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Pulsed laser deposited Cr2O3 nanostructured thin film on graphene as anode material for lithium-ion batteries

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Pulsed laser deposition technique was used to deposit Cr_2O_3 nanostructured thin film on a chemical vapour deposited few-layer graphene (FLG) on nickel (Ni) substrate for application as anode material for lithium-ion batteries. The experimental results show that graphene can effectively enhance the electrochemical property of Cr_2O_3. For Cr_2O_3 thin film deposited on Ni (Cr_2O_3/Ni), a discharge capacity of 747.8 mA h g-1 can be delivered during the first lithiation process. After growing Cr_2O_3 thin film on FLG/Ni, the initial discharge capacity of Cr_2O_3/FLG/Ni was improved to 1234.5 mA h g-1. The reversible lithium storage capacity of the as-grown material is 692.2 mA h g-1 after 100 cycles, which is much higher than that of Cr_2O_3/Ni (111.3 mA h g-1). This study reveals the differences between the two material systems and emphasizes the role of the graphene layers in improving the electrochemical stability of the Cr_2O_3 nanostructured thin film.

Scientific Talks / 3

Angle Resolved Photoemission Spectroscopy Study of Sr4Ru3O10 single crystals and Intrinsic Bi2Te3 Topological Insulator Thin Films

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In the first half of this talk will focus on three-layered strontium ruthenate single crystals. Strontium ruthenates of the Ruddlesden-Popper (R-P) series $Sr_{n+1}Ru_nO_{3n+1}$ have been subject to intensive research since they exhibit distinct collective physical phenomena that are due to the change of the number n of the RuO_6 octahedra layers in the unit cell. The phenomena observed range from unconventional spin-triplet superconductivity in Sr_2RuO_4 (n=1) [1], quantum critical metamagnetism in $Sr_3Ru_2O_7$ (n=2) [2]; and anisotropic ferromagnetism and proposed orbital-dependent metamagnetism in$Sr_4Ru_3O_{10}$ (n=3) [3].

Little is known in literature about the microscopic origin of the metamagnetic transition in $Sr_4Ru_3O_{10}$. Previous experimental and theoretical work on $Sr_3Ru_2O_7$ (n=2) have suggested a band structure-based model of metamagnetism to explain its phase diagram [4]. According to this model, it is expected to find van Hove singularities in the density of states near the Fermi level. The same scenario is expected to be valid for $Sr_4Ru_3O_{10}$ [5]. Experimental information on the near Fermi level electronic structure of $Sr_4Ru_3O_{10}$ is thus needed to investigate the origin of magnetic fluctuations in $Sr_4Ru_3O_{10}$. In this presentation, I will show the first electronic structure measurements on $Sr_4Ru_3O_{10}$ performed at synchrotron using angle resolved photoemission spectroscopy (ARPES) [6]. In particular, I will discuss the near Fermi level band dispersion and the Fermi surface topology of $Sr_4Ru_3O_{10}$ single crystals. Next, I will discuss band dispersions of $Sr_4Ru_3O_{10}$, which reveal a complex density of states that is susceptible of giving rise to van Hove singularities near the Fermi level; a situation expected to be the origin of the magnetic fluctuations in $Sr_4Ru_3O_{10}$.

In the second half of this talk, I will discuss ARPES data on intrinsic Bi_2Te_3 topological insulator thin films. Topological insulators (TIs) are materials with an insulating bulk interior and spin-momentum-locked metallic surface states as a result of a band inversion from large spin-orbit interaction [7]. Bismuth telluride (Bi_2Te_3) is one of the 3D topological insulators (TIs) that have received a considerable amount of attention as potential candidates for room temperature spintronics and quantum computational devices[7]. However, despite significant progress in TI material preparation, growing high-quality TI materials for transport experiments is still a major challenge. Often, bulk carrier conduction complicates direct observation of surface effects in transport measurements.

Here, I will give a brief overview of our current research on thin films of topological insulator [8]. Our combined in-situ spectroscopy, especially angle resolved photoemission spectroscopy study of molecular beam epitaxy grown Bi_2Te_3 reveal topological surface states without a contribution from the bulk bands at the Fermi energy[8]. Investigation of the effect of pure oxygen exposure at atmospheric pressure; and the effect of ex-situ contamination in air show that the surface electronic band structure of our Bi_2Te_3 films are not affected by in-vacuo storage and exposure to oxygen; whereas major changes are observed when exposed to ambient conditions [8]. In future, we might perform these investigations at synchrotron in order to cover a wider spectral range with an intense and highly polarized continuous spectrum with the purpose of making detailed study of the valence photoemission spectra of our topological insulator thin film samples.

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Scientific Talks / 5

Beta-cyclodextrin decreases the aggregation rate of prion proteins induced by metal-catalyzed oxidation

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Prion diseases, also called transmissible spongiform encephalopathies (TSEs), comprise a group of fatal neurodegenerative disorders that affect both humans and animals. Human forms of prion disease include Creutzfeldt-Jakob disease (CJD), Gerstmann-Sträussler-Scheinker syndrome (GSS), fatal familial insomnia (FFI), and kuru. Prion diseases affecting animals include scrapie in sheep and goat as well as bovine spongiform encephalopathies (BSE) in cattle. The histopathological features of TSEs such as spongiform degeneration of the brain, neuronal vacuolation, and astrocytic gliosis, represent the main consequences of the cerebral deposition of the misfolding isoform (PrPSc) of the cellular prion protein (PrPC) into amyloid plaques. At present, there is no effective therapy to treate prion diseases. One of the major obstacles in the treatment of TSEs by anti-prion compounds is the low ability of these compounds to cross the blood brain barrier (BBB) that renders their accessibility to the CNS. In addition, most of these compounds did not exhibit any therapeutical effect when administered after the appearance of
neurologic signs into an animal model. Therefore, the development of optimized and effective therapies against TSEs is urgently needed. β-cyclodextrin (β-CD) has been successfully used by the pharmaceutical industry owing to its complex-forming ability. This ability is due to the structural orientation of the glucopyranose units, which generate a hydrophobic cavity that can facilitate the encapsulation of hydrophobic moieties. In this study we investigated the inhibitory effect of β-CD on the in vitro oxidative aggregation of the structured C-terminal domain of both mouse and human prion proteins induced metal catalyzed oxidation (MCO). β-CD gained attention in the field of anti-prion compounds due to its ability to clear PrPSc from infected cell cultures. Small angle X-ray scattering (SAXS) measurements revealed that the delaying effect of β-CD on the structural conversion of human PrP is rather due to the caging of copper ions generated by MCO than to a direct interaction with PrP. Moreover, the observed pathway switch in the presence of β-CD from unspecific denaturation to specific oligomerization strongly supports the theory that aggregation pathways are determined by the population of specific intermediate states. The results obtained in this study provide new insights toward the developing of a lead structure against TSEs.

Poster Session / 6

Biosynthesis, characterization and nonlinear nonlinear optical properties of copper oxide nanoparticles

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The present research introduces an environment friendly and rapid method for synthesis of CuO nanoparticles [1-3] for potential NLO applications. Copper oxide nanoparticles were synthesized from copper sulphate in the presence of natural saffron dye extracts at room temperature. TEM, SEM and EDX were initially used to characterize the biosynthesized nanoparticles. Spherical nanoparticles with an average diameter <7 nm were also identified. Cu and O which are the main constituents of CuO-NPs were found to be dominant. The NLO properties study in the femtosecond regime showed two-photon absorption behaviour.

Keywords: Biosynthesis, copper oxide nanoparticles, femtosecond regime, NLO, two-photon absorption

Poster Session / 7

Mapping the Epitope: Defining the Structure of the Highly Immunogenic Env-CD4 Complex

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The HPRU has focused on the development of an effective prophylactic HIV vaccine which utilizes a novel immunogen called gp120-2dCD4S60C that consists of a human two domain CD4 with a S60C mutation covalently bound to monomeric gp120. This covalent complex acts as a "super immunogen" in pre-clinical studies in rabbits, where it elicits potent and broadly protective neutralizing antibody responses against HIV-1 Tiers 1, 2, 3, HIV-2 and SIV pseudoviruses. Prior to initiating further preclinical development of the gp120-2dCD4S60C vaccine immunogen in rhesus macaques, it would be critical to characterize and define the structure of the immunogenic HIV-1 gp120-2dCD4S60C complex, and ultimately fine map the specificities of the potent, broadly neutralizing antibodies elicited by the gp120-2dCD4S60C complex in rabbits. The broad aim of this study is therefore to characterize the structure of gp120-2dCD4S60C as compared to gp120 bound to 2dCD4WT. Resolving the architecture of the immunogenic gp120-CD4S60C complex will ultimately be important for defining the structures of the exposed target epitopes of potent neutralizing antibody responses, as compared to those of native non-covalent complex formed with wild-type CD4. Both low-resolution (small-angle x-ray/neutron scattering – SAXS/SANS) and high-resolution (synchrotron X-ray crystallography) structural information will be obtained in collaboration with the Institut Laue-Langevin and European Synchrotron Radiation Facility (ILL-ESRF), both based in Grenoble, France. Only preliminary data has been gained thus far, but it will ultimately assist in gaining insights into the underlying mechanisms of the antiviral activity that will guide strategies for optimizing CD4-based immunogens that will likely provide protection from infection.

Scientific Talks / 8

Structural Analysis of L-asparaginase from novel source as a Promising Drug Target in the Treatment of Childhood Acute Lymphoplastic Leukemia

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Protein Crystallography is a highly throughput technique used to assess the structure-function relationship of biological macromolecules. Obtaining accurate and reliable three-dimensional structures are the basic prerequisites for rational drug design. Childhood Acute Lymphoblastic Leukemia (ALL), cancer of white blood is our goal. It comprises the most common kind of childhood cancer. Many underdeveloped lymphocytes are found in a blood and bone marrow; it can spread to other parts of the body including the lymph nodes, liver, spleen and central nervous system (CNS). Among the drugs used in the treatment of ALL are bacterial-derived enzymes called asparaginases that catalyze the conversion of asparagine into aspartic acid and amonia. L-asparaginase has been considered as a unique chemotherapeutic agent against cancer. Leukemic cells and some other suspected tumor cells are unable to synthesize the asparagine, whereas normal cells can synthesize their own asparagine. This deprives the leukemic cell of circulating asparagine, which leads to cell death. The clinical utility of L-asparaginase is often limited by the Asparaginase immunogenicity, developing of drug resistance and toxicity due to repeated dose. Despite the universal inclusion of asparaginase in treatment protocols, there is much debate regarding the optimal formulation and dosage. Therefore, we are planning to investigate the 3D-structure of L-asparaginase from a novel source (chicken liver) as a promising drug target against ALL. Results are expected to provide new insights for: 1) Identifying the structural environment of the substrate binding sites, 2) Enhancing the drug efficacy by immobilization on biocompatible nanoparticles and hence decreasing the aforementioned obstacles that face the therapeutic treatment of ALL, and 3) Increasing the variety of the drug source as there are only two sources (E. coli & Erwinia sp.) available in the market.

