

Monday Morning, October 28, 2013

Actinides and Rare Earths Focus Topic

Room: 102 C - Session AC+MI+SA+TF-MoM

Actinides and Rare Earths: Experiment and Electron Correlation

Moderator: T. Durakiewicz, Los Alamos National Laboratory

8:20am AC+MI+SA+TF-MoM1 Our Understanding of the Condensed-Matter Physics of Actinides: What have we Learned in 50 Years?, G. Lander, ITU, Karlsruhe, Germany **INVITED**

By 1950 the Manhattan Project and the early nuclear industry had a large legacy of new materials that were poorly understood from a physics perspective. The physics of uranium and plutonium are good examples.

By the mid-1960s progress had been made in applying many physical techniques (many of which, such as sensitive transducers to measure elastic constants, had also been a development of WW II) on the actinide elements and many of their compounds, particularly the simple dioxides. Most theoretical treatments considered the elements and their metallic compounds within the framework of *d* transition-metals, as many properties seemed to follow these metals, rather than those of the *4f* lanthanide series.

By the mid-1970s the group at Argonne National Laboratory had shown, *inter alia*, that a large orbital moment existed in the actinides even if many properties followed itinerant-electron behavior, and the first band-structure calculations showed how difficult it was to resolve this dichotomy.

The discovery of so-called heavy-fermion superconductors, such as UBe₁₃, at Los Alamos National Laboratory in the early 1980s brought considerable prominence to the field and was a precursor, although not recognized at the time, to the discovery of high-T_c materials in 1986. The further discovery (in 2001) of superconductivity at 18 K in PuCoGa₅, also at Los Alamos, shows the key importance of the electronic ground state of the *5f* electrons and how this drastically affects the physical properties.

Theory has always been “behind” experiments in the actinides; however, the experimental results have proved a sensitive test to the most advanced electronic-structure calculations, such as dynamical mean-field theory (DMFT) within the local-density approximation, so that in some respects the actinides have become a “test bed” for the newest theoretical models.

60 years after some of the pioneering condensed-matter experiments on these materials, we have a far better picture of the actinides, the importance of the orbital moments, the relevance of intermediate coupling, and the criterion that determine whether the *5f* states behave as localized or itinerant. However, we do not have *predictive* theories – they are all *reactive*. This implies that we still need to maintain an experimental capability, as these materials will be with us a very long time, even if we abandon nuclear energy.

The challenge today is how to maintain and nurture that experimental capability in a climate where even depleted uranium is regarded with suspicion and its handling demands kilograms of paperwork? Without experiments will theory follow?

9:00am AC+MI+SA+TF-MoM3 5f Electron Localization, J.L. Smith, Los Alamos National Laboratory **INVITED**

The light actinide elements show a large number of crystal structures and low-melting points. At the element americium, this *5f*-electron series finally settles down and looks like the rare-earth series. This occurs because the *5f* electrons have ceased to form energy bands and have localized. The superconductivity of americium proved this. I will review how the tug of war between itinerant and localized behavior leads to all of the interesting properties and touch on such things as quantum critical points. This has impact on the understanding of the other long rows in the periodic table.

9:40am AC+MI+SA+TF-MoM5 Historical Aspects and Perspectives of X-Ray Spectroscopy in Lanthanide and Actinide Materials, G. Kaindl, Freie Universität Berlin, Germany **INVITED**

The talk addresses some aspects in the use of tunable x-rays in studies of electronic and magnetic properties of lanthanide and actinide materials by x-ray absorption fine-structure (XANES) and resonant elastic x-ray scattering (REXS), emphasizing related features of these *4f* and *5f* materials.

Based on early applications of L- and M-edge XANES to lanthanide valence studies, the method was applied to U and Th compounds, exploring XANES at various thresholds (L, M, N, O) [1], and then to the more

radioactive actinides Np, Pu, and Am as well as to high-pressure studies. Subsequently, the method has been improved both experimentally (e.g. high-resolution XANES [2]) and theoretically [3], and even compounds of Pa, Cm, and Cf in solid and aqueous environments have been investigated by now.

Resonant magnetic x-ray scattering was first applied to Ho metal, where the magnetic scattering cross-section is enhanced by a factor of 50, when the x-ray energy is tuned across the L_{III} absorption edge of Ho [4]. Subsequently, much larger enhancements up to 5 magnitudes were observed at the M_V edges of U in UAs [5] and of Eu in the antiferromagnetic (AFM) semiconductor EuTe [6]. In the latter, an epitaxial thin EuTe(111) film was studied, and virtually background-free magnetic Bragg-peaks with pronounced Laue oscillations were found. From these, the AFM order in the EuTe(111) film could be derived with atomic-layer resolution. The magnetization of the outermost layer was found to decrease significantly stronger with temperature than that of the bulk layer [6]. In a further pioneering experiment that employed a synchrotron slicing source for the production of tunable soft x-rays with pulse widths as short as 100 fs (probe pulses) and synchronized pump pulses of 400 nm wavelength, the dynamics of the AFM order could be studied by fs soft x-ray diffraction [7].

References

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11:00am AC+MI+SA+TF-MoM9 High Energy Resolution X-ray Spectroscopy of f-electron Systems, K.O. Kvashnina, European Synchrotron Radiation Facility (ESRF), France, J.G. Tobin, Lawrence Livermore National Laboratory

This contribution will provide an overview of the possible spectroscopic techniques and experiments that become available for f-electron systems using high energy resolution X-ray emission spectrometer^[1]. As an example we will show the studies of the electronic structure of cerium (Ce) and uranium (U) nanostructured materials by means of high energy resolution fluorescence detection (HERFD) and resonant inelastic X-ray scattering (RIXS) via transitions between core levels and between core and valence levels^[2-5]. The experimental spectral features will be characterized using a variety of theoretical codes including the LDA+*U* approximation within DFT^[6], atomic multiplet theory^[7] and full multiple scattering FEFF^[8].

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11:20am AC+MI+SA+TF-MoM10 Signatures of the γ - α Volume Collapse in Cerium, *M.J. Lipp*, Lawrence Livermore National Laboratory
INVITED

High-pressure x-ray emission measurements of the $L\gamma_1$ (L_2N_4) emission line were used to decide the longstanding debate over the nature of the famous iso-structural (γ - α) volume collapse at 0.75 GPa in elemental cerium that ends in a critical point at 1.5 GPa and 480 K. The satellite structure of this line offers direct access to the total angular momentum observable $\langle J^2 \rangle$ as shown by extended local atomic model calculations and experiences a 30% step-like decrease across the volume collapse. This validates the Kondo model in conjunction with previous measurements of the equation of state at high temperature that were also well fit by the Kondo volume collapse model plus a quasiharmonic representation of the phonons - but could also be reproduced within the Hubbard-Mott framework. The remaining satellite in the α -phase after the volume collapse does not change significantly over the pressure range studied. Direct comparison is made with previous predictions by dynamical mean field theory.

