Abstract Booklet

“Research at European Neutron and Synchrotron Facilities by Austrian Scientists”

11th & 12th of November 2013
Vienna University of Technology

organized by NESY

hosted by
Vice Rector for Research
Prof. Dr. Johannes Fröhlich
Vienna University of Technology
Venue

Vienna University of Technology
Karlsplatz 13
A-1010 Wien
Austria

Host:
Vice Rector for Research Prof. Dr. J. Fröhlich

Editorial Team
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Christina Streli (TU Wien)
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Angelika Graumann (TU Wien)

Cover: Picture provided by K. Hradil (TU Wien), Scattering of a decagonal quasicrystal (Al$_{72.5}$Co$_{15.5}$Ni$_{11}$), measured at ESRF, beamline BM02.
Back-cover: Picture provided by K. Hradil (TUW): 5D-Patterson map of a quasicrystalline single crystal data set (Al$_{72.5}$Co$_{15.5}$Ni$_{11}$), measured at ILL/D19
Financial Support
Travel Information

Main Entrance hall; lift to Kuppelsaal (4th Floor)
Underground 4- exit Resselpark
Main Entrance TU Wien
Tram 1, 62 Resselstrasse
Seminar room AA 04 28 (4th floor)

Travel Information:
http://www.tuwien.ac.at/en/contactsearch/visit_us_travelling_information/

Main Building TU Wien
Karlsplatz 13
1040 Wien

Meeting room for NESY meeting:
seminar room AA 04 28
next to Kuppelsaal

Underground 4- Exit Resselpark
Route to Venue

GPS coordinates: (48.198931, 16.369805)
http://www.tuwien.ac.at/en/contactsearch/visit_us_travelling_information

Main Locations of TU Vienna (location maps)

Plane
The Vienna International Airport (VIE) in Schwechat is about 20 km away in the south-east of Vienna.
On the airport’s web site you find flight information as well as transportations into the city center:

- train S7 to Landstraße/Wien Mitte
- **Bus** Service Vienna Airport Lines:
  - VIA to Wien Schwedenplatz: Travel time 20 minutes,
  - VIA to UNO-City: Travel time 20 minutes,
  - VIA to Wien Südtiroler Platz : Travel time 20 minutes,
  - VIA to Wien Südbahnhof: Travel time 25 minutes,
  - VIA to Wien Westbahnhof: Travel time 35 minutes,
- **City Airport Train (CAT)**
- A **Taxi** stand is right in front of the Arrival Hall.

Train/bus
If you prefer travelling by train you will find necessary information at [http://www.oebb.at](http://www.oebb.at) (Austrian Federal Railways) or via phone +43 05-1717.

Public transport in Vienna
The main building of Vienna University of Technology is reachable with the underground lines U1, U2, U4 and the "Badner Bahn" (**station = Karlsplatz**) and also with the trams D, J, 1, 2 and 62 (**station = Opernring**).
Tickets are available at the airport, at the subway stations and in tobacco shops (so-called Traffik’s).

search: city map / search: public transport (Wiener Linien)

Car
**From the South and East:** Südbahn (A2) - Südosttangente - Exit Gürtel - Südbahnhof - Prinz Eugenstraße - Schwarzenbergplatz – Karlsplatz
**From the West:** Westautobahn (A1) - Hietzinger Kai - Schönbrunner Straße - Rechte Wienzeile - Karlsplatz
**From the North:** Donauuferautobahn (A22) - Südosttangente - Exit Gürtel - Südbahnhof - Prinz Eugenstraße - Schwarzenbergplatz - Karlsplatz

Please bear in mind to include the official highway toll label for Austrian motorways ([http://www.vignette.at](http://www.vignette.at)).
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Morphology effect of Co$_3$O$_4$ nanostructures on the reducibility and catalytic performance for CO oxidation

Structural Characterization of Substrate Binding in Monoglyceride Lipase

Direct Observation of Atomic Diffusion in Glass Systems

Structural and functional studies of a ClpC-MecA unfoldase

InAs$_{1-x}$P$_x$ segment in an InAs nanowire: A characterization with nano-focused X-ray diffraction

Studies of atomic-scale diffusion by x-ray photon correlation spectroscopy

In-Situ Synchrotron investigation of the changes of the microstructure of nanocrystalline Pd during deformation using X-Ray Line Profile Analysis

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Shape Retrieval from Colloidal Nanocrystals by SAXS

