9th MaMaSELF Status Meeting 2017

Report of Contributions

https://indico.psi.ch/e/mamaself.rigi.2017

Contribution ID: **0** Type: **not specified**

Photocatalytic properties of TiO2@Fe3O4 nanocomposite surfaces deposited by combined Langmuir and Atomic Layer Deposition techniques

Thursday, 18 May 2017 08:45 (30 minutes)

Since solar energy is the most abundant and sustainable reservoir of energy on earth, there is a tremendous scientific effort to find an efficient way for it to substitute our strong dependency on fossil energy. This is where photocatalytic reactions such as hydrogen/oxygen evolution reaction (Photo Water Splitting) have shown important improvements and hold great expectation. The efficient conversion solar energy into molecular hydrogen, in a cheap and reliably way, is at the forefront of energy research to this date, demanding the fabrication of competitive and reliable nanomaterials with tunable properties. Titanium dioxide (TiO2) and magnetite (Fe3O4) composites have been previously shown promising results in simple mixtures, although showing poor stability overtime and rapid degradation.
Herein, the study aims to investigate the photocatalytic properties of the synthesized TiO2@Fe3O4 nanocomposites. Magnetite Nanoparticles were deposited by Langmuir technique on ITO substrates, TiO2 coating (3 nm) was deposited by ALD technique. Optical (UV-VIS) and structural (XRD, TEM) studies were carried out in order to assess the quality of the samples, While their photocatalytic performance was studied by cyclic and linear voltammetry (CV/LV) and electrochemical impedance spectroscopy (EIS). As a result, it was observed that the synthesized TiO2@Fe3O4 nanocomposite annealed in nitrogen at 300˚C showed the highest stability over time, as well as a clear decrease on resistance upon its irradiation, allowing efficient photoinduced charge separation and transport to the collecting ITO substrate. Results show the promising aspects of the nanocomposites and the deposition techniques used, clearly showing the importance of thermal annealing on the overall performance of nanocomposites prepared.

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Presenter: Mr BARBÉ, Enzo (MaMaSELF Student)

Session Classification: Student Session

Contribution ID: **1** Type: **not specified**

Industrial Applications and Basic Research with Neutrons at the Heinz Maier Leibnitz Zentrum (MLZ)

Tuesday, 16 May 2017 20:30 (1 hour)

The Heinz Maier-Leibnitz Zentrum (MLZ) is a scientific association of the Technische Universität München (TUM) and some Helmholtz centers (Jülich Centre for Neutron Science, JCNS, and GKSS, Geesthacht) with the participation of various universities (for instance RWTH Aachen University) for studies with neutrons and positrons on hot topics from applied and basic research. The groups involved operate in total about 30 powerful instruments at the research neutron source Heinz Maier-Leibnitz (FRM II) in Garching to explore as many scientific cases as possible in physics, chemistry, biology, materials sciences and earth sciences as well as for medical applications. For the energy and information sector, the characteristics of new ionic conductors, superconductors and magnetic systems are analyzed in detail. The presentation gives an overview of the neutron source itself and some of the available tools and applications there.

Primary author: Dr MEVEN, Martin (RWTH Aachen)

Presenter: Dr MEVEN, Martin (RWTH Aachen)

Session Classification: Lectures

Contribution ID: **2** Type: **not specified**

Trailblazing New Paths: A MaMaSELF Alumna's Story

Thursday, 18 May 2017 21:15 (1 hour)

With the aim to share insights about possible career opportunities for MaMaSELF students, my talk will focus on my personal experiences as an alumna of the program, giving emphasis on my educational background and my current profession.

I will tell you about the path I had taken, from being a MaMaSELF student to being an Experimental Physics doctoral researcher at the Paul Scherrer Institute and the University of Zurich, and about my current job (which is also my first job after PhD) at the Biotechnology Space Support Center (BIOTESC - ESA USOC) and at the Hochschule Luzern (Lucerne University of Applied Sciences and Arts, Switzerland).

I will also highlight the interesting field of study and endeavor that I and my group are involved in, what we do at BIOTESC, my recent and on-going projects at BIOTESC, and some of the future projects that I will be undertaking.

Primary author: Dr PASCUA, Gwendolyne (Biotechnology Space Support Center / Hochschule Luzern)

Presenter: Dr PASCUA, Gwendolyne (Biotechnology Space Support Center / Hochschule Luzern)

Session Classification: Lectures

Contribution ID: **3** Type: **not specified**

Research and Development in the Industry.

Wednesday, 17 May 2017 17:45 (30 minutes)

Kurita Europe GmbH is located in Ludwigshafen, Germany and has more than 500 employees and is operating in Europe, Middle East and frica. It was founded 1989 and is an affiliate of the Kurita Water Industries Ltd with headquarters in Tokio. Founded in 1949 the Kurita group achieved a turnover of ca. 1.8 Billion US-$ with worldwide 5400 employees. The Kurita Group produces chemicals and equipment for water treatment and water purification and provides services to their customers.
Research and development is done both in Japan and Germany in the technical centers. The topics are mainly related to all kinds of phenomena related to water, such as corrosion, scaling, microbiological growth and purification. There are co-operations with universities, research centers and institutes.
A key difference to academic research is the focus on markets and economy and the protection of the know-how (intellectual property) by patents and trademarks. This has also a strong impact on the publishing strategy. Furthermore, time to market is a more critical issue in industry.
The researcher in industry has to have a broad spectrum of capabilities besides his scientific knowledge, just to mention high communication skills and to be able to work in an international environment. Furthermore, legal aspects and salesmanship play an important role in his work. In the ever changing world still an efficient and innovative R&D is a key for the long-term success of the company.