This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 and funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 12-LW-014. Portions of this work were performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA under Award No. DE-NA0001974 and DOE-BES under Award No. DE-FG02-99ER45775, with partial instrumentation funding by NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

Monday Afternoon, October 28, 2013

Actinides and Rare Earths Focus Topic

Room: 102 C - Session AC+MI+SA+TF-MoA

Actinides and Rare Earths: Theory and Electron Correlation

Moderator: L. Havela, Charles University, Czech Republic

2:00pm AC+MI+SA+TF-MoA1 **Structural and Electronic Relationships Between the Lanthanide and Actinide Elements, B. Johansson**, Uppsala University, Sweden **INVITED**

The similarity and difference between the solid state properties of the 4f and 5f transition

metals are pointed out. The heavier 5f elements show properties which have direct

correspondence to the early 4f transition metals, suggesting a localized behaviour of the

5f electrons for those metals. On the other hand, the fact that Pu metal has a 30% lower

volume than its neighbour heavier element, Am, suggests a tremendous difference in the

properties of the 5f electrons for this element relative to the heavier actinides. This change

in behaviour between Pu and Am can be viewed as a Mott transition within the 5f shell

as a function of the atomic number Z. On the metallic 5f side of the Mott transition (i.e.,

early actinides), the elements show most unusual crystal structures, the common feature

being their low symmetry. An analogous behaviour for the lanthanides is found in cerium

metal under compression, where structures typical for the light actinides have been observed

experimentally. A generalized phase diagram for the actinides is shown to contain features

comparable to the individual phase diagram of Ce metal. The crystal structure behaviour of

the lanthanides and heavier actinides is determined by the number of 5d (or 6d) electrons

in the metallic state, since for these elements the f electrons are localized and nonbonding.

For the earlier actinide metals electronic structure calculations – where the 5f orbitals

are treated as part of the valence bands – account very well for the observed ground state

crystal structures. The distorted structures can be understood as Peierls distortions away

from the symmetric bcc structure and originate from strongly bonding 5f electrons occupying

relatively narrow 5f states.

2:40pm AC+MI+SA+TF-MoA3 **Signature of Strong Correlations in Actinides and its Compounds: A Dynamical Mean Field Theory Perspective, G. Kotliar**, Rutgers University **INVITED**

Plutonium is a unique element, poised at the edge of a localization delocalization transition. Its compounds exhibit

remarkable phenomena, ranging from insulating behavior with a topologically non trivial band structure in PuB₆ [1]

to high temperature superconductivity PuCoGa₅ [2].

In the last decade a new paradigm for understanding, modeling and predicting physical properties of these materials

has emerged based on realistic implementations of dynamical mean field theory (DMFT) concepts [3][8] [9]. This theory

treats the wave (band-like) and the (particle-like) multiconfigurational aspects of the f-electrons on the same

footing. This theory accounts for the volume of δ Pu in a paramagnetic configuration [6] and predicted its phonon

spectra [7].

In DMFT, an underlying self consistent impurity model can be used to reconstruct local observables of a material.

An illustrative example is the valence histogram, describing the weight of each atomic configuration in the ground

state of the solid. This important concept, and the resulting prediction for Pu can now be probed experimentally

using resonant XES [5] and neutron form factor measurements [11].

There are now many applications by many groups which have extended the reach of this approach to many actinide

based compounds. We will review the basis of the DMFT approach and compare some results with selected experiments

on 5f electron system. We will conclude with some new directions to face the challenge for material design in this

field [10].

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3:40pm AC+MI+SA+TF-MoA6 **Towards a Better Understanding of Low-Energy Excitations in Heavy-Fermion Systems, G. Zwicknagl**, Technische Universität Braunschweig, Germany **INVITED**

Metals containing lanthanide or actinide ions have been at the focus of interest in condensed matter physics during the past decades. The presence of the partially filled f-shells leads to unexpected "anomalous" behavior such as heavy fermions, unconventional superconductivity, unusual magnetism as well as their co-existence.

The f-electron systems lie at the intersection of a large number of long-standing problems in the physics of metals. In metals containing ions with partially filled inner shells, we immediately face the fundamental question which picture provides the better starting point for theoretical models, a delocalized description in terms of energy bands or a localized representation which accounts for the atomic properties. The answer to the question which of the above-mentioned pictures is the appropriate starting point seems to depend on the physical quantities under consideration. This fact is a consequence of electronic correlations which prevent to describe the influence of the f-states over the entire temperature and energy range in terms of a unique simple model. While the high-temperature (high-energy) properties of lanthanide compounds can be understood in terms of localized f-moments it is generally accepted by now that the f-electrons should also be described in within a band picture as delocalized states as far as the low-energy excitations are concerned.

Concerning the underlying microscopic picture, it is generally accepted that the formation of strongly renormalized 4f-bands in lanthanides is a consequence of the Kondo effect where the degrees of freedom of the 4f-shell form a collective singlet ground state with the conduction electrons. The Kondo model, however, does not apply to actinide compounds where the situation is more complex. In some compounds, experiments suggest the co-existence of both localized atomic-like 5f-degrees of freedom with itinerant 5f-band states at low temperatures/ low energies. Microscopic model calculations suggest that partial localization of 5f-electrons may result from the intra-atomic Hund's rule-type correlations.

In the present talk, I shall give an overview over our present understanding of the "Dual Nature" of f-electrons. I present recent results on the suppression of the Kondo state in YbRh₂Si₂ [1]. I discuss microscopic

calculations for electron spectroscopies in actinide compounds emphasizing the consequences of strong intra-atomic correlations of the 5f-shell [2,3].

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4:20pm **AC+MI+SA+TF-MoA8 Electronic Structure of EuO under Pressure**, *L. Petit, D. Szotek, M. Lueders, W.M. Temmerman*, Daresbury Laboratory, UK, *A. Svane*, Aarhus University, Denmark

We present results of an ab-initio study of EuO under pressure. The calculations are based on a first-principles methodology that adequately describes the dual character of electrons, itinerant versus localized by correcting for the unphysical self-interaction that underpins the local spin density approximation. We find that EuO, which at ambient conditions crystallizes in the NaCl structure, undergoes an isostructural insulator to metal transition around 35 GPa. The transition is associated with a change in the ground state valency configuration from $\text{Eu}^{2+}(f^7)$ to $\text{Eu}^{3+}(f^6)$. At even higher pressure we observe a transition to the CsCl structure. The ground state valency configuration remains Eu^{3+} , i.e. this latter transition is isovalent. We compare our results to a recent experimental investigation that postulates a reentrant valence transition to a nearly divalent Eu^{2+} configuration at high pressures.

