AOFKA 2023

21st Conference on Applied Surface and Solids Analysis

«Shine a Light Between Surface and Bulk»

Insightful Data with Light-Sample-Interaction

ETH Zurich – Campus Hönggerberg
11. – 13. September 2023
Program and Abstracts

AOFKA

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21st AOFKA 2023

«Shine a Light Between Surface and Bulk»
Insightful Data with Light-Sample Interaction

ETH Zurich , 11. - 13. September 2023

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Event Endorsement

Division Analytical Chemistry (Swiss Chemical Society)
Haus der Akademien, Laupenstrasse 7, Postfach
3001 Bern
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Conference Venue

ETH Zurich, Campus Hönggerberg
HIL-Building
Stefano- Franscini, Platz 5, 8049 Zürich
8092 Zurich
Switzerland
https://ethz.ch/en/campus/erreichen/hoenggerberg.html

Car Parking

Parking charges at ETH are not included in the fee 24/7-Parking spaces are available in the underground garage on the Hönggerberg campus. You can reach the parking area following the signs from Emil-Klötli-Strasse. See also map below. You are responsible for a valid ticket.

Public Transportation

If you arrive from Zurich airport you will require a ticket valid for 3 zones.

If you are travelling by public transport in Zurich City at least twice a day, it is worth buying a day pass (valid for 24 hours).

Walking into ETH Hönggerberg is uphill from all directions.

You can reach ETH Hönggerberg with public transport by bus from four directions:

- From **Zurich Oerlikon** train station. Take the bus 80 from Oerlikon-Nord bus station in the direction of Triemlispital to "ETH Hönggerberg"
- From **Milchbuck** or **Bucheggplatz**, take the bus 69 in the direction of "ETH Hönggerberg" until the end of the line
- From **Zurich Altstetten** train station or **Meierhofplatz**, take the bus 80 in the direction of Oerlikon to "ETH Hönggerberg"
- From **Zurich Affoltern** train station take the bus 37 (every 30 min) to "ETH Hönggerberg"

During the day, busses leave every 7 minutes from Hönggerberg and there is a regular service until approx. midnight, see below.

Live Departure Timetable from ETH Hönggerberg:

Further information, prices and timetables of Zurich public transport: www.zvv.ch

Further information on Swiss public transport: www.sbb.ch

Networking Events

Lunch

With the badge, you receive lunch vouchers, which are valid **only at "Food Market"** on ETH campus (HPH building see campus map). The Food Market offers a wide range of options, sorted into "Grill & BBQ", "Green Day", "Pizza & Pasta". Click on the links below to check out the daily menus (in German). You will find the menu in English at the entrance.

Grill & BBQ (dishes with meat)

Green Day (vegetarian and vegan dishes)

Pizza & Pasta

If you like to enjoy other catering facilities during the conference, the campus offers a variety of options. Those include a small grocery shop and a bistro (HPI building), a café which also offers different lunch options (HCI building), a bar (HIL building, below the conference area) and an Asia style canteen (HIT building). Opening hours may vary due to the semester break during the conference.

Conference Dinner

The AOFKA Dinner is included in the registration fee. It will be held *at the Restaurant Bellavista (on Campus)* as a *flying service* to enable as much discussion and interaction between the AOFKA participants. It takes place on Tuesday from 19.00 at Bellavista Restaurant at Hönggerberg Campus. Take your badge with you.

Discussion Forums

Two panel discussions gather experts from academia and industry to debate hot topics. The feedback from the participants is welcome. The forums are:

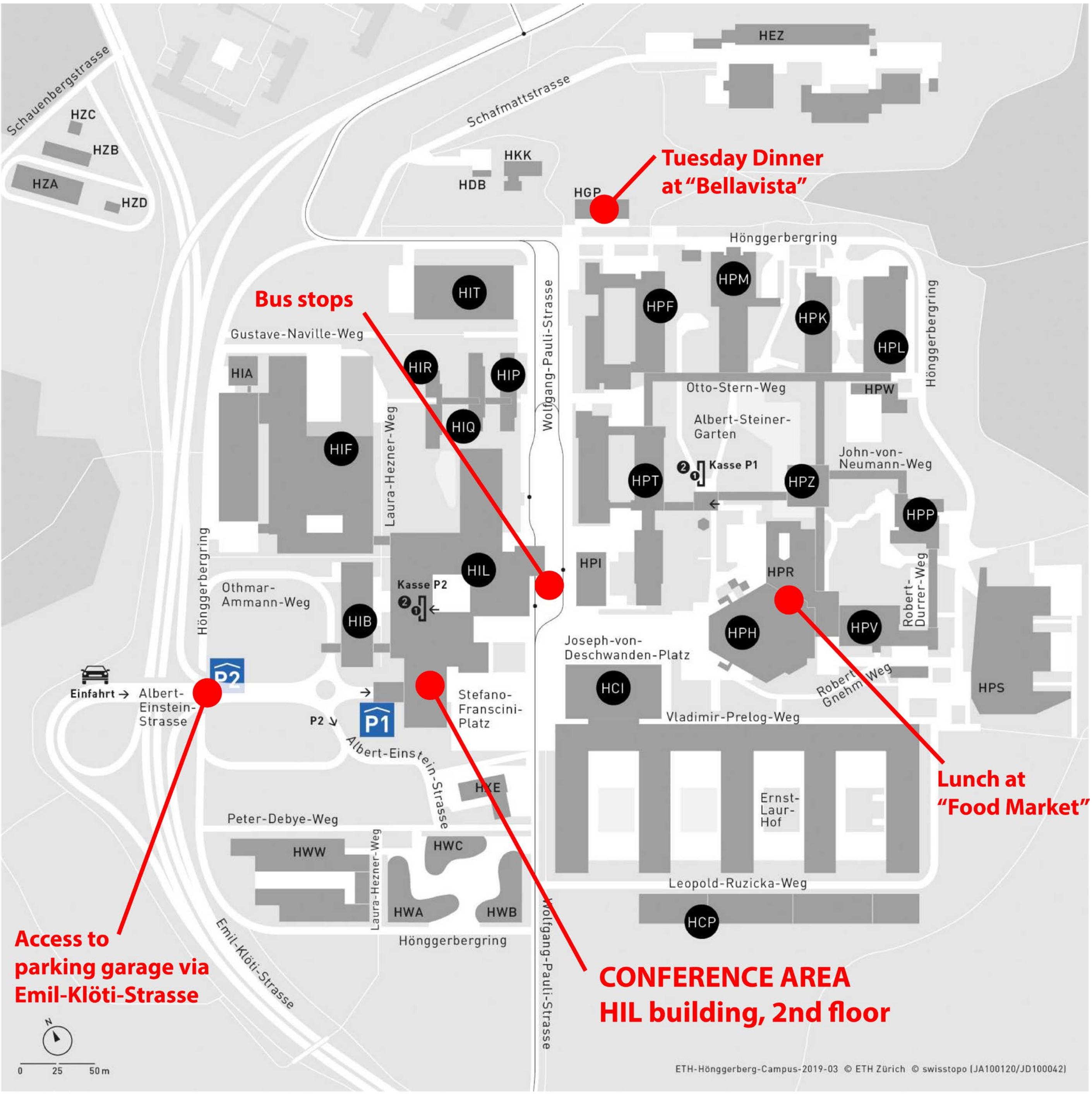
- Analytics in the industry (Monday 11/9 at 14:00 in room E4)
- Teaching Solid Analysis (Tuesday 11/9 at 14:00 in room E4)

Lab Tours

Three Lab Tours are offered on Wednesday after Lunch. The participants should register for one. The lab tours are:

1. Electron Microscopy Center of the ETH Zürich (ScopeM)
2. Zenobi Group, with highlight on organic mass spectrometry and TERS
3. Günther Group, with highlight on elemental microanalysis with LA-ICP-MS

Map Campus Hönggerberg



Tuesday Dinner at "Bellavista"

Bus stops

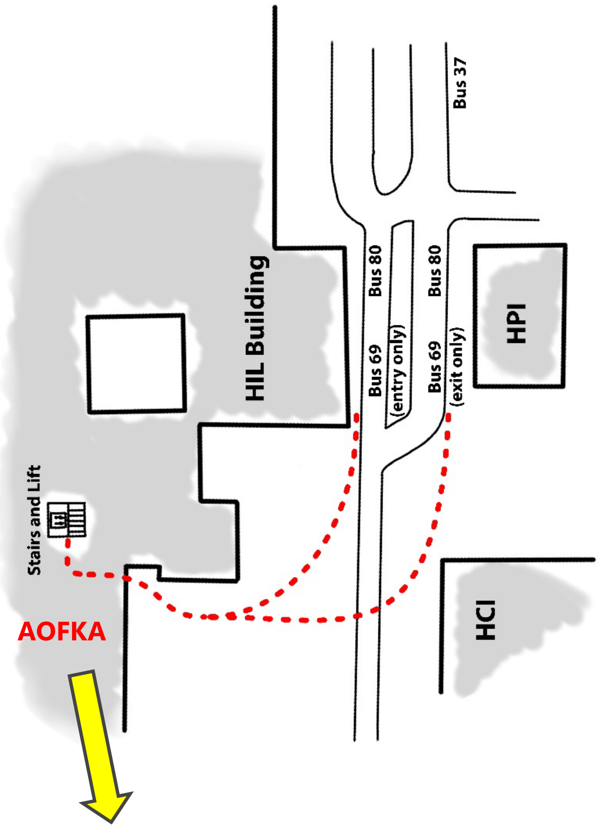
Lunch at "Food Market"

Access to parking garage via Emil-Klöti-Strasse

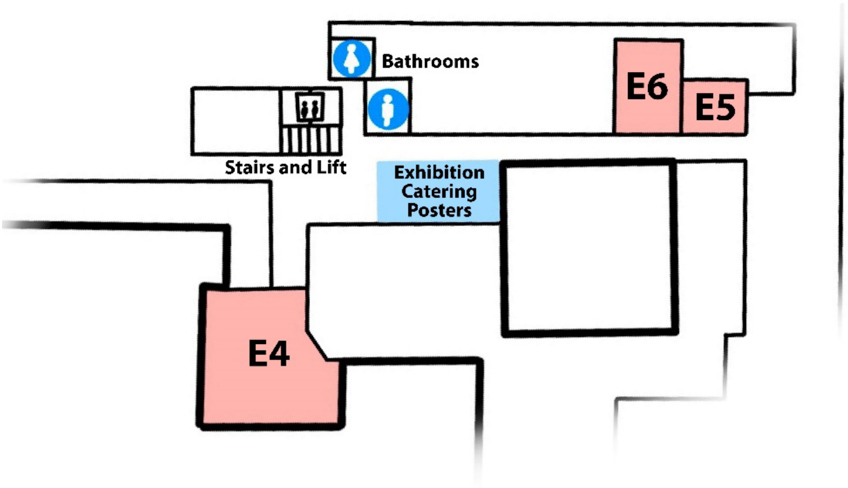
CONFERENCE AREA
HIL building, 2nd floor

Detailed Maps for the AOFKA Neighborhood

AOFKA is in the HIL Building (E Floor). Next to the Bus Stop in the Campus



Schematic map of the lecture halls location (E Floor inside HIL)



Invited Speakers

Dr. Mikhail Agrachev, ETH Zurich
Prof. Gian-Luca Bona, ETHZ & EPFL, Empa CEO 2009-2022
Prof. Alessandro De Giacomo, Uni Bari
Prof. Rolf Erni, Empa
Prof. Ian Gilmore, NPL London
Dr. Daniel Grolimund, PSI
PD Dr Sigve Haug, University of Bern / Einstein Museum
Dr. Vasile-Dan Hodoroaba, BAM Berlin
Prof. Rebecca Ingle, UCL
Prof. Uwe Karst, Uni Münster
Dr. Christine Müller-Renno, TU Kaiserlautern
Prof. Astrid Pundt, KIT
Dr. Arno Schintlmeister, Uni Vienna
Prof. Alexander Shengelaya, Ivane Javakhishvili Tbilisi State University
Prof. Roland Wiesendanger, Uni Hamburg

List of Short Courses

1	Andreas Borgschulte	Electrons and molecules at interfaces - a love affair
2	V. Merk, A. Winckelmann, T. Langner, T. Sieber, A. Rietig, J. Acker, C. Abad and L. Pfeifer	What can we learn about lithium-ion battery materials from the combination of LIBS and Raman?
3	Fabio La Mattina	Spin as a Spy: Investigating Material Properties through Electron Paramagnetic Resonance (EPR)
4	Naresh Kumar	Surface Raman

List of Posters

1	Alessia Cesarini, Marin Nikolic, Pavel Trtik, Jeroen A. van Bokhoven, Andreas Borgschulte	Combinatorial neutron imaging for in-situ alkane adsorption analysis over C1-C4 coupling catalysts
2	Tamás Fodora, Viktor Takátsa, József Hakla, Sándor Molnára, Márton Sohaa, Attila Csíka, Zoltán T. Gaála, Zoltán Halásza, István Rajtaa, Márton Benkeb, Kálmán Vada	Boride layers prepared on iron surfaces by ion implantation
3	Swen Ehnert, Michael Wahl and Michael Kopnarski	The Surface Inspection Pad (SIP) for non-destructive and in-process surface analysis of components
4	S. Molnar, V. Takats, E. Bodnar, T. Fodor, J. Hakl, M. Soha, K. Vad	Investigation of Si island formation through Cu grain boundaries by SPM and SEM methods
5	Marin Nikolic Alessia Cesarini Pavel Trtik Andreas Borgschulte	Neutron insights into nickel metal hydride batteries
6	Johannes D. Pedarnig N. Giannakaris M. Niebauer R. Kleštinec , G. Gürtler and T. Stehrer	Surface Cleaning with Atmospheric Pressure Plasma Jets investigated by Optical Emission Spectroscopy and LIBS
7	Maximilian Podsednik, Maximilian Weiss, Silvia Larisegger, Michael Nelhiebel, Andreas Limbeck	Improved online-laser ablation of solids in liquids (LASIL) cell design: the stethoscope cell
8	Sharath Rameshbabu, Davide Bleiner	Pulsed Laser Deposition of "Röntgen Nano Films"
9	Billy Salgado, Sven Passlack, Swen Ehnert, Michael Kopnarski	Quantitative Analysis of the Hydrogen Concentration on Surfaces using SNMS
10	Martin Arndt	Characterization of the formation of the Zn/Fe intermetallic phases at the surface of 2 galvannealed steels with different Si concentrations
11	Zuqiang Xu, Bodo Hattendorf, Detlef Günther	fs-LA-ICPMS for high throughput analysis
12	R. Hesse, R. Denecke	UNIFIT 2023/UNIFIT 2024 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy
13	Michał Góra, Paula Navascués, Urs Schütz, Dirk Hegemann, Manfred Heuberger	Surfaces forces on nano-porous materials

Detailed Oral Program (by day)

	Monday 11 September		
Room	**ETH HIL E4 Auditorium**	**ETH HIL E5**	**ETH HIL E6**
8:30	Registration		
9:00	**Welcome Opening**		
	Davide Bleiner Gernot Friedbacher		
9:30	**Gianluca Bona (K), ETHZ, EPFL, Empa**		
	Analytics - understanding materials		
10:00	**Sigve Haug (K)**		
	On the photoelectric effect and its contribution to a successful divorce of a prominent marriage		
10:30	Morning Break		
11:00	**Chair Gernot Friedbacher** **Detlef Günther (I)**		
	Laser Ablation-Inductively Coupled Plasma Mass Spectrometry – Mature and Widely Applied		
11:30	**Technology Lectures** Thermo-Fisher LTB		
12:00	**Haider Butt**		
	Multimaterial 3D Printed Smart Contact Lenses		
12:20	**Filippo Longo**		
	Giant magneto-electrocatalytic effect in Ni-based electrodes		
12:40	**Maximilian Podsednik**		
	Improved online-laser ablation of solids in liquids (LASIL) cell design: the stethoscope cell		
13:00	Lunch		
14:00	**Forum 1/ Analytics for Industry** **Lars Sommerhäuser**	**Short Course** **Electrons and molecules at interfaces** Andreas Borgschulte	**Short Course** **Raman LIBS** Virginia Merk
15:00	**Chair Renato Zenobi** **Ian Gilmore (I), National Physical Laboratory**		
	A “molecular uncertainty principle” – can we simultaneously identify and localize molecules with high confidence?		
15:30	**Matea Krmpotić**		
	MeV SIMS as an emerging nuclear analytical technique for surface analysis of paint materials in cultural heritage		
15:50	**Nguyen T. N. Ha**		
	Magnetization switching on self-assembled structure of alpha-helix-polyalanine molecules observed by ambient STM		
16:10	**Viktor Takáts**		
	Diffusion coefficient measurement by LEIS in Cu/Si grain boundary systems		
16:30	Afternoon Break		
17:00	**Chair Detlef Günther** **Uwe Karst (I), Uni Münster**		
	Multimodal Elemental and Molecular Bioimaging for Tissue Analysis		
17:30	**Christine Müller-Renno (I)**		
	Fluid-FM – a versatile method in biomaterials research		
18:00	Apero + Poster		
19:00			
20:00	AOFKA Board		