Hierarchical biotemplating in nanometer scale

Violation of Heisenberg’s Error-Disturbance Uncertainty Relation in Neutron Spin Measurements

Determination and speciation of Rh in cancer cells by TXRF and K-edge SR TXRF XANES

The Differential accumulation of S, Ca, Fe and Zn in human osteosarcoma tissue

SR µ-XRF Imaging of Human Osteoporotic Bone

X-ray strain microscopy of inhomogeneously strained Ge micro-bridges

Phase shift measurements with a neutron interferometer close to the Bragg condition

Crystal structures of the pestiviral protease Npro imply distinct roles for the catalytic water in catalysis

Ultracold neutron detectors based on Boron-10 converters used in the qBounce experiments

Cu doped ZnO – X-ray Absorption Near Edge Spectroscopy (XANES) and SQUID Magnetometry studies

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Neutron Radiography and Tomography at the Atominstitut

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Europe with its strong European neutron and synchrotron radiation sources, but also competitive national sources, has a prominent position to meet the society relevant key challenges concerned with health, sustainable energy supply, mobility, information and communication technology and innovative materials development.

It is a pleasure to host this symposium bringing together the Austrian community of Synchrotron and Neutron radiation scientists. This symposium highlights not only new scientific results from a broad community of the different user groups distributed over Austria. It should not only review the current status but also present an outlook and perspectives on the future trends and needs. Moreover, it provides a good platform to interchange innovative ideas concerning the future developments both in scientific experiments and instrumental techniques specifically offered at new ongoing source projects like ESS and XFEL. Hence, my special thanks go to the European guests from the synchrotron and neutron radiation facilities presenting the newest developments of their facilities.

Regarding an acknowledgement above all my sincere thanks go to the authors of the abstracts, the speakers, and all the participants of the symposium who as a matter of fact are the “essential ingredients” to make this symposium a resounding success. Last but not least I will not miss to mention the great work done by the organization committee and all the “helping hands” in the background that made possible that the idea of a symposium came into being.

I wish the conference every success and to all participants and guests fruitful discussions and insights.
Welcome address organizers

Motivated by the success of the first Austrian Synchrotron Radiation User Meeting in 2011 hosted by the BMWF, it was suggested by the Neutron and Synchrotron Radiation (NESY) section of the Austrian Physical Society (ÖPG) to organize a common symposium of the Austrian neutron- and synchrotron radiation users. The TU Wien (VR Fröhlich) kindly offered to host such a meeting and to provide also some additional financial support. The rest - perfectly coordinated by TU Wien and supported by the program committee - was straight forward, and is summarized in this abstract booklet of the first Symposium “Science at European Neutron and Synchrotron Facilities by Austrian Researchers”. But we did definitely not expect such a big interest in the symposium, and we can proudly announce that 135 participants have registered for the meeting, and 78 abstracts have been submitted for oral and poster contributions.

The meeting is pre-eminently dedicated to science. Keynote lectures by the scientific directors of the facilities with direct Austrian association will provide an overview of current and future possibilities at ESRF, ILL and ELETTRA. Two more keynote lectures will address the two most important future sources, represented by the scientific directors of the European X-ray Free Electron Laser (X-FEL) and of the European Spallation Source (ESS). Moreover 17 oral contributions from established scientists and 56 posters will give a broad overview of the Austrian research at large scale NE&SY facilities. The scientific program will be complemented by short information from the BMWF, from NESY, as well as from the Austrian representatives within the European Synchrotron User Organization (ESUO) and the European Neutron Scattering Association (ENSA). An open discussion about user needs and future wishes will conclude the symposium.

We are very proud that we could realize this symposium without having to collect a conference fee. In this respect, we are deeply indebted to the TU Wien for providing all facilities for free, and besides other Austrian universities for bestowing in addition the most substantial financial contribution. We are also very thankful that the keynote speakers were ready to travel on their own costs, and we wish to thank ELETTRA, ESRF, ILL, ESS and X-FEL explicitly for their contribution. We are also grateful to the ÖPG and the TU-Austria for financial support and to the companies PANalytical and ROFA/Rigaku, for sponsoring the meeting. In addition, we thank all the Austrian scientists for their contributions, being aware that the date in the middle of the semester and the missing financial support makes it quite challenging for some to attend. Finally, we wish to acknowledge the continuous support from the BMWF, with particular thanks MR Dr. Weselka for his sedulous dedication for the NE&SY community. We are confident that this meeting will help to make the Austrian NE&SY user community better visible in the public and within the decision making units in the ÖAW and the University Rectorates, and to achieve also in the future the necessary support from the BMWF for the Austrian memberships at large scale facilities.