Tuesday Afternoon, October 29, 2013

Synchrotron Analysis Focus Topic

Room: 203 C - Session SA+AS+MG+SS-TuA

HAXPES Studies on Interfaces and Buried Layers

Moderator: A. Rossi, University of Cagliari

2:00pm **SA+AS+MG+SS-TuA1 Past and Present of Synchrotron Radiation, from Hard X-ray Photoemission to Soft X-ray and Back, P. Pianetta**, Stanford University **INVITED**

Synchrotron radiation has proven to be a very important tool for the study of materials in applications including earth sciences, energy and semiconductors. Most of the early applications focused on the study of surface phenomena using valence and core level spectroscopies using soft x-rays. Although one of the first studies at a multi-GeV synchrotron used hard x-rays, its practical use was limited by low counting rates. With the advent of high brightness synchrotron sources along with highly efficient electron energy analyzers, x-ray photoelectron spectroscopy using multi-keV x-rays has seen a rebirth for the study of buried interfaces and bulk materials properties. This talk will discuss the evolution of synchrotron radiation photoelectron spectroscopy from the early experiments to the present day.

2:40pm **SA+AS+MG+SS-TuA3 Practical use of Photoemission with Synchrotron Radiation in Nanotechnology: From Soft to Hard X-rays, O.J. Renault, E. Martinez, CEA-LETI, France, N. Barrett, Cea Dsm Iramis Spcsi, France**

Over the past 15 years, due to intrinsic limitations of laboratory X-ray sources, photoemission using synchrotron radiation has played an increasing role in solving issues of technologically-relevant materials and systems. With narrow spectral widths, synchrotron sources enable photoemission at uncomparable effective energy resolutions for refined assessment of chemical states at interfaces [1]. The broad energy range offers ultimate surface sensitivities with soft x-rays [2], and also much deeper photoelectron escape depths in the hard x-ray range which is crucial to investigate buried interfaces intrinsically found in devices. This contribution will highlight the advantages and achievements of hard x-ray photoemission (HAXPES) compared to soft x-ray photoemission, through a selection of recent studies performed on nanotechnological materials and devices (CMOS high-k/metal gate stacks, memory devices) [3]. Finally, we will briefly mention new developments: first, the extension of photoelectron spectroscopy (XPEEM) from chemical state and band structure imaging, to hard x-rays excitation (HAXPEEM) [4]. Second, the application of inelastic background analysis of HAXPES spectra.

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3:00pm **SA+AS+MG+SS-TuA4 Effective Attenuation Length for Titanium Nitride, Hafnium Oxide, Silicon, Silicon Dioxide, Lanthanum Lutetium Oxide, Lanthanum Calcium Manganite, and Gold from 1 keV up to 15 keV, J. Rubio-Zuazo, G.R. Castro**, SpLine Spanish CRG beamline at the European Synchrotron Radiation Facility, France

Material composites, which combine different materials mostly multilayer hetero-structure, with specific and defined properties, are a promising way to create products with specific properties. In these materials the interfaces define many of their properties. The surfaces and interfaces play a fundamental role, and are the source of a great variety of new, and even unexpected, physical phenomena due to the existence of step changes in the structure and the electronic coordination. Third generation synchrotron radiation sources enables the extension of photoemission spectroscopy to higher electron kinetic energies (HAXPES, Hard X-ray Photoelectron Spectroscopy) compensating the decrease of the photoionization cross-section for excitation energies in the hard X-ray region. HAXPES allows the accessibility to buried interfaces and bulk materials due to the dramatic increase of the effective attenuation length (EAL). Electronic, compositional and chemical depth profiles can be then performed in a non-destructive way over the tens-of nanometers scale with nanometer depth resolution. Such an important application of HAXPES is crucial for many condensed matter experiments and requires reliable EALs for high kinetic

energy. EALs are well established for electrons with kinetic energies up to 2 keV. Even if EALs can be obtained by extrapolating well-known formulae, there is a lack of experimental data in the energy range between 1 and 15 keV. In the present study we have determined the EAL dependency on kinetic energy for titanium nitride (TiN), hafnium oxide (HfO₂), silicon (Si), silicon dioxide (SiO₂), lanthanum lutetium oxide (LaLuO₃), lanthanum calcium manganite (La_{0.66}Ca_{0.33}MnO₃), and gold (Au) from 1 keV up to 15 keV. A correlation between the EAL energy dependence and the material density is established. The EALs have been obtained by following either core level peak intensity dependence for a fixed kinetic energy as a function of the overlayer thickness or the core level peak intensity dependence with the photoelectron kinetic energy (i.e. photon energy) for a fixed overlayer thickness. The experimental set-up used is devoted to the combination of X-ray Diffraction (XRD) and HAXPES. Hence, we are able to determine the exact thickness and roughness of the layer from a fit of the X-ray reflectivity (Kiessig fringes) and simultaneously to obtain the EALs from the HAXPES signal evolution. It is important to stress that due to the simultaneous detection of the diffracted and photoemitted signal, the EALs, thickness and roughness determination correspond exactly to the same sample region.

4:00pm **SA+AS+MG+SS-TuA7 Hard X-ray Photoelectron Spectroscopy (HAXPES) Investigations of Electronic Materials and Interfaces, J.C. Woicik**, National Institute of Standards and Technology (NIST) **INVITED**

Photoelectron spectroscopy is a widely used technique that can uniquely measure the chemical and electronic structure of solids. Owing, however, to the historical use of low-energy photons and the resulting limited photoelectron inelastic mean-free path, the technique has found only general application to surfaces and shallow interfaces. With advances in both photon-source and electron-spectrometer instrumentation, hard x-ray photoelectron spectroscopy (HAXPES), where the photon energy is typically in the 2.1 – 10 keV range, has consequently emerged as a powerful tool for studying the bulk and interfacial properties of complex materials systems.

In this talk, we will discuss developments of the HAXPES technique at the NIST beamline X24A at the National Synchrotron Light Source for the study of electronic materials. Examples will include nitrogen treatment of HfO₂ gate stacks on Si, depth profiling of the HfO₂/SiO₂ interfaces, Ga and As “out-diffusion” at semiconductor/oxide interfaces, band offsets and Schottky barrier heights at semiconductor/oxide and diamond/metal interfaces, and oxygen vacancies in N doped TiO₂ and solid-oxide fuel cells. In all cases, the increased probing depth of HAXPES over traditional lab based XPS is crucial to study the electronic structure of entire overlayers and/or buried interfaces with thicknesses of industrial significance.