	Tuesday 12 September		
Room	**ETH HIL E4 Auditorium**	**ETH HIL E5**	**ETH HIL E6**
8:30	Registration		
9:00	Chair Michael Kopnarski **Roland Wiesendanger (K)**		
	Magnetic-sensitive Atomic-scale Surface Analysis by Spin-Polarized Scanning Tunneling Microscopy and Spectroscopy		
9:30	**Vasile-Dan Hodoroaba (I)**		
	Correlative Analysis of Nanostructured Materials		
10:00	**Werner Goedel (I)**		
	Atomic Layer Deposition of protective coatings onto Bundles of Technical Fibres		
10:30	Morning Break		
11:00	Chair Gunnar Schwarz **Alessandro De Giacomo (I)**		
	Nanoparticle-Enhanced Laser Induced Breakdown Spectroscopy		
11:30	**Technology Lectures** Bruker Prevac		
12:00	**Laura Kronlachner**		
	Further developments in sample preparation strategies for nanoparticles analysis		
12:20	**Salome Gruchola**		
	Implementations and Applications of Laser Ablation and Ionisation Mass Spectrometry for Earth and Space based Research		
12:40	**Nikita Boeren**		
	Laser Desorption Ionisation Mass Spectrometry for in situ Molecular Biosignature Detection		
13:00	Lunch		
14:00	**Forum 2/ Teaching Solid Analysis** **Gunnar Schwarz**	**Short Course** **Electron Spin Resonance Spectroscopy** Fabio La Mattina	**Short Course** **Surface Raman** Naresh Kumar
15:00	Chair Andreas Borgschulte **Astrid Pundt (I)**		
	Hydrogen in thin films: controlling stress release paths by microstructure and size		
15:30	**Reinhard Denecke (I)**		
	Insights into the structural modification of electrochemically synthesized layered double hydroxides by X-ray photoelectron spectroscopy		
15:50	**Benedikt Wolfsjäger**		
	Reduction of iron oxides as indirect hydrogen detection method in XPS		
16:10	**Tobias Berger**		
	Unlocking the Mystery of Catalytic Design for Methanol Steam Reforming		
16:30	Afternoon Break		
17:00	Chair Fabio La Mattina **Alexander Shengelaya (K)**		
	Solid-State Electron Paramagnetic Resonance Spectroscopy		
17:30	**Michail Agrachev (I)**		
	EPR spectroscopy in heterogeneous catalysis: combining in-situ and ex-situ approaches		
18:00	**Lars Jeurgens**		
	Chemical state analysis of functional oxide thin films by combining soft and hard X–ray Photoelectron Spectroscopy		
19:00	**AOFKA Gala Dinner**		
20:00			

Wednesday 13 September

Room	ETH HIL E4 Auditorium		
8:30	Registration		
9:00	**Chair Davide Bleiner** **Rebecca Ingle (I)**		
	Are there applications of ultrafast spectroscopy in the analytical sciences?		
9:30	**Daniel Grolimund (I)**		
	Multimodal Chemical Imaging: Linking Microscopic Chemistry to Materials Properties and Reactivity		
10:00	**Alexander Winckelmann**		
	Study of lithium-ion battery aging using laser-induced XUV spectroscopy (LIXS)		
10:30	Morning Break		
11:00	**Chair Naresh Kumar** **Rolf Erni (K), Empa**		
	Nucleation of metallic nanoparticles in liquid phase		
11:30	**Technology Lectures** IonTOF Specs Agilent		
12:00	**Stefan Grünberger**		
	Discrimination of technical polymers via laser and electric spark discharge based optical		
12:20	**Christian Commenda**		
	Diffraction Studies of Medium Manganese Steel Grades		
12:40			
13:00	Lunch		
14:00	**Lab Tour 1** **E-Microscopy Labs**	**Lab Tour 2** **Zenobi Labs**	**Lab Tour 3** **Günther Labs**
15:00	**Chair Christine Müller-Renno** **Arno Schintlmeister (I)**		
	Strength and challenges associated with SIMS-based visualization of single cell physiology		
15:30	**Fabian Göhler**		
	Unraveling Interlayer Interactions in Multilayered Ferecrystalline Thin Films via Photoemission Spectroscopy		
15:50	**Stefan Emrich**		
	Transport of solid lubricants in tribological systems - measurement of transfer rates to improve service life models		
16:10	**Yevhenii Havryliuk**		
	Influence of thermal annealing and CuxS secondary phase on the electrical and		
16:30	thermoelectrical properties of Cu2ZnSnS4 nanocrystals		
17:00	**Closing: Awards, Announcement AOFKA 2025**		

ABSTRACTS

Short Courses

(Alphabetical order of first authors)

Electrons and molecules at interfaces - a love affair

Andreas Borgschulte

Empa - Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129,
Dübendorf CH-8600, Switzerland
andreas.borgschulte@empa.ch

Gas - surface and liquid - surface interactions are at the basis of future sustainable energy technologies [1]. The improvement and understanding of the underlying interface reactions gained great attention by scientists. The analysis of such interfaces by the established electron spectroscopy methods is challenging, in particular for reactions in liquids or with gases at high pressures. Over the years, various approaches have been developed with specific advantages as well as disadvantages.

In this tutorial, I will discuss the fundamentals of electron spectroscopy methods including basic vacuum technology, photon- and electron sources, electron optics and -detection. Newest developments such as near ambient pressure photoemission and membrane electron spectroscopy are introduced and discussed along applications relevant to sustainable energy conversion.

Examples will include:
- From gas handling and analysis in reaction engineering at high pressure to ultra-high vacuum
- UHV-based soft and hard X-ray photoelectron spectroscopy for catalyst characterisation [2]
- Near ambient pressure photo-electron spectroscopy of oxygen evolution reaction [3]
- Metal hydride formation followed by membrane electron spectroscopy [4]

[1] A. Borgschulte, et al., Front. Energy Res. **2022**, *9*, 784082.
[2] O. Sambalova, et al,. Surf Interface Anal. **2020**,*52,* 811–817.
[3] F. Longo, et al., submitted (2023)
[4] E. Billeter, et al., Adv. Mat. Interfaces **2022**, *9*, 2200767.

Non-destructive and label-free chemical analysis using Raman spectroscopy at the micro- and nano-scales

Naresh Kumar

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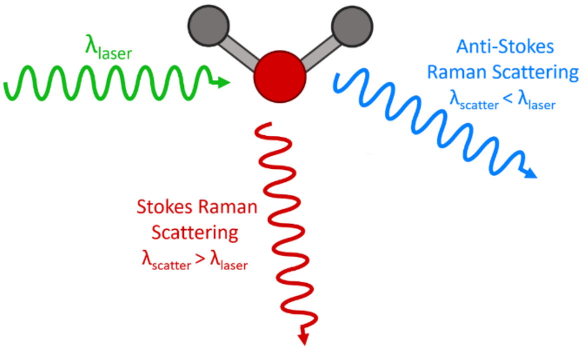


Principle of Raman scattering

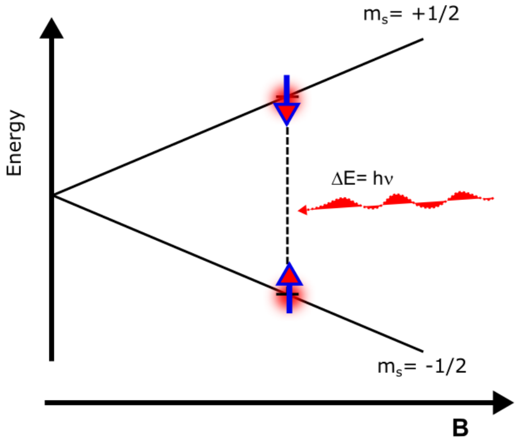
This short course lecture will provide an overview of the primary linear and non-linear Raman spectroscopy methods. Specifically, the following techniques will be covered: confocal Raman spectroscopy, resonance Raman spectroscopy, stimulated Raman spectroscopy, and tip-enhanced Raman spectroscopy. The focus of this lecture will be on the fundamental principles of these major Raman spectroscopy techniques and their applications in non-destructive and label-free chemical analysis of biological samples at the micro- and nano-scales.

Spin as a Spy: Investigating Material Properties through Electron Paramagnetic Resonance (EPR)

Fabio La Mattina

Empa, Swiss Federal Laboratories for Materials Science and Technology,
Überlandstrasse 129, 8600 Dübendorf, Switzerland

Electron paramagnetic resonance (EPR) spectroscopy, also known as electron spin resonance (ESR), is a powerful technique that detects transitions between magnetic states of electronic structures with unpaired electrons. This tutorial aims to provide a comprehensive theoretical framework and experimental examples to illustrate the broad applications of EPR spectroscopy in solid-state physics. In particular, selected cases will be reviewed to demonstrate how the unpaired electrons act as probing agents, investigating interactions within the surrounding matrix. In addition, the review highlights the versatile nature of EPR spectroscopy in unveiling a multitude of material properties, encompassing crystal field symmetry, magnetic ordering, spin dynamics, and identification of defects or impurities. By delving into these aspects, this tutorial review seeks to enrich the understanding of the capabilities of EPR spectroscopy and its valuable contributions to the field of solid-state physics.



Schematic representation of the Electron Paramagnetic Resonance (EPR) in a system with a spin S=1/2. The magnetic field B generates an energy splitting between two spin projections (ms=±1/2). Transitions between these projection states can be induced by a photon matching their energy difference..

Outline of the lecture:

- Magnetic resonance phenomenon : Zeeman effects and phenomenological Block equations
- Effective spin Hamiltonian
- Examples:
  - Transition metal ions in oxides
  - Ferromagnetic resonance
  - Magnetoelectric effects in multiferroics

What can we learn about lithium-ion battery materials from the combination of LIBS and Raman?

V. Merk[1], A. Winckelmann[2,4], T. Langner[3], T. Sieber[3], A. Rietig[3], J. Acker[3], C. Abad[2] and L. Pfeifer[1]

1 LTB Lasertechnik Berlin GmbH, Berlin, Germany
2 Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany
3 Brandenburg University of Technology Cottbus-Senftenberg, Department of Physical Chemistry, Senftenberg, Germany
4 Humboldt-Universität zu Berlin, Department of Chemistry, Berlin, Germany
virginia.merk@ltb-berlin.de

Lithium-ion batteries have become the dominant technology for storing electrical energy in recent decades. For quality control, development of new materials and recycling it is very important to get information about the initial structure and elemental composition but also to understand the processes of aging and degradation of the materials. Therefore, a demand for analytical methods for the investigation of those materials arises. Due to the fact that changes during aging and degradation can occur very locally[1] chemical imaging methods are preferred over bulk analysis methods.

The combination of LIBS and Raman is very promising in this context because LIBS delivers information about the elemental composition and with Raman structural and chemical information about the metal ions, degradation products and the graphite layer can be obtained.[2] From the structure of the graphite layer information about the intercalation of the metal ions into the graphite layer can be derived.[3]

We will present first results on the combination of LIBS and Raman for the investigation of different lithium-ion battery materials, among others lithium nickel manganese cobalt oxide (NMC), lithium cobalt oxide (LCO) and lithium iron phosphate (LFP). This includes the development of models for the quantification of metal content, investigations on the correlation of metal ion content and the graphite structure as well as the investigation of the degradation processes on cathode foils in air.

[1] T. Langner, T. Sieber, J. Acker, Scientific Reports, **2021**, *11*, 6316.
[2] T. Langner, T. Sieber, A. Rietig, V. Merk, L. Pfeifer, J. Acker, Scientific Reports, **2023**, *13*, 5671
[3] C. Sole, N.E. Drewett, L.J. Hardwick, Faraday Discuss, **2014**, *172*, pp. 223-237

Oral Presentations

(Alphabetical order of first authors)

Invited

(Alphabetical order of first authors)

EPR spectroscopy in heterogeneous catalysis: combining in-situ and ex-situ approaches

Mikhail Agrachev, Gunnar Jeschke

Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 2, 8093, Zurich, Switzerland
magrachev@ethz.ch

Electron Paramagnetic Resonance (EPR) is a spectroscopic technique which selectively detects paramagnetic (and more generally magnetic) species. It is therefore widely used for in-depth characterization of heterogeneous catalysts and provides valuable and detailed information about paramagnetic centres, which are frequently encountered in these systems and often represent the active sites for the catalytic reaction. These include transition metal ions, defects, magnetic nanoparticles and photoexcited states.

The present overview covers a series of applications of EPR in the field of heterogeneous catalysis which are being investigated in our group. Several of them focus on the characterization of single atom catalysts, consisting of metal centres atomically dispersed on a surface, which may consist in a metal oxide (alumina, ceria)[1] or a carbon-based support.[2] With continuous wave (CW) EPR we are able to track subtle changes in oxidation states and geometries of the paramagnetic sites, aggregation and redispersion processes and possibly identify and characterize the active sites. Advanced pulsed hyperfine techniques, such as Hyperfine Sublevel Correlation Spectroscopy (HYSCORE) and Electron Nuclear Double Resonance (ENDOR) provide further structural details about the local environment of the paramagnetic centres by detecting weak hyperfine couplings with nearby magnetic nuclei, which are typically not resolved by CW-EPR. A combined HYSCORE-DFT approach allowed us to characterize the changes in composition of heavy polyaromatic compounds (coke) inside the zeolites channels during the methyl coupling reaction.[3]

Moreover, what makes EPR particularly appealing for catalysis is the possibility to use it in situ or in *operando* mode, allowing to monitor the evolution of the catalyst in real time in the operational reaction conditions. With this approach we investigated In_2O_3 and Zn/ZrO_2 based catalyst for CO_2 reduction to methanol, in which the catalytic performance is determined by oxygen vacancies.[4,5]

This overview shows the potential of EPR to solve crucial and challenging problems in heterogeneous catalysis thanks to its high sensitivity and a unique ability to detect fine structural details of paramagnetic and magnetically coupled systems.

[1] I. Surin, Z. Tang, J. Geiger, S. Damir, H. Eliasson, M. Agrachev, F. Krumeich, S. Mitchell, V. A. Kondratenko, E. V. Kondratenko, G. Jeschke, R. Erni, N. López, J. Pérez-Ramírez, *Adv. Mater.*, **2023**, 2211260.

[2] V. Giulimondi, S. K. Kaiser, M. Agrachev, F. Krumeich, A. H. Clark, S. Mitchell, G. Jeschke, J. Pérez-Ramírez, *J. Mater. Chem. A*, **2022**, *10*, 5953-5961.

[3] A. Cesarini, S. Mitchell, G. Zichittella, M. Agrachev, S. P. Schmid, G. Jeschke, Z. Pan, A. Bodi, P. Hemberger, J. Pérez-Ramírez, *Nat. Catal.*, **2022**, *5*, 605–614.

[4] T. P. Araújo, C. Mondelli, M. Agrachev, T. Zou, P. O. Willi, K. M. Engel, R. N. Grass, W. J. Stark, O. V. Safonova, G. Jeschke, S. Mitchell, J. Pérez-Ramírez, *Nat. Commun*. **2022**, *13*, 5610.

[5] T.P. Araújo, J. Morales-Vidal, T. Zou, M. Agrachev, S. Verstraeten, P.O. Willi, R.N. Grass, G. Jeschke, S. Mitchell, N. López, J. Pérez-Ramírez, *Adv. Energy Mater.*, **2023**, *13*, 2204122.