Primary author: Dr HATER, Wolfgang (Kurita Europe GmbH)

Presenter: Dr HATER, Wolfgang (Kurita Europe GmbH)

Session Classification: Lectures

Contribution ID: **4** Type: **not specified**

Structural investigation of two pH-responsive block copolymers using synchrotron-SAXS

Wednesday, 17 May 2017 09:15 (30 minutes)

Multi-responsive polymers have gained a lot of attention, mainly due to the huge array of applications [1] they can be used for, such as sensors, drug delivery systems or tissue engineering. In this work, core-shell micelles with a pH-responsive shell, whose shell blocks undergo a phase transition from expanded to collapsed as a response to changes on the pH, are investigated. At higher concentration, network formation is found, and the phase transition results in strong changes of the mechanical properties [2,3]. Here, we focus on the structural changes.

Two block copolymers were investigated in this work PMMA-b-PDMAEMA-b-PMMA (PMMA and PDMAEMA are poly(methyl methacrylate) and poly[2-(dimethyl amino) ethyl methacrylate]) and PMMA-b-PDMAEMA-b-P2VP-b-PDMAEMA-b-PMMA (where P2VP stands for poly(2-vinylpyridine)). Both block copolymers have similar architectures, ABA and ABCBA, with small hydrophobic blocks A in the outer part of the chain and large pH-responsive blocks B and C in the inner part. While PDMAEMA is a weak polycation, P2VP is a strong one and becomes hydrophobic at high pH values.

To study structural changes under different conditions, solutions of the polymers were prepared in D2O at different concentrations (0.1-1 wt%) and pD values (1, 4 and 7). Synchrotron small-angle X-ray scattering experiments were carried out at the beamline D1 at CHESS to investigate the structure of the micelles.

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[3] G. Gotzamanis, C. Tsitsilianis, S. C. Hadjiyannakou, C. S. Patrickios, Macromolecules, 2006, 39, 678.

Primary author: Mr OLIVEROS COLÓN, Victor (Mamaself)

Co-authors: Dr PAPADAKIS, Christine (TUM); Mr TSITSILIANIS, Constantinos (University of Patras); Dr SMILGIES, Detlef (Cornell University); Mr JUNG, Florian (TUM)

Presenter: Mr OLIVEROS COLÓN, Victor (Mamaself)

Session Classification: Student Session

Contribution ID: **5** Type: **not specified**

Pressure dependence of the crystal and electronic structure of iridium fluorides studied by XRPD and RIXS

Thursday, 18 May 2017 11:45 (30 minutes)

In the last decade, iridium oxides (iridates) have been heavily studied due to their unexpected cor- related behavior induced by the strong spin-orbit coupling (SOC) and crystal field. Their novel ground state arises from the superposition of the Ir outermost orbitals and is often referred to as jeff =1/2 state. Recently, Birol and Haule[1] predicted the realization of similar spin-orbit induced correlated physics in another class of materials namely iridium fluorides. Recent work by Pedersen et al.[2] and Rossi et al.[3] seem to validate this theoretical study by means of x-ray magnetic circular dichroism (XMCD) and resonant inelastic x-ray scattering (RIXS), respectively. The main goal of this thesis is to study the pressure dependence of the electronic ground state of iridium fluorides and its relation with SOC and trigonal distortion which are the two main parameters governing the ground state. The pressure dependence of the electronic states of these compounds was mapped by RIXS measurements, which were performed at beamline ID20 of the European Synchrotron Radiation Facility (ESRF, Grenoble). From these measurements we observe an increasing splitting of the jef f =3/2 excited states, and a shift of the center of mass of these levels. X-ray powder diffraction (XRPD) measurements will later be performed at beamline ID27 of the ESRF to obtain the corresponding pressure dependence of the crystal structure.

Primary author: Ms YAO, YI (University of rennes 1)

Presenter: Ms YAO, YI (University of rennes 1)

Session Classification: Student Session

Contribution ID: **6** Type: **not specified**

Graphene/Ferromagnetic fundamental structures investigated at the atomic level using advanced synchrotron X-ray spectroscopies and STM/AFM scanning microscopy

Thursday, 18 May 2017 13:45 (30 minutes)