4:40pm **SA+AS+MG+SS-TuA9 HAXPES Study of Full High-κ/Metal Gate Stacks Deposited on Ge Substrates, C. Fleischmann, I. Kalpyris, T. Conard, C. Adelman, S. Sioncke**, IMEC, Belgium, J.P. Rueff, J. Ablett, Synchrotron SOLEIL, France, W. Vandervorst, IMEC, KU Leuven, Belgium

The introduction of Ge in CMOS devices beyond the 14 nm technology node requires effective passivation of the Ge gate stack. Besides the interface passivation, a highly scaled gate stack is needed for the next generation of CMOS devices. Scaling of the gate stack can be achieved by several means, for instance by changing process conditions. In this work, we investigate the influence of both the high-κ stack and the metal gate on the properties of a GeO_xS_y interfacial passivation layer by Hard X-ray Photoelectron Spectroscopy (HAXPES). Using high energy x-rays (4 to 8 keV), we are able to probe the buried interface between the high-κ layer and the Ge substrate, and hence to reveal direct information on the chemistry and the thickness of the GeO_xS_y passivation layer. Note that such a buried interface is not accessible using a “standard” XPS tool relying on Al K_α x-ray radiation.

In this study, we considered three high-κ materials (Al₂O₃, HfO₂ and an Al₂O₃/HfO₂ bi-layer) and three metal gates (TiN, TiW and Pt). Samples have been measured both directly after atomic layer deposition and after forming gas anneal, to investigate the effect of a thermal treatment on the interfacial properties. To disentangle the impact of the particular metal gate, comparison is made to a high-κ stack sample without metal gate.

We first demonstrate the importance of analyzing full stacks, as no effect of annealing was observed on the stacks without metal gates, while clear modification of the Ge/high-κ interfacial layer thickness is observed when a gate is present. We then show that this effect on interfacial layer thickness depends on both the high-κ and the metal gate material used. This can lead

for example to an increase (i.e. HfO_2/TiN) or to a decrease (i.e. $\text{Al}_2\text{O}_3/\text{TiN}$) of the interfacial layer thickness after annealing. As a global trend, the thinnest interfacial layers are obtained for pure Al_2O_3 . However, the interfacial layer thickness appears to be more sensitive to variations in the metal gate rather than the high- κ material. We also show that the introduction of a very thin Al_2O_3 layer ($\sim 2 \text{ \AA}$) between the Ge substrate and the HfO_2 layer strongly influences this observed sensitivity of the interfacial layer properties to the metal gate and forming gas anneal. Aside from quantifying the interfacial layer thickness, we will also analyze changes in the interfacial layer from a chemical point of view. As a conclusion, the final layer structure (hence, the Equivalent Oxide Thickness of the gate stack) is thus a complex interplay between the initial GeO_xS_y thickness before forming gas anneal and the chemistry of the high- κ and metal gate materials.

5:00pm **SA+AS+MG+SS-TuA10 X-ray Absorption Spectroscopy of Magnetic/Ferroelectric Complex Oxide Interfaces**, *M.B. Holcomb, J. Zhou, D. Chen*, West Virginia University, *C. Jenkins, M.A. Marcus*, Lawrence Berkeley National Laboratory, *Y.-H. Chu*, National Chiao Tung University, Taiwan, Republic of China

Magnetolectric coupling (the electrical control of magnetic properties or vice versa) has promising applications in computer memory and logic, magnetic sensing and energy scavenging. Magnetolectric interfaces are a potential new method to improving magnetolectric coupling strength and controllability. We utilize x-ray absorption spectroscopy, photoemission electron microscopy, and second harmonic generation to understand both the order parameters of the individual layers and the resulting interface. This talk will focus on bilayers composed of ferromagnetic $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) and ferroelectric $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ (PZT). Through photoemission electron microscopy imaging, ME coupling was confirmed at the interface. X-ray absorption spectroscopy of Mn was taken across wedged samples of varying ferroelectric and ferromagnetic thicknesses. The change of Mn valences at different thicknesses of LSMO and PZT helps to understand ME coupling and impact of thickness on the ME properties. This work suggests a strategy for improving not only magnetolectric devices, but also magnetic systems. This work is supported by West Virginia's Higher Education Policy Commission.

5:20pm **SA+AS+MG+SS-TuA11 Local-Structure Determination Using Combined Fitting of EXAFS and Neutron Total Scattering Data**, *I. Levin*, National Institute of Standards and Technology **INVITED**

The functional responses of many industrially-relevant materials are controlled by their *local structure* – a term that refers to the atomic arrangements on a scale ranging from atomic (sub-nanometer) to several nanometers. Today, multiple experimental techniques exist for probing the local atomic order. Nonetheless, finding accurate comprehensive structural solutions still remains a challenge, because any one of the existing methods yields only a partial view of the structure. In this talk, we will discuss recent advances in local-structure determination using simultaneous fitting of EXAFS, X-ray/neutron total scattering, and electron diffuse scattering data. Examples will include several representative perovskite systems that find use as dielectrics and ferroelectrics.

Tuesday Afternoon Poster Sessions

Synchrotron Analysis Focus Topic

Room: Hall B - Session SA-TuP

[3] Hönicke et al., *Anal. Bioanal. Chem.* **396**, 2825 2010

[4] Hermann et al., *Optics Express* **21**, 2913 2013

Synchrotron Analysis Poster Session

SA-TuP1 Mesoscale and Microstructural Changes in HMX Measured with Synchrotron-Based USAXS and Microtomography, T.M. Willey, L. Lauderbach, T.W. van Buuren, I.C. Tran, Lawrence Livermore National Laboratory, **J. Ilavsky,** Argonne National Laboratory, **H.K. Springer,** Lawrence Livermore National Laboratory

HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) is a relatively insensitive high explosive at room temperature. Mesoscale voids are thought to influence sensitivity and detonation properties in polymer bound explosive compositions, where HMX crystals are mixed with, for example, ~5% Viton. HMX molecular crystals undergo a solid-solid phase transition from the so-called beta- to delta- phases at elevated temperatures around 170 Celsius, an prior to this study, little was known about how this phase transition affected mesoscale voids and microstructure. We have measured the ultra-small angle x-ray scattering (USAXS) as the explosive was heated through this phase transition. The USAXS is sensitive to structure from about 10 nm to about 5, and shows how the porosity in these size regimes evolves during the phase change. X-ray computed microtomography was also performed before and after temperature cycling to observe changes on length scales larger than a micron. These results enable studies to determine how the mesoscale porosity affects detonation properties in heated HMX-based explosives.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

SA-TuP4 Grazing Incidence X-ray Fluorescence Analysis for the Characterization of $\text{Ge}_{1-x}\text{Sn}_x$ Thin Films, P. Hönicke, Physikalisch-Technische Bundesanstalt, Germany, **C. Fleischmann,** IMEC, Belgium, **P. Hermann,** Physikalisch-Technische Bundesanstalt, Germany, **S. Zaima,** Nagoya University, Japan, **B. Beckhoff,** Physikalisch-Technische Bundesanstalt, Germany, **O. Nakatsuka,** Nagoya University, Japan

Crystalline GeSn alloys have triggered enormous research efforts in the last decade for future optoelectronic devices. The $\text{Ge}_{1-x}\text{Sn}_x$ material system exhibits a tunable direct energy gap in the composition range $0 < x < 0.15$, enabling its use in light emitting/absorbing components. In addition, GeSn alloys are predicted to show enhanced carrier mobility when compared to elemental Ge, a necessary prerequisite for high-speed semiconductor devices.