Policy and Strategy Talks / 9

The Impact of Synchrotron Radiation on Science and Society in Developing Countries

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The more than 50 light sources now in operation around the world include facilities in Brazil, Korea, and Taiwan which started their programs in the 1980's when they were developing countries. They came on line in the 1990's and have since trained hundreds of graduate students locally, without sending them abroad and losing many of them. They have also attracted dozens of mid-career diaspora scientists to return. Their growing user communities have demanded more advanced facilities, leading to the funding of high performance new light sources that are now coming into operation.

Poster Session / 10

Structural studies of the dynamic host-pathogen interaction underlying HIV infection

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Cluster of differentiation 4 (CD4) plays an important role in the adaptive immune response. CD4 is also the primary receptor for the HIV-1 envelope glycoprotein 120 (gp120). CD4 contains a metastable disulphide bond in its second domain which enables this protein's redox activity. CD4 binds the gp120 component of the viral envelope protein in a partially reduced state as shown by biochemical analyses carried out at the HIV Pathogenesis Research Unit (HPRU) at the University of the Witwatersrand, South Africa.

A collaboration exists between the ILL, ESRF and HPRU to use high and low resolution X-ray and neutron scattering techniques to determine the local and global conformational changes of CD4 as a result of its redox state and how this impacts its ability to bind gp120. We predict that this data will result in previously uncharacterised structural realignment within the CD4 protein which will aid in rational design of anti-CD4 directed immunogens for HIV-1 vaccination development.

Scientific Talks / 11

The Use of Diffraction to Determine the Residual Stress of HVOF WC-17Co Coatings

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The investigation was conducted to determine the residual stresses of thermally sprayed HVOF WC-17Co coatings on different alloy substrates by non-destructive techniques. Non-destructive determination of residual stresses in the WC-Co coated systems was exceptionally challenging because coatings were only about 200 microns thick. The best-suited techniques for investigation of the WC coatings were diffraction-based strain scanning, using penetrating radiation such as thermal neutrons (most penetrating), high energy synchrotron X-rays (100 keV enables 20 micron penetration) and laboratory X-rays (limited to 5 micron penetration). Laboratory X-rays (Necsa, using Co radiation), thermal neutrons (ANSTO, Australia) and X-ray synchrotron (ESRF, France) were successfully employed to resolve the stress conditions. The influence of heat treatment was assessed by understated stress relief heat treatment of the grit-blasted substrates and coated substrates.

The surface stresses of the coatings exhibited both small compressive and low tensile stresses on the as-sprayed coated samples. After annealing, the stresses became substantially more compressive. The near-surface trends of the grit-blasted substrates were completely relaxed after annealing, with thermal stresses being the dominant mechanism for residual stress induced due to the large difference in the coefficients of thermal expansion (CTE) between the WC coatings and the substrates.

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Scientific Talks / 12

Reviewing the value of synchrotrons for Sasol; relevance of research at synchrotrons for African Industries

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Sasol is an international integrated energy and chemical company that develops and commercializes chemical technologies. The company is listed on the Johannesburg and New York stock exchanges. Sasol's experience and understanding of Fischer Tropsch synthesis provides us with a unique reliable energy value proposition nationally and internationally. Sasol's global presence includes a number of African countries, for example Botswana, Zambia, Nigeria and Egypt. Sasol's financial results showcases our focus on sustainable value creation and our South African energy cluster listed an operating profit of R41.7 billion for the 2014 financial year. One of the keys to Sasol's success is corporate social investment that maximizes social development and value for our stakeholders in the communities where we operate. The Sasol Global Foundation was established in 2013 to coordinate and optimize these investments.

Our in-house technology development capacity includes more than 300 employees with PhD's and an intellectual property portfolio of more than 500 registered patent families. Our analytical technologies include advanced analysis of hydrocarbon synthesis streams and atomic scale resolution characterization of catalysts. Our research facility makes use of synchrotron and neutron techniques and we have the in-house capability to design experiments and interpret high resolution data. In-house training of scientists on synchrotron data manipulation and interpretation is an on-going activity. We encourage our post-graduate bursary holders to apply for academic beam time and often assist with proposal writing. The XRD and synchrotron group participates in the South African synchrotron strategy, roadmap, conferences, workshops, beam times (academic and commercial) and publishing. We provide a world-class catalyst characterization and fundamental understanding [1] in support of our Coal-To-Liquids (CTL), Gas-To-Liquids (GTL) and new catalyst development partners. A few published examples including synchrotron and neutron results will be presented: γ-alumina [2-4] and in situ synchrotron powder X-ray diffraction of the reduction of a model catalyst [5].

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Trabecular architecture in the distal hallucal phalanx - implications for understanding loading history at toe off

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Unlike African apes, human experience very high loads on their hallux just prior to toe-off at the end of stance phase of locomotion. Because of this difference, trying to determine the habitual loading regime of the hallux in fossil hominins would prove to be a useful endeavour to better characterize the evolution of human locomotor biomechanics. A few studies have successfully shown that cortical bone cross-sectional properties in the hallucal metatarsal differ between apes and humans, with fossil hominins tending to have an intermediate morphology. While these finding are valuable, they do not necessarily reflect the loading history of the hallux at toe-off since it is the distal hallucal phalanx (DHP) that bears the majority of weight (in humans) at this point in the gait cycle. In the current study, we investigated trabecular bone architecture of the DHP in a small sample of humans (n=10), African apes (n=8 each for gorilla and chimpanzee) and fossil hominins. The fossil hominin sample included specimens attributed to Au. africanus, early Homo, and H. erectus. We predicted that modern humans would differ from African apes, and that fossil hominins would have an intermediate morphology between these extant groups. The following properties were calculated: bone volume fraction, trabecular number, trabecular thickness, trabecular separation and degree of anisotropy. Estimated body mass was used for scaling purposes. Our preliminary results demonstrate that humans are different from African apes in most trabecular properties. But, the principal orientation of trabecular bone struts between groups run in a similar direction - The Homo erectus specimen is most similar to modern humans, while the other hominin DHPs show different patterns. However, neither of these are ape-like. These findings allow us to discuss possible scenarios of the evolution of human locomotor biomechanics, especially the toe-off mechanism specialized in humans.

Poster Session / 14

X-Ray Diffraction Use fo PZN-PT Single Crystal's Synthesis and Microscopic Thermal Dilatation Coefficient Determination

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The performance of transducers can be significantly increased by the use of active materials with large piezoelectric coefficients (dij) and large coupling factors (kij) [1]. Recently, high levels of piezoelectricity have been published in $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) and $Pb(Zn_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PZN-PT) single crystals: d33 > 2500 pC/N, d31> -1500pC/N, k33> 90%, k31> 80% and kt> 60% [1-5].

X-Ray Diffraction is an excellent technique to follow and analyze structures and crystallographic phases of solid materials.

In this paper we use the X-Ray powder Diffraction technique to control the different steps for the synthesis of precursors ($PbTiO_3$ and $ZnNb_2O_6$) and single crystals such as PZN-PT and PMN-PT.

X-Ray powder Diffraction was performed on ground single crystals with the help of a Philips X'pert Pro diffractometer using a monochromatic selecting CuKα radiation (λ = 1.5418 Å). Measurements for XRD characterization were realized by using a HTK16 high temperature chamber. The DRX diffraction patterns confirm a pure perovskite phase for the two crystals, within the X-ray powder diffraction's sensitivity. It means that $Pb(Zn_{1/3}Nb_{2/3}))O_3$ and $PbTiO_3$ have formed a perfect perovskite structure solid solution. Generally, XRD diagrams are carried out over narrow angular regions centered about the six pseudo-cubic reflections (100), (110), (111), (200), (220) and (222), from which it is possible to determine unambiguously the crystal's symmetry [6]. In the rhombohedral symmetry, the (h00) pics are all singulets while the (hhh) pics become doubled. In our case, from the peak profiles of the pseudo-cubic (200) and (222) reflections, the symmetry is clearly seen to be rhombohedral. The lattice parameters were determined in ambient and non-ambient conditions for the rhombohedral and cubic structure respectively. The plot of the lattice parameter and the lattice volume versus temperature in the cubic phase was performed to determine the dilatation coefficients a and v by calculating the slope as indicating in the following equations:

Scientific Talks / 15

Application of iron L3 edge XANES spectroscopy to colloid speciation

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L-edge XANES spectroscopy has been used to identify the speciation of iron (Fe) in natural samples. The majority of previous analyses are limited to the identification of Fe(II) versus Fe(III) speciation in complex natural samples however, these spectra are rarely used to identify different mineral phases in soils and sediments. Using the fine spectral variations between different crystalline and amorphous Fe phases, we developed a technique to evaluate the local coordination environment of Fe in in natural samples. The technique makes use of splitting of the main electronic transitions in the L3 edge region, and the ratio of their peak intensities. These spectral parameters are sensitive to the valence state, electronegativity of the coordinated ligands and the degree of distortion of the polyhedra of Fe.

Based on our findings of the Fe L3-edge spectral responses to variations in Fe mineralogy, we have applied this spectroscopic tool to colloids and nanoparticles suspended in the Southern Ocean. Here, Fe is known to be limiting to phytoplankton primary productivity, and Fe speciation and thus bioavailability, impacts global biologically-mediated air-sea carbon dioxide exchange. Our findings classify five broad categories of suspended Fe rich particles including ferric oxides, magnetite, other mixed valence species and at least two ferrous species. The distribution of these phases in the Southern Ocean is discussed in terms of primary productivity and in terms of their association with organic carbon.

Scientific Talks / 17

One hydrogen bond does not a separation make, or does it?-The importance of high resolution structural data

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The enantiomeric purity of a chemical entity is important in various industries, such as analytical, food, pesticide and pharmaceutical. When a compound is produced as a racemic modification typically only one of the enantiomers exhibits the required biological effect. One of the main resolution method is based on the formation of diastereomeric salts. The full understanding of the mechanism of chiral discrimination may lead us to design the 'perfect' resolving agent for a given racemic modification.
In order to understand the molecular recognition during the resolution process we have studied a series of inclusion compounds [1] and diastereomeric salt formations [2] to map the correlation between structure and the success of the enantiomeric resolution. One of our latest publications [3] discusses a series of experiments when a sugar derivative was employed to resolve racemic chiral amines. The non-bonding interactions which give rise to the structures of the diastereomeric salts were analyzed and the selectivity was explained by the formation of one additional hydrogen bond between the ion pairs. This result emphasizes the importance of high resolution structural data to obtain accurate hydrogen atom positions.

