SDS micellar solutions. The micelles structure changed to be more rodlike in major axis and then crossed the critical phase transition from micellar solution into liquid crystal phase as lamellar structure emerged by further addition of alcohols. The inter-lamellar distances were also depending on the hydrocarbon chain length and concentration of alcohols. While the persistent micellar structures occurred in addition of medium chain of *n*-alcohol, pentanol at all concentrations.

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Keywords: small-angle neutron scattering, micellar solution, micelles, liquid crystals, lamellar structure

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Structural investigation on InAs/GaSb thin films

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In the present work, InAs-GaSb super lattice thin films have been prepared and characterized. These thin films are widely used in detector technology because of their long carrier lifetimes and high detectivities. While the Molecular Beam Epitaxy (MBE) method is used for the synthesis of the studied thin films, X-ray diffraction (XRD), Dynamic X-ray simulation and X-ray scattering (SAXS and WAXS) methods have been also used to access structural knowledge. Molecular and nano scale structural information such as thickness, density, internal structure, inhomogenities, inner surfaces, repeat distances in partially ordered nano aggregations etc. have been obtained from thin film samples with surface area of 5x8 mm². The rocking curves related GaSb substrate (004), InAs and InAs-GaSb layers and the transmitted scattering profiles of the thin films have been recorded by using CuK_a. Fig.1. shows the XRD pattern and the simulation results of a studied sample. At the end of the structural characterizations, the well prepared samples have been determined.

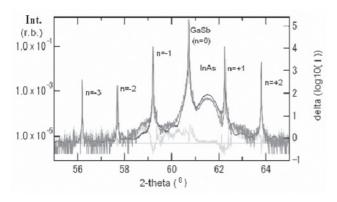


Fig.1. XRD pattern (red color) and dynamic simulation result (blue color) of a studied InAs-GaSb thin film

Keywords: thin films, InAs/GaSb, XRD, SAXS

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Examination of structural changes in the tendons during the healing process

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Tendons are bands of dense connective tissues which connect muscles to skeletal elements and transmit force generated by muscles to bones. Structurally, tendon is composed of tenoblasts and tenocytes lying longitudinally in a network of different collagen molecules. Tenocytes are responsible for the production of extracellular components of tendon that consists of collagen type I, III, V, proteoglycans, fibronectin and elastic fibrils. The largest component of tendon tissue is primarily collagen type I (COLI) and III (COLIII) which are providing unique tensile strength properties. Cross-linking between Type V collagen (COLV) and fibrils improves the forming a core structure for type I fibrils to bind and form a more stable/compact fibril package.

In the experimental researches, adult male Wistar albino rats (8-10 weeks old) were used. The reconstruction processes with/without application of tendon grafts were examined after the main phases of the acellularization of flexor tendons, reseeding of acellularized tendons *invitro*, *in-vivo* implantation of reseeded tendon constructs. The sutured Achilles tendons were isolated, and their 0.2-cm-long sections were used in structural analysis and mechanical tensile testing.

Before and after the mechanical testing, the structural analyses of the tendons were carried out by SAXS and WAXS methods. Molecular and nanosized structural details tried to investigate by the scattering data analysis and the constructed structural models. Structural parameters were refined by fitting experimental data with theoretical results.

At the end of the data evaluation, the present researches have showed that the native tendons may be used in improving biomaterials for tissue engineering.

Keywords: SAXS, WAXS, collagen

MS05.P01

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In situ diffraction studies into the formation of jarosites

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Jarosites, AFe₃(SO₄)₂(OH)₆ (where A is typically K, Na or H₃O), and related minerals are of great importance to a range of mineral processing and research applications. They are deliberately precipitated in order to remove unwanted iron from process solutions in hydrometallurgical circuits. They also form in bioleaching systems and flotation circuits involving bacterial conditioning, but here they form kinetic barriers to further reaction. They occur in acid mine drainage environments and there has been a recent resurgence in interest in jarosite since its identification on Mars by the MER rover Opportunity. Jarosites are also of considerable theoretical interest as model compounds for spin frustration in kagomé-Heisenberg antiferromagnetic materials. Knowledge of their nucleation and crystallisation mechanisms is an indispensable prerequisite for the understanding of conditions which enhance or inhibit their formation thus allowing control of their occurrence in a range of environments.