On behalf of the program committee

Oskar Paris (NESY chairman)
Program
# Program: 11th November 2013, Morning

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<tr>
<td>10:00 — 11:00</td>
<td>NESY Meeting</td>
<td>AA 04 28 “Kuppel Seminar-Raum” 4th floor</td>
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<th>Time</th>
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<th>Name</th>
<th>Chair: J. Fröhlich</th>
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<tr>
<td>11:00 – 11:10</td>
<td>Welcome address: TU Wien</td>
<td>Johannes Fröhlich (TU Wien)</td>
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<tr>
<td>11:10 – 11:15</td>
<td>Welcome address: organizers</td>
<td>Klaudia Hradil (TU Wien), Christina Streli (TU Wien)</td>
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<tr>
<td>11:15 – 11:25</td>
<td>Welcome address: ÖAW</td>
<td>Günther Bauer (Uni Linz &amp; ÖAW)</td>
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<tr>
<td>11:25 – 11:35</td>
<td>Welcome address: BMWF</td>
<td>Daniel Weselka (BMWF)</td>
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<th>Chair: O. Paris</th>
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<th>Chair: O. Paris</th>
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<tr>
<td>12:20 – 12:45</td>
<td>Ronald Miletich- Pawliczek (Uni Wien)</td>
<td>In very tight places – Solids and their mechanical response at high pressures</td>
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| Time | Lunch Break/Poster, Kuppelsaal |
# Program: 11\textsuperscript{th} November 2013, Afternoon

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<th>Name</th>
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<th>Chair: H. Abele</th>
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<tr>
<td>14:15 – 15:00</td>
<td></td>
<td>Talk scientific director ESS</td>
<td>ESS: A source of discovery</td>
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<td>15:00 – 15:25</td>
<td></td>
<td>Peter Fierlinger (TU München)</td>
<td>Neutrons and the early Universe</td>
<td>H. Abele</td>
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<td>15:50 – 16:15</td>
<td></td>
<td>Thomas Loerting (Uni Innsbruck)</td>
<td>X-ray and neutron studies on amorphous ices</td>
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<tr>
<td>16:15 – 16:40</td>
<td></td>
<td>Roland Resel (Uni Graz)</td>
<td>Dynamical scattering effects in grazing incidence x-ray diffraction experiments: examples from organic thin films</td>
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**16:15 – 17:10**  
**Coffee Break, Kuppelsaal**

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<tr>
<td>17:10 – 17:55</td>
<td></td>
<td>Talk scientific director Elettra</td>
<td>The Future of Elettra and FERMI</td>
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<tr>
<td>17:55 – 18:20</td>
<td>Kristina Djinovic-Carugo (Uni Wien)</td>
<td>X-ray induced radiation damage on macromolecular crystals</td>
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<td>18:20 – 18:45</td>
<td>Nicola Hüsing (Uni Salzburg)</td>
<td>Synchrotron radiation based X-ray scattering: a powerful tool in materials chemistry</td>
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<td>18:45 – 19:10</td>
<td>Christoph Rameshan (TU Wien)</td>
<td>Synchrotron based AP-XPS for obtaining correlations between surface structure and catalytic selectivity</td>
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<tr>
<td>19:10 – 19:35</td>
<td>Michael Schöbel (MLZ/FRM II)</td>
<td>Multiscale tomography and diffraction for stress measurements and damage characterization in cast components</td>
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**19:35 – open end**  
**Dinner, Kuppelsaal**
**Program: 12th November 2013, Morning**