Hybrid Graphene/magnetic structures display a variety of physical phenomena and properties such as room-temperature long-spin lifetimes, spin filtering and tunnel magneto-resistance [1-2], which could yield a range of innovative graphene spintronic technologies [3]. In views of developing spintronic devices incorporating FM1/graphene/FM2 systems, assessing the possibility to realize exchange coupled magnetic thin-films across a single graphene layer appears of primary importance. Here we present a XAS and XMCD results investigating the magnetic properties of Co/Gr/Co structures on Ir (111) and Pt (111)/Al2O3 (0001) substrates. We have also pointed out the orbital and spin moments of the intercalated Cobalt layer that were found using sum rules analysis. The hybrid magnetic heterostructures were in-situ fabricated via molecular beam epitaxy (MBE) and using intercalation procedures [4, 5].Our results demonstrate an antiferromagnetic exchange coupling across the Graphene spacing layer in the Co/Gr/Co/Ir (111), in good agreement with a recent theoretical prediction [6] and similarly to our previous results for Co/Gr/Fe/Ir (111) structures [7]. Additionally, early results on the study of the magnetic properties of Co/Gr/Co/Pt/Al2O3 (0001) structures will be discussed. Finally, the presentation will briefly outline the work planned for the next months, which includes: i) the completion of the on-going set-up of two UHV deposition and AFM-STM analysis chambers, ii) the in-situ study by AFM-STM of FM1/Gr/FM2 trilayer structures, iii) the fabrication and investigation of other related hybrid structures on alternative substrates such as Silicon and a stepped single crystal surface.

Primary author: Mr BLEU, Yannick Mexon (University of Montpellier-ALBA Synchrotron Light Facility)

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Presenter: Mr BLEU, Yannick Mexon (University of Montpellier-ALBA Synchrotron Light Facility)

Session Classification: Student Session

Contribution ID: **7** Type: **not specified**

Understanding Mechanical Response Mechanisms of Modern Engineering Alloys

Wednesday, 17 May 2017 14:45 (30 minutes)

Shape memory alloys (SMA) are stimuli-responsive materials which have the ability to return to their original shape and size after induced deformation. Ni-Ti (nitinol) is a SMA which presents several interesting properties for engineering applications, such as shape memory effect (SME) and superelasticity (SE). In both effects, the Ni-Ti deformation occurs by a diffusionless martensitic phase transformation. The name originates from the steel (Fe-C) system, where the transition occurs from austenite (face-centered cubic) phase to martensite (body-centered tetragonal). In the case of nitinol the martensitic transition occurs from a high symmetry, high temperature cubic structure (austenite, B2 type cubic) to a low symmetry, low temperature monoclinic structure (martensite, B19'type).

Superelasticity also called pseudoelasticity is an isothermal property where the deformation or transformation, respectively, is carried out just with applied stress, whereas the shape memory effect can be done in a one-way and/or a two-way mechanism. In one-way SME the alloy has the ability to return to its original shape via a heat treatment. Two-way SME is the ability of the Ni-Ti to "remember"its shape at high and low temperature which can be achieved by the application of thermo-mechanical processing treatment.

For this work in-situ neutron diffraction data from a Ni-Ti alloy as function of temperature was collected at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in Garching, Germany with the high resolution powder diffractometer SPODI. The aim of this research is to analyze the thermal structural changes in the alloy taking processing-induced texture (crystallographic preferred orientation) properly into account by refinement of the data by a new Rietveld software called MAUD.

Primary author: Mr MARTINEZ CORTES, Guillermo (MaMaSELF)

Co-author: Prof. W. SCHMAHL, Wolfgang (LMU)

Presenter: Mr MARTINEZ CORTES, Guillermo (MaMaSELF)

Session Classification: Student Session

Contribution ID: **8** Type: **not specified**

Exploring oxygen diffusion mechanisms of Pr2NiO4+δ as a function of oxygen partial pressure at high temperature via single crystal neutron diffraction

Wednesday, 17 May 2017 14:15 (30 minutes)

The development of new oxide materials for high energy conversion devices continues to be an area of strong interest. Oxides displaying nonstoichiometry due to Oxygen interstitial species have become one of the most promising alternatives in this field of study [1].

The aim of this project is to study the oxygen diffusion mechanisms of Pr2NiO4+δ as a function of the oxygen partial pressure by means of high resolution single crystal neutron diffraction. With this new perspective, one can expect to explore both the structural changes during the orthorhombic to tetragonal phase transition and the superstructure reflections that have been already observed to appear in this compound in previous high brilliance X-ray measurements [2-6].

This will be achieved by realizing comparative studies of the diffraction patterns obtained when increasing the temperature in atmospheric air conditions and after exposing the sample to a vacuum environment, studying the maximum and minimum apical Oxygen displacements. After this measurement, the atmosphere surrounding the sample will be controlled by means of a gas mixture of Argon and Oxygen allowing the study of the oxidation state inside the structure. Finally, pure Oxygen will be introduced to analyze the changes with maximum Oxygen content. Once finished, data refinement methods will be carried out and maximum entropy modelling will be fulfilled thanks to MaxEnt.

Due to the complexity of the experiment, a dedicated furnace has been constructed together with the gas system that will be implemented. Theoretical models have been done using SolidWorks and Comsol software simplifying the whole process. Once the fabrication process was completed, testing and safety procedures were hold in order to be able to perform the experiment.