The growth of single crystalline GeSn thin films is very challenging due to the limited solubility of Sn in Ge and the large lattice mismatch. Progresses made in the last years using epitaxial growth techniques such as molecular beam epitaxy (MBE), GeSn thin films can be grown with high crystal quality and Sn concentrations above 1 at.% [1]. However, as these films are highly metastable with respect to their equilibrium conditions, sustaining their quality, and hence their electrical and optical properties upon further processing will be as demanding as their growth. As such, the applicability of GeSn in electronic devices will depend on their stability upon e.g. thermal treatment.

We report on the thermal stability of strained GeSn (4-6 at.% Sn) thin films grown by low-temperature MBE on Ge. We discuss degradation mechanisms observed in these layers and the thermal budget that can be derived from this. The samples were characterized using synchrotron-based, reference-free X-ray fluorescence analysis [2] in grazing incidence mode (GIXRF). This technique is based on the in-depth intensity variations within the X-ray Standing Wave (XSW) field which arises between primary and reflected beam. During a GIXRF measurement, the depth distribution of Sn is combined with the intensity distribution of the XSW field, resulting in a distribution specific angular fluorescence curve [3]. This method enables us to gain information about the *in depth* and the *integral changes* of the Sn concentration in the layer.

A relative comparison of GIXRF profiles recorded on pristine and annealed GeSn indicates significant diffusion of Sn and compositional changes in the GeSn layer for high annealing temperatures. Complementary analysis reveal morphological changes on the surface of the annealed films, e.g. the formation of large islands. IR-based scattering type scanning-near-field optical microscopy (s-SNOM) [4] measurements show that these islands exhibit distinctively different optical properties than the GeSn layer.

[1] Shimura et al., *Thin Solid Films* **518** 2010

[2] Beckhoff et al., *Anal. Chem.* **79**, 7873 2007

Wednesday Morning, October 30, 2013

Synchrotron Analysis Focus Topic

Room: 203 C - Session SA+AS+MI+SS-WeM

Synchrotron and Imagery: PEEM, Nano-ARPES and Others (8:00-9:40 am)/Synchrotron TXRF and Related Techniques (10:40 am-12:00 pm)

Moderator: M.C. Asensio, Synchrotron SOLEIL, France, J. Kawai, Kyoto University, Japan

8:00am SA+AS+MI+SS-WeM1 LEEM, PEEM and ARPES Studies of Epitaxial Graphene on SiC(0001), *U. Starke*, Max Planck Institute for Solid State Research, Germany **INVITED**

Large area epitaxial graphene (EG) can be grown on SiC(0001) by heating in Ar atmosphere [1]. However, such graphene layers are *n*-doped due to the influence of a covalently bonded carbon interface layer. This influence can be completely eliminated and the graphene layers be decoupled from the substrate by atomic intercalation. The electronic structure can be tuned in various ways for these decoupled graphene layers. Detailed investigations of the π -band structure, the spatial arrangement, chemical bonding and local surface order are shown based on angle-resolved photoemission spectroscopy (ARPES), low-energy electron microscopy (LEEM), photoemission microscopy (PEEM) combined with microscopic X-ray photoelectron spectroscopy (μ -XPS) and low-energy electron diffraction (μ -LEED), as well as scanning tunneling microscopy (STM) experiments.

By annealing the EG samples in atmospheric H₂, atomic hydrogen reacts under the interface layer, so that the underlying SiC layer becomes passivated [2]. The interface layer alone transforms into a quasi-free standing monolayer while monolayers and bilayers turn into decoupled bilayers and trilayers [3,4]. As a result, charge neutral quasi-free standing graphene layers can be obtained. By intercalation of Germanium the graphene layers can also be decoupled. In this process both *p*- and *n*-doping can be produced, depending on the amount of Ge material intercalated. By preparing both phases in coexistence on the surface, lateral *p-n* junctions can be generated on a mesoscopic scale [5]. Intercalation of Cu induces a coincidence superstructure on top of the SiC surface, which originates from periodic regions of different bond configuration for the carbon atoms in the graphene layer. As a result, a long range periodic potential is imposed onto the graphene layer, which leads to a profound modification of its electronic spectrum. A surprisingly strong doping and the development of mini-Dirac cones are observed [6].

References:

- [1] K.V. Emtsev, et al., Nat. Mater. 8, 203 (2009).
- [2] C. Riedl, C. Coletti, T. Iwasaki, A.A. Zakharov, and U. Starke, Phys. Rev. Lett. 103, 246804 (2009).
- [3] S. Forti, K.V. Emtsev, C. Coletti, A.A. Zakharov, C. Riedl, and U. Starke, Phys. Rev. B 84, 125449 (2011).
- [4] C. Coletti, K.V. Emtsev, A.A. Zakharov, T. Ouisse, D. Chaussende, and U. Starke, Appl. Phys. Lett. 99, 081904 (2011).
- [5] K.V. Emtsev, A.A. Zakharov, C. Coletti, S. Forti, and U. Starke, Phys. Rev. B 84, 125423 (2011).
- [6] K.V. Emtsev, S. Forti, A.A. Zakharov, C. Coletti, and U. Starke, in preparation.

8:40am SA+AS+MI+SS-WeM3 An Imaging NEXAFS Detector for Compositional and Structural Analysis, *C. Weiland*, Synchrotron Research, Inc., *Z. Fu, C. Jaye, D. Fischer*, National Institute of Standards and Technology (NIST), *K. Scammon*, University of Central Florida, *P. Scobol, E. Principe*, Synchrotron Research, Inc.

We present the development of the second generation Large Area Rapid Imaging Analytical Tool (LARIAT MKII) for near edge x-ray absorption fine structure (NEXAFS) surface chemical and structural analysis. This analyzer utilizes magnetostatic electron optical elements to maintain the lateral distribution of electrons into a 16 mega channel detector, while providing a near 180° collection angle for high collection efficiency enabling rapid parallel imaging. A series of electrostatic lenses can be used to tune the energy and depth sensitivity of the imaged electrons allowing for 3D analysis of the near surface region (<7nm). The first LARIAT MKII will be installed on the NIST SST beamline at NSLS II; initial testing is currently being performed at NSLS beamline U8B.