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<th>Chair: G. Bauer</th>
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<tbody>
<tr>
<td>09:00</td>
<td>Report BMWF</td>
<td>Daniel Weselka (BMWF)</td>
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<tr>
<td>09:10</td>
<td>Report NESY</td>
<td>Oskar Paris (chair NESY, Montanuni Leoben)</td>
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<tr>
<td>09:15</td>
<td>Report ENSA</td>
<td>Hartmut Abele (chair ENSA, TU Wien)</td>
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<tr>
<td>09:20</td>
<td>Report ESUO</td>
<td>Julian Stangl (chair ESUO, Uni Linz)</td>
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<tr>
<td>09:25</td>
<td>Talk scientific director ILL</td>
<td>Helmut Schober (ILL)</td>
<td>A short walk through recent ILL science highlights</td>
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<td>10:10</td>
<td>Coffee Break, Kuppelsaal</td>
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<tr>
<td>10:30</td>
<td>Talk scientific director Eu-</td>
<td>Thomas Tschentscher (European XFEL)</td>
<td>Science capabilities at European XFEL</td>
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<tr>
<td>11:15</td>
<td>Neutron scattering – from</td>
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<td>12:05</td>
<td>Overview on the application</td>
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<tr>
<td>11:15</td>
<td>Silke Bühler-Paschen (TU Wien)</td>
<td>Neutron scattering – from phonons to magnetic excitations</td>
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<tr>
<td>12:05</td>
<td>Martina Grieser (Kunsthistorisches Museum Wien)</td>
<td>Overview on the application of neutron and synchrotron techniques for studies connected to the Cultural Heritage</td>
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<tr>
<td>12:30</td>
<td>Michael Zehetbauer (Uni Wien)</td>
<td>In-situ Synchrotron Multi-Reflection X-ray Line Profile Analysis of Semicrystalline Polymers</td>
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<td>12:55</td>
<td>Mario Stefanelli (Materials Center Leoben)</td>
<td>X-ray Nanodiffraction Characterization of Residual Stresses and Microstructure in Thin Films</td>
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<td>12:55</td>
<td>Lunch Break/Poster, Kuppelsaal</td>
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## Program: 12th November 2013, Afternoon

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<tr>
<td>14:15 – 14:40</td>
<td>Martin Fally (Uni Wien)</td>
<td>Neutron optics using holographic gratings</td>
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<tr>
<td>14:40 – 15:05</td>
<td>Peter Geltenbort (ILL)</td>
<td>Particle Physics at the high-precision/low-energy frontier with Ultracold Neutrons at the Institut Laue-Langevin in Grenoble</td>
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<tr>
<td>15:05 – 15:30</td>
<td>Hinrich Grothe (TU Wien)</td>
<td>Inelastic Neutron Scattering and Neutron Diffraction of Nitric Acid Hydrates</td>
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### 15:30 – 15:40

**Coffee Break, Kuppelsaal**

### 15:40 – 17:00

**Moderated Discussion with Austrian users of large facilities**

- H. Abele (Austrian ENSA representative, TU Wien)
- G. Bauer (ÖAW representative, Uni Linz)
- J. Fröhlich (discussion leader, TU Wien)
- G. Krexner (chairman ILL Beirat, Uni Wien)
- O. Paris (chairman NESY and ESRF Beirat, Montanuni Leoben)
- J. Stangl (Austrian ESUO representative, Uni Linz)
- D. Weselka (BMWF representative)
- A. Franciosi (scientific director Elettra)
- A. Hiess (ESS, on behalf of D. Argyriou, scientific director ESS)
- H. Reichert (scientific director ESRF)
- H. Schober (scientific director ILL)
- T. Tschentscher (scientific director European XFEL)
Oral contributions: Keynote
The Upgrade of the ESRF: Science with Synchrotron Radiation from a 6 GeV Source

Harald Reichert

(1) European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, B.P. 220, 38043 Grenoble Cedex 9, France

The European Synchrotron Radiation Facility is Europe's premier hard X-ray synchrotron radiation source serving 45 experimental stations for public use. The facility is currently engaged in Phase I of an ambitious upgrade program (2009-2015) covering all aspects of the facility: photon production, experimental facilities for users, user service, and X-ray technology development. The upgrade benefits all areas of X-ray applications: Imaging, Spectroscopy, and Diffraction. 19 new or upgraded beamlines provide new opportunities for the study of materials with probing beams down to the nanometer scale. Selected examples will be used to demonstrate first results of the ongoing upgrade.

In parallel we have started work on the technical and scientific case for Phase II of the upgrade program focusing on a major upgrade of the storage ring with the goal to reduce the horizontal emittance by at least a factor of 30. The associated linear increase in brilliance and coherence caters for new applications of X-rays for the study of soft and hard condensed matter. Current planning aims for the realization of Phase II from 2015 to 2019.
ESS: A source for discovery