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Poster Session / 19

Structural Studies on the Purified Cxcr4 Expressed by Cell-Free

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Membrane proteins constitute up to 30% of the genome and have extremely important roles in many biological processes such as signal transduction, or the substrate transport energy production. Economically, existing drugs targeting GPCRs generate annually nearly $ 25 billion in the world economy. It is therefore essential to have a thorough understanding of their structures and their dynamics to understand their functions and / or their failures to develop new specific active molecules of these receptors.

CXCR4 is a membrane protein of the family of G-coupled receptors (GPCR) which we are using as a well-characterised model system for this project. CXCR4 is a chemokine receptor for the SDF-1 (CXCL12), which is involved in chemotaxis of lymphocytes. Additionally, CXCR4/SDF-1 is known to be important regulator of haematopoiesis, and deregulation of its function has been linked to carcinogenesis. Of most interest however, is the role of CXCR4 as a co-receptor required for HIV infection.

Recombinant GPCR proteins are typically extremely difficult to produce in cellular expression systems due to namely, poor yields, aggregation and misfolding. Using the cell free technology and the experience of Synthelis, we aim to remove these barriers. Using CXCR4 as our model, the first objective of the project is to obtain a proof of concept of the feasibility of effectively purifying GPCRs from proteoliposomes. Upon purification, CXCR4 shall be characterised both structurally and functionally using techniques available at Synthelis and ILL/ESRF. We shall for instance assess its binding to its native ligand, SDF-1. Additionally, with the expertise of the University of Witwatersrand (Johannesburg, South Africa), we also shall seek to demonstrate the binding of gp120 viral protein, and viral particles, to CXCR4. Ultimately, we wish to obtain structural insights of the protein using SANS/SAXS and potentially, X-ray crystallography. In parallel with the work on the CXCR4 model system other, but uncharacterised, proteins benefitting from the unique capabilities of cell-free expression will be studied.

Scientific Talks / 20

Fabrication and characterisation of high temperature operating light emitting diodes from Silicon Carbide

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Light-emitting diodes (LEDs) are semiconductor devices that emit light in a narrow-band spectrum with wavelengths ranging from the infrared to the ultraviolet. This paper will look at the fabrication techniques and characterisation of high temperature operating LEDs from silicon carbide (SiC). SiC has a wide band gap and high thermal conductivity. These unique properties make SiC an ideal candidate for fabricating high-temperature operating semiconductor devices. Most of the LED technology at present uses gallium nitride (GaN) with phosphors. Phosphors have a short life-time and contain rare-earths which are very expensive. In order to overcome these shortcomings, the technology of producing highly efficient SiC-based LEDs has to be explored so as to make them a viable alternative to GaN-based LEDs.

Scientific Talks / 22

African Synchrotron Science : A personal perspective

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Synchrotron radiation has and will undoubtedly continue to play a vital role in the advancement of many important scientific and technological endeavours. However there remain huge obstacles and limitations to it becoming more generally usable, especially to this African researchers.

Poster Session / 23

In-situ synchrotron X-ray diffraction study of TiC/Ni-Al2O3 composites obtained by SHS

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Combustion synthesis commonly called SHS (for self-propagating high-temperature synthesis) is a promising method employed for the synthesis of many advanced materials, such as ceramics, composites, intermetallics, etc. This method is based on the use of the heat released during exothermic reactions in order to preheat raw materials and to obtain a self-sustained system.
The main advantages of the SHS technique are the high cost-effectiveness associated with the low energy requirement, short processing time, simplicity of facilities, and formation of high-purity products. However, the SHS composites obtained had poor mechanical properties due to the coarse-grained microstructure exhibited.
As a model system for SHS processes, the Ti-C system, has been widely studied. The heat generated by the reaction between titanium and carbon is large enough to sustain a combustion wave propagation, once the reaction is initiated. However, the reaction is extremely fast and the final product is highly porous. The addition of diluents is sometimes required to lowering combustion temperature and decreasing the reaction rate, which help achieve the appropriate microstructure.
In this study, 5 and 10 wt% of thermite mixture NiO-Al, were added to the stoichiometric mixture Ti-C to produce TiC-Ni-Al_2O_3 composites. The formation of a by-product alumina-nickel could be sought for the hardness of the final product, since Ni is known to be a good sintering aid for titanium carbide and the presence of Al_2O_3 is usually not a drawback as it is usually considered as a reinforcement.
to monitor in situ the structural and thermal evolutions taking place during the SHS reactions, a time-resolved X-ray diffraction (TRXRD) experiments using an X-ray synchrotron beam (ID11, ESRF Grenoble) was carry out with a short acquisition times (35ms/scan). This analysis enable us to observe several steps including intermediate phases' appearance-disappearance, aluminum melting and thermite reaction before obtaining the final product. Those results were then, compared with earlier study results on the Ti-C-Ni system, where the Ni was a part of the reactive mixture.
Tracking the evolution of the lattice parameters of TiC during its formation enabled us to estimate the critical temperatures for those SHS reactions.
Products, were analyzed by SEM observations.

Poster Session / 24

Synchrotron Light Sources: Working with and for industry

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The creation and tailoring of new materials are at the heart of current industry challenges. New materials must meet ever more stringent requirements of performance, whilst fitting into the modern cradle-to-grave cycle of material production, use, and recycling. The properties and function expected of materials depend heavily upon their composition and their micro- or even nano-structure. Their "ultimate" characterisation is possible down to the atomic scale using the tools and techniques of large-scale facilities such as synchrotron X-rays.

Synchrotron X-rays are a non-destructive probe of material structure at length scales ranging from centimetres to the size of an atom. Special properties such as element selectivity offer a variety of analytical tools for characterising materials under in situ conditions (heat, cold, pressure, chemical, stress/tension, electrical/magnetic fields....) and in real time that are not accessible with traditional techniques. Synchrotrons therefore provide the ability to visualise the atomic, nano, and macro-structure of a huge range of complex real-world materials, often under processing or end-use conditions and in real time. This capability lends itself to an equally wide range of industrial R&D; problems which, in particular, have been adopted by the healthcare industry. Beyond drug discovery and development, synchrotron facilities are also very active in providing analysis for micro- and nano-electronics, energy and smart materials, transport, chemistry and catalysis, engineering materials, and home and body care amongst others.

In this context, new business models are springing to life, with more partnerships, more services, and nimble small start-ups bridging the gap between the oft "ivory tower" nature of research infrastructure and the commercially driven industry world.

This poster will present how ESRF works with industry in delivering advanced materials characterisation for innovative industrial and applied R&D;.

Scientific Talks / 26

XAS investigation of 'invisible' gold impurities in synthetic sulfide minerals

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Gold in ores of hydrothermal and magmatic origin deposits in the form of its own crystalline phase (usually in the form of an alloy with the silver - electrum) or dispersed in sulfides as isomorphic impurity, nanosized particles Au° or chalcogens and compounds with semimetals (As, Sb, Bi, Te). Scattered ("invisible") form of gold is much more difficult to remove when ore processing, and most part of it becomes waste. To determining the structural and chemical state (degree of oxidation and structural position) of "invisible" gold atoms we synthesized gold minerals systems Cu-S, Fe-S, Cu-Fe-S and Fe-As-S. Synthesized minerals were studied by X-ray spectroscopy at the LIII edge of gold. Measurements were made at ESRF and “Kurchatov synchrotron center”. Data treatment were made using computational methods for optimization geometry of gold inclusions in mineral structure (Quantum Espresso) and finite difference method for XAS calculation (FDMNES).

EXAFS spectra were measured for several model systems at “Kurchatov synchrotron center”. Fitting of EXAFS data has provided information concerning local atomic structure around absorbing Au atoms.

HERFD-XANES spectra were collected ID26 beamline at ESRF for several reference samples and minerals with gold inclusions. Comparison with standards and modeling spectra, calculated using FDMNES, showed that in covellite Au atoms incorporated into disulfide groups. This form of "invisible" gold is stable in a wide range of temperatures and does not break during the quenching system. In other minerals of Cu-Fe-S gold is in the form of a solid solution, stable only at high temperatures .

Scientific Talks / 27

Optimization of Renewable Energy Processes: Projects at the Synchrotron Radiation Facility PETRA III

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Today's societies are eminently depending on the access to permanently available energy sources. However, more than 80% of the worldwide energy consumption is based on ultimately finite resources such as fossil fuels and nuclear power. Therefore, huge efforts are taken to provide the growing world population with permanent sustainable energy.

One of these energy sources is the sunlight which could deliver 10,000 times the power at present consumed by mankind. However, to efficiently harvest and store the energy from sunlight on large scales is still a great challenge as the technology of efficient and cost-effective solar cell based power plants is still not developed. Furthermore, the sun power has to be buffered to bridge the sunless gap during the night, and new and optimized battery technologies with high duty cycles is required.

It will be presented how 3rd generation synchrotron radiation sources such as PETRA III in Hamburg, Germany, uniquely contribute to the engineering process of deveoping new solar cells and batteries. With their capability for in-situ investigations of energy generating and storing systems on microscopic and atomic scales, synchrotron radiation based measurements such as element specific imagaging and tomography of highest resolution are crucial for the advancements in energy technology.

Policy and Strategy Talks / 28

International cooperation schemes at the research center DESY

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The Deutsches Elektronen-Synchrotron DESY in Hamburg is one of the world's leading research centers for photon science, particle and astroparticle physics as well as accelerator technologies. It offers many exciting possibilities for excellent research programs and international science collaborations. In photon science three user facilities are available: the 3rd generation synchrotron radiation source PETRA III, the soft x-ray laser FLASH and the NanoLab providing access to a suite of sophisticated tools in nano-
characterization, structuring and synthesis. Opportunities at all three facilities for international cooperation exist. At PETRA III three international partnership programs on a strategic level are already in place: The India/DESY cooperation, the Sweden/DESY cooperation and the Russian/German beamline. Each of the partnership programs is uniquely tailored to fit the scientific needs of the national communities in order to maximize the benefits for the partners.

This talk will summarize existing collaborative models at DESY and will report on opportunities for international cooperation - taking into account future upgrades and extensions of DESY's light sources.