Analytics - understanding materials

Gian-Luca Bona

ETH Zürich; EPF Lausanne & Empa

Überlandstrasse 129; CH-8600 Dübendorf, Gian-luca.bona@empa.ch

In the last decades, advancements in analytical methods and tools have progressed enormously. Methods that are ever more precise and tools have been demonstrated and developed to a level of maturity that allows rapid collection of large amounts of data with high precision. Be it by using electrons, photons, neutrons or quasi particle interaction at various energy levels data that give insights into the materials, its surfaces and interfaces is obtained. Understanding and driving the 'right' conclusions from this data remains the challenge given that the laws of physics, in particular, quantum mechanics govern the interaction between material under investigation and the probe. Hence, understanding the materials around us also required the diligent use of the computational concepts and the modeling toolbox. Modern machine learning algorithms – also known as AI – are a rapidly growing filed supporting the deeper understanding of analytical data. While we start to grasp on the atomistic level materials interactions, the world seems to get ever more complex. Trans- and interdisciplinary collaborative work of scientist of various domains is required. It is at the boundary of the various disciplines that new insights can be found. Driven by creativity and imagination of open-minded researches new insights in materials will lead us to novel applications and solutions for the well-being of our society.

Insights into the structural modification of electrochemically synthesized layered double hydroxides by X-ray photoelectron spectroscopy

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Layered double hydroxides (LDHs) are important and versatile two-dimensional nanomaterials with a variety of application fields such as energy storage, environmental protection and remediation, medical treatment, drug delivery, electronics and catalysis [1]. Ex situ XPS experiments have been carried out with the aim to better understand the modifications of Co based LDHs in alkaline media which seem to appear during the first anodic segment of a cyclic voltammogram. The Co LDHs have been prepared with Al and Fe in order to investigate the role of trivalent cation on the redox behaviour. XP spectra of the different core levels recorded after stopping the first anodic potential sweep at different potential values display drastic and irreversible changes starting at a particular voltage for each system studied (Co/Al and Co/Fe). These changes are related to changes in oxidation state which in turn signal structural changes.

Fig. 1 displays Co 2p spectra for the Co/Al system obtained after a certain potential has been applied during the first voltammetry cycle. The spectra start with a clearly Co(II) state for the pristine situation which switches to Co(III) above 0.525 V. This is in line with a change from a $Co^{II}(OH)_2$ to a $Co^{III}O(OH)$ configuration [2]. Similar changes are also found in the other core levels. The situation for Co/Fe is similar but not as clearly observable. Subsequent cathodic potentials and repeated cycles do not cause significant changes.

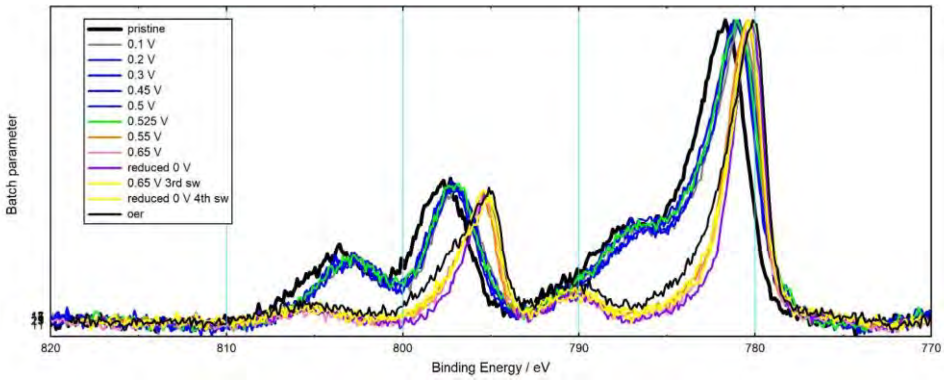

Fig. 1: Co 2p spectra recorded after the first anodic potential sweep was stopped at the marked voltages or preparation steps.

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Nanoparticle-Enhanced Laser Induced Breakdown Spectroscopy

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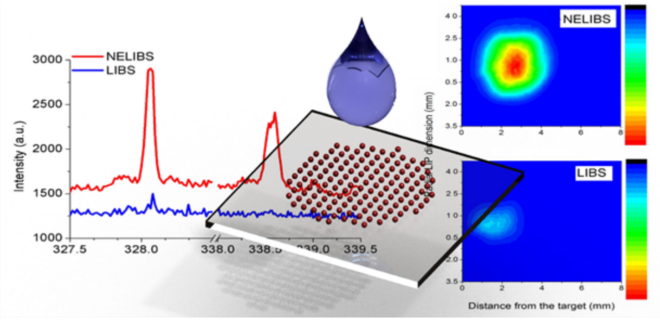
During last decades, plasmonic systems based on metallic nanoparticles (NPs) have been largely employed for analytical spectroscopy since they can help to reach an extremely high sensitivity and very low limits of detection. Nanoparticle Enhanced Laser Induced Breakdown Spectroscopy (NELIBS) has been successfully employed for enhancing the emission signal obtained with Laser Induced Breakdown Spectroscopy (LIBS), in order to reach LOD down to ppb level [1]. The main mechanism of signal enhancement occurring during the NELIBS has been recently reported in Ref. [2] and it is based on the coupling of the NP plasmonic system with the ablated matter at the initial stage and the electromagnetic field of the incoming laser pulse. NELIBS has been applied to several applications spacing from elemental analysis of metal alloys [1], biological fluids and tissues [3] as well as to precious sample that need to be preserved from laser sampling [4]. Finally NELIBS has also shown to be used a sensor for protein-NP conjugates [6].



In this lecture starting from fundamental aspects some important applications will be shown as examples and the comparison of NELIBS with traditional LIBS will be discussed on the basis of experimental observations.

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Nucleation of metallic nanoparticles in liquid phase

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Little is known about the detailed mechanisms that trigger the growth of particles in liquid phase, even for simple elemental metal nanoparticles that are routinely synthesized in such environments. The LaMer particle-growth model most simply considers nucleation to occur instantaneously. The classical nucleation theory, at least, provides guidelines about energy hurdle and critical cluster size. Yet, both of these models describe particle growth by attachment of single molecules or single atoms, whereas particle interactions are entirely ruled out. Particularly for more complex systems, like $CaCO_3$, there is plenty of evidence that these simple theoretical models fail to describe the multi-step mechanisms experimentally documented.

We have developed liquid-phase in-situ approaches in the scanning transmission electron microscope to uncover nucleation and growth mechanisms of simple metallic elements, such as Au, Pt or Pd or alloys thereof. Our approaches are based on employing either graphene-based liquid cells (see, e.g. [1,2]) or liquid nanoreactors of vacuum compatible ionic liquids (see, e.g., [3]), both allowing atomic scale observations to be done with single atom sensitivity (see Fig. 1).

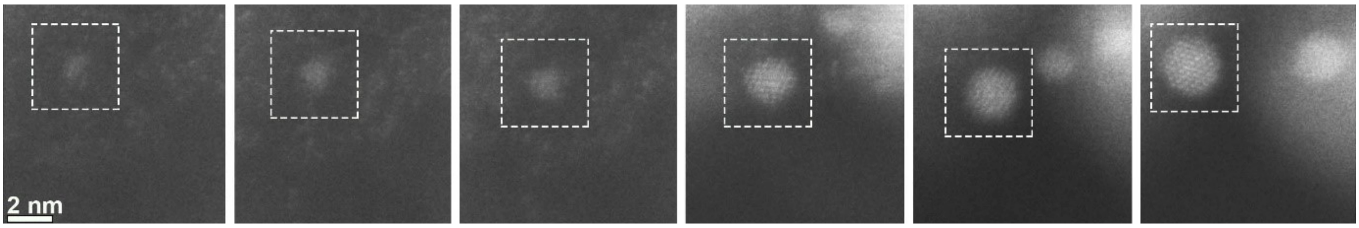

Fig. 1 Nucleation of a Pt particle in an aqueous solution in a graphene-based liquid cell. Reproduced from reference [4].

Our experiments reveal that even the simple metal systems investigated in our studies do not follow an ordinary one-step mechanism. These nucleation and particle-growth reactions consist of several steps where, for instance, particle interactions are of critical importance in the growth process [3]. In the case of gold nucleating in aqueous solution, we see that the immediate environment of a growing particle can be described as a cluster cloud that dynamically acts as source and drain of matter during the growth and crystallization steps [1]. Based on volume and surface energies of the corresponding bulk materials, we developed a systematic model that allows different steps in nucleation and particle-growth reactions to be predicted.

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A “molecular uncertainty principle” – can we simultaneously identify and localize molecules with high confidence?

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Nuclear magnetic resonance (NMR) and high-performance liquid chromatography mass spectrometry (HPLC-MS) are the “gold standards” for molecular identification. However, they have limited spatial information. A multitude of mass spectrometry methods with different probes have been developed to attain high spatial resolution but this has been achieved with the sacrifice of mass spectrometry performance. Generally, from an analytical perspective, this creates what can be termed the “Metabolite Uncertainty Principle”, where the more certain we are about a metabolite’s identity, the less certain we are about its localization. This is a frustrating barrier for measurements at the frontiers of scientific discoveries and for next generation technologies.

In 2017, we introduced the OrbiSIMS technology [1] bringing the mass spectrometry (MS) performance found in high-end proteomics laboratories to UHV surface and interface analysis studies at the mico (spatial) and nanoscale (depth). The OrbiSIMS, uses a hybrid approach where the high mass resolution of the Orbitrap MS, but slow speed, complements the high-speed, but low mass spectrometry performance, of a time-of-flight (ToF) MS. The OrbiSIMS was originally designed for single-cell metabolomic studies to reduce drug attrition and improve drug efficacy in pharmaceutical research and development. Since then, the ability to escape the confines of the “molecular uncertainty principle” has enabled many laboratories around the world to push scientific boundaries from in situ protein identification in biomaterials [2] to the design of new photoresists in next-generation Extreme Ultra-Violet Photo-Lithography [3].

The capability of the OrbiSIMS will be illustrated for metabolite imaging with sub-celluar spatial resolution and nanoscale depth resolution for organic electronic and inorganic semiconductors. The next generation Cryo-OrbiSIMS will be introduced for native state biological imaging preserving cellular structure and chemical integrity as well as new detection concepts for improved signal to noise.

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Atomic Layer Deposition of protective coatings onto Bundles of Technical Fibres

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Atomic Layer Deposition (ALD) is a very useful tool to apply to a surface thin, uniform and conformal coatings way down into complex structures. Here we use atomic layer deposition to coat 'endles' bundles of technical fibres (carbon, siliconcarbide) with inorganics coatings (alumina, titania, phosphates, carbonaceous hybrid materials) that may serve as oxidation protection and modify the mechanical coupling between fibres and matrix in fibre reinforced ceramic composites. Our focus is on oxidation resistant coatings and 'soft' coatings and multilayers of several materials the combine their properties in an advantageous way. [1–4]

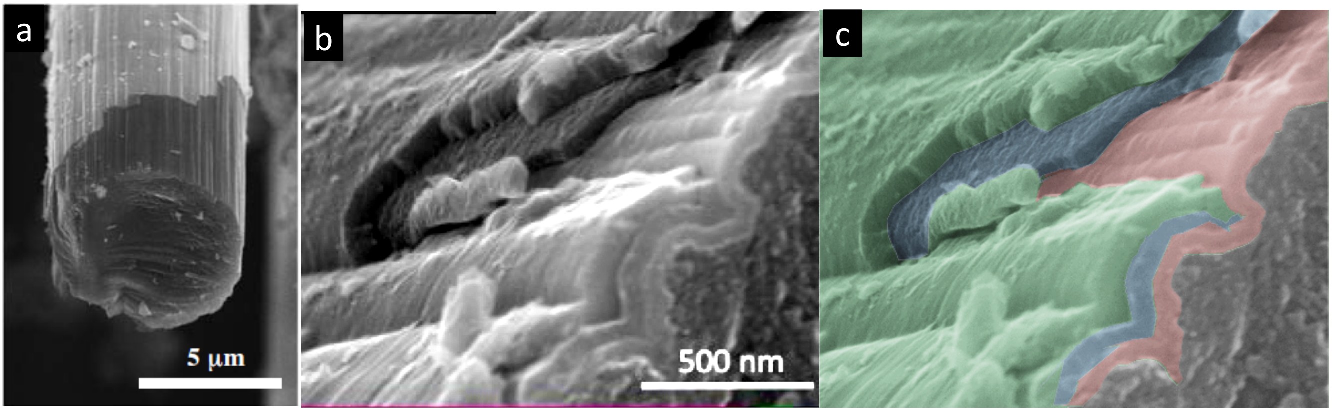

Figure 1: a: end of a carbon fibre cut after coating with a monolayer of alumina via ALD, close to the cut the coating splintered off, further up the fibre the coating is visible as brighter region [1]. b: close up image of the edge of a fibre coated with a multilayer and then cut. The multilayer splintered off, forming several distinct steps.[4] c: the same image as in b, manually coloured according to elemental composition.

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Multimodal Chemical Imaging: Linking Microscopic Chemistry to Materials Properties and Reactivity

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Nearly all natural and engineered materials exhibit pronounced physical and chemical heterogeneities at various length scales. These heterogeneities potentially dictate the physical properties as well as the chemical reactivity of the macroscopic material. Consequently, being able to image and visualize spatial variations of physicochemical characteristics is fundamental to advance our understanding of the properties, function, and reactivity of materials. Quite commonly though, imaging analysis is limited to ‘physical imaging’ providing information related to physical properties such as morphology or physical structure. Often however, in particular in the context of materials reactivity, microscopic chemical properties and their spatial framework turns out to be determinative.

Over the most recent years, micro-analytical facilities based on synchrotron X-ray beams advanced to be indispensable instruments in the context of micro-analytical imaging in general. The exceptional brilliance of modern synchrotron sources in combination with advanced design and production of hard X-ray focusing optics allowed the construction of dedicated high-flux microprobe beam lines. Opportunely, concerning chemical imaging, such synchrotron-based X-ray microprobe facilities possess several intrinsic advantages. Most important, the element-specific absorption resonances accessible within the X-ray energy range provide an element-specific chemical sensitivity. The fine structure of an absorption edge reveals specific chemical information of the target atom such as molecular structure and electronic state. These speciation-dependent features provide a chemical contrast that can be used for chemical imaging going beyond elemental composition mapping. Several X-ray techniques providing chemical contrast, including X-ray fluorescence (XRF), X-ray absorption or emission spectroscopy (XAS, XES) or X-ray diffraction (XRD), can be applied synchronously allowing the recording of multimodal datasets.

Due to the considerable penetration power of (hard) X-rays, not only two-dimensional scanning studies (‘chemical images’) based on spectro-microscopy and/or XRD-imaging. investigations in 3D (‘chemical tomography’) are feasible. Combining computed tomography approaches with the afore mentioned chemical X-ray techniques provides means to derive local chemical information from within intact, undisturbed objects or materials. Moreover, in most cases X-ray techniques can be considered as being non-invasive and non-destructive. This important feature allows the undisturbed recording of multiple, consecutive three-dimensional chemical and structural images of an evolving reactive system – corresponding to a 4D visualization of chemistry in space and time. Time-resolved chemical imaging allows diverse scientific communities to gain unrivalled insights into the chemical complexity of hierarchical, heterogeneous materials, including corresponding chemical reaction pathways and kinetics (‘reactivity’).

In this presentation, recent progress and achievements in the field of 2D/3D chemical imaging and speciation analysis using various synchrotron radiation microprobe techniques will be demonstrated. Examples from a wide range of scientific disciplines, including materials science and energy systems, will be used to illustrate the potential of chemical imaging. Recent progress in time-resolved chemical imaging will be detailed based on *in-situ* observations of physicochemical processes occurring during advanced manufacturing and machining[1,2].

Example of relevance of multimodal chemical imaging: Degradation of Solid Oxide Fuel Cell.