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Neutrons have been called beautiful because of their varied and unusual properties. The Nobel Laureate Bertram Brockhouse said of neutrons that if we did not have them, we would need to "invent them" in order to study novel states of matter. The basic advantage of neutrons are that they are charge neutral and thus highly penetrating, they obey conservation laws that allow us to probe both the time and spacial domains of materials, they possess a magnetic moment that makes them a probe of choice to investigate magnetism in materials and finally the exhibit sensitivity to light elements. These properties allow us to use neutron in a large variety of ways to examine materials from both the fundamental and technological perspective. It is for this reason that neutrons are deployed on diverse scientific areas such as archeology to ecology, from high-temperature superconductors to lipid membranes and proteins. The ESS will offer the brightest neutron fluxes in the world opening new horizons to materials research and fundamental physics. We shall look at our crystal ball (with some risk) at current trends in science that ESS can potentially impact and discuss some of the likely experiments that it will carry out. The European Spallation Source (ESS) is a joint project sponsored by 17 European countries, to build the world’s brightest neutron source for the study of materials and fundamental physics.
The Future of Elettra and FERMI

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The third-generation synchrotron radiation source Elettra in Trieste was upgraded with a full-energy injector and operates now routinely in top-up mode. Of the 26 operating beamlines the second highest in-demand from the international user community is the Small-Angle X-ray Scattering (SAXS) facility owned and operated by the Technical University of Graz. Starting next year, the SAXS facility will join the Central European Research Infrastructure Consortium (CERIC-ERIC), a new European entity of multi-disciplinary large scale facilities with statutory seat in Trieste, which will include institutions from Austria, Croatia, the Czech Republic, Hungary, Italy, Poland, Romania, Serbia and Slovenia.

We look forward to involve the Austrian user community in the exploitation of FERMI, the only seeded free-electron laser (FEL) user facility currently available worldwide. The FERMI FEL-1 line is open to users for wavelengths down to 10 nm, while the FERMI-FEL-2 laser line, optimized for 3 nm operations, is currently under commissioning. The seeded character of the source allows for unprecendented control in FEL pulse intensity, wavelength and linewidth and the APPLE-II undulators afford full control of the polarization. Some 25 international institutions are currently involved in the implementation of beamlines for diffraction and projection imaging, low density matter, elasting and inelastic scattering, terahertz and magnetic dynamics studies at FERMI.
In the year 2000 the ILL has embarked with the Millennium Programme a rigorous course of modernisation. Profiting from the most recent technological innovations the performance of the ILL instrument park could be enhanced enormously. Significant gains could be obtained from improvements in the neutron transport, the tailoring of the beams via adapted optics and the neutron detection.

The instrument and infrastructure upgrades have provided ILL users with completely new possibilities for conducting research. In my talk I will try to convey a flavour of recent scientific achievements in the broad field of research inherent to ILL ranging from a fundamental physics to biology and health.
European XFEL is a large international research infrastructure currently under construction in the Hamburg Metropol region, North Germany. This infrastructure will provide researchers with free-electron laser (FEL) radiation in the x-ray range from 0.25 to 25 keV. Six science instruments dedicated to a variety of x-ray techniques and applications will be available initially. The facility layout allows increasing the number of science instruments up to fifteen. In contrast to other FELs the x-ray beam delivery system at European XFEL foresees the parallel operation of three (later five) science instruments. This will dramatically increase the availability of hard x-ray FEL radiation for user experiments and therefore will allow broadening the user base of short-wavelength FEL science significantly. Another difference to existing FEL facilities is the possibility to generate and utilize a much increased pulse rate of up to 27,000 pulses per second. An overview of the related R&D efforts and the prospects for using such high repetition rates will be given in the talk. The construction of the European XFEL facility advances rapidly. Civil construction is nearing completion and the installation of the electron accelerator has begun. The design of the first x-ray instruments is almost complete and construction is about to start. First experiments are scheduled for 2016 and a brief status report is given.

The European XFEL facility addresses a large variety of science areas such as physics, chemistry, structural biology, materials sciences, or plasma and planetary physics. Hard x-ray FEL radiation is available since 2009 at the LCLS (SLAC, U.S.A.) and since 2011 at SACLA (Spring-8, Japan) and has since been applied in a broad scientific program. Highlight experiments will be described during the talk in order to demonstrate the new science capabilities provided by hard x-ray FEL radiation. In addition, new methods for generating FEL radiation with improved performance have been proposed and were partly tested. A brief overview of these new schemes allows extrapolating possible developments of these extremely brilliant x-ray sources in coming years.
Oral contributions
In very tight places – Solids and their mechanical response at high pressures