Poster Session / 29

Towards a crystal undulator

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A crystal undulator is similar to a normal undulator as typically found at a synchrotron for the production of extremely brilliant X-ray beams. The difference is the magnetic lattice is realized by the periodic electrostatic potential of a crystal lattice seen from the reference frame of the GeV range electron or positron beam. The extremely relativistic incident particle beam is captured in a high index crystallographic channel of a crystal superlattice. The particle beam will then "see" a many Tesla range periodically varying magnetic field with a few micron pitch.
This method could theoretically lead to an MeV range gamma ray laser by the FEL principal. We have investigated a prototype diamond superlattice (produced by Element Six) using x-ray diffraction topography. The undulator fabrication principle involved CVD growth of diamond on a diamond substrate while varying the concentration of boron in the gas phase during growth. This leads to the periodic variation of the lattice dilatation by the varying concentration of the single substitutional boron impurity atom.

Poster Session / 30

Ultra smooth surface of diamonds, towards Å scale roughness for the (111) orientation

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Synthetic diamond of exceptional quality is required for many high technology applications. An example from high performance electronics is the so-called δ-doped diamond envisaged as an electrical switch in FETs, operating at high power and high frequencies. Another example is 111-oriented diamond plates that are needed at synchrotrons such as the ESRF to serve as a beam splitter monochromator working in reflection geometry (Bragg case).
In these applications, the surface is of special interest. It should be smooth, flat and defect free. For the diffraction application, the requirements is in addition a low miscut for the 111 surface. The various communities for the high tech applications of diamond are therefore seeking a surface processing step to remove the scaife polishing damage (200nm depth), improve roughess (few Å) and flatness (1m) and to also process the diamond 111 surface, the hardest known surface (~0.20 miscut).
We present a summary of the different polishing techniques as well as their advantages and limits:
* Mechanical polishing with nano diamond powder.
* Oxygen electron cyclotron resonance (ECR) etching, oxygen radio frequency etching or microwave etching (ICP) in a O_2+SF_6+Ar gas mixture.
* Oxygen implantation, followed by annealing in vacuum at 950°C. ‘‘Lift-off’’ resulted from either a hydrogen plasma or an acid etch, and the final anneal in air at 500°C provided an additional soft isotropic etch.
* Hot metalling 1: The diamond is moved with low speeds over a surface of pure Fe at 1000°C in vacuum for at least 3 hours
* Hot metalling 2: Mechanical diamond-grit-less sciafe polishing at high speeds, high temperatures and high loads

Policy and Strategy Talks / 31

Our plan of schools and practical trainings to contribute to the African Light Source project

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Introduction
We would like to take part in to proceed and support the African Light Source project.
We had the schools for the SESAME staffs and users to study synchrotron sciences at the Middle East region several times. Many lectures were given on the fundamentals of synchrotron radiation, beamline diagnostics, and synchrotron experiments. There were also some tutorials to analyse data such as XRD, XPS, XRF, XAFS or others. In addition, researchers and students had come to Japan to study synchrotron radiation and to have practical trainings at synchrotron facilities.
We believe that these programs would be effective and useful to make the African Light Source project get forward. We hope you may get interested in these schools and practical trainings. Here, we would like to talk on the overview of the programs, and have collaborators to operate.

Our Plan Overview
The school on synchrotron radiation would be held once a year at an African institute. Lectures would be given widely on the fundamentals of synchrotron radiation, beamline diagnostics, and synchrotron experiments. We could accept about one hundred partici- pants for the class.
Tutorial lessons to learn how to analyse data of synchrotron experiments would be also given. These tutorials would be operated in relatively small groups in order to make the lessons effective, and about fifty members could be acceptable.
We would invite researchers and students to Japanese synchrotron facilities to study synchrotron radiation and to have practical trainings of measurements. They could be stay a few month at maximum. These practical trainings would help them to become beamline scientists and leaders of synchrotron sciences at the African Light Source.
We are glad that collaborative researches will be performed.

Invitation to be collaborators
Collaborators at African nations are required to operate the program of the schools and practical trainings. We would like to apply to Japanese funding agencies to operate the programs, and some funding programs require collaborations of Japanese and African organizations. Also, collaborative researches should be carried out. Those who will be interested in our proposal, please contact me.

Scientific Talks / 32

Kurchatov synchrotron: present state and upgrade program

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Synchrotron source of NRC “Kurchatov Institute” has a long story. It was found as a light source for microelectronic production later it was transformed into scientific facility. Years of development led to multidisciplinary scientific institution. The upgrade Phase-I gave possibility extend experimental hall and supporting labs, install new, modern beamlines and insertion devices. During the years 2007-2010 Kurchatov synchrotron was the fetus of the NBICS-Center, center for converging technologies in Nano-Bio-Informative-Cognitive- Social sciences and humanities.
At the present date the synchrotron organize annually 2-3 national and international conferences, accept every year many users from all over the Russia and some international ones. The ongoing stage of upgrade is the construction of 10 new beamlines, including beamlines for soft regime.
The launch of CREMLIN (Connecting Russian and European Measures for Large-scale research Infrastructures) project – will push forward development of Russian synchrotron community.

Scientific Talks / 33

Organic and inorganic layered systems study by X-ray standing wave technique

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The grazing incidence x-ray standing wave technique (XSW) is widely used for thin layered structure investigation. It is based on simultaneous analysis of x-ray reflectivity and x-ray fluorescence yield modulated by standing wave field formed due to the interference of the incident and reflected beams. While the reflectivity is sensitive to general distribution of electron density the angular dependence of fluorescence yield is sensitive to the position of selected atom along the normal to the surface [1, 2].
In this report the XSW technique was used for the determine of the preferential molecular orientation in organic monolayers of porphyrin(Zn)-fullerene dyad ZnDHD6ee on the water surface and solid substrate [3], for the investigation of diffusion process in thin layered structures during the thermal quasicrystal film formation [4] and of the growth mechanisms in the Si–Ge heterostructures [5]. It is well-known that XSW is very promising to study of the planar systems different nature – organic, bioorganic and inorganic, including self-organizing macromolecule or lipid-protein systems on water surface [1]. This technique also can be used for “in vitro” study of transport, barrier and protective functions of cell-membrane model.

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Scientific Talks / 34

Non-mechanical ultrafast tunable X-Ray optics (X-Ray acoustic elements and bending crystals): advantages and possibilities.

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My report focuses on the proposal, development and successful testing of the controlled elements for X-ray optics based on the lithium niobate crystals structures. Using such elements allows to achieve a scanning range of hundreds of angular seconds, even at low supply voltage. In addition, experiments that demonstrate the absence of hysteresis in such elements were performed. In this case it gives us a reason to use it as controlled X-ray optics element with the ability to pricisly control the angular displacement. It is important to note that the bending elements based on lithium niobate crystals are characterized by very small values of rearrangement time, which will allow using X-Ray optics elements based on them for fast experimentation, such as using in synchrotron beam stations.

Scientific Talks / 35

X-ray study of nanosized multilayer heterosturctures

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X-ray methods for diagonostic of nanosized heterostructures are long proved reliable instrument for analysis of real structure of multilayer heterocompositions and determination of parameters for single layers and interfaces.

In given work we used high-resolution x-ray diffraction and x-ray reflectivity methods for the analysis of spintronic maultilayer heterosystems. Spintronic is a new technological approach based on management of spin degrees of freedom in solid structures. Semiconductor spintronic systems which are the basis for the creation of spin transistors allow to manage spin currents. It is also important to mention that traditional electronic systems based on electric charge transfer have high power consumption and heat generation while in the semiconductor spintronic systems heat dissipation is minimal. X-ray diffraction rocking curves and x-ray reflectivity curves measurements were held in laboratory x-ray equipment of Kurchatov complex of NBICS technologies.

Joint analysis of x-ray diffraction and reflectivity data from semiconductor magnetic 2D structures with quantum dots GaAs/δ-Mn/InGaAs/GaAs allowed to determine structural parameters of all layers including very thin δ-layers of Mn and these of interfaces. The were established layers parameters of magnetic impurity allowed to find interrelation between structure of the samples with their magnetic and transport properties.

For the metallic superlattices Fe/Cr/Gd/Cr on Si substrates there were determined parameters of layers inside the superlattice period and interfaces between them. It allows to clarify real structural parameters of given heterocomposition and explain some peculiarities on their magnetic properties.

Such complementary approach for study of spintronic heterosystems like cap-layer/EuO/Si allowed to analyze modification of structural parameters on interfaces. As a result of study it was established that at the average thickness of interface ~25 Å the transfer from strained lattice EuO to a fully relaxed one takes place.

Joint analysis of x-ray methods data allows to analyze real structure including all of it peculiarities for different objects. In combination with data from other methods it gives the opportunity to establish interconnection between the structure of nanosized heterosystems and their electrophysical, magneto-trasport and other properties.

Scientific Talks / 36

Integrating synchrotron technology into the palaeosciences in South Africa

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While possibilities exist for using high resolution X-ray based technology (e.g., microCT) in South Africa, synchrotron technology offers a number of additional, crucial advantages to palaeoscientists that create unique opportunities for addressing scientific questions. Its non-destructive nature and high resolution imaging capability (e.g., submicron spatial resolutions) are especially important among these. Here, examples of successful partnerships between beam line scientists at the ESRF and palaeoscientists from South Africa are highlighted. These collaborations span investigations being performed on South African heritage objects that are hundreds of millions of years old up to relatively more recent times. Typically, fossil internal structure is targeted because it reveals otherwise unavailable evidence on organismal biological processes, growth trajectories, and structural details. Moreover, the intersection of synchrotron technology and palaeoscientific research is proving to be a rich area for developing new types of biological investigations.

The Department of Science and Technology (DST) and the National Research Foundation (NRF) of South Africa are acknowledged as primary funding agencies in this area of South African palaeoscientific research.

Poster Session / 37

Crystal structure and thermoresponsive studies of porous and non-porous borophosphates.