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Presenter: Mr MAGRO, Fernando (MaMaSELF)

Session Classification: Student Session

Contribution ID: **9** Type: **not specified**

Making Ptychography and CDI comparison

Wednesday, 17 May 2017 08:45 (30 minutes)

In the last decade, coherent X-ray diffraction imaging has become a high resolution lens-less imaging technique for materials characterization. In a number of fields, such as neutron/X-ray/electron diffraction, astronomy, X-ray crystallography and remote sensing, one can measure only the magnitude of the Fourier transform but not its phase which is lost at the detector. The phase problem is normally tackled by using iterative phase retrieval algorithms. This is achieved by projecting back and forth between a real space constraint (ie. Support) and a Fourier space constraint in which we replace the amplitude with measured data. Another technique is Ptychography which allows the sample to be larger than the beam. By scanning the beam relative to the sample, we can reconstruct both the probe function and the sample if there is sufficient overlap area (normally > 60%) between adjacent probes. During this presentation, I will illusrtate some widely used iterative phasing algorithms (eg. Error reduction, Hybrid Input-Output, Difference map)with a Python code which is able to reconstruct a ESRF logo from its diffraction pattern. Then I will present the result of 3D reconstruction of the same gold nanocrystal using both CDI and Ptychography.

Primary author: Mr YANG, Ziye (ESRF)

Presenter: Mr YANG, Ziye (ESRF)

Session Classification: Student Session

Contribution ID: **10** Type: **not specified**

Seeing atoms and electrons in motion

Wednesday, 17 May 2017 11:15 (30 minutes)

Pump-probe electron diffraction and microscopy with ultrashort electron pulses allow directly observing the atoms and charges in motion on their fundamental length and time scales (picometers and femtoseconds/attoseconds). Such imaging is essential for understanding light-matter interaction from a fundamental perspective. My current research group has developed an all-optical control approach for compressing electron pulses to extremely short duration (Science 352, 429, 2016). With such pulses, we succeeded in measuring sub-light-cycle electromagnetic phenomena in photonic device structures (Science 353, 374, 2016). The next step in this endeavor is to establish our electron pulse control ideas into a commercial electron microscope, in order to combine our world-leading experience with ultrashort time resolution with the unprecedented spatial resolution capabilities of a state-of-the-art microscopy device.

This study involves design, simulation, realization and first characterizations of a transmission electron microscope in which the beam is modulated by a coherent laser beam. With this contribution, we will establish a novel type of electron microscopy facility that will for the first time be suitable for sub-cycle imaging of light-matter interaction in space and time.

Primary author: Mr IBRAHIM, Mohamed (Ludwig-Maximilians-Universität)

Presenter: Mr IBRAHIM, Mohamed (Ludwig-Maximilians-Universität)

Session Classification: Student Session

Contribution ID: **11** Type: **not specified**

CVD Growth and Characterization of Atomically Thin Transition Metal Dichalcogenides

Wednesday, 17 May 2017 11:45 (30 minutes)

Monolayer Transition Metal Dichalcogenides (TMDs) has attracted great interest due to its special band structure, very high electronic conductivity, high photoluminescence intensity and spin-valley polarization, which made it good candidate for sensors, energy storage devices, electronic and optoelectronic devices.

Synthesis of controlled, uniform, defect free single domain TMDs is main challenge for in practical application. The property and shape of synthesized TMDs also depends on the synthesis process. Chemical Vapor Deposition (CVD) is commonly accepted synthesis process for high quality and controlled growth TMDs. The temperature, time and pressure of the growth process, precursor (WO3 or MoO3, S) amount, carrier gas (Ar, H2) flow rate, Substrate and its position are important parameter to optimize the growth process for CVD TMDs.

In this presentation I will like to talk about the CVD growth of monolayer TMDs with size 3-50 μm in our lab and how the shape and size of TMDs varies with growth parameters. I will also talk about the characterization of these samples using Optical microscopy, Atomic Force Microscopy and Raman Spectroscopy.

Primary author: Ms BISWAS, Banani (Master student)

Presenter: Ms BISWAS, Banani (Master student)

Session Classification: Student Session

Contribution ID: **12** Type: **not specified**

Use of synchrotron radiation at the University of Helsinki

Thursday, 18 May 2017 17:00 (1 hour)

The history of x-ray physics at University of Helsinki, Finland, dates back to the 1960's when systematic x-ray crystallographic studies were started at the Department of Physics. In the 1970's, x-ray Compton scattering spectroscopy [1] was introduced, then using the home-lab based x-ray sources. Synchrotron radiation use in Helsinki started already in the 1970's since the work of prof. Pekka Suortti (now emeritus) at Brookhaven's National Synchrotron Light Source (NSLS). He worked with synchrotron radiation techniques including designs of beamlines and their application to spectroscopy, x-ray diffraction, including the resonance phenomena, and medical imaging. In the 1980-1990 period many researcher visits were made to Daresbury and HASYLAB as well. In the early 1990's Keijo Hämäläinen (currently vice-rector of University of Helsinki) developed various x-ray scattering spectroscopies at NSLS, and became well known in the field of x-ray spectroscopy from his utilization of resonant x-ray emission spectroscopy to yield much more information on the electronic structure than regular x-ray absorption spectroscopy can yield [2]. The "Hämäläinen method"was based on the recording of resonant x-ray emission peak intensity when incident photon energy is tuned across an x-ray absorption edge. The variations of the intensity could be interpreted as x-ray absorption spectra with an elimination of the deep core-hole lifetime broadening. This is even now a modern tool for x-ray spectroscopy, often called these days as high-energy-resolution fluorescence-detected (HERFD) x-ray absorption spectroscopy [3].