Poster Sessions

The results of *in situ*, synchrotron X-ray powder diffraction experiments conducted during the (i) the synthesis and (ii) the dehydration of $\mathrm{Na^+/H_3O^+}$ and $\mathrm{K^+/H_3O^+}$ jarosites will be presented. These time-resolved studies provide information regarding the kinetics of formation over temperatures ranging from 80°C to 120°C and also show the occurrence of cation exchange on the A site with time. The synthesis reactions show that samples can be prepared in which the ironsite vacancies are ordered. The ordering is accompanied by a lowering of symmetry, from rhombohedral, space group *R-3m*, to monoclinic, C2/m. This has implications for the variability of magnetic properties reported for synthetic iron-deficient jarosites.

Keywords: jarosite, in situ, synchrotron

MS05.P02

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Crystal structure and magnetic transition in $Mn_{2\text{-}x}Fe_xP_{1\text{-}y}Ge_y$ magnetocaloric compounds

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Magnetic refrigeration based on the magnetocaloric effect (MCE) is becoming an alternative technology to replace the conventional gas-compression refrigerators. The compounds of the $\mathrm{Mn_{2x}Fe_xP_{1,y}Ge_y}$ system exhibit a reversible giant magnetic-entropy change, adjustable Curie temperature and hence make this material system an excellent candidate for working material in magnetic refrigeration.

Structure and magnetic properties of $Mn_{2-x}Fe_xP_{1-y}Ge_y$ compounds as a function of temperature, and applied magnetic field were investigated using neutron powder diffraction. It noted that temperature and magnetic field can induce the first order phase transition between the paramagnetic phase and ferromagnetic phase in the materials. The paramagnetic and ferromagnetic phases have two very distinct crystal structures and the magnetic-phase transition is accompanied by structural transition. In addition, the magnetic-entropy changes as a function of magnetic field or temperature being directly controlled by the phase fraction of this first-order transition. We also found that the crystallites below a threshold size inhibit the paramagnetic to ferromagnetic transformation.

Keywords: neutron_diffraction, magnetic_refrigerant, crystallography

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In Situ Energy-Dispersive Diffraction Studies of Reaction Layers in Inert Anodes

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Many important light metals - including aluminium, magnesium and titanium - can be produced via electrowinning involving the use of carbon anodes in the reduction of solid metal oxides in a molten salt bath (for example, cryolite, $\mathrm{Na_3AlF_6}$ or calcium chloride, $\mathrm{CaCl_2}$) operating at ~1000°C. The carbon anodes can contaminate the light metal product and are consumed at a rapid rate, necessitating frequent replacement and producing carbon dioxide emissions, all of which affects cell stability and reduces cell efficiency.

Inert anodes are a potential replacement for carbon anodes as they are not consumed and evolve only pure oxygen from the melt. As well as reducing costs and greenhouse gas emissions, the inert anode provides greater cell stability and avoids carbon contamination of the product.

Ex situ studies suggest that passivating layers form on the inert anode surface upon immersion in the molten bath and wear away during cell operation. These layers are thought to be the key to electrode longevity as they protect the anode from the molten bath. Fundamental study of these layers in situ in operating cells is imperative in understanding the mechanism of their formation and wear, and hence, to developing genuinely breakthrough inert anode technology.

To this end, we have developed an experimental facility and analysis methodologies in order to study layer formation in operational electrochemical cells. The facility and methodologies may also be applied to other systems where time-resolved *in situ* measurements of materials in challenging environments are important.

An *in situ* energy-dispersive diffraction study of operational electrochemical cells to observe passivation layers formation on model inert anodes was conducted on beamline I12 (JEEP) at the Diamond Light Source. The diffraction data has been quantitatively analysed by the Rietveld method yielding layer thickness as a function of time, and a kinetics analysis of these results shows that the layer growth is diffusion controlled with a decreasing nucleation rate.

Keywords: X-ray diffraction, in situ, electrochemistry

MS05.P04

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Crystal and magnetic structures of inorganic-organic frameworks using powder diffraction

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The fascinating structures and properties of inorganic-organic hybrid frameworks have made them the focus of extensive study, with much of the focus placed on the nanoporous metal-organic frameworks [1], [2]. Recently denser frameworks with extended inorganic (e.g. metal-oxygen-metal) connectivity have become of increasing interest [1], [3]. These compounds exhibit electronic and magnetic properties more commonly found in purely inorganic compounds. The structure-directing effect of the organic ligands on the framework, however, enable them to adopt unusual structures with unique and often low dimensional properties. The vast majority of structural studies of framework materials are performed using single crystal diffraction but, using a combination of neutron and synchrotron Xray sources, powder diffraction can be used to examine the details of these architectures with greater precision. Neutron diffraction also allows the magnetic structure of frameworks to be examined in detail, revealing more complex behaviour than often found in purely inorganic compounds.

In this work we present two structural studies of hybrid frameworks with extensive inorganic connectivity, which have been explored using a combination of powder and single crystal diffraction. In the