The first generation LARIAT has demonstrated capabilities in determining simultaneously the concentration and orientation of single-strand DNA micro array sensors, organic electronic combinatorial device arrays, and

semifluorinated molecular gradients. Additionally, LARIAT MKI was used to identify cancerous versus non-cancerous dermal tissue through spectroscopic analysis. LARIAT MKII advances these capabilities by improving the lateral resolution of the analyzer to below 7 μ m and improving collection efficiency through a series of gridless electrostatic lenses. Here we will present an overview of LARIAT MKII and its capabilities, as well as some of the initial data recorded from the system.

9:00am SA+AS+MI+SS-WeM4 Recent Advances in High Resolution Real and Reciprocal Space Photoelectron Emission Microscopy, *K. Winkler, B. Kroemker*, Omicron NanoScience, Germany, *N.J. Weber, M. Escher*, FOCUS GmbH, Germany, *N. Barrett*, Cea Dsm Iramis Spesi, France

Conventional electron spectroscopy methods are limited in providing simultaneous real and reciprocal or *k*-space information from small areas under laboratory conditions. Therefore, the characterization of materials with only micron scale sample homogeneity requires new instrumentation. Recent improvements in aberration compensated energy-filtered photoelectron emission microscopy (PEEM) can overcome the known limitations in both synchrotron and laboratory environments.

We present first results from real and reciprocal space photoelectron emission microscopy (PEEM) e.g. on Ag (111) showing high *k* and high energy resolution using a laboratory based He I and II radiation at room temperature and temperatures below 40K. The combination of a recently developed LHe cooled sample stage with an improved aberration compensated energy-filter allows 30 meV energy resolution while a new type of event counting detector improves the signal to noise ratio of the detector.

9:20am SA+AS+MI+SS-WeM5 Quantum Material Spectroscopy Center at the Canadian Light Source, *S. Gorovikov, B. Yates*, Canadian Light Source, *A. Damascelli, H. Davis*, University of British Columbia, Canada, *R. Reiningger*, Advanced Photon Source, *K.I. Blomqvist*, Consultant, *M. Sigrist, S. Chen, E. Hallin*, Canadian Light Source

We report on the concept and design features of the Quantum Material Spectroscopy Center (QMSC), a state-of-the art XUV and soft X-ray beamline facility currently under construction at the Canadian Light Source. The QMSC will operate within the photon energy from 15 to 1200 eV and is intended for spin- and angle-resolved photoemission spectroscopy (SARPES and ARPES).

A distinctive feature of the QMSC is the combination of two independent end stations dedicated to SARPES and ARPES experiments with a unique source consisting of a pair of 4 m long APPLE type undulators. The low- and high-energy undulators will be installed side by side in a switch yard arrangement and will provide the highest possible photon flux within this photon energy range. Complete polarization control in both linear and circular modes will be available. Moreover, the quasiperiodic magnetic structure of the low-energy undulator will result in optimized suppression of the higher order harmonics.

The optical design of the beamline is based on the Variable Line Spacing Plane Grating Monochromator (VLS PGM) design and will deliver 10¹² - 10¹³ photons/second at the experimental stations with a resolving power higher than 10⁴ over the full photon energy range.

The theoretical performance of the beamline will be presented. Research capabilities of the beamline will be illustrated.

9:40am SA+AS+MI+SS-WeM6 Nano-ARPES Beamline at SOLEIL: A Powerful and Innovative Probe for Nanoscience, *M.C. Asensio*, Synchrotron SOLEIL, France

Over the last decades, we have witnessed exponential advances in a wide diversity of new nanotechnologies. These advances, seen particularly in nanoelectronics, nanomagnetism and nanochemistry, among others, affect almost every aspect of our lives. Following the fundamental step in the creation of nano-objects and even if these "building blocks" have shown remarkable properties, they would have remained unexploited if, at the same time, we had not developed new tools capable of analyzing, viewing and scrutinizing objects on a wide range of scales, from a few microns to a few tens of nanometers.

Recently, great progress has been made as a result of the rapid expansion in the range of modern microscopies. However, if they have achieved nanometer spatial resolution, the challenge still remains to provide powerful high-energy-resolution spectroscopic tools for probing nano- and micro-areas. The challenge then, is to quantify and analyze the electronic properties of advanced materials on a nano- and mesoscopic-scale. For such a result, analysis of the electronic structure must be comprehensive, not

only with regard to detection of core levels, but especially to study the structure of electronic states of the valence bands, directly responsible for chemical bonds, electrical transport and the thermal and mechanical properties.

In this presentation, the latest results of the ANTARES microscope beamline at the synchrotron SOLEIL will be disclosed. In particular, nano-ARPES findings describing the electronic band structure of mono-atomic thick graphene films grown on copper substrates by chemical vapor deposition will be presented¹. This end-station, with a spatial resolution of several tens of nanometers, has already been able to carry out direct imaging of core levels, their chemical shifts and the band electronic structures of several ordered materials. High precise Chemical images and valence band information of nano-objects like exfoliated graphene, granular materials and Nanowires will be reported.

1.- J. Avila et al., *Sci. Rep.* 2013, 14, August 3 : 2439 | DOI: 10.1038/srep02439

10:40am **SA+AS+MI+SS-WeM9 Grazing Incidence and Grazing Exit X-ray Spectroscopy of Ultra Shallow Arsenic Implants in Silicon.** *F. Meirer*, Utrecht University, Netherlands **INVITED**

Grazing incidence (GI) and grazing exit (GE) geometries exhibit exotic geometries in x-ray fluorescence (XRF) spectroscopy and are mainly used to restrict the information depth of the analysis to the sample surface. For samples with sufficiently small surface roughness, variation of the angle of incidence within the range of the critical angle of total (external) reflection of x-rays allows obtaining information about the depth distribution of elements within the sample's surface. In total reflection x-ray fluorescence analysis (TXRF) the effect of total reflection is utilized adjusting the measurement angle below the critical angle. TXRF offers excellent detection limits and is routinely used for chemical trace analysis and surface contamination control.

The use of synchrotron radiation (SR) is highly beneficial for TXRF and for angle-dependent XRF in general, because its properties (e.g., high intensity, linear polarization, small source size, and natural collimation) make it ideally matched to the requirements of these techniques. Furthermore, when using SR as x-ray source these methods can be combined with x-ray absorption spectroscopy (XAS) analyzing the local coordinate structure of an element of interest in the sample. This extends XAS to the trace element level (ppb) in samples where only small amounts are available or where the sample is confined in or on the surface of a substrate material.