Currently the x-ray and synchrotron science in Helsinki is led by prof. Simo Huotari who is a frequent visitor to, e.g., European Synchrotron Radiation Facility and has specialized in inelastic x-ray scattering spectroscopy and other x-ray spectroscopies.

Some of this history and recent Helsinki research activities in the field of synchrotron as well as home-lab x-ray spectroscopies and imaging will be shown.

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Primary author: Prof. HUOTARI, Simo (University of Helsinki)

Presenter: Prof. HUOTARI, Simo (University of Helsinki)

Session Classification: Lectures

Contribution ID: **13** Type: **not specified**

The Electronic Structure of Mononuclear Manganese Compounds: Insights from Experimental and Theoretical X-ray Absorption Spectroscopy

Thursday, 18 May 2017 16:30 (30 minutes)

As one of the most abundant transition element in earth materials, manganese occurs in different oxidation states and among them, Mn(II), Mn(III), Mn(VI) are the most encountered redox states involved in biochemical process such as photosynthesis. It is a challenging issue to determine the reaction mechanism where the valence of manganese is not straightforward to evaluate with chemistry alone. X-ray absorption spectroscopy (XAS) is an element-specific spectroscopic method that can reflect the electronic structure information of the element. After the absorption of an X-ray photon, a core electron is excited to empty or partially filled orbital which is just below the ionisation threshold, giving an absorption edge. This unique energy provides fingerprint information about the oxidation state, site symmetry, spin state, and crystal field splitting of the targeting materials.

High-Energy Resolution Fluorescence Detected (HERFD) XAS spectra of nine Mn compounds were collected on the ID26 beamline of the ESRF at the temperature of 10 K. In this technique, the emitted energy is tuned to a fluorescence line and the incident energy is scanned through Mn K-edge (6535–6546 eV). The samples present a range of manganese symmetry environments (Oh - octahedral, D4h - distorted octahedral C3v - trigonal bypyramidal), and valences (II, III, and IV).The acquired experimental data was processed using Python codes. The pre-edge features of the XAS are shifted towards higher energy with higher oxidation states, and gain intensity in complexes of lower symmetry.

Theoretical simulations using the Quanty package were conducted to obtain deeper insight of pre-edge features. In this work the Hamiltonian included the Coulomb repulsion, spin-orbit coupling, crystal field splitting, and metal 3d ligand orbital hybridization. For compounds having lower symmetry the calculations were done by considering also the hybridization of the 3d and 4p metal orbitals to study the intensity enhancement observed experimentally. Compared with symmetries that present a center of inversion such as Oh, where only the 1s to 3d quadrupole transitions are allowed, in non-centrosymmetric structures the mixing of 4p character gives rise to a enhancement of the pre-edge intensity thanks to the contribution from 1s to 4p dipole transitions.

Resonant Inelastic X-ray Scattering (RIXS) spectra were also measured for these compounds. The resonance occurs when the incident energy is tuned close to an absorption edge, resulting in an energy transfer reduced to a few eV. By interpreting in terms of a second energy transfer axis, one can find new spectral features and this opens up possibilities for more detailed studies of the electronic structure. Data processing and simulations for RIXS measurements will be done in order to reveal more detailed information about electronic configuration concerned in Mn compounds. It would also be interesting to conduct an ab initio calculation by ORCA package to compare with the results obtained by Quanty.

Primary author: Ms HUANG, Juanjuan (Mamaself)

Presenter: Ms HUANG, Juanjuan (Mamaself)

Session Classification: Student Session

Contribution ID: **14** Type: **not specified**

Ordering mechanism in NiMn-based Heusler alloys

Wednesday, 17 May 2017 13:45 (30 minutes)

The characteristic length scale of the L21 anti-phase domain (APD) structure has been observed to have a significant influence on the magnetic properties of Ni2Mn-based Heusler alloys. Specifically, a small scale APD structure leads to a decrease in ferromagnetic properties. Up to this point, the fundamental mechanism of this relation is not understood. Yet, it is conjectured that either chemical segregation effects at the APD boundary or a magnetic coupling across the boundary play an important role in the observed property degradation. The ideal systems to study this phenomenon are the full-Heusler compounds Ni2MnAl0.5Ga0.5 and Ni2MnAl where the phase transition temperatures and diffusion kinetics allow to adjust a variety of APD dimensions. In the scope of this proposal, we intend to perform small angle neutron scattering experiments on samples from both alloy systems with a range of APD sizes. By recording diffraction patterns at a variety of temperatures in the paramagnetic and ferromagnetic regime, we intend to reveal and distinguish potential segregation and magnetic coupling effects at the APD boundary.