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In this work we present the synthesis and structure-property investigation of anhydrous non-porous borophsophates BPO_4 and hydrated porous $(NH_4)0.5Co1.25(H_2O)2(BP_2O_8)(H_2O)0.5$ phases. Cristobalite-type BPO_4 crystallizes in the tetragonal lattice, space group I-4 (No. 82) [1]. Variable-Temperature Powder X-ray diffraction (VT-PXRD) patterns of this material were analysed by the sequential Rietveld refinement protocol. This method was used to determine the temperature dependency of the lattice parameters and linear thermal expansion coefficient. The refinement reveals significant anisotropy along the a- and c- crystallographic axes as a function of temperature, with thermal expansion coefficients of 10.6 x 10-6 /°C and 2.83 x 10-6 /°C, respectively. Structural changes accompanying this thermoresponsive behaviour will be discussed, including the variation of the interatomic distances and P-O-B (inter-polyhedral angle) with temperature. The open framework borophosphate $(NH_4)0.5Co1.25(H_2O)2(BP_2O_8)(H_2O)0.5$ was synthesized under mild hydrothermal conditions at 180°C. The crystal structure was refined in the hexagonal lattice, space group P65 (no. 170) [2]. The compound is composed of NH_4+ and H_2O molecules located within the helical channels running along the [001] direction. Thermoresponsive investigation conducted by TGA analysis reveal a four step mass loss process, with the final step observed at 500-700°C range. Preliminary VT-PXRD results of this compound will also be presented.

Poster Session / 39

Stress assisted diffusion of krypton ions in polycrystalline titanium

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Stress migration of point and open-volume defects in materials is an important problem in a wide variety of applications, including radiation damage and ion beam modification of materials. This study aims to contribute to a better understanding of the basic processes underlying the effects of stress-assisted diffusion and ion-beam induced stress relaxation in metals. The stress profile in polycrystalline titanium has been determined using synchrotron radiation diffraction, for different krypton implantation doses. For each dose, the krypton profile has been experimentally determined using Rutherford backscattering geometry, and compared to model calculations using SRIM 2008. A strong stress relaxation was found for high dose implantation. It was further observed that for the titanium samples implanted at low fluence, ion implantation modifies the pre-existing residual stress through the introduction of point and open volume defects. The stress fields resulting from the ion implantation act to drift the krypton inclusions towards the surface of titanium.

Poster Session / 40

Fossorial adaptations of the functional morphology and internal structure of the forelimb of the Early Triassic cynodont Thrinaxodon liorhinus.

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Therapsids were severely affected by the Permian-Triassic mass extinction event and only a few lineages were able to survive. One of the main behavioural responses that may have aided in Therapsid survival across the extinction was fossorialism. Several fossilized skeletons of the non-mammaliaform cynodont, Thrinaxodon were found in curled up position and assumed to have died in a burrow, leading to the idea that this taxon was perhaps a digger. To date, limb morphology of Thrinaxodon has not been systematically compared to extant burrowing specialists. Besides exhibiting potential burrowing adaptations, the limbs of Thrinaxodon have been described as exhibiting a transitional phase between classic sprawled limbs of reptiles and mammalian parasagittal postures. The present research investigates the internal and external morphology of Thrinaxodon liorhinus in comparison to a fossorial mammal and reptiles that exhibit different behavioural patterns. The study uses Geometric Morphometric analyses, forelimb indices, torsion and cortical thickness in order to determine the extent to which Thrinaxodon forelimb illustrates modifications due to gait versus a fossorial lifestyle. This indicates that Thrinaxodon retained the reptilian skeletal configuration and began adaptation to resemble a parasagittal gait. These results advance present understanding of Thrinaxodon limb structure, mobility, habitat and ecological preference.

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Towards Structural Characterization of Novel Bacteriophage Proteins

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Towards Structural Characterization of Novel Mycobacteriophage Proteins

Interest in bacteriophages- viruses that infect bacterial hosts- has been increasing as the potential for bacteriophages to serve as alternatives to antibiotics is being investigated once more. Isolation and genomic annotation of mycobacteriophages that infect Mycobacterium smegmatis, a closely related strain of the clinically relevant Mycobacterium tuberculosis, has revealed novel phage genes not found in any other phages or organisms. These novel genes, termed “orphams”, and the proteins they encode are the focus of this study. In particular, the M. smegmatis. phage Butters has a very compact genome compared to other phages in its class, yet still possess several orphams. How these novel proteins function in an infection cycle that results in bacterial destruction is unknown. Here, we present biochemical and biophysical data on several of the proposed orphams from Butters including a putative membrane protein, and steps towards structural characterization.

Poster Session / 42

Targeting transthyretin amyloidosis: Neutron and X-ray diffraction analysis of a pathogenic protein

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Transthyretin (TTR) amyloidosis is the most common hereditary form of amyloidosis that is characterised by extracellular deposition of insoluble amyloid fibrils derived from misfolded protein in one or more organ systems in the body. It is an irreversible and progressive disease and is fatal within 10 years of onset. Autosomal dominant mutations in the TTR gene alter the protein stability leading to tetramer dissociation and favouring an abnormal monomeric structure, which in turn polymerises into unknown intermediates and finally into amyloid fibrils. [1,2]

Up to date, around 200 X-ray crystal structures are available for TTR, but there is no consistent model to conclude the molecular assembly of the fibril building blocks and the triggering factors for this process. Neutron protein crystallography is a powerful tool that strongly complements X-ray structural studies by revealing key details of hydrogen atom interactions within the protein. Looking at the differences in hydrogen bonding, protonation states and hydration of two TTR mutants – S52P and T119M, which play opposite roles in the protein stability, will provide key insights into how they destabilise the tetramer and promote amyloidotic aggregation. Neutron analysis of the TTR in complex with various ligands will also provide useful information for improved drug design for the treatment of TTR amyloidoses.

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Poster Session / 43

A seed protein from Moringa oleifera used in traditional water purification: structural and in vivo studies

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Moringa oleifera is a tropical plant that belongs to the Moringaceae family and is native to northern India. The tree grows quickly and is cultivated in tropical areas. Moringa oleifera is also called The Miracle Tree1 because many of its parts have valuable applications. In particular, seed extracts from the plant have been used in traditional water treatment throughout Africa. The application of this extract to untreated water causes a 95% reduction of turbidity, and a decrease in particle and bacterial content. Numerous laboratories have demonstrated these effects but the precise nature and properties of the active components in the extract has been unclear. Small-angle neutron scattering has demonstrated the unusually dense nature of flocs formed with seed extract2 and reflection studies have been carried out, to determine the arrangement of protein adsorbed at model interfaces3

We have analysed seed extract from Moringa oleifera and separated a major component protein that has a molecular mass of 11.8 kDa. The protein was purified in a two-stage process and crystallised. A recent crystallographic study yielded data to a resolution of 1.6 Å, and the molecular structure was solved using sulphur SAD. The structure contains 4 disulphide bonds, and the analysis has yielded a substantial part of the amino acid sequence. These data are being correlated with results from N-terminal sequencing, in combination with trypsin digestion.The pure protein is also being studied to probe a rational basis for the nature of the activity of the crude extract in traditional water treatment. Initial tests have demonstrated a bacteriostatic/bacteriocidal effect on living E.Coli cells. In future, we will use a recombinant expression system to produce a deuterated protein for a neutron crystallographic analysis aimed at understanding the nature of hydration interactions and protonation states in the structure.

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Synchrotron imaging and the African fossil reccord: a decade of collaboration

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Palaeontologists have always sought for new techniques aiming to retrieve more and more information from the fossils they discovered. Until recently, one of the most difficult problems to overcome was the non-destructive visualization of inner structures, to access the numerous information for the understanding of life evolution on Earth. Using X-rays to scrutinize fossils rapidly appeared as an obvious non-destructive solution. From early medical scanner to synchrotron, Computed Tomography has revolutionized palaeontology opening new possibilities in all its branches.
African researchers were not an exception in this exploration of the unseen. The richness of the African fossil record was offering abundant and important material and more questions to answer. One of the first uses of synchrotron in palaeontology was the study an early member of the hominid lineage from Chad, Sahelanthropus tchadensis, also known as Toumaï, studied by a Tchad-French team. This incredibly important fossil paved the way for many collaborations of African researchers with the European Synchrotron: Ethiopia, Kenya, Morocco, Cameroon, Mozambique and South Africa, to name a few and the list keep growing.
South Africa is a remarkable example of collaboration with the ESRF. From the first palaeontological experiment in 2008, South African researchers pushed forward to take advantage of their two cultural heritage treasures: the Karoo, first, land of the longest most extended continuous continental fossil record, documenting the most dramatic of all mass extinction, but also the rise of mammal forerunners and their fall at the dawn of dinosaurs; the second, the UNESCO world heritage site known as the Cradle of Humankind, where more fossil hominids have been discovered than anywhere else. The palaeontological community actively participated to the agreement with the ESRF, making South Africa the first African country to join the European Synchrotron. This endeavour made it possible for South African researchers to take advantage of their incredible fossil record and of the best tool available in the world for imaging of fossils.

Policy and Strategy Talks / 45

The ESRF model: history, governance, access, key facts and figures and socio-economic impact

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The ESRF is one of the very few cases where a synchrotron light source has been constructed under an Intergovernmental Convention. The ESRF governance, access, budget, procurement, communication, etc. are all framed by this internationality. The aim of the presentation is therefore to outline the ESRF model: how it operates in terms of governance and funding, key facts and figures, the ESRF access system, the return to its partner countries and its socio-economic impact.

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Science and Technology Development at Light Source Facilities around the World

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The 12th International Conference on Synchrotron Radiation Instrumentation (SRI2015) was hosted by National Synchrotron Light Source II (NSLS-II) and held in New York City, July 6-10, 2015. This triennial conference brought together scientists and engineers from around the world to highlight the most exciting science and technology developments in the synchrotron and free-electron laser light source community. This presentation will attempt to provide a summary of these advances and will highlight the current trends in scientific research and in facility development.

