural, optical and photoluminescence properties of Ni substituted CeO₂, which has potential applications in photocatalysis etc. was reported. (Ref: Saurabh Tiwari et al, J. Alloys and compounds, Vol. 782, p 689 (2019)). The role of nickel doping in Fe₂O₃ dendrite nanostructure for bandgap modulation to enhance photo-electrochemical water splitting was also published. (Ref: Soniya Gahlawat et al, Phys. Chem. Chem. Phys., Vol. 21, p20463 (2019)). The role of structure on the Li⁺ conductivity in LiSnZr(PO₄)₃ ceramics for applications in high performance rechargeable all-solid-state lithium batteries (Ref: Tanvi Pareek et al, J. Alloys Comp, Vol. 777, p602 (2019)), and the dependence of the energy storage properties in lead-free (1-x)Na_{0.5}Bi_{0.5}TiO₃ - xAgTaO₃ ceramics as a function of composition and structure, were studied and published (Ref: Anita Verma et al, J. Appl. Phys., Vol. 125, p054101 (2019)). The gas trapped in shale rocks are a clean source of energy. The fractal dimensions and characteristics of natural shale rock were analyzed using small angle x-ray scattering to determine the gas-storing capacity of natural shale from two regions in India. (Ref: Debanjan Chandra et al, Int. J. of Coal Geology, Vol. 228, p103556 (2020)). In a study of Na₃ZrSi₂PO₁₂-polymer hybrid composite (NASICON), high ionic conductivity is observed, the mechanism of which is explained using X-ray Abs. Spec.(XAS) and found to be due to the decoupling of the Na⁺ ions from the polymer matrix, thereby providing pathways for ionic conduction. (Ref: M. Dinachandra Singh et al, Mat. Lett., Vol. 262, p127022 (2020)). Studies on atomic scale reshuffling during oxygen ion conductivity in doped ceria lattice are investigated by in-situ XAS and XRD measurement for solid oxide fuel cell applications (Ref: Shraddha Shirbhate et al, Solid State Ionics, Vol. 345, p115157 (2020)). Studies on metal doped natural rubber/polyethylene oxide block copolymer were reported, that have applications in the development of polymer electrolyte in lithium ion batteries (Ref: M.S. Mrudula et al, J. Polymer Research, Vol. 26, p191 (2019)). Studies have also been carried out and published to understand the mechanism of lithiation/delithiation in Li:MoS₂/C/CNT composite based electrode materials, and its reversible Li-storage capacity, rate capability, and cycle life. (Ref: Kruti K. Halankar et al, J. Alloy Comp., Vol. 844, p156076 (2020)). Technologically important p-type high temperature thermoelectric material Dy filled CoSb₃ and Fe_{1.5}Co_{2.5}Sb₁₂ has been studied and a correlation between their physical and structural properties have been reported. (Ref: Keshav Dabral et al, ACS Appl. Energy Mater., Vol. 3, p6644 (2020)). Photoelectron spectroscopic (PES) studies of oxygen state in nanostructured Zn_{1-x}(Ga_{0.5}Al_{0.5})_xO and its effect on electrochemical properties for applications in super capacitors have been published. (Ref: S. Ayaz et al, ACS Appl. Nano Mater., Vol. 3, p4562 (2020)). The role of chemical state

and surface composition of graphene oxide supported Cu/Cu_xO nano-electrodeposits, which can efficiently and selectively electro-reduce CO₂ into ethylene with high efficiency, has been published. (Ref: Nusrat Rashid et al, RSC Adv., Vol. 10, p17572 (2020)).

Studies on materials and structures related to possible future applications for devices have also been reported. Studies on materials for applications in transparent all oxide p-n junctions α -Cr₂O₃/ β -Ga₂O₃ (Ref: Sahadeb Ghosh et al, Appl. Phys. Lett., Vol. 115, p251603 (2019)), and studies on the correlation between the electronic structure and disorder in amorphous TiO_{2-x} films and their effect on the resistivity of films for applications in resistive memory devices have been reported (Ref: D. Das et al, J. Phys. Chem. C, Vol. 123, p26812(2019)). Thin films of ZrO₂, in its cubic and tetragonal form, which has attracted immense attention as a key engineering material because of its excellent mechanical and thermal properties, were studied and published. (Ref: Parswajit Kalita et al, Phys. Chem. Chem. Phys., Vol. 21, p22482 (2019)). The structure of Ni/NiO based catalysts for hydrogenation of cashew nut shell oil into value-added products like cyclohexane, cyclohexanol etc. was also published (Ref: Hari Singh et al, Energy Fuels, Vol. 296, p112 (2019)). In view of the importance of graphene and graphite structures in several applications, the degree of graphitization of carbon black during the synthesis stage using ferrocene as an organometallic additive into olive oil precursor has been studied (Ref: S. S. Reddy et al, Diamond and related materials, Vol. 101, p107539 (2020)). Studies on the luminescence properties and its mechanism in carbon mediated centers in porous alumina as a potential futuristic luminescence material has been reported. (Ref: S. Bhowmick, et al, J. Appl. Phys., Vol. 126, p164904 (2019)). XAS studies in SrZnO₂ nanophosphors to understand the mechanism behind the excitation energy dependent emission for possible applications in solid state lighting and white light emitting devices are also reported. (Ref: Manju et al, J. Mater. Chem. C, Vol. 8, p3147 (2020)).