Primary author: Ms CHIU, PINYI (TUM)

Presenter: Ms CHIU, PINYI (TUM)

Session Classification: Student Session

Contribution ID: **16** Type: **not specified**

Nanoporous titania/silica hybrid electrodes for lithium ion batteries

Thursday, 18 May 2017 10:45 (30 minutes)

Light-weight, high energy density, stable and flexible solid-state lithium-ion micro batteries are of great importance due to its applications for miniature medical devices such as capsule endoscopes, implantable heart pumps and biosensors. However low energy density of commercial graphite anodes of lithium ion batteries limit their applications. Titania/silica ultrathin hybrid electrodes with different ratios have been designed aiming to obtain advantages of titania's high charge/discharge rate, stability and good cyclability as well as silica's high gravimetric capacity and low potential vs Li/Li+.

The hybrid electrodes are synthesized by sol-gel method. Simultaneously Polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer (DBC) was applied as a guiding template for production of nanoporous structure, which leads to higher charge/discharge rate. Spin-coating was then applied to obtain ultrathin film and samples were spin coated on silicon wafer and mica window following by calcination to remove DBC. Samples spin-coated on the mica windows are possible to be peeled off from mica window and get free standing ultrathin hybrid electrodes.

The electrodes coated on silicon wafers have been characterized by X-ray diffraction (XRD) and all peaks contributed from silicon, which suggested that the hybrid electrodes are in amorphous state.

Later on scanning electron microscopy (SEM) and small angle X-ray scattering (SAXS) will be applied for further investigation of nanostructure of the hybrid electrodes. Simultaneously the peeling off process needs to be improved to obtain entire electrode films. Finally the electrode will be coated of a layer of gold, assembled into liquid electrolyte lithium batteries and characterized of its capacity and cyclability.

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Session Classification: Student Session

Contribution ID: **17** Type: **not specified**

Characterization of doped GaAs-AlGaAs core-multishell nanowire lasers

Thursday, 18 May 2017 14:15 (30 minutes)

Electrically driven III –V semiconductor nanowires (NWs) are wildly considered to be a potential frontier in small and coherent light sources for photonic integrated circuits. One of most essential characters of semiconductor nanowires is that its active mediums of lasing are surrounding by dielectric shells which forming an innate optical cavity and waveguide due to 1-D geometry. However, for fabrication of electrically driven nanowires laser, there are 4 key factors to be utilized, high carrier density, low contacting resistance, homogeneous etching and carrier confinement in active mediums, respectively. Hence, we are going to develop methods to resolve these 4 topics and achieve electrically driven nanowire lasers.
In this work, the GaAs nanowires with multi-shells structure are grown in silicon (111) substrate using both vapor-liquid-solid and selective area methods by Molecular beam epitaxy (MBE). Then for n-type GaAs nanowires, GaAs nanowires are heavily doped with Si which incorporating on Ga sites and acting as a donor during MBE growth. Similarly, heavily Carbon doped GaAs nanowires function as a p-type semiconductor due to Carbon occupying arsenic sites as an acceptor.
In the first part, the doping concentration is determined by Photoluminescence spectroscopy (PL) and nanowires field effect transistor (NWs-FET). For Photoluminescence spectroscopy (PL), the shape of spectrum is proportional to the occupied states in conduction band (CB) in degenerated semiconductor and the carrier density is deduced from the edge of conduction band (CB), Fermi level (EF) and lattice temperature by fitting Photoluminescence spectra with density of state function. For nanowires field effect transistor (NWs-FET), the top-gate geometry and 4 probes measurement are adopted in measuring carrier mobility and conductivity in nanowires for solving carrier concentration.
In second part, in order for Ohmic contact to n-type GaAs, there are several papers reporting different metallization including Ge/Ni/Au, Co/Ge or AuGe/Ni/Au. Here we perform the good Pd/Ge/Au ohmic contact on n-type GaAs nanowires.
In third part, the simplest structure for electrically driven nanowire laser is p-i-n core-shell structure (p-type core, intrinsic shell and n-type shell respectively) and due to electrically driven purpose, there is a metallic connection on core and shell individually. Thus, it is necessary for us to develop homogeneous etching to metallic contacting on core.
In last part, we will simulate the propagation mode of laser and optimize the thickness of active medium within core-multi-shells structure in nanowires.

Summary

In summary, the study of Photoluminescence spectra show that the highest carrier concentration in n-type GaAs nanowires is n=2.1×10ˆ18 cmˆ-3. Second, the contact resistance on n-type GaAs nanowires is around 10ˆ9 Ω before annealing and 10ˆ3 Ω after annealing. Third, the homogeneous etching is performed by citric acid (CA) and H2O2 solution. And the etching rate of CA/H2O2 solution is 0.2 Å⁄s on GaAs multi-shells nanowire structure.