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Biosciences using synchrotron infrared microspectroscopy

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Infrared spectroscopy and microscopy may look an exotic analytical tool in biology. It's rather known for identification of molecular vibrational motion in chemistry , physics, geology, space science…. But, the technique has clearly showed its potential when a synchrotron source was thought to be used instead of a traditional thermal source (also called lab-source).
Vibrational spectroscopy identifies the resonant vibrational motion of molecular groups, as each of them has a single, or multiple resonant frequency, called also absorption bands, characteristic of their identity.in addition, the resolution is such that any perturbed environment (for example ordered / disordered beta sheets) can be identify at sub-micron level. Infrared spectroscopy use the IR photons emitted by a thermal source, in the energy domain 2-200 microns (which are long wavelength compared to the most known X-ray photons).
Originally, an active field of research has been developed around the changes of motion of the main component of an human cell or tissue (protein, lipids, DNA, RNA etc.), in order to identify any evolution or disease. When the synchrotron radiation was identified as a bright source that can be coupled with such an instrument, one has realized that the brilliance advantage of such a source makes possible to probe tissues and cells at sub-cellular resolution. This has held a big promise in detecting any change in the nucleus of individual cells, with a fast data recording at high lateral resolution, with very good spectral quality(S/N) . There exist several biological and biomedical applications which emphasize on the promising future of synchrotron infrared micro-spectroscopy in these scientific disciplines. This will be the main objective of this talk. In particular, I will details the following examples:
• Urinary stone disease, constitutes a major health problem and is affecting an increasing number of people. Calcium oxalate, calcium phosphate, uric acid, ammonium hydrogen urate and magnesium ammonium phosphate are the main components of stones. Very small crystals in the kidney biopsy sample, of 2,8-dihydroxyadenine (2,8-DHA) were identified , and this has direct relevant therapeutic implications. Doctors from Hospital for a rapid screening of kidney sections actually routinely use IR synchrotron microscopy. This results in a direct implication in the patient therapy and recovery.
• The potential changes occurring in hematopoietic cells expressing BCR-ABl and BCR-ABL carrying T3151 mutation, conferring resistance to most tyrosine kinase inhibitors currently used has been evaluated using IR micro-spectroscopy. The use of the synchrotron is fully justified due to the small dimension of human leukemia cells .
• Stem cells research is a very important research topic nowadays. Several studies have shown that IR microscopy can determine the differentiation state of the stem cells. But more importantly, we have been able to show that synchrotron IR microscopy can assess unambiguously the reprogrammation of stem cells, which is more difficult otherwise.
• Liver steatosis is a severe disease that can lead to hepatosteatosis, cirrhosis and cancer. The precise determination of the steatosis content during the liver transplant is crucial with recommendation to select livers exhibiting no more than 20% steatosis. This drastic recommendation contrasts with the incapacity of usual histological methods to rigorously provide an objective and non-biased assessment of steatosis. Synchrotron infrared microspectroscopy has helped determining the presence of micro vesicle with lipids content that can be directly related to the lipidomic HPLC tests. The database established with the synchrotron source is actually used to condition an IR thermal source based microscope, to be set up in hospital for direct diagnostic during liver transplant.

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X-ray Physicochemical Imaging of Catalysts Under Working Conditions

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The imaging of catalysts and other functional materials under reaction conditions has advanced significantly in recent years. The combination of the computed tomography (CT) approach with methods such as X-ray diffraction (XRD), X-ray fluorescence (XRF), and X-ray absorption near edge spectroscopy (XANES) now enables local chemical and physical state information to be extracted from within the interiors of intact materials which are, by accident or design, commonly inhomogeneous. The spatially resolved signals obtained can reveal information that would otherwise be lost in bulk measurement. Such local signals are simpler to interpret since they are highly likely to contain fewer phases. Studying intact materials rather than idealised powders allows for behaviour under industrially relevant conditions to be observed. Furthermore the background signal from in situ apparatus / cell can be readily separated.

We show how such methods have been applied to understanding the behaviour of a number of catalytic systems at a range of length scales. Crucially we demonstrate that the obtained chemical and physical information can be correlated to catalytic activity and selectivity. At the small length scales, sample size and density allow for transmission of comparatively low energy signals allowing combination of XRF-CT and XANES-CT in conjunction with XRD-CT, enabling simultaneous multi-technique imaging. This combined approach has been used to characterise intact single catalytic particles (a 100 μm Mo promoted Pt/C catalyst under liquid phase hydrogenation operating conditions) and packed bed micro-reactors enabling identification of active species and correlation to performance. High energy XRD-CT enables large/dense objects to be studied. We show how this has been used to study the behaviour of industrial pellets (e.g. following the evolution of the cobalt phases in 3 mm diameter Co/Al_2O_3 catalyst under industrial conditions) and also to see inside working bulk reactors (6 mm catalytic membrane reactor device used for the oxidative coupling of methane; the reactor consists of a dense ceramic oxygen transport membrane containing a packed bed of $Mn\text{-}Na\text{-}W/SiO_2$). In the latter case the active state is captured and material is observed to form that is likely to impact on the long term performance of the reactor. Such information is vital to rational catalyst and reactor design that cannot be obtained by conventional bulk measurements.

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Synchrotron Radiation and Structural Biology

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An overview will be given of how synchrotron radiation has revolutionized structural biology. To day the experiments are facilitated by the highly automated beamlines for diffraction and small angle scattering, and through partnerships like the PSB (Partnership for Structural Biology) in Grenoble complementary techniques are made available. These advances will be illustrated by our studies of PfEMP1 malariaproteins by diffraction and small angle scattering. The impact of experiments with free electron lasers on the future developments of structural biology at the synchrotron facilities will also be addressed.
In relation to the creation of ALS I shall report on my personal experience with creating a network of researchers in the nordic countries supported by the EU funding.

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Brazilian Synchrotron Light Laboratory – LNLS: from scratch to a state-of-the-art machine in 30 years

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The first discussions to build a synchrotron light source in Brazil started in the early 80's. At that time, Brazil had no knowledge in either building or operating a synchrotron machine. Moreover, only a handful of researchers in the country had already used a synchrotron somewhere else in the world. Strategies were taken both to train young physicists, engineers and technicians in the different fields needed to build a synchrotron accelerator and its beamlines, as well as to educate researchers for their usage. The overall design and construction of UVX, the name of the Brazilian second generation machine, took from 1987 up to 1997, when it was opened to users. It was the first synchrotron light source in the southern hemisphere, as it is still today the only one in Latin America. It opened with 7 beamlines, and it evolved to have 17 today. The number of users grew from less than two hundred to more than a thousand per year. They come today from a community of approximately 3.000 users that have at some point visited LNLS. The development of such a community placed a natural demand for a better machine. Thus, LNLS started to work on a project of a new synchrotron light source. The first proposal to initiate the studies of such a machine was presented to the Minister of Science and Technology in 2008. From then on many developments were made, and today Sirius, the nickname of the new synchrotron, is starting to become a reality. It is a very challenging light source, one of the first fourth generation machines, designed to have one of the highest brightness among the 3 GeV synchrotron sources in the world. Besides the scientific impact, Sirius is also having a positive effect on the industrial sector, involving both small and large Brazilian companies in the production and development of its components. Construction of the building started in December of 2014, and the first beam is expected by 2018.

Poster Session / 51

Interfacial reactions and surface analysis of W thin film on 6H-SiC

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Tungsten (W) thin film was deposited on bulk single crystalline 6H-SiC substrate and annealed in H2 and Ar ambient at temperatures ranging from 700 to 1000 °C for 1 hour. The resulting solid-state reactions, phase composition and surface morphology were investigated by Rutherford backscattering spectroscopy (RBS), grazing incidence X-ray diffraction (GIXRD) and scanning electron microscopy (SEM) analysis techniques. As-deposited RBS results indicate the presence of W and O_2 in the deposited thin film, the XRD showed the presence of W, WO_3, W_5Si_3 and WC. RBS results indicated the interaction between W and SiC accompanied by the removal of oxygen at 700 °C for the samples annealed in H_2 ambient. The XRD analysis indicated the presences of W_5Si_3 and WC in the samples annealed at 700 °C. At temperatures of 800 °C, 900 °C and 1000 °C, W further reacted with the SiC substrate and formed mixed layer containing silicide phases and a carbide phase. That is, W_5Si_3, WSi_2 and WC for the Ar ambient and W_5Si_3, WSi_2, WC and W_2C for H_2 ambient. The SEM micrographs of the as-deposited samples indicated the W thin film had a uniform surface with small grains. Annealing at 800°C led to the agglomeration of W grains into clusters for the H_2 annealed samples. SEM micrographs of the Ar annealed samples at 800 °C indicated randomly orientated large crystals growing on top of each other on the surface.

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Overview : Synchrotron Light Source Machines

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The general layout of a synchrotron light source will be given with the description of the different accelerator areas like linac, booster synchrotron and storage ring as well the description of the different components like magnets, vacuum system, RF-system, etc. As an example the layout the of MAX-IV and the ESRF-EBS will be discussed in order to reach a small emittance and high brilliances for the users. The project SESAME will be used to describe a roadmap for the establishment of the synchrotron light source in Africa.

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African projects at the IPANEMA research platform for ancient materials. Perspective within the European research infrastructure for Heritage science.

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IPANEMA, the research platform for ancient materials located in Paris-Saclay, is a centre for the development of advanced methodologies of material characterization in archaeology, past environments, paleontology and cultural heritage, and the support of synchrotron research through external users hosted on the platform. IPANEMA develops and provides a set of techniques for preparing specimens, to study artifacts and samples, and statistically analyze collected datasets.
For the last ten years, several initiatives and research projects were carried out with teams from several African countries. Results regarding the analysis of rock art samples, characterisation of palaeontological specimens, and study of archival documents will be presented. Perspectives of advanced partnership within the European research infrastructure for Heritage science will be discussed.

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Residual stress analyses using diffraction techniques

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Residual stress is a double-edged sword since tensile stresses, especially when existing close to surfaces, can lead to component failure due to stress corrosion cracking, whist compressive stresses mitigate against crack formation and propagation. Diffraction techniques enable analyses of the prevailing residual stress conditions from direct investigation of the lattice plane spacing. By combining this property with penetrating radiation such as hard X-rays and thermal neutrons, depth-resolved information can be obtained.

Using hard X-rays (energies larger than 65 keV) produced in synchrotron facilities has made possible the elucidation and quantification of depth influences resulting from:
• Surface stress modification treatments such as shot peening to enhance fatigue lifetimes in steel samples;
• WC-Co hard metal coatings on substrates that rendered extensive differences in the coefficient of thermal expansion between such coating and the substrates. This leads to interactive thermal stresses that may be beneficial to both the coating and the substrate.
Notwithstanding the capability of depth profiling to typically 50 μm resolution, data quality is strongly influenced by grain statistics. With neutron diffraction investigations larger gauge volumes need to be employed that largely mitigates the latter effects.

We shall report on the complementary use of X-ray and neutron strain analyses towards depth-resolved investigations of these systems.

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Policy and Strategy Talks / 55

The role of International Physics Organizations

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I will review existing programs and describe the potential role of the International Union for Pure and Applied Physics (IUPAP) and of the International Centre for Theoretical Physics (ICTP) in support of the strengthening of the African community of users of synchrotron light sources.

Scientific Talks / 56

Depth-resolved and fatigue studies of thermal sprayed hydroxyapatite coatings

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Hydroxyapatite coatings (HAp composed of $Ca_{10}(PO_4)6OH_2$), deposited by air-plasma spray onto cylindrical Ti_6Al_4V rods were investigated in the as-coated and fatigued conditions. Through-thickness characterisation was carried out using conventional X-ray (near surface in reflection mode) and Synchrotron radiation (depth dependence in transmission mode) diffraction of the phase composition, percentage crystallinity, and residual stress. Fatigue investigations were performed on samples submerged in simulated body fluid maintained temperature around 37°C. Samples were mechanically loaded to 150, 500 and $750x10^3$ tension-compression cycles.