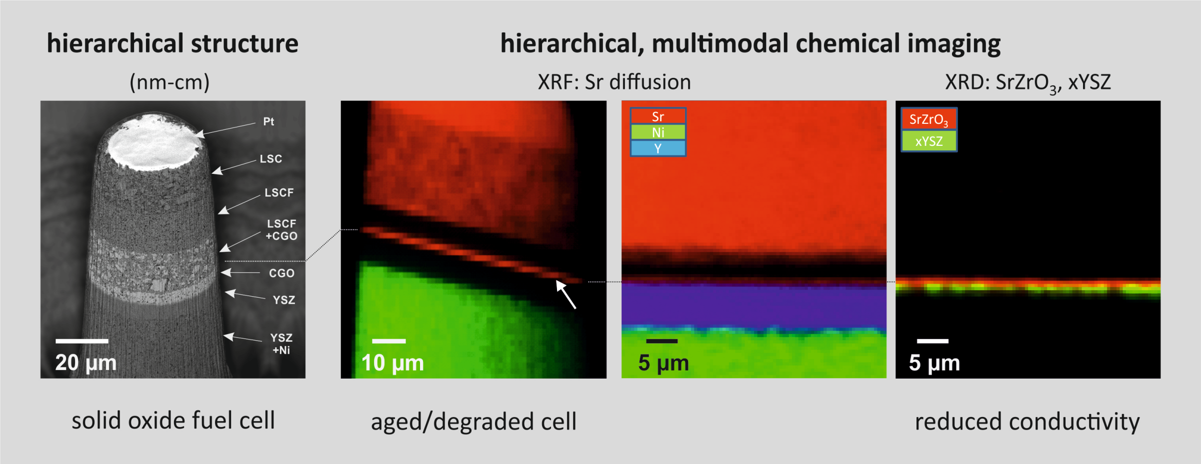

Figure 1: XRF based imaging identifies unexpected Sr-diffusion process. Simultaneous XRD imaging reveals $SrZrO_3$ precipitation and a linked chemical modification of YSZ at the electrolyte/diffusion barrier interface. These reaction products build a thin resistor layer, drastically reducing the device performance[3, 4].

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Laser Ablation-Inductively Coupled Plasma Mass Spectrometry – mature and widely applied

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Laser ablation-inductively coupled plasma mass spectrometry has entered many research areas and the community of users is continuously growing. The direct solid sampling capabilities, the high spatial resolution, low limits of detection and the large linear dynamic range of modern mass spectrometers make the technique (introduced by A. Gray in 1985) very attractive today for major, minor and trace element analysis and isotope ratio determinations. In the last years, research has focused on simultaneous detection capabilities for imaging using ICP-Time of Flight-mass spectrometers (ICP-TOFMS), which requires different aerosol transport systems. Some examples with respect to resolution, detection capabilities and acquisition speed will be given. Furthermore, some interesting and precious samples cannot be transported into the laboratory which led to the development of portable laser ablation. The capabilities using such devices will be discussed. Finally, the re-introduction of nitrogen plasmas (MICAP) opened some new capabilities for aerosol transport and analysis. A prototype nitrogen plasma has been developed in our lab and has been coupled to LA. Some of the fundamental studies will be reported and their future perspectives will be discussed.

On the photoelectric effect and its contribution to a successful divorce of a prominent marriage

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“Let there be light, and there was light.” Some millennia later, Newton and colleagues referred to both particles and waves for the description of light. Then the cognitive model became that of a wave only. In the year 1905 a young man at the patent office in Bern submitted an article to the “Annalen der Physik”, delivering an interpretation of the experimentally known photoelectrical effect, suggesting again that light could be a particle. The young man probably didn’t anticipate that this article would become an initiator for the development of quantum mechanics, a Nobel Prize, a vast number of applications and a rather secular help in his personal life. In this little talk we reflect on the science of light, the photoelectric effect, Albert Einstein and some of his more profane aspects.

Correlative Analysis of Nanostructured Materials

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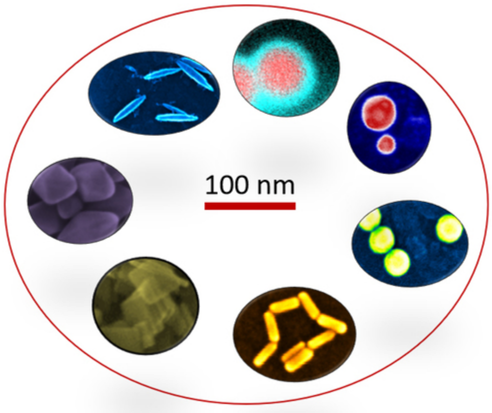
Newly developed methodical approaches with an emphasis on correlative analysis of morphology and chemistry of nanomaterials will be presented. Correlative imaging by STEM-in-SEM with high-resolution SEM and EDS, and further with AFM, or with the new technique TKD (Transmission Kikuchi Diffraction) will be explained on various examples of nanostructures, both as starting materials and as embedded/functionalized nanoparticles in products [1]. The unique analytical benefits of the Auger electron probe as a veritable nano-tool for the surface chemistry will be highlighted. Examples of hybrid analysis of the bulk of nanomaterials by X-ray Spectroscopy and the highest surface-sensitive methods XPS and ToF-SIMS as advanced surface characterization methods available in the Competence Centre nano@BAM [2] will be offered. Particularly for the spatially resolved analysis of the chemistry of nanostructures, such in-depth and lateral gradients of chemistry within mesoporous thin layers, or the completeness of the shells of core-shell nanoparticles, the latter methods are inherent.



Other dedicated developments like approaches for the quantitative determination of the porosity of thin mesoporous layers by electron probe microanalysis (EPMA) with SEM or for the quantitative determination of the roughness of particle surface by electron microscopy will be also presented.

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Are there applications of ultrafast spectroscopy in the analytical sciences?

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Ultrafast spectroscopies with sub-picosecond time resolutions allow for real-time measurement of many of the fastest processes in chemical dynamics, including bond breaking and formation, charge redistribution and energy transfer.[1-3] These spectroscopies have revolutionised our understanding of how molecules interact with light and how chemical reactions occur at the atomistic level as well as how fast.

Most ultrafast experiments are performed in a pump-probe configuration, where an ultrashort pulse photoexcites the sample. Then, a second pulse, the probe, is used to record a spectrum at varying time delays to map out the reaction of the molecule and how fast it occurs. The advantage of pump-probe schemes is that they are highlight flexible – the probe could be a broadband white light continuum for absorption spectroscopy, or a highly energetic X-ray pulse for performing time-resolved X-ray emission measurements. However, many of these techniques face a number of experimental challenges that mean they are far from being standard analytical measurement tools.

In this talk, I will give an overview of some of the state-of-the-art methods in ultrafast spectroscopy and present some of the challenges of these techniques, both in terms of experimental implementations and data analysis. I will then show some applications of transient electron absorption spectroscopy and its use for materials design and development and some of our work and future possibilities of bringing these methods towards robust analytical tools.

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Multimodal Elemental and Molecular Bioimaging for Tissue Analysis

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To study the distribution and the biological effects of metallopharmaceuticals and other metal species in the human, animal or plant organism, imaging methods at the tissue scale with lateral resolution in the lower micrometer range have been found to be particularly valuable.

Traditionally, pathologists use formalin fixation and subsequent paraffin embedding as standard method for sample preparation prior to optical microscopic investigation of the tissue samples. (Immuno)histological staining may provide additional valuable information on the samples. However, rinsing steps during these procedures may either remove analytes or add contaminations. While this is not an issue for optical microscopy, chemical imaging techniques often require the use of fresh frozen tissue samples instead.

Elemental imaging of tissue samples is performed using micro X-ray fluorescence (µXRF) spectroscopy for pre-screening and imaging of analytes in the high ppm concentration range and above, while laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) provides quantitative imaging of (ultra)trace elemental concentrations. Complementary molecular information on functional groups is provided by infrared microscopy, and compound-specific images are generated by matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS). A workflow for multimodal tissue imaging based on all of these methods was developed under consideration of the fact that some of these methods are non-destructive, while others are destructive.

Applications of the multimodal workflow include a study of the distribution and the biological effects of metal nanoparticles in rat lungs as well as studies using gadolinium-based contrast agents for magnetic resonance imaging (MRI) and platinum cytostatics for cancer chemotherapy.

Fluid-FM – a versatile method in biomaterials research

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The scanning force microscope (SFM), respectively scanning force spectroscopy (SFS) are powerful tools for investigating the interaction of biological molecules and organisms with surfaces. The Fluid-FM add-on was introduced recently, giving access to many new applications. It consists of special micro- and nanopipettes, which serve as hollow cantilevers with openings between 300 nm and 8 µm. They are combined with a fluid reservoir and a pump. This combination allows it to suck and to spot, all under imaging conditions and force control.

In this contribution, particular emphasis will be given to applications of the Fluid-FM in the field of biomaterials and nanobiotechnology. These comprise, e.g., single-cell adhesion measurements, colloidal particle adhesion, and nano spotting [1-5]. The advantages and challenges of this versatile technique will be discussed.

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Hydrogen in thin films: controlling stress release paths by microstructure and size

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Metal-hydrogen (M-H) systems offer great opportunities for research studies on fundamental metal systems properties. This is due to the high diffusivity of the smallest of all atoms which allows alloying even at room temperature. When the system size is reduced to the nano-scale, microstructural defects as well as mechanical stress significantly affect the thermodynamics and kinetics properties of the system.[1-6] Effects will be demonstrated on Niobium-H and Palladium-H thin films.

Hydrogen absorption in metal systems commonly leads to lattice expansion. The lateral expansion is hindered when the metal adheres to a rigid substrate, as for thin films. Consequently, high mechanical stresses arise upon hydrogen uptake. In theory, these stresses can reach about -10 GPa for 1 H/M. Usually, metals cannot yield such high stresses and deform plastically. Thereby, maximum compressive mechanical stress of -2 to -3 GPa is commonly measured for 100 nm Nb thin films adhered to Sapphire substrates.

It will be shown that phase transformations change in the coherency state upon film thickness reduction. The coherency state affects the nucleation and growth behaviour of the hydride phase as well as the kinetics of the phase transformation.[1] It will be further demonstrated that plastic deformation can be hindered and even suppressed upon film thickness reduction. In this case the system behaves purely elastic and ultra-high stress of about -10 GPa can be experimentally reached.[2] These high mechanical stresses result in changes of the materials thermodynamics. In the case of Nb-H thin films of less than 8 nm thickness, the common phase transformation from the α-phase solid solution to the hydride phase is completely suppressed, at 300 K.[3,4,5] The stress-conditions can be modulated by using additional lateral confinement [6]. The experimental results go in line with the σDOS model that includes microstructural and mechanical stress effects on the chemical potential [7].

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Strength and challenges associated with SIMS-based visualization of single cell physiology

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The dynamic development of ‘omics’ approaches has enabled high-throughput exploration of microbiomes with respect to phylogenetic characterization, identification of functional genes, transcription, translation and metabolism on the bulk level. Though, deciphering the complex interplay between individual members in highly diverse microbial consortia necessitates interrogation of (sub)micron sized single cells in their natural environment. Fluorescence in situ hybridization (FISH) has become the workhorse for phylogenetic identification of microbial cells, but cannot answer the question about their metabolic activity. Feeding microbes with isotopically labelled nutrients leads to tagging of metabolically active cells by isotope enrichment, but necessitates isotope-specific imaging with high spatial resolution for identification. For this purpose, the Large-instrument facility for environmental and isotope mass spectrometry of the University of Vienna runs a NanoSIMS 50L, which has unravelled previously unrecognised physiological properties of bacteria and archaea thriving in soils, microbial mats, activated sludge, deep groundwater samples and within symbiotic relationships in marine ecosystems as well as the mammalian gut. In the second core-field of applications, the instrument is utilized for investigating the uptake, subcellular distribution and metabolization of therapeutic agents, in particular metal-based anticancer drugs. In this context, the high sensitivity and precision obtained in elemental and isotopic analysis is exploited to explore the mechanisms underlying their efficacy, selectivity and side effects.

Though appearing as straight-forward from the applicant’s point of view, (Nano)SIMS analysis necessitates careful consideration of measurement-process related effects for selection of the most appropriate analysis strategy. For complex shaped samples, does depth profiling or cross sectional scanning better preserve the correlation between structure and composition? How to obtain maximum secondary ion yields in analysis of thin sections required for ultrastructure characterization by transmission electron microscopy? In how far can preferential sputtering, redeposition of sputtered sample material and atomic mixing lead to bias in determination of local isotope compositions by depth profiling? The intention of this talk is to illustrate these aspects based on NanoSIMS analysis results obtained from a variety of biological samples and approaches for optimization of measurement parameters as well as minimization of systematic error will be discussed.

Solid-State Electron Paramagnetic Resonance Spectroscopy

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Since the discovery of the electron paramagnetic resonance (EPR) by E. K. Zavoisky in 1944, it has been used in a vast variety of applications and fundamental research. EPR is a powerful method which can provide in-situ and non-destructive information on electron spins, orbitals, and nuclei at the microscopic scale. In this lecture basic principles of EPR spectroscopy will be described and examples of the application of EPR in solid state physics and materials science will be presented. Different examples will be shown starting from the single paramagnetic centers in perovskite crystals to collective effects in magnetically concentrated compounds. It will be demonstrated how EPR helps to understand microscopic properties of these materials. Important recent development of EPR combined with scanning tunneling spectroscopy (STM) will be also discussed.

Magnetic-sensitive Atomic-scale Surface Analysis by Spin-Polarized Scanning Tunneling Microscopy and Spectroscopy

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The development of magnetic-sensitive surface analysis methods with atomic-scale spatial resolution, such as Spin-Polarized Scanning Tunneling Microscopy (SP-STM) [1-3] and Magnetic Exchange Force Microscopy [4], has become of significant importance in the fields of advanced magnetic materials and nano-scale spintronic devices. In particular, the atomic-resolution mapping of 3D spin textures by vector-resolved SP-STM [5] has led to the discovery of chiral magnetic domain walls [6], chiral spin spirals [7], and chiral magnetic skyrmions [8,9] in ultrathin magnetic films. Nano-scale magnetic skyrmions offer great potential for future magnetic data storage technologies, such as MRAM and racetrack-type memories [10]. Recent advances in the optimization of SP-STM probe tips offering 100% spin polarization have led to high spin-contrast mapping of artificially constructed arrays of magnetic atoms on surfaces of superconducting substrates [11]. Such magnet-superconductor hybrid systems were recently demonstrated to exhibit Majorana quasiparticles which offer great potential for robust topological quantum computation [12-15]. It will be shown how the optimization of the various materials platforms for novel types of quantum devices is guided by the unprecedented insight into the combined atomic-scale electronic, magnetic, and superconducting properties as revealed by spatially, energy- and spin-resolved scanning probe techniques.

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Contributed

(Alphabetical order of first authors)

Unlocking the Mystery of Catalytic Design for Methanol Steam Reforming

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Perovskite-type oxide materials (ABO_3) are a very versatile class of materials. Their ability to exsolve metallic nanoparticles on their surfaces has drawn an increasing interest of the scientific community for their application as catalysts in complex reaction conditions. Via doping the A- and B-sites of these materials the socketed, exsolved nanoparticles on the surface can be specifically tuned to fit the requirements needed for any reaction. [1], [2] A deep understanding of the impact of the elements used for building the perovskite structure are of crucial importance for an intelligent design of perovskite-based catalysts. Therefore, several perovskite-typed oxides, with varying A- and B-site elements were examined in this study. We focused on two points in particular. One, the influence of the chosen elements for the A- and B-site on the capability of catalysing the reaction of **M**ethanol **S**team **R**eforming (MSR). Second, the impact of varying concentrations of B-site dopants (e.g. Cu) on particle growth and formation of the exsolved nanoparticles. For this, *operando* **X**-**R**ay **D**iffraction (XRD) were performed at DESY (***D**eutsches **E**lektronen **Sy**nchrotron*) Beamline P02.1 combined with **S**canning **E**lectron **M**icroscopy (SEM) as well as catalytic test measurements in a fixed bed reactor. The experiments revealed that all investigated materials displayed catalytic behaviour towards MSR. However, we were able to demonstrate that the observed catalytic activity was highly dependent on the elements used for the A-site as well as the concentration of the B-site dopants. Furthermore, the impact of the Cu-content used for the B-site on the formation of nanoparticles could also be proven.