In this presentation I will review strengths and weaknesses of SR induced TXRF, GI-XRF and GE-XRF and their combination with XAS on the basis of the analysis of state-of-the-art ultra shallow arsenic implants in silicon produced by plasma immersion ion implantation and deposition (PIIID) and subsequent LASER annealing.

11:20am **SA+AS+MI+SS-WeM11 Basic Principles and Applications of Time Resolved Grazing Incidence EXAFS Experiments for Surface Studies in the 50 ms Range.** *D. Lützenkirchen-Hecht, J. Stötzel, O. Müller, R. Frahm*, Bergische Universität Wuppertal, Germany

The surfaces of materials play a decisive role for many fundamental physico-chemical processes such as e.g. aqueous and gaseous corrosion, catalysis, or coating procedures. Many of those processes proceed in non-vacuum environments, so that classical surface analytical techniques like XPS or scanning electron microscopy are not suited for in-situ investigations. Furthermore, all of the above mentioned processes are strongly time dependent, so that fast surface sensitive in-situ probes are necessary to study the respective phenomena. EXAFS can be made surface sensitive by using the grazing incidence geometry: For incidence angles below the critical angle of total reflection, the penetration depth of the X-rays amounts to only some few nanometers, and the reflected X-ray beam only contains information about the near surface region of the studied samples. Here we have combined the grazing incidence geometry with the Quick-scanning EXAFS (QEXAFS) data collection. Recent experimental developments of QEXAFS have substantially improved the time resolution to about 50 ms for a single spectrum, thereby enabling completely new surface science experiments.

In this contribution, we will briefly discuss the experimental setup and present results obtained in-situ during the film deposition by sputtering. The growth of gold and copper thin films on float glass substrates and Si wafers were investigated as examples. We will show that the evolution of the film structure can be followed with a subsecond time resolution, and a detailed modelling of the experimental data using the distorted wave Born approximation yields e.g. the film composition, thickness and roughness as a function of time. First experiments showed the need for an automated analysis, and we will also introduce appropriate software solutions for the processing of huge amounts of data acquired in a typical time resolved experiment with several thousands of spectra. Furthermore, we will also discuss the oxidation of the Cu thin films by their exposure to ambient air at

different temperatures. The results clearly show that the dynamics of the oxidation are strongly depending on the actual temperature of the samples.

11:40am **SA+AS+MI+SS-WeM12 Portable versus Synchrotron TXRF Analysis.** *J. Kawai, Y. Liu, S. Imashuku*, Kyoto University, Japan

Total reflection X-ray fluorescence (TXRF) analysis is a micro (absolute amount is less than pg) and trace (relative concentration is less than ppb) analysis method. When synchrotron X-rays are used, the minimum detection limit becomes down to fg for transition metals. However the synchrotron radiation is an elemental selective method, and thus overall elements are not detectable. On the other hand, synchrotron radiation can eliminate the interference of elements whose analytical lines overlap, such as Ba and Ti, As and Pb. The TXRF spectrometers can be classified into three categories: (i) synchrotron radiation TXRF, (ii) high power X-ray tube (kW) TXRF, and (iii) low power (1-50 W) desk top TXRF. Type (i) achieves highest sensitivity, with WD-TXRF spectrometer (wavelength dispersive), down to fg, however ED (energy dispersive type) is also used, where polarization is additionally used to reduce the scattering of incident X-rays. Type (ii) is used for routine analysis of Si wafer analysis (ISO standard methods), but due to the recent progress of the semiconductor processing, the detection limit is not enough for the advanced semiconductor processing systems. Type (iii) is again classified into monochromatic and non-monochromatic types. Monochromatic type needs 50 W X-ray tube (cooling by fan), but non-mono type is possible only by 1 W X-ray tube. The sensitivity is comparable. Type (iii) is mainly used for environmental analysis, toxic elements analysis, and water quality analysis. We must also consider the sensitivity of elements for mass spectrometry such as SIMS and ICP-MS. These methods are sometimes more sensitive than synchrotron radiation TXRF. Most versatility method is the non-monochromatic X-ray tube (1 W) type portable TXRF spectrometer, by which we can analyze something toxic materials, whether it is truly toxic or not toxic. Several examples which show the ability of the low power TXRF, such as laboratory hazard analysis, will be presented.

Friday Morning, November 1, 2013

Nanoparticle-Liquid Interfaces Focus Topic

Room: 201 B - Session NL+AS+BI+SA-FrM

Emerging Methods to Identify and Measure Nanomaterials in Biological Environments

Moderator: G. Ceccone, European Commission, Joint Research Centre, IHCP, Italy

8:20am **NL+AS+BI+SA-FrM1 3D Views of Hydrated Biological Cells with Soft X-ray Tomography.** *C.A. Larabell*, University of California, San Francisco **INVITED**

SXT is similar in concept to the well-established medical diagnostic technique, computed axial tomography (CAT), except SXT is capable of imaging with a spatial resolution of 50 nm, or better. We examine whole, hydrated cells (between 10-15 μm thick), eliminating the need for time-consuming and potentially artifact-inducing embedding and sectioning procedures. Cells are rapidly frozen then imaged using photons with energies between the K shell absorption edges of carbon (284 eV, $\lambda=4.4$ nm) and oxygen (543 eV, $\lambda=2.3$ nm). In this energy range, photons readily penetrate the aqueous environment while encountering significant absorption from carbon- and nitrogen-containing organic material. Consequently organic material absorbs approximately an order of magnitude more strongly than water, producing a quantifiable natural contrast image of cellular structures. By collecting images from multiple angles through 360 degrees of rotation, SXT reconstructions yield information at isotropic resolution.

Images are formed using unique optics called zone plates (ZP). An X-ray ZP optic consists of a number of concentric nanostructured metal rings, or zones, formed on a thin X-ray transmissive silicon nitride membrane. The width of the outermost ring determines the spatial resolution of the ZP lens, whereas the thickness of the rings determines the focusing efficiency. In our microscope, we use a condenser ZP lens with an overall diameter of 1 cm and an outer zone width of 50 nm. The high-resolution objective ZP lens has a diameter of 63 μm , 618 zones, a focal length of 650 μm at 2.4 nm wavelength, and an outer zone width of 50 nm.

Because SXT is fast (~ 5 min per tomographic data set), we can examine large numbers of cells. Since organic material absorbs approximately an order of magnitude more strongly than water, a unique and quantifiable natural contrast image of cellular structures is generated. X-ray absorption follows Beer's Law, therefore the absorption of photons is linear and a function of the biochemical composition at each point in the cell. As a result, a linear absorption coefficient (LAC) value of each voxel can be calculated. For example, lipid drops with high concentrations of carbon are more highly absorbing ($\text{LAC}=0.7 \text{ mm}^{-1}$) than fluid-filled vesicles ($\text{LAC}=0.2 \text{ mm}^{-1}$). We can determine the position of specific molecules by overlaying fluorescence microscopy signals on cell structures obtained with x-ray imaging. In addition, we can directly determine the locations and numbers of metal probes throughout the cell.