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Session Classification: Student Session

Contribution ID: **18** Type: **not specified**

Lithium-ion containing block copolymer electrolytes for rechargeable lithium batteries

Thursday, 18 May 2017 11:15 (30 minutes)

Current rechargeable Li-ion batteries are important constituents of portable electronics, stationary grid-energy storage components, and hybrid/electric vehicles. Solid-state polymer electrolytes (SPEs) is one of the most promising candidates for replacing conventional liquid electrolytes, ensuring better safety, higher theoretical storage capacity and longer calendar and cycle life. However, most solid-state polymer electrolytes exhibit lower ionic conductivity at room temperature, this is where this study coming from.
In this study, diblock copolymer (PS-b-PEO), lithium salt (LiTf) and ionic liquid (EMIMTf) are used to composite SPEs, LiFePO4 serves as the active material for the cathode, lithium metal is employed as the anode. In the previous study taken by our group, the relationships between the conductivity performance and the morphology of the ternary hybrid solid-state polymer electrolytes, as well as the crystalline nature of this doped PS-b-PE have been investigated by employing SAXS/WAXS, DSC and impedance measurements for different temperatures and ionic liquid ratios. Whereas the lithium-salt concentration was kept constant at a molecular ratio of [Li]/[EO] = 0.1. The highest ionic conductivity value of 1.710−3 S/cm at room temperature was found with a ratio of [IL]/[EO] = 0.3, which is very competitive with other systems like high ionic conductivity gel-like electrolytes. Complete Li/SPE/LiFeO4 batteries were then assembled in an argon glovebox as my work. Hereafter, DC electrochemical measurements were performed, wherein, current, voltage, capacity, and energy were collected.
The follow up works include optimising the hand made full cell to achieve a more stable cycling performance, from where the in situ SAXS/WAXS can be carried out for the investigation of the morphology changing during cells charging and discharging.

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Session Classification: Student Session

Contribution ID: **19** Type: **not specified**

Fabrication of LaMnO3 epitaxial films via electron beam physical vapor deposition

Wednesday, 17 May 2017 10:45 (30 minutes)

The fabrication of ReBa2Cu3O7-δ (Re: rare earth element) (ReBCO) high temperature superconductor (HTS) based coated conductors requires development of intermediate layers between a metal tape and a superconductor which are called buffer layers. These buffer layers have to fulfill a list of requirements among which are chemical stability and compatibility with adjacent films. Inclined substrate deposited MgO and cap layer MgO are used as incident buffer layers, because they create a biaxial texture on metal substrate for growth of oriented HTS film and serve as a diffusion barrier for harmful substrate elements, respectively. However, MgO is a hygroscopic material and has high lattice misfit with ReBCO, which reasons limitations in superconducting properties such as critical temperature and critical current density. LaMnO3 (LMO) is a perspective candidate as a terminal buffer layer because of its good chemical stability with MgO and low lattice misfit with ReBCO which provides good template for HTS growth.

In this study, electron beam physical vapor deposition technique is adopted to deposit LMO on MgO film. LMO was evaporated at different substrate temperatures and O2 gas/H2O vapor flows in addition to varied layer thicknesses in order to optimize LMO film quality. Surface morphology of the films were observed using field emission - scanning electron microscopy and so far some samples were structurally and compositionally investigated using x-ray diffraction and inductively coupled plasma - atomic emission spectroscopy, respectively. Several samples with LMO layer were already deposited with DyBCO, and also critical temperature and critical current density were measured to figure out the growth quality of HTS layer on the buffer layer.

In the future work, the influences of powder particle size, deposition rate and film stoichiometry on LMO layer quality and superconductivity properties will be investigated. In plane and out of plane texture measurements of LMO layer will be done and pole figures will be plotted. Finally, reproducibility experiments will be conducted using the optimal deposition parameters.

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Session Classification: Student Session

Contribution ID: **20** Type: **not specified**

Processing and characterization of diamond nanocrystals for applications in biosensing

Thursday, 18 May 2017 09:45 (30 minutes)

Due to its unique physical properties (transparency, bio-compatibility, chemical inertness, availability of stable luminescent centers, etc.), artificial diamond is a promising material for applications in cellular biosensing. In particular, nanometer-sized diamond crystals offer unique opportunities for optical labeling and drug delivery in living cells, due to their low toxicity.

The samples in this thesis work are produced through either detonation or fragmentation of samples grown by HTHP synthesis, with particle size ranging between 5 nm and 1 μm. Thermal processing techniques are applied to graphitize the amorphous carbon component, which is then removed by a subsequent etching process.

The optical labeling properties of the nanocrystals are based on the Nitrogen-Vacancy defect, which can be introduced in the lattice by means of ion-beam-induced damaging. The samples were implanted with a 2MeV H+ ion broad beam at the accelerator facility of the INFN Legnaro National Laboratories.

The characterization of the structural modification on the nanoparticles was carried out through Diffuse Reflectance Infrared Fourier Transform and Raman spectroscopies during each step of the processing. SEM imaging provided an estimation on the size of the nanodiamonds.

Subsequently both cellular imaging and (possibly) drug delivery will be explored as a final goal of the activity.

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Presenter: Ms MARTINEZ CANTU, Brenda Berenice (Student)

Session Classification: Student Session

Contribution ID: **21** Type: **not specified**

Microstructural and electrical characterization of superconducting MgB2 thick films produced by aerosol deposition technology

Wednesday, 17 May 2017 09:45 (30 minutes)

The project consists of producing superconducting magnesium diboride (MgB2) thick films deposited by special film formation process called aerosol deposition method. They will be used in power generators of wind turbines. Within the project, MgB2 layers are formed on various substrates like metal or glass. The focus is on two problems about MgB2 production using aerosol deposition method. First challenge is the high affinity of magnesium to oxygen. The second is low connectivity and porosity. The former makes it hard to manufacture MgB2 without MgO formation even if high purity boron, magnesium and protective atmosphere are used. The latter leads to poor superconducting current density (Jc) and risks the reproducibility, as varied Tc and Jc are obtained even under the same conditions.