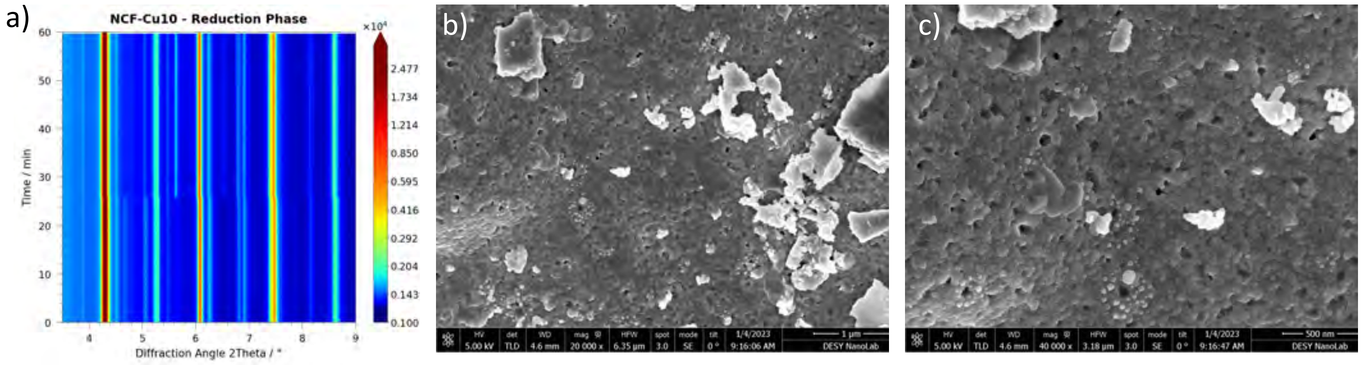

Fig. 1 a) Operando XRD measurement during reducing conditions at Beamline P02.1 at DESY (Hamburg) for $Nd_{0.6}Ca_{0.4}Fe_{0.9}Cu_{0.1}O_3$. Formation of metallic Cu after 25 minutes under reducing conditions. b) and c) SEM images of $Nd_{0.6}Ca_{0.4}Fe_{0.9}Cu_{0.1}O_3$ after reaction conditions of methanol steam reforming proving the formation of nanoparticles on the surface of the material.

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Laser Desorption Ionisation Mass Spectrometry for in situ Molecular Biosignature Detection

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Humanity has long been wondering about the presence of extinct or extant life elsewhere in the Solar System and beyond. Currently, searching for signs of past or present life on other planetary objects has become feasible by means of spacecraft landing and the application of novel measurement technologies. Therefore, the detection of signatures of life, so-called biosignatures, has become a high priority topic for future space exploration missions.

Several groups of compounds are marked as potential targets in the search for signs of life, including but not limited to lipids (e.g. prenols), amino acids and nucleobases. Reliable in situ detection and identification of these molecules poses a challenge for instrumentation. The instruments should be flight-capable, imposing restrictions on size, weight and energy consumption; i.e., laboratory size instruments cannot be flown. Also, the detection capabilities should not be limited to one specific compound or compound group, but ideally several different compounds should be able to be detected simultaneously. Lastly, a high sensitivity and broad dynamic range coverage are required to detect trace abundances, as well as the highly abundant compounds.

A space prototype Laser Ionisation Mass Spectrometer (LIMS) operated in laser desorption mode was designed and constructed at the University of Bern [1]. The instrument, named ORIGIN (ORganics Information Gathering INstrument), was designed for the detection and identification of biomolecules on future space exploration missions to e.g., Mars or the icy moons of Jupiter and Saturn. ORIGIN's compact and simple design makes it a robust and lightweight system, which complies with the requirements for space instrumentation [1]. Currently, the system consists of a nanosecond pulsed laser system (λ = 266 nm, 20 Hz, τ ~ 3 ns) and a compact reflectron-type time-of-flight (R-TOF) mass analyser (160 mm x Ø 60 mm) [2].

Measurements are performed on a solid sample film (residue), which is obtained by drop-casting 1 µL of solution and subsequent solvent evaporation. Thereafter, a laser desorption measurements are performed on a single sample by rastering over the sample surface. Molecules are desorbed and ionised by the laser pulse, where after the positive ions are separated based on their mass-to-charge ratio by the mass analyser. For each laser shot, a single mass spectrum is obtained.

Several studies were conducted to investigate the current measurement capabilities of ORIGIN regarding molecular biosignature detection, as well as laser desorption conditions and the influence of the sample substrate [1,3,4]. In our contribution, the ORIGIN setup and measurement procedures will be discussed in detail, including sensitivity and dynamic range. In addition, we will show the latest results regarding sample substrate influence and the detection of nucleobases.

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Multimaterial 3D Printed Smart Contact Lenses

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Multimaterial 3D printing is a novel technology with exciting potential. This study explores the use of vat photopolymerization-based 3D printing to build multimaterial hydrogel based contact lenses, which exhibit multiband optical filtering properties (amongst other sensing application). Such hydrogel devices can be useful for treating ocular diseases including Color Vision Deficiency (CVD) or color blindness. There are several types of CVDs and they occurs in patients with varying degree of severities.[1,2] The 3D printing of multimaterial and multi-filtering contact lenses (Fig. 1), delivers a promising approach for providing a customised solution to colour blind patients – tinted lens tailored to each patient's needs. The printed multimaterial lenses were examined for their optical and mechanical characteristics, along with hydration behaviour. The optical qualities of the contact lenses were found to be unaffected by the multimaterial printing technique. Due to multiple tinting dyes that were utilized, the printed multimaterial contact lenses provided a combined multi-band filtering property for color blindness correction (Fig. 2). The obtained optical spectrum closely matched the color blindness correcting glasses that are readily available on the market.

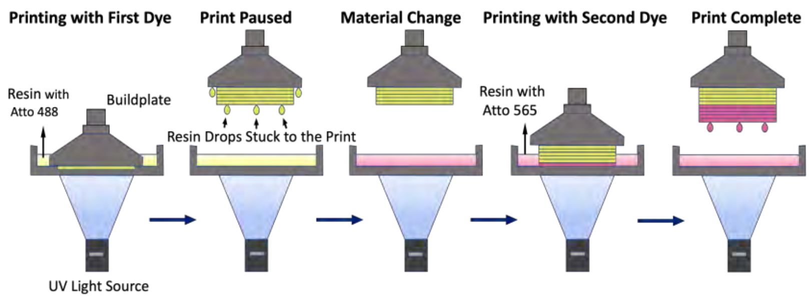

Fig 1: Multimaterial DLP printing process used in this study.

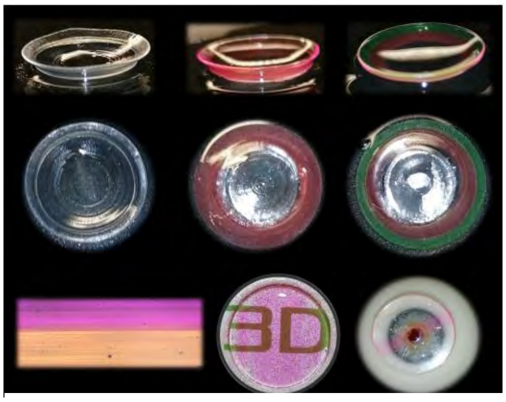

Fig 2: Multimaterial 3D printed contact lenses. Rigth top: clear contact lenses. Middle: clear + pink lenses. Left: clear, pink and yellow lenses.

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Diffraction Studies of Medium Manganese Steel Grades

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Samples from a medium manganese thermomechanical processed steel sheet show strongly preferred crystallographic orientations far from the random distribution. For the quantification of the retained austenite phase a novel X-Ray diffraction (XRD) based method is presented that calculates the phase fraction from the measured texture data. By a geometrical averaging procedure in a large area of the reciprocal space it is possible to define an orientation dependent phase fraction that can be related to the mechanical and magnetic properties along different directions. The structural information from XRD of the phases ferrite, retained austenite and epsilon martensite is used to setup a combined Electron Backscatter Diffraction (EBSD) and Energy Dispersive X-Ray detection (EDX) measurement on the scanning electron microscope (SEM). The distribution, shape and chemical composition of the phases is obtained with a high lateral resolution. The local misorientation of the EBSD data is calculated with a kernel averaging method for each phase and correlated to the experimental data of the residual stresses measurement by XRD along different directions. The results of this orientation dependent analysis can be used to improve the understanding of the physical phenomena and mechanical strengthening mechanisms of medium manganese steels. There is an attempt to describe the magneto-elastic interaction in the complex microstructure with ferromagnetic matrix and non-ferromagnetic retained austenite. Measurements of the residual stresses of the individual phases are compared before and after magnetization.

Transport of solid lubricants in tribological systems - measurement of transfer rates to improve service life models

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A common task for the surface analysis of solids is the quantitative and spatially resolved measurement of the elemental composition. But also the determination of the absolute amount of substance on surfaces is a goal-oriented approach for many questions in technology, which can be pursued reasonably with suitable analytical methods. One example is the quantitative characterization of mass transport in various tribological systems. In combination with gravimetric measurements to determine wear rates, it is possible, for example, to measure the material flows in rolling bearings with liquid-free lubrication. The transport of solid lubricants from specially developed sacrificial components into the respective tribocontacts plays a decisive role here and is intended to significantly increase the service life of the bearings [1]. On the surfaces of the components in the respective tribological system, a certain mass thickness dynamically adjusts itself in the equilibrium of new building and degradation processes, which is measured at selected points along the service life in order to determine the associated transport rates. The aim is to develop a model for calculating the service life of rolling bearings or to measure the solid lubricant rate that can be provided by suitable tribological subsystems [2]. Depending on the geometric shape and the existing total mass density of the component surfaces, suitable analytical methods must be selected. For example, for spherical rolling elements, the measurement of representative mass coverages with the plasma-assisted Secondary Neutral Mass Spectrometry SNMS is advantageous, which, when using absolute sensitivity factors, allows the measurement of element-specific mass thicknesses directly from the total flux of the sputtered particles. In addition to the local geometric measurement of layer coverages with the Focused Ion Beam method FIB or electron microscopy, energy-dispersive X-ray analysis EDX can also be used to find the associated mass thicknesses from the attenuation of the substrate signal. In rolling bearings, we were able to show through the use of surface analysis methods that the element-specific lubricant transfer factors reach values of up to 10%. For molybdenum disulfide as a solid lubricant, the associated mass flows are then, for example, in the range of several 10-5 µg per revolution. In the article, the respective procedure for different tribological systems is described and comparative measurements for validation of the methods are presented together with the results obtained.

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Unraveling Interlayer Interactions in Multilayered Ferecrystalline Thin Films via Photoemission Spectroscopy

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The stacking of two-dimensional sheets provides a pathway towards the study of interlayer interactions, emergent properties, and subsequently novel applications for 2D materials. Common approaches to create these heterostructures are the manual stacking of exfoliated sheets, or sequential layer-by-layer growth via chemical or physical vapor deposition. However, the achievable complexity of the layering sequence is often limited by available stable constituent layers or compatible growth conditions.

In contrast, the self-assembly of artificial layered precursors, which is known as the Modulated Elemental Reactants (MER) technique, offers unparalleled flexibility in the composition and layering sequence of thin films. In this two-step synthesis, amorphous elemental precursors are first deposited via sequential physical vapor deposition. By calibrating the thicknesses and layering sequence of the constituents to mimic the targeted structure, it is possible to crystallize the precursors into a layered thin film via annealing in inert atmosphere. Due to the structuring of the precursors on an atomic level, the necessary energy input as well as layer intermixing during crystallization is reduced, enabling the synthesis of metastable structures with almost arbitrary complexity. The increased structural freedom of MER thin films comes at the expense of epitaxial alignment, as layers are generally showing turbostratic rotational disorder along the crystals *c*-axis. [1]

We will discuss how by controlling the nanoarchitecture of the precursor, one can create systematic series of heterostructures to facilitate the growth of certain metastable constituent layers such as rock-salt structured BiSe or metallic 1T-$MoSe_2$ [2], and investigate the effects of modulation doping to tune charge transport [3], superconductivity, or charge density waves. The contribution will focus on recent results on two classes of heterostructures built up from BiSe, Bi_2Se_3, and $MoSe_2$ [2], as well as PbSe and VSe_2 [3], respectively.

While the thickness of MER thin films is usually on the order of 50 nm spanning multiple unit cells, we were able to push the MER synthesis towards the two-dimensional limit by preparing a one monolayer thick, nanocrystalline layer of $MoSe_2$ on a substrate of epitaxial graphene on silicon carbide [4]. Building on these results, we are now exploring the growth of more sophisticated, one unit cell thick heterostructures by also incorporating bismuth selenide. Preliminary results suggest that these films are at least partially aligned with respect to the graphene, indicating that the main drawback of the MER synthesis could be eliminated by the choice of an appropriate growth substrate.

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Implementations and Applications of Laser Ablation and Ionisation Mass Spectrometry for Earth and Space based Research

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In this contribution, we present two laser ablation and ionisation mass spectrometers (LIMS) developed at the University of Bern. The systems are used for the spatially resolved chemical analysis of solids, ranging from materials used in the semiconductor industry to geological samples that host old life forms. Both LIMS instruments use short laser pulses for the ablation and ionisation of the sample material, have a co-linear ablation geometry and are coupled to a time-of-flight mass analyser. However, the instruments differ in size and therefore have different performance and application characteristics. While one of the instruments is a compact space-prototype instrument developed for in-situ analyses of solids on other planetary bodies in our Solar System[1,2], the other instrument is a laboratory scale version intended for Earth-based chemical composition analysis[3,4].

We will present technical details of the setups, specifications, and applications of the two LIMS instruments. Both instruments are currently coupled to a femtosecond laser source. In the past nanosecond lasers operated at different wavelengths were used as well. We will therefore discuss the observed influence of the laser pulse width on measurement performance[1]. Furthermore, the impact of the laser wavelength on quantification based on measurements conducted with three different wavelengths ranging from IR to UV[5] will be discussed. Finally, we will show how the instruments' measurement capabilities were improved through small changes to the setup, including the installation of a double pulse system and a mass selective beam blanking device[6–8].

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Discrimination of technical polymers via laser and electric spark discharge based optical emission

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Spark Optical Emission Spectroscopy (spark OES) and Laser-Induced Breakdown Spectroscopy (LIBS) are advanced element analysis methods that are widely used in the metal industry (spark OES) and in many different industry branches (LIBS [1]). While spark OES requires samples that are electrically conductive, LIBS can be employed to nearly all kinds of materials. However, LIBS is suffering from the matrix effect, i.e. the sensitivity and limits of detection depend on the structure and composition of the sample matrix. We combine electric spark discharge and laser ablation for the excitation of analytical plasma and optical emission spectroscopy (Laser Ablation Spark Discharge OES, LA-SD-OES). This combination has been shown to overcome the matrix effect for high alloyed steel samples [2]. Here, we report on further advancements of the LA-SD-OES method to measure also non-conductive samples. A low-to-mid energy laser pulse is applied to the sample inducing a faint plasma that triggers an electric spark discharge between two electrodes. The optical emission of the laser-induced/spark plasma is measured.

Different technical polymers (PA6, PC, PE-HD, PET, PMMA, POM, PP, PS, PTFE, PVC, UHMWPE, etc.) are measured by LIBS and LA-SD-OES aiming to distinguish the materials by distinct spectral features. Molecular emission bands of CN and C_2 as well as atomic lines of O, N, H, and of some specific elements are measured and the correlation of intensities is used for materials discrimination. Halogenation of polymers as well as signs for flame retardants etc. can be easily detected with LA-SD-OES while LIBS is not able to identify these additives. The damage of the polymer sample surfaces stays minimal as the electric spark discharge does not contribute to the ablation process.

ACKNOWLEDGEMENTS

Financial support by the Austrian Research Promotion Agency FFG is gratefully acknowledged (K-project PSSP 871974, COMET Competence Center CHASE GmbH K1-Center 868615).

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Influence of thermal annealing and Cu_xS secondary phase on the electrical and thermoelectrical properties of Cu_2ZnSnS_4 nanocrystals

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Among the alternative energy sources, which attract attention of the researchers, one of the most promising is solar energy. But despite the great achievements in this field, one of the main issues is reduction of solar panel efficiency due to overheating. One of the approaches of solar panel cooling and using the usually waste heat to create additional electrical energy is hybrid photovoltaic-thermoelectric devices. This is why materials with thermoelectric and photovoltaic properties gain popularity in recent years. Research especially focuses on materials that are cheap, easy to produce, and environmentally friendly. One of such materials is the Cu_2ZnSnS_4 (CZTS) and related compounds. Owing to its good absorption properties and a bandgap around 1.3 eV, this material is promising for photovoltaic applications. The ability to produce CZTS nanocrystals (NCs) by „green” synthesis in colloidal solutions makes it even more attractive for use in so-called third generation photovoltaics. In addition, recent studies show good thermoelectric properties for CZTS-like materials. This fact makes CZTS NCs very promising for hybrid photovoltaic-thermoelectric devices and can enable an improved overall conversion efficiency.