In the as-coated condition, HAp and its thermal decomposition products, tetracalcium phosphate (TTCP), tricalcium phosphate (TCP) and calcium oxide exist throughout the coating thickness. Chemical phase quantification with Rietveld refinement indicates HAp and TTCP to be the major phases. The HAp content is maximum at the coating mid-thickness from where it systematically reduces with depth. The decrease in HAp composition is compensated by an increase in the TTCP content. The coating is most crystalline at the near-surface region, from where it decreases as the coating-substrate interface is approached.

With fatigue treatment, the HAp phase content increases with number of cycles, whereas the TTCP phase content decreases. Residual stress results indicate that the principal components 11 and 33 are respectively tensile and compressive at the surface; both components relax with depth. With further depth a change in stress state at the midpoint for both components is observed.

Policy and Strategy Talks / 57

Outline of Policy Session and the AfLS Vision

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The origins of this event have been the long history of a global conversation around the need for a Light Source in Africa. After a consultative process, the Interim Steering Committee for the African Light Source was formed in August 2014. This Committee has organized this week's deliberations. The Conference section of he event has just been completed where the delegates have heard talks outlining the tremendous impact that light sources have had on quality research in a range of interdisciplinary fields. Ultimately, the impact is also on human and infrastructural capacity building and on sustainable economic development more generally. We have also just seen, in the Conference section of the event, many examples of research conducted by African scientists using the light source as a premier research tool. It is now our task to think deeply and strategically, and engage each other with the aim of laying the foundations towards the goal of establishing a light source in Africa. We have planned several talks as input for discussion, followed by plenaries, where we will workshop the ideas. Finally , we will have concrete outcomes, developing the Roadmap for a Light Source an Africa, as well as establishing a fully mandated Steering Committee, to guide the journey along this Roadmap. In this presentation, we can consider both the vision, and the process, to facilitate our coming deliberations.

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The African Laser Centre: A Model for African Collaborations

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The African Laser Centre (ALC) is a network of laser researchers in Africa that has grown to involve more than thirty (30) laboratories across the continent. It is an African Union/NEPAD flagship programme that seeks to achieve the following: (1) promote laser-based research, development, and innovation, as well as laser-related education and training on the African continent, (2) foster collaborations among laser researchers and institutions across the continent, as well as facilitate collaborations of these with their international counterparts, (3) contribute to the advancement of African countries' economies and global competitiveness for the welfare of their people. We describe the genesis of the ALC since its launch in 2003 and its programs and major successes over the past ten years. Finally, we discuss how the ALC could serve as a model of an African light source.

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Remote Access at the ESRF's Structural Biology Beamlines

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I will demonstrate various modes of remote access on the structural biology beamlines at ESRF. What I show should be of use for the operation of an eventual Africal Light Source.

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TANGO - a mature Open Source collaborative framework for building control systems

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TANGO is a toolkit for building control systems. It started originally at the ESRF in 1999 and has reached maturity since a while but keeps on being improved. It is a Free Open Source toolkit which can be downloaded and installed on Linux, Windows or Macintosh. Binary packages exist for Debian Linux and Windows. TANGO is used on many sites in Europe including synchrotrons, lasers, wind tunnels, gravitational observatories and other types of installations. It can be used on a small system like a Raspberry PI to control a single device. TANGO has recently been chosen for the Square Kilometer Array (SKA) to be built in South Africa and Australia. TANGO is a modern system with a clear roadmap. TANGO represents a great opportunity for the African Light Source to create synergy with SKA.

For more information about TANGO got to http://www.tango-controls.org

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Review of synchrotron-based activities in South Africa

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Synchrotron radiation has revolutionized basic and applied research in many fields of science and technology. South African, like most countries, has seen an ever larger number of scientists accessing synchrotrons for their research. South African synchrotron radiation usage has correspondingly increased steadily over the last decades despite spiralling cost and long distance travel. This talk aims to give an overview of synchrotron-based activities currently undertaken in South Africa, provide some examples of successes achieved thus far including government support and commitment for accessing international synchrotron facilities; highlight some challenges experienced by the community and outline the long-term goals for the country and the region for the use of synchrotron radiation. We will outline current efforts of building momentum towards the realisation of a future African light source.

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Role of the African Physical Society Towards an African Light Source

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The paper gives a brief profile on African Physical Society and discusses the role African Physical Society can play towards the establishment of a light source centre in Africa and future planning of workshops and conferences on light sources.

It presents how an interface with appropriate Governments officials and ministers will encourage African Countries to investigate their suitability for hosting the facility and assist with a program that sends light source users to various Universities and other institutes to the light source Centre.

It discusses how African Physical Society can identify companies in various African countries that could benefit from the use of light sources, and how African Physical Society could facilitate students and researchers visit to international Light sources for training and research.

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4D in situ microtomography in materials science

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X-ray tomography is becoming a standard characterisation in a numerous materials science research field : room or high temperature damage in composites of metals, solidification, sintering ...[1] More than 3D images it is possible since several years to perform 4D investigation providing dedicated experimental set up are developed. For example 4D studies were performed in various domains : bubble growth and foam setting during breadmaking, solidification of aluminium alloys, damage in metals at room or high temperature, sintering ... The main improvement in the last 10 years in 4D analysis with X-ray tomography lie in the improvement in images quality, field of view, spatial resolution, scan time and multiresolution possibilities. We will present possibilities and limits of the techniques with some application in various fields of material science (solidification, damage in materials, phase transformation ...).
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International Co-operation

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Pore Scale Investigations of Forced Imbibition/Drainage in Porous Media Studied by in situ X-Ray Microtomography

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The forced imbibition or drainage of an aqueous phase into an initially oil filled bead matrix is studied. The advancement of the water front is imaged in real-time using ultrafast x-ray tomography. The 3d time series are analysed in terms of oil saturation, front area and morphology of the pore-throat filling behaviour. The displacement behaviour hardly depends on gravitational effects and details of the pore space, as was explicitly tested. For flow rate of the invading phase or viscosity of the defending phase below a certain threshold the dependence of both viscosity and velocity can be also neglected. For typical front velocities of about 3 μm/s, as e.g. relevant for oil recover, the multiphase flow is dominated by capillarity and the wettability of the porous matrix with the invading phase is the key parameter to understand the displacement behaviour. We could identify a wetting and a non-wetting regime for small and low contact angles of the invading phase with a transition region of about $\theta \sim 30^\circ$ separating both regimes. Within each regime the displacement behaviour is fairly insensitive to the exact contact angle.

A compact front develops for early times for a wettable invading phase whereas a branched front develops for a non-wettable invading phase. The two regimes and the developing front shapes can be explained by local instabilities as introduced by Cieplack and Robbins [1]. In particular the absence or the appearance of 'Burst-Instabilities' where the local instability occurs when the pressure in a throat exceeds the required filling pressure can be used to distinguish the transition between both wetting regimes. For the non-wetting system where the local front progression occurs mainly by 'Burst-Instabilities' an interconnected and very extended network of invading and defending phase develops at later times. The interconnected network of the defending phase is slowly drained by gutter flow leading to an increased residual saturation which is reached only after a substantial flush of the invading phase.

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XRF and FTIR Analysis of certain African historical documents

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The aim of this was work was to assess the oxidative degradation risk and suggest conservation methods of certain historical documents. All the documents studied were obtained from the National Library of South Africa except one that was obtained from a private library at the city of Timbuktu, Mali. The Abbey pH pen method was used to check the pH level of all the samples. It was found that all the samples except two were acidic. The sample from the Timbuktu manuscripts was found to be extremely acidic with a pH level of below 5.0. It is recommended that all the acidic samples be de-acidified using the Bookkeeper process in order to retard the process of degradation due to hydrolysis. XRF technique was used to study the elemental composition of the samples. In all the samples six elements namely Fe, Cu, Mn, Ca, K and S were detected. It was found that older documents had higher concentrations of Ca and hence have a considerable alkaline buffer than recent documents. It was also observed that the levels of Ca dropped significantly in the samples dating between 1800 and 1890 coinciding with the period during which paper making technology changed. The concentrations of K and S also decreased around 1890. Iron remained considerably high and was detected in all the samples. Copper and manganese were found to be at very low concentrations compared to Fe. The nature of the fibres that make up the samples studied was determined using FTIR. It was found that all the samples were made of cellulose. The Courier sample also had lignin and hemicellulose. The Total Crystallinity Index (TCI) of each of the samples was also calculated in order to determine the susceptibility of cellulose to degradation agents. This index is the ratio of the integrals of the FTIR band at 1372 cm-1 to that at 2900 cm-1. The integrals were taken over the ranges 1390 – 1339 cm-1 and 2959 – 2830 cm-1 for the bands at 1372 cm-1 and 2900 cm-1 respectively. The Lateral Order Index (LOI) was also calculated using the ratio of the integrals of the absorption bands at 1420 cm-1 to that at 898 cm-1. These bands are known to be sensitive to the relative amounts of crystalline versus amorphous structure in the cellulose. It was also observed that all the samples had clay but none of the samples had gypsum as a filler material. Traces of calcium carbonate were found in four of the samples studied. Kaolin was also found in all the samples except two. Only one sample showed the presence of gelatine.

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Investigation of Letlhakane Mine DK/1 mudstones using diffraction methods

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Letlhakane Mine DK/1 belongs to a cluster of about 85 kimberlite pipes, Orapa Kimberlitic Cluster, located approximately 240km west of the Francistown in the Boteti District of Central Botswana. It is one of the Orapa (AK/1) Letlhakane and Damtshaa (OLDM) diamond mines operated by Debswana Diamond Company.
The OLDM are experiencing a huge variance coefficient of rock strength within the same lithology of which the cause has not yet been established. Several authors have investigated strength variation of the rock within the same lithology and formation on different geological setups and environments. However this variation of strength within the same lithology has not been linked to the petrographical parameters such as how grains are packed, grain size, grain shapes, cementing material and minerals. In addition the OLDM are faced with an issue of red-mudstone especially in the A/K1 and D/K1 pits. Upon exposure the red-mudstones crumble causing the top Mosolotshane sandstones to topple because the lower support has been weakened or removed. The objective of this work was to further explore the use of diffraction (X-ray diffraction, Synchrotron XRD and neutron diffraction) to determine the residual strain in country rock, as well to investigate the influence on the chemical composition and mineralogy.