Regarding studies on materials related to manufacturing applications Grazing incidence XRD studies to determine the suitability of Ar⁺ irradiated pure V and V-Cr-Ti alloy as a structural material for fusion reactor application have been reported. (Ref: S Mandal et al, Fusion Engg. Design Vol. 154, p111518 (2020)). The porosity and microstructure of additively manufactured graphene reinforced AlSi₁₀Mg composite were studied using 3D x-ray imaging and the correlation between the mechanical properties of these materials with the microstructure was established. (Ref: Jitendar Kumar Tiwari et al, Additive Manufacturing, Vol. 33, p101095 (2020)),

Other materials science studies include work on finding the correlation between the crystal structure and AC conduction mechanism in bulk delafossite CuFeO₂ (Ref: P. Pokhriyal et

al, J. Appl. Phys., Vol. 125, p164101(2019)) and the role of crystallographic strain in determining the Urbach tail in PrFe_{1-x}Cr_xO₃ system. (Ref: Anil Kumar et al, J. Phys.: Condens. Matter, Vol. 31, p275602(2019)). Studies on the correlation between lattice structure and magnetic spin order α -Fe_{1.4}Cr_{0.6}O₃ oxide as a function of heat treatment for possible applications in magnetic memories, has been reported. (Ref: R.N. Bhoumik et al, J. Mag. and Mag. Mat., Vol. 484, p42 (2019)). Temperature-dependent XRD measurements of novel rare earth ferrite, SmFeO₃ confirm an anomaly in various structural parameters which suggest spin-lattice coupling in the system. (Ref: Warshi et al, Chem. Mater., Vol. 32, p1250 (2020)). PES studies have been carried out to determine the electronic structure of itinerant ferromagnet SrRuO₃, specifically the charge and spin state of Ru ions in order to understand the large magnetic moment on Ru ions in these thin films. (Ref: S. Tyagi et al, J. Phys.: Condens. Matter, Vol. 32, p305501(2020)). Studies to explain the electronic structure of CrSi, a possible thermoelectric and spintronic material, have also been reported. (Ref: Soma Banik et al, Sci. Rep., Vol. 10, p12030 (2020)). Studies to understand the mechanism of occurrence of electronic topological transition which improves the mechanical and superconducting properties when Re is added to Mo, have also been reported. (L. S. Sharath Chandra et al, J. Appl. Phys., Vol. 127, p163906 (2020)).

Some of the important publications related to biology using the protein crystallography beamline are as follows: The structure of M1dr protein and its mutant, which regulate processes like tumor growth, hormone regulation, immune cell development etc. was determined (Ref: R. Agrawal et al, J. Struct. Bio., Vol. 208, p51 (2019)), and the structure of Nosto cphycocyanin protein and its correlation with its optical absorption properties that have implications on organic based solar energy harvesting, have also been published. (Ref: R. Sonani et al, Sci. Rep., Vol. 9, p9863 (2019)). Crystal structures of coronin protein domain mutants of Leishmania donovani, a causative organism for kala-azar, have been determined. This study shows crucial role of some residues in stabilizing the asymmetry in the protein which is useful for specific biological function of Leishmania (Ref: Karade et al, Int. J. Biol. Macromol., Vol. 143, p785 (2020)). Crystal structure of FK506-binding protein C-terminal domain has been determined at 1.1 Å resolution. The study shows that the protein has strong activity for interconversion of cis and trans isomers of proline peptide bonds and no role in histone chaperoning. (Ref: Singh et al, Nucleic Acids Res. Vol. 48, p1531 (2020)) Structural basis for the unusual substrate specificity of unique two-domain M1 metalloproteinase has been unmasked by a series of crystal structures, determined at the beamline. (Ref: R. Agrawal et al, Int. J. Biol. Macromol., Vol. 147, p304 (2020)).

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