One of the most common methods to tune the properties of CZTS materials is thermal annealing, which allows not only the crystallinity to be improved but also transitions between disordered and ordered kesterite structures to be induced. However, thermal annealing can cause changes in the NC films, which are deteriorating the photovoltaic performance, namely the appearing of Cu_xS secondary phases.

Here, we investigate the effect of thermal annealing up to 350 °C on spin-coated thin films of CZTS NCs obtained by “green” colloidal synthesis. In the temperature range up to 200 °C, despite improved surface morphology, as confirmed by atomic force microscopy, and crystalline quality, as confirmed by Raman spectroscopy, the electrical conductivity of CZTS NCs films is very low and does not allow us to determine the Seebeck coefficient. At the same time, the appearance of the Cu_xS secondary phase at annealing temperatures of 250 °C and 300 °C provides a significant improvement in the conductivity, making these films suitable for thermoelectric measurements. The change of Seebeck coefficient and conductivity with the content of Cu_xS phase is revealed. This lets us conclude that thermoelectrical properties of the films obtained are predominantly determined by the Cu_xS phase. Therefore, being deteriorative for photovoltaic effect, the Cu_xS phase can be beneficial for good thermoelectrical performance of thin films based on CZTS NCs.

Chemical state analysis of functional oxide thin films by combining soft and hard X–ray Photoelectron Spectroscopy

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As demonstrated in the present study, the recent development of commercial lab-based HAXPES systems, equipped with both a soft Al-Kα and hard Cr-Kα scanning X-ray source, opens up unique opportunities for monitoring the local chemical states of the cations and anions in functional oxides and catalysts, in a routine laboratory environment [1,2]. Surface-sensitive deep core-level photoelectron lines and respective Auger transitions can be measured using the hard X-ray source, whereas more bulk-sensitive shallow core-levels can be excited using either the hard or soft X-ray source. As demonstrated for thin Al_2O_3 films, the local chemical state of the constituting ions in the oxide may even be probed at near constant probing depth by smart selection of sets of photoelectron and Auger lines, as excited with the combined soft and hard X-ray sources [1]. Exemplary cases are given for the combined chemical state analysis of cations and anions in different amorphous and crystalline TiO_2 and Al_2O_3 polymorphs, as prepared in the form of a thin film (~10-50 nm) by various synthesis methods, including thermal oxidation, anodization and atomic layer deposition (ALD) [1,3]. By careful selection of sets of photoelectron and Auger lines, as excited with the combined soft and hard X-ray sources, the Auger parameters (AP) for the respective cations and anions were derived at various probing depths [1]. The depth-resolved AP values for the thin (amorphous) oxide films were compared to their respective bulk crystalline reference phase(s). The resolved shifts in the cation and anion AP values as function of the synthesis conditions could be linked to tiny changes in the local electronic polarizability around the core-ionized atoms between the different oxide polymorphs, which originate from differences in the local coordination spheres (short-range order) around the constituting cations and anions. Moreover, the local chemical state of oxygen in various techologically-relevant oxides could be correlated to the optical/dielectrical properties, such as the refractive index (see Fig. 1).

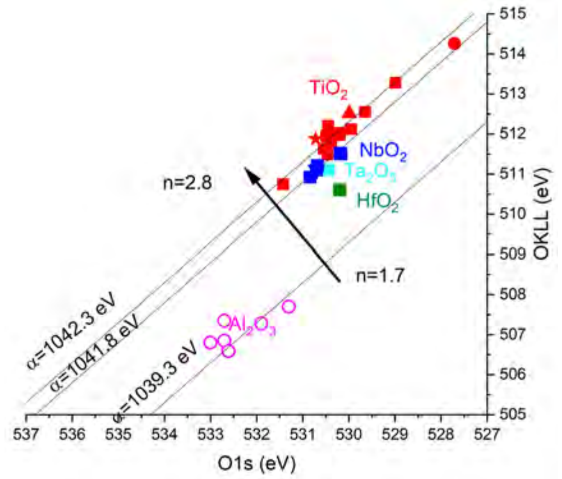

Fig.1 *Oxygen Auger parameter derived for different oxides, showing a clear correlation with the respective refractive index.*

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MeV SIMS as an emerging nuclear analytical technique for surface analysis of paint materials in cultural heritage

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The preservation of works of art as cultural heritage requires sensitive analytical techniques that can help identify the materials that were originally used by the artist. Accurate determination of major constituents of paints as well as understanding their chemical stability provides invaluable information to restorers and curators, and usually requires a multi-analytical approach for chemical characterization.

Secondary ion mass spectrometry with MeV primary ions (MeV SIMS) is an accelerator-based nuclear analytical technique that has great potential for studying organic materials in cultural heritage objects due to its high surface sensitivity, higher secondary molecular ion yields, lower fragmentation, and higher mass range than conventional (keV) SIMS, as well as chemical imaging capability [1–3]. This technique allows investigating the chemical composition and degradation phenomena that occur in the uppermost layers of materials without the need for sample preparation [4]. This is an added value as surface layers cannot be analyzed by e.g., standard chromatographic methods coupled to MS. In addition, MeV SIMS can also be considered as non-destructive since primary ion doses are well below the so-called static limit, so the sample may be preserved for subsequent characterization by other techniques.

The use of MeV SIMS to study the works of art is only beginning to be recognized as currently only a few accelerator laboratories around the world develop and utilize this method. In this work we will present current research on artists' paints performed at the Ruđer Bošković Institute accelerator facility, where two MeV SIMS setups have been developed for the analysis and molecular imaging of organic materials [2,3]. The focus is on the analysis of a wide selection of pigments, binders, mock-up paint mixtures and commercial products that fall into categories of both traditional and modern materials. The aim is to investigate the ability of detecting and identifying individual components in complex paint mixtures by building an MeV SIMS mass spectra database that would facilitate material characterization in surface analysis and chemical imaging of real art samples, aged paints, or paint cross-sections. To this end, several examples of real samples analysis are also presented and discussed.

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Further developments in sample preparation strategies for nanoparticles analysis using laser ablation single particle−ICP-MS

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Nanoparticles are utilized in diverse fields, such as material manufacturing, energy production, food processing, consumer goods, and life sciences. The physicochemical properties of materials in the nanometer size range differ significantly from those of bulk materials, resulting in unique characteristics useful for various products such as medical products, catalysts, cosmetics, food technology, and household items. [1], [2] However, the widespread use of nanoparticles in consumer goods raises concerns about their impact on the environment and human health. To address this issue, single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) has been developed as a powerful tool for investigating nanoparticles. [1] However, conventional SP-ICP-MS, which enables the simultaneous determination of particle size and number concentration, is limited to nanoparticles in suspension. Further limitations of this approach include difficulties in the sample storage because of the low stability of suspensions as well as limited efficiency of sample introduction and the potential negative impacts of the solvent on the quality of ICP-MS analysis.

To overcome these limitations, the measurement of solid samples is recommended. The combination of laser ablation as the sampling technique and SP-ICP-MS for the analysis was introduced to incorporate the benefits of solid sampling. [2] [3] This approach allows the sizing and counting of nanoparticles directly in a solid matrix with the advantage that embedded nanoparticles can be stored without changes in particle size. Similar to conventional SP-ICP-MS, laser ablation SP-ICP-MS (LA-SP-ICP-MS) also requires nanoparticle standards for signal evaluation. In the literature, the commercially available nanoparticle standards were prepared in a gelatine matrix and investigated with LA-SP-ICP-MS. [3] The use of gelatine is related to drawbacks such as the need for heating, which can affect the dissolved fraction of the nanoparticles. Moreover, gelatine is a natural biological substance which results in a complex sample matrix containing several nutrients and trace elements. Application of techniques for fabrication of even thin films with controllable thickness, such as spin coating, is not possible with gelatine.

In this study, dispersions of metallic nanoparticles in polymer matrices were produced by spin coating using different types of polymers. The aim was to achieve a random distribution of isolated nanoparticles within the generated polymer thin film without particle agglomeration. This spin coating approach gives the vital advantage of creating even and uniformly thin polymer films, which can be used as standards for signal evaluation if a specified quantity of solute analyte is added to them and an exact area of the film is completely ablated. The impact of the sample preparation procedures and the effect of the different polymer matrixes, as well as the influence of the laser energy in the ablation process, were investigated and compared to assist in the further development of LA-SP-ICP-MS.

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Giant magneto-electrocatalytic effect in Ni-based electrodes

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Alkaline water electrolysis represents one of the simplest methods employed for renewable hydrogen production [1]. In contrast to acidic electrolyzers (e.g., PEM), alkaline electrolyzers reach high conversion efficiency with low-cost abundant transition metals such as Ni-Fe alloys [2]. In addition to its intrinsically high electrolytic activity for oxygen evolution reaction (OER), we show that the activity can be enhanced by more than 20% simply applying a magnetic field (Fig. 1). The understanding of the phenomenon is complex as the surface of these catalysts is subject to a dynamic equilibrium, and the presence of specific phases depends on the presently applied conditions including the magnetic field as well as on the history of the sample. Using APXPS [3] and a combination of soft- and hard x-ray photoelectron spectroscopy with electrochemical impedance spectroscopy we find that the high intrinsic electronic conductivity comes together with an increasing water intercalation into the oxy-hydroxide, which is experimental evidence for a water mediated OH- diffusion mechanism. Our hypothesis is that this pore structure is affected by the presence of a magnetic field to minimize the local stray field. The (re-)orientation requires restructuring of the surface, explaining the time dependence of the effect.

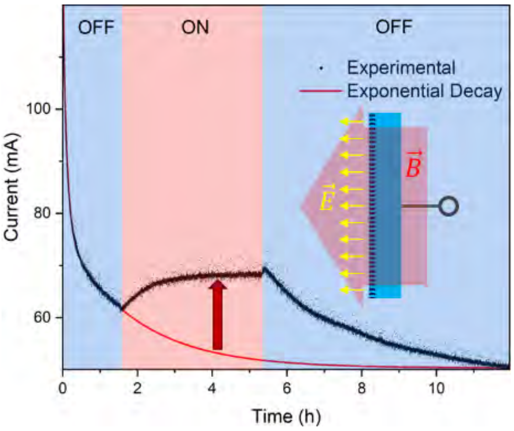

Fig. 1. OER enhancement of Ni-based electrode under applied magnetic field.

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Magnetization switching on self-assembled structure of alpha-helix-polyalanine molecules observed by ambient STM

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Polyalanine (PA) with an α-helix conformation has gathered recently a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization of the transmitted electron. However, studies on a molecular scale are still rare, although this length scale provides direct insight into the role of molecular properties. We studied now in detail with STM the self-assembly of PA molecules on magnetic $Au/Co/Au/Pt/Al_2O_3$ substrates and probed the transmission by local spectroscopy (STS). Because of the high spatial resolution, our setup allows to study this CISS effect on the nanoscale and probe the importance of cooperative effects. By switching the out-of-plane magnetization of the heterostructure, the transport of electrons can be controlled depending on molecule's specific handedness. Furthermore, for various lengths of molecules with and without a cysteine termination, we studied the spin polarization in detail. The phase separation into well-ordered enantiopure hexagonal phases and hetero-dimer structures of the right (L) and left handedness (D) allow for the analysis of the spin polarization of PA molecules in different environments. Our results clearly demonstrate that both the coupling as well as the ordering and coordination are important in order to achieve a high spin-polarization in chiral systems.

Improved online-laser ablation of solids in liquids (LASIL) cell design: the stethoscope cell

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In online-LASIL, a solid sample is ablated under a continuous stream of a liquid carrier medium, which is then introduced into the plasma of an ICP-MS. This approach circumvents the laborious sample digestion step required for conventional ICP-MS analysis but enables liquid standards for quantification in contrast to other solid sampling techniques. [1, 2] For this reason, online-LASIL was mainly applied to analyze thin films deposited on standardized substrates; therefore, the cavity for the sample was optimized for 5x5x0.5 mm3 samples. However, due to the online-LASIL cell design, the analysis of bigger samples required a previous cutting or thinning step.

To overcome the limitations regarding the sample geometry, the online-LASIL cell was redesigned, resulting in the development of the stethoscope cell, allowing the analysis of flat samples with a minimum length of 7 mm. This work will present the new cell design compared to the previous one. It will be demonstrated how the new cell design offers more freedom in terms of sample geometry, while also remaining limitations will be discussed. The applicability of the stethoscope cell will be demonstrated on quantitative measurements of the SRM NIST 612.

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Diffusion coefficient measurement by LEIS in Cu/Si grain boundary systems

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Surface islands formed by grain-boundary diffusion has been studied in Cu/Si and Ni/Cu nanolayers by in-situ low energy ion scattering spectroscopy (LEIS), X-ray photoelectron spectroscopy (XPS), scanning probe microscopy (STM) and ex-situ depth profiling based on secondary neutral mass spectrometry (SNMS). A new experimental approach of the measurement of grain boundary diffusion coefficients is presented [1]. It is based on appearing time measurement of silicone atoms diffused through a few nanometers thick copper layer and detected by surface sensitive LEIS method. The temperature range of 423–463 K insures the pure C-type diffusion kinetic regime. Grain boundary diffusion coefficients were estimated by the relation used for calculation of diffusant distribution from a constant source in assumption that the diffusion path equals to the film thickness at the moment of appearing Si atoms on the Cu surface. At 453 K we estimated the surface segregation factor and detected formation of Cu–O–Si atomic bonds on the Cu film surface [2] measured by XPS. Depth distribution of Cu in Ni layer has been determined by SNMS depth profile analysis. A combined measurement technique of LEIS and SNMS gave a unique possibility to measure the fast diffusion in nanolayers at low temperatures. Furthermore, the advantage of this technique was that determination of grain boundary diffusion coefficient did not require a complicated calculation with segregation factors in order to remove the effect of B-type diffusion kinetic and, as a result of this, the diffusivity could be studied in a simply way, only by measurement of the appearing time.

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Study of lithium-ion battery aging using laser-induced XUV spectroscopy (LIXS)

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Laser-induced XUV spectroscopy (LIXS) [1] is an emerging technique for elemental mapping. In comparison to conventional laser-induced breakdown spectroscopy in UV-vis (LIBS), it has a higher precision and wider dynamic range, and it is well suited for the quantification light elements like lithium and fluorine. Further it can spot oxidation states. The XUV spectra are produced at a very early stage of the plasma formation. Therefore, effects from plasma evolution on the reproducibility can be neglected. It has been shown, that high-precision elemental quantification in precursor materials for lithium-ion batteries (LIBs) can be performed using LIXS.[2] Based on these results, LIXS mapping was used to investigate aging processes in LIBs. Different cathode materials with varying compositions of fluorine containing polymer binders were compared at different stages of aging. Due to effects comparable to X-ray photoelectron spectroscopy but in reverse, monitoring of changes in the oxidation state is envisioned, which makes information about the chemical environment of the observed elements accessible. The combination of elemental distribution and structural information leads to a better understanding of aging processes in LIBs, and the development of more sustainable and safe batteries.

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Reduction of iron oxides as indirect hydrogen detection method in XPS

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Challenges of analysing hydrogen must be addressed to keep up with increasing interest of hydrogen effects in the field of material science. In contrast to other elements, most characterization methods are not able to detect hydrogen directly which necessitates alternative detection techniques. X-Ray photoelectron spectroscopy XPS can be used to indirectly prove hydrogen diffusion through bulk steel samples. To prove this concept, we electrochemically charged high strength dual-phase steel DP1000 on one side (hydrogen entry side) with hydrogen and monitoring the reduction of iron in oxide layers on the opposite side (hydrogen exit side) due to diffused hydrogen. This reaction is resolvable in the high-resolution Fe2p$_{3/2}$ peak (see Fig. 1) and was shown for native and artificially grown oxide layers. A shift in the order of few eV towards lower binding energies as well as the position of the shake-up satellites are used to resolve the reduction of oxide layers. The amount of iron transitioned from the third to the second oxidation state was estimated through an appropriate fitting procedure. Additionally, a layer model of the most common iron oxide species is presented for the reduction processes and re-oxidation experiments that quantitatively represents the volume ratios of the species.