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The overall majority of matter exists at pressures different from 1 bar atmospheric condition. Non-ambient conditions shape our planets and turn everyday liquids and gases into condensed solids, exotic metals or unexpected molecular compounds. Solid materials exhibit a broad spectrum of polymorphism and polyamorphism, both in the crystalline and amorphous states, driven by the changes of electronic structures and chemical-bond interaction, which originate from densification and energy input at mechanical loads. Apart from state-of-the-art computational approaches, the experiment plays a key role in understanding chemical and physical properties of condensed matter under non-ambient and extreme conditions. Research has evolved into a strongly inter-disciplinary field at the intersection of various fields of sciences. The pioneering developments by Percy W. Bridgman (Nobel Prize in Physics 1946) initiated the successful era of experimental in-situ techniques, which nowadays allow to directly probe materials exposed to pressure and temperature, coupling static and dynamic techniques. Access to advanced in-situ characterization tools is provided through a large extent through dedicated large-scale facilities. Among them are high-intensity synchrotron radiation sources, high-flux neutron sources. These sophisticated tools can now be used to examine materials exposed to multi-megabar pressures at several thousands of Kelvin elucidate structures and dynamics over broad length and time scales.
The use of X-ray absorption and synchrotron based micro-
X-ray fluorescence spectroscopy to investigate anti-cancer
metal compounds in vivo and in vitro

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X-ray absorption spectroscopy (XAS) and micro-synchrotron based X-ray fluorescence (micro-SXRF) are element specific spectroscopic techniques and have been proven to be valuable tools for the investigation of changes in the chemical environment of metal centres. XAS allows the determination of the oxidation state, the coordination motif of the probed element, the identity and the number of adjacent atoms and the absorber–ligand distances. It is further applicable to nearly all types of samples independent of their actual physical state (solid, liquid, gaseous) down to μM concentrations. Micro-SXRF can provide information on the distribution and concentration of multiple elements within a sample simultaneously, allowing for the chemical state of several elements within subcellular compartments to be probed. Modern third generation synchrotrons offer the possibility to investigate the majority of the biologically relevant elements. The biological mode of action of metal-based compounds often involves interactions with target and/or transport molecules. The presence of reducing agents may also give rise to changes in the coordination sphere and/or the oxidation state. XAS and micro-SXRF are ideal techniques for investigating these issues. This review introduces the use of XAS and micro-SXRF techniques into the field of inorganic medicinal chemistry. The results obtained for platinum, ruthenium, gallium, gold and cobalt compounds within the last few years are presented.

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The neutron’s unique properties offer fascinating pathways to address fundamental questions in particle physics and cosmology. With extreme measurement precision at very low energies, neutrons are used to search for diluted traces of effects that once dominated the early Universe, some of them far beyond the reach of accelerators. Next generation flagship experiments are being enabled by strong sources like the ESS, but also at the FRM-II in Munich or the ILL in Grenoble. Also in the context of the recent discovery of the Higgs particle and the possible completion of the Standard Model of particle physics (SM), these efforts gain even more attention as highly promising approaches to find new physics. A prominent class of experiments are interferometric spin-precession measurements with trapped ultra-cold neutrons, developed to search for the time-reversal symmetry breaking electric dipole moment of the neutron. Such a phenomenon would be a manifestation of yet unknown broken symmetries above the TeV scale and is required to explain the matter-antimatter asymmetry in the Universe, as a natural consequence of most theories beyond the SM. Via such clock-comparison measurements, also Lorentz-Invariance and the CPT theorem, both foundations of our description of nature, will be probed with sensitivities close to Grand-Unified-Theories. This type of experiments is advancing technology with spin-offs in different fields of science, e.g. ultra-low field magnetic resonance. With the recent invention of a gravity resonance spectroscopy technique with neutrons, very sensitive searches for new gravity-like or spin-dependent interactions at short distances and selected dark matter candidates became feasible, also addressing physics closer than a nanosecond after the big-bang. Within the scope of these new techniques, also the equality of the electric charges will be investigated, one of very few possibilities to connect string theory to measurable quantities. Next to punctually probing quantities far beyond the reach of most other techniques, the investigation of the decay of the neutron and the properties of the decay products is a very valuable technique to deepen our understanding of the weak interaction. Implications of these experiments are for example the explanation of the formation and the relative abundance of the light elements hydrogen, deuterium, helium and small amounts of lithium and beryllium in the Universe during the so-called primordial nucleosynthesis. From angular correlations of the decay products momentum and polarization in neutron decay, also the validity of fundamental symmetries can be tested. An overview of the potential reach of such fundamental physics searches involving neutrons will be discussed in this presentation, based on selected examples supported by the German DFG priority program SPP 1491, which was initiated to pursue the above goals.
Neutron optical studies of fundamental phenomena in quantum mechanics