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EU-Africa collaboration on cutting edge research challenges

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The dialogue on Research Infrastructures between Africa and the European Union is strategically valuable and builds on a number of relevant initiatives such as the European Commission 7th Framework Programme project -PAERIP– aimed at Promoting African- European Research Infrastructure Partnerships, which mapped the RI context and its potential as well as the Square Kilometre Array (SKA) initiative which represents a clear example of how African and EU interests can converge around a cutting edge scientific challenge.

The development of a roadmap for the African Light Source could pave the way for a further enhancement of the scientific cooperation between European and African scientists in line with the "Open to the World" priority promoted by the European Commission.
European lessons learned and best practices derived from ongoing and past activities in the domain of Research Infrastructures, including the SESAME initiative could provide valuable input in the frame of the African Light Source initiative. An analysis of the key aspects for Research Infrastructure long term sustainability, road-mapping, user needs analysis, multidisciplinary approach and strategic governance will provide the basis for a wider international debate.

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The Vision of Egypt for the AfLS

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SESAME started a long journey since 1997 when it was only a thought to construct the first light-source in the Middle-East. Current members are: Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. Where, Brazil, China, the European Union, France, Germany, Greece, Italy, Japan, Kuwait, Portugal, the Russian Federation, Spain, Sweden, Switzerland, the United Kingdom and the United States are the observers. SESAME, the third generation light source seeks Excellency of Science, as well as, bridging the gaps between its diverse -culturally and politically- conflicting societies. Huge obstacles were faced, and more challenges are still there, but soon with its planned commissioning in 2016, the dream of so many people will become a reality.

Since its foundation under the auspices of UNESCO and up till now, SESAME -which is still under construction- receives in-kind support from several international organizations, the observers, as well as, its members. Resembling SESAME, the African Light Source (AfLS) embodies the first synchrotron-light facility for African countries. The progress is going forward with international support. However, with the preliminary studies, it is expected that the machine will be into operation not before 10-15 years. On the other hand, SESAME could be into operation within the next year with 2 day-1 beamlines, and more to be added, having secured the necessary fund of a few millions of dollars. For this, a joint strategy and urgent work plan is mandatory.

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The contribution of the IUCr to the development of scientific education, research and infrastructure in Africa

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The International Union of Crystallography (IUCr) is a scientific union adhering to the International Council for Science (ICSU). Its objectives are to promote international cooperation in crystallography and to contribute to all aspects of crystallography, to promote international publication of crystallographic research, to facilitate standardization of methods, units, nomenclatures and symbols, and to form a focus for the relations of crystallography to other sciences. The IUCr fulfils these objectives by publishing primary scientific journals, the series of reference volumes International Tables for Crystallography, distributing the quarterly IUCr Newsletter, maintaining the online World Directory of Crystallographers, awarding the Ewald Prize and organising the triennial Congress and General Assembly. In addition to all this, the IUCr carries out a wide program of outreach activities aimed at improving public awareness of the field, boost access to instrumentation and high-level research, nurture “home-grown” crystallographers in developing nations, and increase international collaborations for the benefit of future generations.

In January 2014, the IUCr and UNESCO launched a year of activities to support the UN Resolution A/RES/66/284 proclaiming the International Year of Crystallography (IYCr2014). With this resolution, the UN recognized that humankind’s understanding of the material nature of our world is grounded, in particular, in our knowledge of crystallography, and stressed that education about and the application of crystallography are critical in addressing fundamental challenges. At a time when scientific endeavour is critical for societal benefit, the importance of crystallography is greater than ever, yet it remains a science that still has lower visibility than it should. Understanding the structure of matter and relating this to the properties and functionality of any kind of compound has given a new path to scientific research, has transformed industries and created new frontiers, from the design of new medicines and materials to assessing the mineral content of Mars. The future global economy will be determined by progress in cutting-edge fields. However, the playing field is not level in crystallography and fundamental courses on crystallography are disappearing from most academic chemistry degree curricula and are almost absent in the developing countries.

Several activities conducted by the IUCr to promote crystallography and science in general in the developing regions will be presented in this talk, with particular emphasis to Africa. Among these:
- the IUCr “Crystallography in Africa” initiative, launched in 1999 and thanks to which crystallographic equipments have been or are being installed in some sub-Saharan African countries;
- the IUCr-UNESCO OpenLab initiative, a network of operational crystallographic laboratories, organized in partnership with industry, which are enabling students in far-flung lands to have hands-on training in modern techniques and expose them to cutting-edge research in the field;
- the IUCr-ICSU "Building Science Capacity in Africa via Crystallography" initiative, a project prepared as a follow-up to the IYCr Pan African Summit meeting (Bloemfontein, October 2014), which will support the 1st Pan African Crystallographic Conference (Dschang, October 2016), the 2nd North African Crystallographic Conference (to be announced) and several other additional actions.

Possible future collaborations with other scientific and international institutions will be also discussed, as well as the role that the IUCr and similar institutions could play to facilitate the discussion about the need and possible implementation of an African Light Source.

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Structural biology: A powerful tool to gain insight into the biology of the malaria parasite, Plasmodium falciparum

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Plasmodium falciparum is responsible for the vast majority of malaria cases and deaths, especially in sub-Saharan Africa. Progress towards malaria elimination is hampered by the lack of an effective vaccine, the rapid development of drug-resistant parasites and insecticide-resistant Anopheles mosquito vectors, and insufficient knowledge of the biology of the parasite, in particular of the proteome and gene regulation. The array of sophisticated structural biology techniques available at ESRF and ILL provides a powerful tool to study critically important P. falciparum proteins and their interactions within the parasite. Two potential therapeutic target proteins are currently being investigated: Erythrocyte Binding Antigen, EBA-181, which is required for the invasion of erythrocytes, and PfMyb2, a DNA-binding protein and putative transcription factor.

Biophysical characterization of the RIII–V regions of EBA-181 (EBA-181$_{945–1097}$) revealed an intrinsically disordered structure. Characterization of the protein at atomic resolution using nuclear magnetic resonance (NMR) spectroscopy showed that it is essentially a statistical coil with several turn motifs but it does not possess transiently populated secondary structures commonly seen in intrinsically disordered proteins that fold via specific, pre-formed molecular recognition elements. Small-angle synchrotron X-ray and neutron scattering experiments confirmed the overall shape of the molecule and suggested also the binding region with its macromolecular receptor.

PfMyb2 localises to the nucleus as demonstrated by an indirect immunofluorescence assay. Gene knockout studies implied that the gene is essential for parasite survival. The N-terminal DNA-binding domains of PfMyb2 were expressed as recombinant his-tagged proteins from a pET-15 vector construct and electrophoretic mobility shift assays (EMSAs) revealed binding to a consensus DNA sequence. To improve solubility of the recombinant PfMyb2, four smaller sections of the DNA binding domains of the gene have been amplified and cloned into pETM-11, a kanamycin-resistant vector, to allow for the production of deuterated protein for structural studies on the PfMyb2-DNA complex.

Envisaged future studies will focus on the role of structural biology in a malaria drug development pipeline. The interaction of lead anti-malarial compounds with their target proteins will provide valuable information to guide optimisation of the lead compounds.

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Light Sources for Materials and the AfLS context

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The discovery of new materials lies at the heart of future technologies, whether they are high energy density batteries for next generation electric cars, or locally sustainably manufacturable photovoltaics for off-grid African villages. Since materials derive their properties from the atomic arrangements, a starting point is characterize the structure and relate it to properties and processing. Modern materials of interest are highly complex, defective and nanostructured, but may have great properties. To solve the detailed structure of such materials we need powerful synchroton based x-ray sources, and novel data analysis methods which I will describe. Access to such facilities is foundational for materials science in the 21st century. I will discuss ways in which African scientists can begin to participate in this activity starting right away, and present a possible path forward towards greater independence and autonomy in the coming years, with the ultimate goal of an African synchrotron.

I will present an overview of the recently built NSLS-II synchrotron light source at Brookhaven National Laboratory, which will be the world's brightest synchrotron when it reaches full power, and the materials diffractometer, XPD, at that facility.

I will also discuss JUAMI, the Joint US-Africa Materials Institute, which is designed to bring together young African and US-based PhD researchers to learn together how to carry out research on materials, and to develop collaborative research activities. There will be a second JUAMI school in Arusha, Tanzania, in June 2016 focused on materials for sustainable energy. There is the possibility for an AfLS presence at that school.

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International Co-operation

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This presentation discusses the topics of international co-operation and large scale research infrastructures from the point of view of the South African Department of Science and Technology. These matters are considered in the context of the roadmap towards a possible light source in Africa.

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AFRICA

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Africa is the only habitable continent without a synchrotron light source. Many African scientists use facilities abroad. Even though South Africa has become a member of ESRF, the number of users is limited by distance and travel cost. A light source in Africa would give many more African scientists access to this tool. Momentum is now building for an African light source, as a collaboration involving several African countries. An interim Steering Committee has been formed, with a mandate to plan a conference. SESAME, now nearing completion in Jordan, is a collaboration of 9 countries in the Middle East (www.sesame.org.jo) is an example to follow. UNESCO became the umbrella organization for SESAME at its Executive Board 164th session, May 2002, as it did in the case of CERN in the 1950s. UNESCO's Executive Board described SESAME as ``a quintessential UNESCO project combining capacity building with vital peace-building through science'' and ``a model project for other regions.'' It is likely that UNESCO, if asked, would play a similar role as a facilitator for an African light source. An interim Steering Committee has been formed. It is now planning a major conference on November 16-20, 2015 at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France to bring together African, policy makers, and stakeholders.

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Neutron Scattering analysis of the bacterial holotranslocon

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In bacteria, up to 30% of all proteins are translocated into or through the bacterial membrane. This mechanism relies on the trimeric SecYEG (translocon) complex, which forms a pore through the membrane and can open laterally in order to integrate trans-membrane protein into the lipid bilayer1. The energy required to perform the translocation is provided either by the ribosome (co-translational pathway) or the secA ATPase (post-translational pathway)2.
Four additional subunits can join the core translocon :
• Sec D and Sec F favor the translocation by using the proton-motive force3
• YidC, a conserved membrane protein insertase
• YajC, a small protein whose function remains unknown.
This seven-subunit membrane complex is called the holotranslocon (HTL). It is thought to interact with the ribosome and secA and is more efficient for membrane protein integration.
A flexible lipid cavity has been described at the center of the holotranslocon (Botte et al., in revision). We are now investigating its function and dynamic.