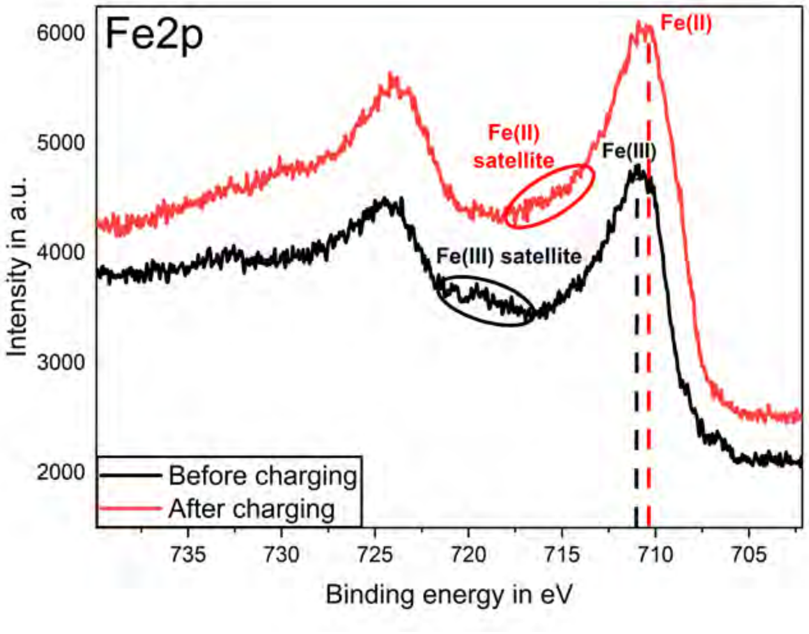

Figure 1. High-resolution Fe2p$_{3/2}$ peak indicating the reduction of the iron oxide layer.

Poster Presentations

(Alphabetical order of first authors)

Combinatorial neutron imaging for in-situ alkane adsorption analysis over C_1-C_4 coupling catalysts

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Hydrocarbons are essential commodity chemicals used in various applications and crucial for our society. However, their dependence on fossil sources puts pressure on the environment. Hence, the production of these molecules from renewable sources is crucial for the advancement of a sustainable society. Currently, the most promising routes rely on the activation and subsequent oligomerization of small molecules (C1-C4) into longer chain hydrocarbons over heterogeneous catalysts. Nevertheless, these systems suffer from poor selectivity towards a single target product,[1] as well as rapid deactivation.[2] These transformations are largely governed by the ability of the reagents and products to diffuse though the catalyst pore network. Therefore, a complete understanding of the sorption kinetics is beneficial for the establishment of descriptors that aid the design of catalytic materials with optimized properties. Such investigations are traditionally performed by infrared radiation (IR) in combination with Raman spectroscopy or by simple gravimetric methods.[3] While these methods provide valuable information on the properties of a system, the in-situ optical visualization of the material changes during the adsorption/desorption process remains challenging due to interferences with the source light. In addition, the design of suitable cells is required for the application of these techniques under realistic temperatures and pressures. Herein, the uptake and desorption kinetics of n-hexane as probe molecule over commercial zeolite catalysts under catalytically relevant conditions is studied using the combinatorial neutron imaging method.[4] The large interaction between neutrons and hydrogen leads to significant changes in contrast when H-containing molecules are adsorbed on the materials. This property enables the in-situ adsorption/desorption visualization, and the quantification of the hydrocarbon species adsorbed. In addition, the custom designed experimental setup used in this study allowed the simultaneous investigation of up to 69 samples.[4] For temperatures below 473 K, the observed radial diffusion profiles in most porous materials indicate that the diffusion of long chain products plays a critical role in the catalyst deactivation under typical reaction temperatures (423 523 K). Overall, these findings provide new insights on the adsorption kinetics of hydrocarbons over systems with varying porosity and pore connectivity, facilitating the design of optimized catalysts for oligomerization reactions.

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The *Surface Inspection Pad* (SIP) for non-destructive and in-process surface analysis of components

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If components are to be surface treated, the cleanliness of the surfaces plays an inherently important role. Thus, checking the surface cleanliness is essential. In principle, expensive inline or online analysis devices can be integrated into the process lines for this purpose. However, small and medium-sized enterprises (SMEs) do not have the financial resources for this. Furthermore, the component geometry or size often does not allow for an inline/online analysis. In such cases, the components to be examined must be removed from the process and given to an analysis institute. Since the components for the surface analysis, which is usually carried out in an ultra-high vacuum system with a small vaccum lock, must be cut into suitable pieces and thus destroyed, they cannot be returned to the process afterwards. If the analysis of large quantities is necessary, this is consequently accompanied by an enormous financial loss. For this reason, we have developed an innovative solution: the *Surface Inspection Pad* (SIP). The SIP allows the surface cleanliness to be checked without having to remove the corresponding components from the process or destroy them. The principle is based on transferring the surface contamination to the SIP with subsequent analysis of the SIP surface instead of the component surface. Suitable materials were identified, and the first prototypes were built and successfully used. Contamination can be transferred in a variety of ways, such as rinsing, wiping, or stamping. Using the highly sensitive ToF-SIMS analysis, even the smallest amounts of contamination can be clearly detected.

An extension of the SIP to other areas of application is also possible. Tribological applications are of particular importance here. With the help of SIPs, the cleanliness of lubricating oils or tribological test benches can be checked, for example after an oil change. For this purpose, the test stand is rinsed with an ideally unalloyed oil and a scratch mark is created on a SIP using a scratch test method (e.g., pin-on-disc). Here, the characteristic surface-active property of additives is exploited, whereby these can be enriched and clearly detected even with very small concentrations. This allows the detection of additive contamination in oils well into the sub-ppm range.

Boride layers prepared on iron surfaces by ion implantation

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Boriding, or boronizing is a surface hardening method that produces protective metal-boride layers on various metal surfaces, such as iron and steel. It increases surface hardness, resistance to wear, oxidation and corrosion. Corrosion resistance is highly sought after in most industrial fields, increasing the lifetime of products and machinery. The wave-forming tips or baffles in wave soldering machines used in the manufacture of printed circuit boards are good examples. There are several methods of boriding, using various media (solid, liquid, gaseous and plasma). Pack cementation boriding is widely employed due to its ease of use and availability. The main drawback of this method is the formation of a double layer of FeB and Fe_2B, due to the amount of boron that diffuses into the various surface depths during the process.[1] There are notable differences in the crystal structures and thermal expansion coefficients of the two borides, making this double layer mechanically weak. FeB is also generally unfavourable due to its brittleness and tendency to spall.[2] We aim to solve this issue by avoiding diffusion dependent methods, instead using ion implantation for inserting boron atoms into the iron matrix under more controlled conditions. High current ion implantation is a well-known method for modifying surface layers of different metals. In this work boron ions were implanted into the surface of high-purity iron samples. We studied the boron distribution in the surface layer by depth profile analysis and the chemical bonds between iron and boron by X-ray photoelectron spectroscopy.

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Surfaces forces on nano-porous materials

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Nano-porous materials are increasingly attracting attention in the field of materials science [1-3] and diverse applications due to their unique properties. The surface forces present on nano-porous materials play a crucial role in determining their interactions with the surrounding environment, involving fluids, solutes, and organisms. The presence of porosity can add a significant amount of internal surface area and additional volume capacity, which can affect the interaction kinetics. This amplification is expected to greatly enhance some so-called confinement effects that can be observed and studied in flat surface confinement. Undertaking a systematic investigation of surface forces on different nano-porous model surfaces thus is a novel approach that offers an opportunity to discover and comprehend previously unknown equilibrium and non-equilibrium processes.

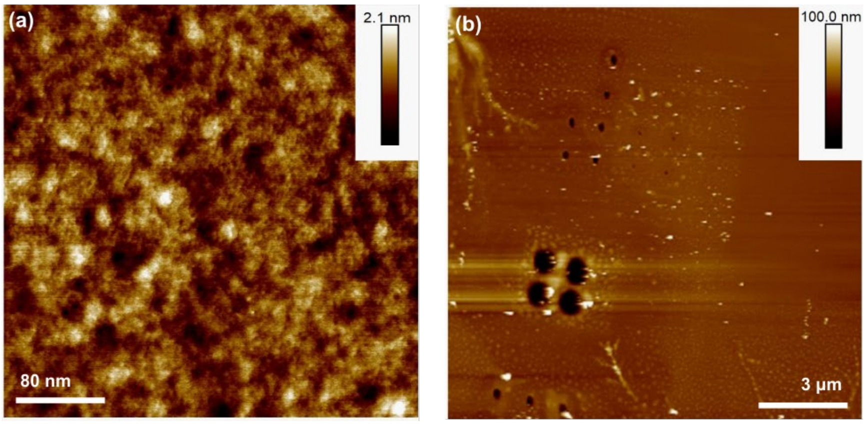

Figure 1: AFM images of porous surfaces fabricated by (a) plasma enhanced chemical vapor deposition and (b) focussed ion beam with various pore diameters.

In this study, we examine surface forces appearing on different nano-porous surfaces using two different techniques, namely atomic force microscope (AFM) and extended Surface Force Apparatus (eSFA) in order to discover physical phenomena occurring at different scales. Nano-porous models are fabricated using two different approaches, such as plasma-enhanced chemical vapor deposition, resulting in highly cross-linked plasma polymer films deposited on muscovite mica with pore sizes below 10 nm. The second model surface with larger pores is fabricated using focused ion beam technique on muscovite mica, resulting in adjustable pore dimensions in range of few hundreds nanometers in diameter. Examining surface forces on these nano-porous models of various sizes offers insights into novel effects that occur in confined fluids.

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Spatially Resolved Corrosion Zone Analysis of Cement Stone Samples by Non-destructive (Confocal) Micro X-Ray Fluorescence Spectroscopy

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Micro X-ray Fluorescence (MXRF) instruments enable non-destructive and elemental analysis of solid samples with a spatial resolution of a few micrometers by implementation of a focusing optic. Here, confocal MXRF (CMXRF) provides additional depth-dependent measurement capabilities. The in-depth sensitivity of CMXRF spectrometers is based on a defined three-dimensional probing volume, which is formed by the confocal arrangement of two focusing lenses in the excitation and detection channel. The spectrometer in this study is a modified commercial MXRF tabletop spectrometer (M4 TORNADO) by Bruker (see Fig. 1a) which is equipped with a micro-focus X-ray tube, a polycapillary full lens for X-ray focusing and a 30 mm^2 silicon drift detector (SDD). Due to the modification a polycapillary half lens was installed in front of a 60 mm^2 SDD providing a confocal overlap of both foci. (see Fig. 1a)

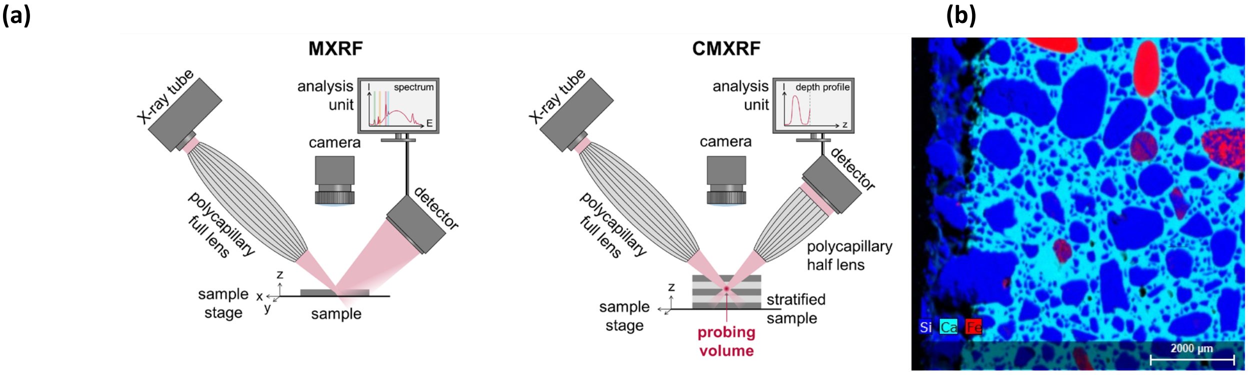

Fig. 1 Scheme of a MXRF and CMXRF (adapted by reference [1]) (a) and element distribution image of a corroded mortar cross-section sample for silicon (blue), calcium (cyan) and iron (red) (b).

In the building materials science, the analysis of corrosion zones in concrete is of significant interest, in order to describe the corrosion processes precisely and to be able to make statements about e.g. concrete durability. In this connection MXRF provides the position-dependent (x and y) investigation of the element composition of corroded and uncorroded zones (see Fig. 1b) and with CMXRF the immediate analysis of the corroded samples is possible. Thus, the necessity of prior sample preparation, like cross-section preparation, which could subsequently manipulate the sample properties, is avoided. Those depth-resolved measurements are executed by moving the sample through the probing volume via a motorized sample stage. The capability of this setup for depth-resolved and three-dimensional element analysis has already been demonstrated for polymeric, biological and mineral samples where elements of medium to high Z numbers have been investigated. [1-5] In this work we will show advantages and disadvantages of this method when analytes of low Z number have to be analyzed.

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Investigation of Si island formation through Cu grain boundaries by SPM and SEM methods

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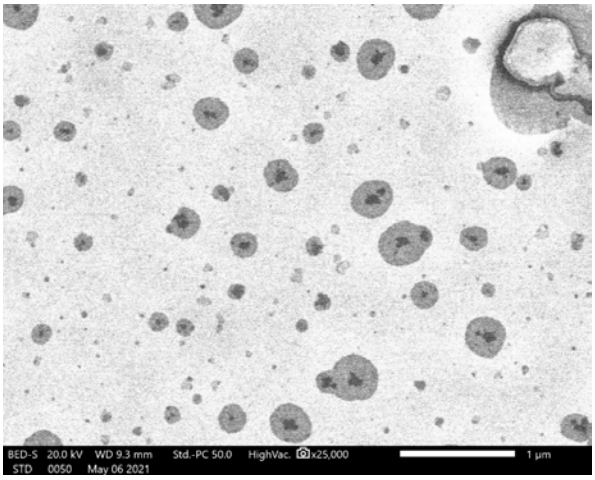
Silicon island formation on top of a polycrystalline copper layer was studied with Scanning Probe Microscope and Scanning Electron Microscope in the 403-453K temperature range. Onto silicon single crystals, 80 nm amorphous silicon and 40 nm copper was deposited successively. Scanning Electron Microscopy and Scanning Probe Microscopy methods experimentally proved, that heat treatment of the samples causes silicon atom migration though the grain boundaries of the upper copper layer, resulting in silicon island formation instead of a continuous Si layer on the Cu surface. Surface coverage of the Si islands were up to 30%. These results show good correlation with our recent Low Energy Ion Scattering measurements, as well as with the previous one [1].



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Neutron insights into nickel metal hydride batteries

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The transition to renewable energy sources relies on seasonal energy. Nickel metal hydride (Ni-MH) batteries, invented at the end of the last century, are established batteries without the use of precious and highly hazardous materials [1]. Despite great advantages such as high power-density and easy scale-up, NiMH battery are currently no option as seasonal storage because of various side reactions leading to great efficiency losses such as self-discharge. The latter stems from the unavoidable hydrogen background pressure of the hydride used. Furthermore, hydrogen/oxygen generation occurs during overcharging or over-discharging. For safety, a vent is installed into the battery to release the excess gas. However, the efficiency loss remains [2].

To minimize these effects, it is beneficial to know the dependence of the external parameters on the hydrogen evolution. It is important to study this on the systems and not on the materials level, because the hydrogen pressure depends on the dead volume and (catalytically active) surfaces present in the battery. We performed neutron imaging and tomography while monitoring the SoC of the battery under operating conditions to observe the reaction processes in the battery. The measurements reveal the hydrogenation states of the electrodes as well as the hydrogen back pressure in the battery in real time as a function of applied potential and current. One of the most contradictory observations is that over-discharge, i.e., the generation of hydrogen gas during discharge, depends on the charging state of the battery as well as current extracted.