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Experiments with Si perfect-crystal neutron interferometers have been established as one of the most ideal method to study foundations of quantum mechanics [1]. In particular, the beam line S18 at the Institut Laue Langevin (ILL) has been serving the most powerful neutron interferometer setup in the world. The present setup at S18 is a multi purpose instrument for neutron interferometry and USANS (Ultra Small Angle Neutron Scattering) spectroscopy with wide range tunability of wavelength. The neutron interferometer setup S18 at the ILL has provided excellent opportunities of interference experiments with matter waves and has won high reputation. Over the last decades many different types of interferometer experiments have been performed, ranging from fundamental quantum investigations to applied measurements, such as precise measurements of coherent neutron scattering lengths. The former exploits the neutron interferometry as a matter-wave interference experiment and the latter is an important basis for other neutron scattering experiments. While matter-wave physics can be studied, e.g. also with electrons, atoms, ions and molecules, the features of neutron interferometry, such as macroscopic-scale experiments, high detector-efficiency, low decoherence-rate, and high-efficiency manipulation rate, make it unique for quantum mechanical investigations [2]. Neutron polarimetry is an alternative method to observe a phase difference between spin eigenstates, namely spin-dependent phase. This method is used various demonstrations of fundamental quantum mechanical phenomena such as non-commutability of Pauli matrices, Pancharatnam/Berry phase. A recent experiment with neutron polarization measurements enables the first test of Heisenberg’s uncertainty relation: this experiment reveals the violation of the original error-disturbance uncertainty relation by Heisenberg and confirms the validity of new formalation by Ozawa [3]. I am going to give an overview of neutron optical approach for investigations of foundation of quantum mechanics.


Figure 1, Neutron interferometer (left) and polarimeter (right) are used for investigations of foundation of quantum mechanics.
X-ray and neutron studies on amorphous ices

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Amorphous ices are the most abundant form of water in the universe, but still not much is known about their properties. Three distinct poly-a-morphic forms of water ice are now known, which can be interconverted by sharp transitions that are accompanied by sudden jumps in density. The low- and the high-density forms of amorphous ice transform by glass transitions to deeply super cooled liquids at ~116 K and ~136 K [1]. We studied the possibility of fast precursor dynamics in this temperature range on the high-Q backscattering spectrometer IN13 at ILL [2]. Thus, ultra viscous liquid forms of water may indeed exist in space and may act as a solvent for chemical reactions and the evolution of molecules under low-temperature conditions, e.g., in the process of planet formation or in cometary ices.

The molecular structure of these amorphous forms of water was deduced from isotope substitution neutron diffraction experiments at the SANDALS instrument at ISIS, with the main result that all the amorphous ices obey the Bernal-Fowler ice rules and that the jump like increase in density is achieved by an increase in coordination number. 0, 1 and 2 interstitial positions are occupied by water molecules in low-, high- and very-high density amorphous ice, respectively [3-6]. Besides the microscopic structure, we have also studied the evolution of the specific surface area and micro- and mesoscale structure in amorphous water-vapour deposits by combined small- and large-angle neutron scattering at the NIMROD instrument at ISIS. These data clearly indicate the presence of non-spherical, interconnected micropores, which experience 3D to 2D collapse upon heating [7]. Guest molecules are trapped irreversibly inside the pores and exert a high internal pressure on the surface, causing them to crystallize to clathrate hydrates. These are elusive guest-host inclusion components, in which volatile molecules are trapped in polyhedra made from water molecules. Such components usually do not appear in the vacuum, but at elevated pressures on the ocean floor [8].

Dynamical scattering effects in grazing incidence x-ray diffraction experiments: examples from organic thin films

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The structural properties of organic thin films are frequently investigated by grazing incidence x-ray diffraction (GIXD) experiments. Several crystallographic properties can be obtained from these investigations: the crystallinity of the organic material, the appearance of polymorph phases, the preferred orientation of the crystals, mosaicity and crystal size. However, dynamical scattering effects can cause considerable shifts of the Bragg peaks, also peaks from multiple scattering can appear. This talk will show examples of molecular crystals on surfaces from Tyrian purple, pentacene and ternaphtalene. Despite the fact that these three molecules are known to be crystalline, differences in the crystal quality are visible. The comparison of the diffraction pattern clearly shows that the dynamical scattering effects are less observable in weakly crystalline materials like Tyrian Purple, while highly crystalline materials like ternaphtalene show a them quite pronounced. Refraction correction has to be taken into account to understand the shift of Bragg peaks and the appearance of split Bragg peaks is explained by multiple scattering.