For high quality film formation, powder treatment is one success factor. As-received powder is milled under different parameters, x-rayed and scanned under SEM to get the required analytics. The prepared powder are dispersed in dry gases and accelerated into vacuum to form a layer on the substrates, where a dense nanograined film is deposited. Several analysis techniques like SEM, FIB-SEM and EDX are used for the analytics of the microstructure of deposited films. Electrical measurements including conductivity, critical current density and critical temperature are done to determine the electrical and superconducting properties. Methods to combine microstructural and electrical properties of approximately 5µm thick superconducting layers are researched.

For future work, after deposition under different parameters, the grain connectivity inside the structure will be investigated with the aim of looking on improvement of it by porosity and crack reduction in the structure as well as MgO content reduction and distribution. Delta resistivity measurements under cryogenic temperatures will also be used to investigate the grain connectivity.

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Session Classification: Student Session

Contribution ID: **22** Type: **not specified**

Ultrafast photo-induced dynamics in bi-stable charge transfer materials.

Thursday, 18 May 2017 09:15 (30 minutes)

Charge transfer materials are bi-stable systems where an external stimulus that can be provided by temperature, pressure or light is capable to induce an electron transfer between two metallic atoms. The resulting change in the electronic configuration can alter the electrical, magnetic and optical properties of these materials. The use of light to trigger these changes is particularly interesting from the point of view of both fundamental science and practical applications.
In this thesis optical pump probe spectroscopy is used to study the dynamics of the charge transfer in various systems. The sample is excited using a laser pulse (pump) and the resulting change in the optical signature is measured by another pulse at a different energy (probe). By changing the optical path of one of the lasers it is possible to introduce a variable time delay between the two and thus measure the evolution of the optical properties of the sample with a time resolution in the order of hundreds of femtoseconds. By changing the pump's energy it is possible to target different absorption bands in the sample and reach different excited states; this can lead to a change in the time evolution of the system's relaxation.
Further developments for the project will include a more thorough investigation of different charge transfer materials in order to study their response as function of the excitation energy and time.

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Session Classification: Student Session

Contribution ID: **23** Type: **not specified**

XANES and EXAFS analysis of LixMn2O4 as thin-film cathode material for lithium-ion batteries

Thursday, 18 May 2017 14:45 (30 minutes)

Owing to their light weight and high energy density, lithium-ion batteries (LIBs) are currently the method of choice for energy storage for numerous applications and are dominating the rechargeable batteries market. However, it is well accepted that the interfaces of the LIBs electrode materials are the source of problems in terms of capacity fading and safety. Atomic layer deposition (ALD) is considered as great technique to address these shortcomings, allowing the production of highly uniform and conformal films with an accurate thickness and growth control at the sub-Å level, making it an enabling technology for 3D all-solid state thin-film LIBs. Among the available cathode materials for these batteries, lithium manganate spinel is a promising candidate due to its low cost, low toxicity, high voltage, high specific capacity for storage of electrochemical energy, and minimal structural changes during charge/discharge cycling. In the present study, thin films of LiXMn2O4 spinel with different level of lithiation were produced by means of ALD. The synthesis process consisted of the deposition of a 100-nm MnO2 parent oxide film on a Si wafer that was subsequently lithiated using a precursor of lithium tert-butoxide and water (LiOt Bu +H2O). To gain fundamental understanding of this lithiation process, the atomic structure of this material was investigated by means of XAS at the CLÆSS beamline from the ALBA synchrotron radiation facility. Signals were collected at the Mn-K edge (6.5 keV) simultaneously in TFY (total fluorescence yield) and TEY (total electron yield) modes. From the XANES region, it was demonstrated that the Mn oxidation state decreases as a function of lithitation cycles, while from the EXAFS analysis, it was shown that there are not corner-sharing octahedral in the spinel cathode material in comparison to the parent oxide MnO2 with rutile structure. Further analysis and interpretation are under way, specially focused on polarization and strain studies (in-plane and out-plane-bond distances and strains).

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Session Classification: Student Session

Contribution ID: **24** Type: **not specified**

Thermodynamics seen through a diffraction experiment

Wednesday, 17 May 2017 18:15 (30 minutes)

Crystallography and diffraction experiments with bright radiation sources offer much more that a structure solution and refinement. Structural data collected as function of pressure, temperature, electric or magnetic field, under laser radiation or in any other in-situ conditions provide with a unique information on the thermodynamics of various processes in solids. In the lecture I illustrate this statement with diffraction probes of phase transitions and Landau thermodynamics, with estimates of relative stability of different polymorphs based on atomic displacement parameters, and with a special focus on thermodynamic of gas adsorption by porous solids seen through a diffraction experiment.

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Session Classification: Lectures