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Surface Cleaning with Atmospheric Pressure Plasma Jets investigated by Optical Emission Spectroscopy and LIBS

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Atmospheric pressure plasma jets (APPJs) are increasingly employed for industrial applications such as surface cleaning, modification of surfaces, deposition of coatings and for bio-medical applications such as skin treatment and bacterial inactivation [1]. In this research, the plasma of an industrial APPJ (Acerios, Fronius International GmbH) is investigated and applied to the cleaning of surfaces [2]. The device operates a spark discharge in Argon gas flow in the few kW power range resulting in a continuous and powerful plasma jet expanding into ambient air. The APPJ plasma parameters are measured by Optical emission spectroscopy (OES) and the plasma cleaning of coated sample surfaces is monitored by OES and Laser-induced breakdown spectroscopy (LIBS). For the characterization of plasma by OES a new methodology is developed [3]. The plasma electron temperature T_e and electron number density N_e are determined accurately by evaluating the Ar (I) and Ar (II) emission lines using the Saha-Boltzmann plot method. For the cleaning experiments samples are coated with organic oil layers of 0.5 to 10 µm thickness. The APPJ plasma cleaning efficiency is calculated from measured spectra and the atomic lines and molecular bands of species originating from the contamination layer. Chemical imaging of samples before and after plasma cleaning is performed by LIBS. Spatial profiles of the cleaning efficiency are measured. We find a strong influence of the APPJ plasma parameters and the type and thickness of contamination layer on the efficiency of the cleaning process. For instance, the cleaning becomes more efficient at higher power of the plasma generator (CN violet band emission measured in situ by OES).

Financial support by the Austrian Research Promotion Agency FFG (project CAPCOAT Plus 872846) and by the European programme for education, training, youth and sport Erasmus+ is gratefully acknowledged.

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Improved online-laser ablation of solids in liquids (LASIL) cell design: the stethoscope cell

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In online-LASIL, a solid sample is ablated under a continuous stream of a liquid carrier medium, which is then introduced into the plasma of an ICP-MS. This approach circumvents the laborious sample digestion step required for conventional ICP-MS analysis but enables liquid standards for quantification in contrast to other solid sampling techniques. [1, 2] For this reason, online-LASIL was mainly applied to analyze thin films deposited on standardized substrates; therefore, the cavity for the sample was optimized for 5x5x0.5 mm3 samples. However, due to the online-LASIL cell design, the analysis of bigger samples required a previous cutting or thinning step.

To overcome the limitations regarding the sample geometry, the online-LASIL cell was redesigned, resulting in the development of the stethoscope cell, allowing the analysis of flat samples with a minimum length of 7 mm. This work will present the new cell design compared to the previous one. It will be demonstrated how the new cell design offers more freedom in terms of sample geometry, while also remaining limitations will be discussed. The applicability of the stethoscope cell will be demonstrated on quantitative measurements of the SRM NIST 612.

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Pulsed Laser Deposition of ''Röntgen Nano Films''

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In 1974, Fisher [1] proposed the concept of utilizing single crystals to generate an incredibly small X-ray laser. Yariv [2] calculated the lasing parameters in the single crystals to achieve distributed feedback. The core of this laser lies in the resonant matching between the wavelength and the interplanar distance of the crystal. Due to the strict requirements of crystal quality and stoichiometry, that theoretical underpinning never made its way to an experimental system.

This work's long term objective is the experimental realization of such a miniature X-ray laser. "Röntgen material" signifies crystals that are active as gain media. Detailed calculations on various ''Röntgen materials'' have been performed to evaluate the performance at various X-ray wavelengths [3]. From those materials, one of the potential candidates was selected for this experimental work, namely Ho_2O_3. The calculated results provided the dimension for the single crystal, which turns out to be around 100 nm. To create such a tiny crystal, we employed pulsed laser deposition (PLD) to grow an epitaxial thin film. PLD is well known for its stoichiometry transfer and epitaxial growth of thin films [4]. This is most important in our case. Ho_2O_3 is a robust candidate to grow as a thin film due to its chemical stability.

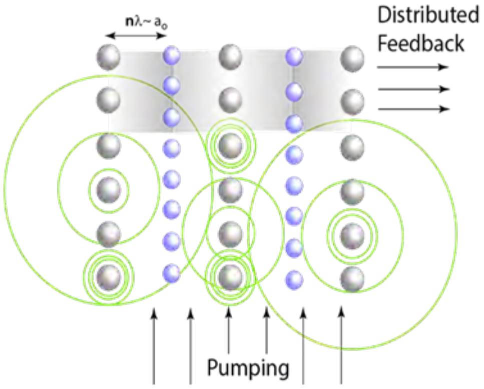

Fig.1 Lasing principle of single crystal X-ray laser.

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Quantitative Analysis of the Hydrogen Concentration on Surfaces using SNMS

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The quantitative characterization of the concentration profile of hydrogen H in technical materials still represents a challenge for analytics and, on the other hand, is of great importance for hydrogen technology, especially with regard to the influence that hydrogen has on the material properties. In particular, the reliable detection of relatively small concentrations, in the range of one atomic percent and below, is difficult and requires the use of suitable measurement methods. This is not only due to the fact that hydrogen is also present as a reactive species in the vacuum of the measuring apparatus and provides a background contribution to the actual measurement signal for the hydrogen intrinsically present in the sample. Hydrogen is not directly detectable for the electron spectroscopic methods of surface analysis and also Secondary Neutral Mass Spectrometry SNMS has the problem that the sensitivity factor for hydrogen, with its high ionization energy of over 15 eV, is very small due to the small electron impact ionization cross section. When using quadrupole mass filters, the so-called zero blast occurs as a further problem, which even more hampers the sensitive and reliable measurement of hydrogen concentration depth profiles. Therefore, for the detection and quantitation of hydrogen with SNMS, deviating from the usual quantitation routine, the dimer neutral particle signal I_{MH} is used instead of the atomic one. This molecule is also emitted during sputtering of the sample surface by co-emission of a matrix atom M together with an adjacent hydrogen atom H. Our measurements show that the relative detection factors are then significantly higher. The basics of a quantitation routine with the MH dimer signal is presented, sensitivity factors and detection limits for the measurement of hydrogen with this method are determined and the application of the method is demonstrated using various sample systems from practice.

Characterization of the formation of the Zn/Fe intermetallic phases at the surface of 2 galvannealed steels with different Si concentrations

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Galvannealing of steel means you first start with hot-dip galvanizing. After the steel strip leaves the liquid Zn bath excessive Zn is blown away by air knives and the strip is annealed for only a few seconds at temperatures between 500 and 565°C in order to create Zn/Fe intermetallic phases. The phase transitions must be completed before the steel strip reaches the first roll. If the amount of Si is increased in modern steels to about 1,5 wt.-% in order to archive better mechanical properties of the steel, it was observed that the annealing process is massively slowed down.

The aim here is therefore understanding what causes this deceleration of the Fe diffusion into the Zn layer. And the first step in order to archive it is to find characterization tools which can show the phase developments in the Zn layer.

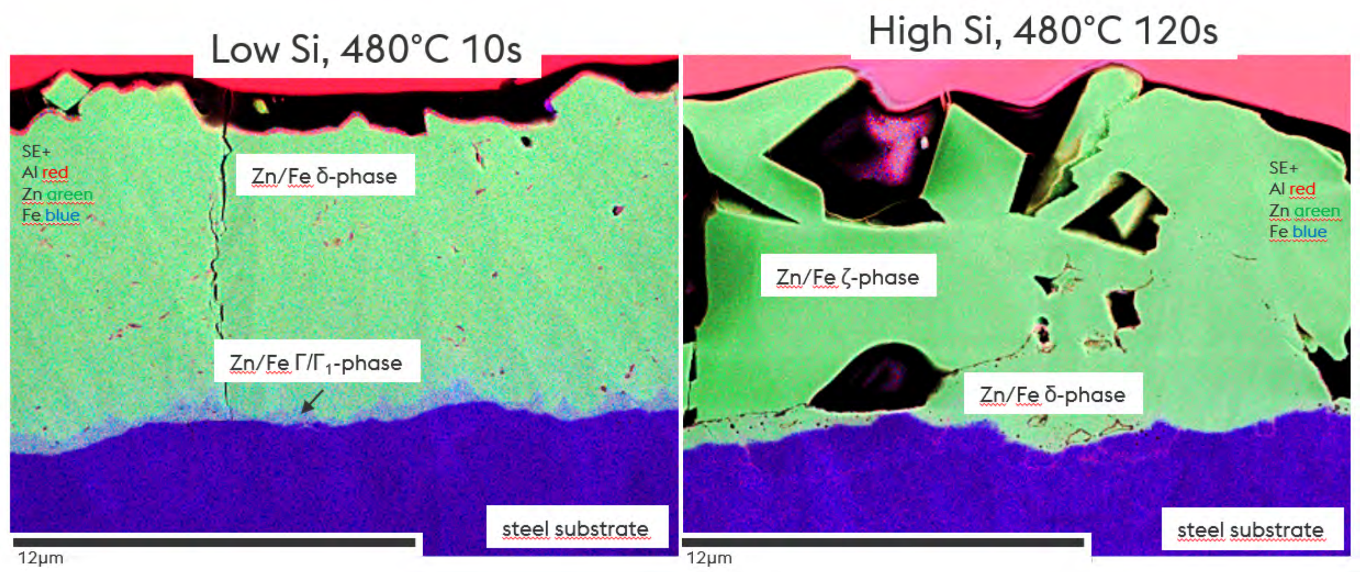

Figure 1 Comparison of 5kV EDX element mappings of cross sections prepared via Ar ion polishing of low and high Si containing steels after annealing at 480°C. The images show an overlay of the secondary electron image with the elements Al, Zn, and Fe in red, green, and blue

So far, the measurement technique of choice is a proper cross section preparation via Ar ion polishing and subsequent EDX-element mapping at low primary beam energy in order to archive a compromise between good lateral resolution and distinguishability between Zn/Fe phases, for example the difference between ζ- and δ- phase is only about 1.5 wt.-%. An example is shown in Figure 1. Other methods were also used for confirmation of the findings like XRD, AES, XPS, GDOES, and TEM.

There are a lot of difficulties and measurement artefacts in EDX when measuring low concentration of elements like Si and Al at that special prepared surface due to geometry and sum peaks and I want to show some of these aspects which I found.
I also want to give an explanation for the different Fe diffusion behavior of the two steels.

Fs-LA-ICPMS for high throughput analysis

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Laser ablation coupled to ICPMS has become a powerful tool in quantitative analysis of solid samples and recently also in imaging and bioimaging applications due to the spatially resolved sampling resolution at μm-resolution and sensitivity [1,2]. However, the application to high throughput analysis and imaging of samples has been limited due to long transport time of laser-generated aerosols to ICP. Thus, a combination of femtosecond laser coupled with fast ablation cell [3] coupled to TOFMS will allow for fast and simultaneous detection of elements with high resolution and accuracy due to the reduced fractionation effects in materials science, geology and biological part for polymers, geological samples and tissues.

Initial experiments were performed using Pharos fs-laser system (wavelength: 257 nm, pulse duration: 190 fs) equipped with HeLex ablation cell [4] and Agilent 8900 ICPMS system. Four reference samples (BCR-2G, NIST SRMs 610, 612 and 614) were used with SRM 610 being the external calibration standard and ^{42}Ca as internal standard element to quantify for other 58 chosen isotopes. Quantification results were obtained and compared to investigate the relationships of quantification accuracies, sensitivities and LODs with different parameters including crater size, output energy and repetition rates.

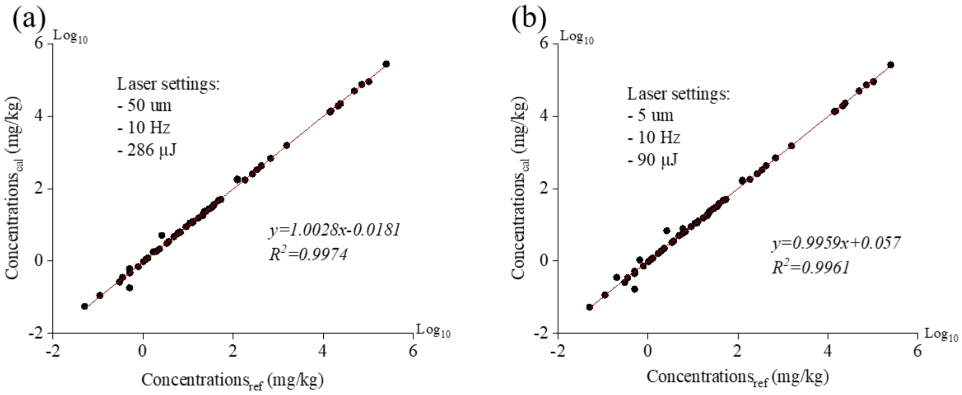

Figure Quantification results of BCR-2G in comparison with reference values with different parameters

Results showed that the quantified concentrations agreed with the certified values with deviations within 10% when using 50 μm and 5 μm in BCR-2G. Deviations occurred mostly for elements like As, Ag and Cd), whose mass fractions are close to the instrumental LODs. Investigation of laser output energy in relation to the spot size showed logarithmic relationship and the measured spot size in comparison with the system settings represented as linear correlation.

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UNIFIT 2023/UNIFIT 2024 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

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Main focus of the advancement of UNIFIT 2023/UNIFIT 2024 are the optimization of the saving and loading procedure of Unifit projects and the batch processing sub-routine. For a better and faster operation of the software the common Windows shortcuts are integrated. The definition and display of the preferences are reworked and newly designed. The dialogue 'Programme Parameters' is redesigned and expanded for easier handling. The definition of the excitation sources and their satellites is reworked completely. The pop-up and pull-down commands are improved. The setting options of the X-axis and Y-axis dialogues are refreshed. New export functions are implemented. In order to increase the processing speed of the software, the programme code is reworked and optimized.

Scientific Program at Glance

	Monday 11 September			Tuesday 12 September			Wednesday 13 September		
Room	ETH HIL E4 Auditorium	ETH HIL E5	ETH HIL E6	ETH HIL E4 Auditorium	ETH HIL E5	ETH HIL E6	ETH HIL E4 Auditorium		
8:30	Registration			Registration			Registration		
9:00	Welcome			Chair Michael Kopnarski			Chair Davide Bleiner		
				Roland Wiesendanger			Rebecca Ingle		
9:30	Gianluca Bona			Vasile-Dan Hodoroaba			Daniel Grolimund		
10:00	Sigve Haug			Werner Goedel			Alexander Winckelmann		
10:30	Morning Break			Morning Break			Morning Break		
11:00	Chair Gernot Friedbacher			Chair Gunnar Schwarz			Chair Naresh Kumar		
	Detlef Günther			Alessandro De Giacomo			Rolf Erni		
11:30	Technology Lectures			Technology Lectures			Technology Lectures		
	Thermo-Fisher			Bruker			IonTOF		
	LTB			Prevac			Specs		
							Agilent		
12:00	Haider Butt			Laura Kronlachner			Stefan Grünberger		
12:20	Filippo Longo			Salome Gruchola			Christian Commenda		
12:40	Maximilian Podsednik			Nikita Boeren					
13:00	Lunch			Lunch			Lunch		
14:00	Forum 1/ Analytics for Industry Lars Sommerhäuser	Short Course Electrons and molecules at interfaces Andreas Borgschulte	Short Course Raman LIBS Virginia Merk	Forum 2/ Teaching Solid Analysis Gunnar Schwarz	Short Course Electron Spin Resonance Spectroscopy Fabio La Mattina	Short Course Surface Raman Naresh Kumar	Lab Tour 1 E-Microscopy Labs	Lab Tour 2 Zenobi Labs	Lab Tour 3 Günther Labs
15:00	Chair Renato Zenobi			Chair Andreas Borgschulte			Chair Christine Müller-Renno		
	Ian Gilmore			Astrid Pundt			Arno Schintlmeister		
15:30	Matea Krmpotić			Reinhard Denecke			Fabian Göhler		
15:50	Nguyen T. N. Ha			Benedikt Wolfsjäger			Stefan Emrich		
16:10	Viktor Takáts			Tobias Berger			Yevhenii Havryliuk		
16:30	Afternoon Break			Afternoon Break			Afternoon Break		
17:00	Chair Detlef Günther			Chair Fabio La Mattina			Closing: Awards, Announcement		
	Uwe Karst			Michail Agrachev			AOFKA 2025		
17:30	Christine Müller-Renno			Alexander Shengelaya					
18:00	Apero + Poster			Lars Jeurgens					
19:00				AOFKA Gala Dinner					
20:00	AOFKA Board								