9:20am **NL+AS+BI+SA-FrM4 Ultrathin Electron Transparent Membranes as a Platform for Scanning Electron and Photoelectron Imaging and Spectroscopy of Fully Hydrated Nanoparticles.** *X.M. Ma, J. Geisler-Lee*, Southern Illinois University Carbondale, *M. Amati, L. Gregoratti*, Sincrotrone Trieste, Italy, *S. Guenther*, Technical University Muenchen, Germany, *M. Kiskinova*, Sincrotrone Trieste, Italy, *A. Kolmakov*, Southern Illinois University Carbondale

The increased use of engineered nanoparticles (ENPs) in biomedical applications and their inevitable release into the environment has prompted considerable need to study of their uptake, accumulation and transport inside biological tissue and in plants. This is particularly true for addressing the ENPs fate on a cellular level which inevitably requires the microscopy approach. For long time optical microscopy with the resolution in the order of 100 nm was the major tool available. Better resolution can be readily achieved with traditional transmission (TEM) or scanning (SEM) electron microscopy. However, it requires histological sample treatments such as fixation, staining, dehydration, freezing etc which excludes *in vivo* (*in situ*) modes of observations and can alter their native morphology, functionality and living cycles. Different from standard environmental SEM, where the near sample pressure is limited by ca few tens of Torr, we are actively working on fabrication and tests of electron transparent membranes for ambient pressure electron spectromicroscopy and its application to fully hydrated samples for phytotoxicity, and materials research. Such enclosed environmental cells, equipped with 50-100 nm windows transparent for 10-20 keV electrons, can maintain the sample at atmospheric pressure and/or

fully hydrated. This approach is beneficial compared with dry methods since *in vivo* SEM/TEM observations at nanoscale can be performed. Using this methodology, we were able to image the uptake of silver (Ag) NPs by living Arabidopsis roots on a cellular level. It was shown that NPs with the sizes larger than 20 nm accumulate preferably on the surface of the cellular walls and do not to traverse the plant cell membrane.

Recent developments in high yield fabrication and handling protocols of ultrathin (~ 1 nm) membranes, such as graphene or graphene oxide sheets with thicknesses comparable to the effective attenuation length (EAL) of 200-1000 eV electrons opened the opportunity to perform traditional XPS (X-ray Photoelectron Spectroscopy) and AES (Auger Electron Spectroscopy) at the interfaces between the membrane and fully hydrated samples. Using model water solutions and NPs, we report here on major design principles of such cells as well on first spectral demonstrations, advantages and limitations of this new technique.

9:40am **NL+AS+BI+SA-FrM5 Small-angle X-ray Scattering Investigation of Functional Materials at Inorganic-Macromolecular Interfaces.** *T.W. van Buuren, T.M. Willey, J.R.I. Lee, I.C. Tran, M. Bagge-Hansen*, Lawrence Livermore National Laboratory

Development in nanoscale engineering has enabled bioelectronics that can mimic and/or interact with the biological systems. Lipid bilayer-functionalized Si nanowires are considered as a promising candidate for the construction of bioelectrochemical devices. These biomimetic lipid bilayers serve as a general host matrix for bio-functional components such as membrane proteins. Though meaningful technological advancement of these materials has been made, critical questions about their structural and chemical composition remain. Small angle x-ray scattering (SAXS) experiments are used to investigate the structure of the lipid bilayers on Si nanowires, which provide information on the overall 1-D bilayer structure, the effect of substrate curvature on the lipid packing and local self-organization. The SAXS derived lateral-averaged characterizations are then corroborated with local arrangements of lipid bilayers on Si nanowires revealed by Scanning Transmission X-ray Spectroscopy (STXM). The results provide insights into a number of unresolved questions that are crucial for the comprehensive understanding this class of materials.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Martinez, E.: SA+AS+MG+SS-TuA3, 5
Meirer, F.: SA+AS+MI+SS-WeM9, 9
Müller, O.: SA+AS+MI+SS-WeM11, 9

— N —

Nakatsuka, O.: SA-TuP4, 7

— P —

Petit, L.: AC+MI+SA+TF-MoA8, 4
Pianetta, P.: SA+AS+MG+SS-TuA1, 5
Principe, E.: SA+AS+MI+SS-WeM3, 8

— R —

Reininger, R.: SA+AS+MI+SS-WeM5, 8
Renault, O.J.: SA+AS+MG+SS-TuA3, 5
Rubio-Zuazo, J.: SA+AS+MG+SS-TuA4, 5
Rueff, J.P.: SA+AS+MG+SS-TuA9, 5

— S —

Scammon, K.: SA+AS+MI+SS-WeM3, 8
Scobol, P.: SA+AS+MI+SS-WeM3, 8
Sigrist, M.: SA+AS+MI+SS-WeM5, 8
Sioncke, S.: SA+AS+MG+SS-TuA9, 5
Smith, J.L.: AC+MI+SA+TF-MoM3, 1
Springer, H.K.: SA-TuP1, 7
Starke, U.: SA+AS+MI+SS-WeM1, 8
Stötzel, J.: SA+AS+MI+SS-WeM11, 9
Svane, A.: AC+MI+SA+TF-MoA8, 4
Szotek, D.: AC+MI+SA+TF-MoA8, 4

— T —

Temmerman, W.M.: AC+MI+SA+TF-MoA8, 4
Tobin, J.G.: AC+MI+SA+TF-MoM9, 1
Tran, I.C.: NL+AS+BI+SA-FrM5, 10; SA-TuP1, 7

— V —

van Buuren, T.W.: NL+AS+BI+SA-FrM5, 10; SA-TuP1, 7
Vandervorst, W.: SA+AS+MG+SS-TuA9, 5

— W —

Weber, N.J.: SA+AS+MI+SS-WeM4, 8
Weiland, C.: SA+AS+MI+SS-WeM3, 8
Willey, T.M.: NL+AS+BI+SA-FrM5, 10; SA-TuP1, 7
Winkler, K.: SA+AS+MI+SS-WeM4, 8
Woicik, J.C.: SA+AS+MG+SS-TuA7, 5

— Y —

Yates, B.: SA+AS+MI+SS-WeM5, 8

— Z —

Zaima, S.: SA-TuP4, 7
Zhou, J.: SA+AS+MG+SS-TuA10, 6
Zwicknagl, G.: AC+MI+SA+TF-MoA6, 3