Figure: Grazing incidence x-ray diffraction (GIXD) pattern of thin films from the molecule ternaphtalene (left) and of Tyrian Purple (right).
X-ray induced radiation damage on macromolecular crystals

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Radiation damage to macromolecular crystals is an inherent problem of X-ray crystallography, especially at the highly brilliant synchrotron sources. Blake and Phillips carried out the first systematic study on radiation damage in protein crystals in 1962 at room temperature on myoglobin crystals. During the last decade the topic of radiation damage in macromolecular crystallography has become an increasing concern for structural biologists. It has become clear that, even with the crystalline sample kept at 100 K during the data collection, not only do the deleterious effects of damage affect the chances of successful structure solution, but they can also compromise the biological information that may be inferred from the results. An overview will be given on the current understanding of X-ray induced radiation damage and explored practical ways of mitigating its effects. Finally, a study will be reported on UV-vis micro-spectrophotometry/X-ray crystallography systematic study of a wide range of potential soaked-in scavengers to assess their capacity to: (i) alleviate photo-reduction of metal centres, (ii) to reduce global and specific radiation damage effects in presence of cryoprotectants and high concentrations of ammonium sulphate employed as a common precipitating agent. The study showed that due to the fast initial reduction of metal-centres it seems improbable that any concentration of the tested scavengers can efficiently protect the metal centres of metallo-proteins from X-ray induced photo-reduction.
Synchrotron radiation based X-ray scattering: a powerful tool in materials chemistry

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Advances in designing materials with well-defined chemical composition, e.g. silica, non-silicate oxides, phosphates or hybrid materials, and structures on different length scales from the nanometer level up to the macroscopic range play a vital role in manifold fields, e.g. adsorbents, protective coatings, biomaterials, heterogeneous catalysis or energy storage applications. Sol-gel chemistry is a remarkably versatile approach for fabricating (multi-)functional inorganic, organic and inorganic-organic hybrid materials ranging from highly porous, light solids, toughest ceramics to bioactive materials in various morphologies (coatings, monoliths, powders, particles). The high level of chemical control in the hydrolysis and condensation reactions of molecular precursors allow the combination and even deliberate positioning of various entities in these solid networks on the nanometer level.

Keeping in mind that nanoscale chemistry yields better materials, the need for techniques that allow for studying \textit{in situ} network formation on the nanoscale is evident. Small angle X-ray scattering has proven to be a very powerful tool to study structural properties of materials on this length scale. In combination with the high brilliance of modern synchrotron radiation sources local and time-dependent phenomena, as for example the network formation of colloidal particles in sol-gel materials can easily be followed [1-3].

In this presentation, examples from our joint work for the successful scientific development of sol-gel based materials supported by the precise structural analysis via small angle X-ray scattering will be presented. The focus will be on examples in which \textit{in situ} measurements have been performed, e.g. in supercritical carbon dioxide, high temperatures, etc, but also topical questions for future projects will be addressed.

Synchrotron based AP-XPS for obtaining correlations between surface structure and catalytic selectivity

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The interface between solids and gas govern many processes in the environment, the heterogeneous catalysis and in energy generation. As examples the removal of harmful components from automotive exhaust streams, the reaction of fuels at the electrodes of solid oxide fuel cells or the cloud droplet nucleation on atmospheric aerosol particles. There are several surface sensitive spectroscopies and microscopies that can be used to study vapor/solid interfaces, such as infrared spectroscopy (IR), vibrational sum frequency generation (VSFG), X-ray emission spectroscopy (XES), surface X-ray diffraction (SXRD), scanning tunneling microscopy (STM), transition electron microscopy (TEM) and scanning electron microscopy (SEM).

X-ray photoelectron spectroscopy (XPS) is one of the most versatile methods for the investigations of surfaces on the atomic scale [1]. It gives quantitative information about the elemental composition and about the chemical specificity (e.g., oxidation state) of the surface. Due to the strong interactions of electrons with atoms at typical electron energies used in XPS (100 eV – 1500 eV) the mean free path of the electrons is only on the order of several monolayers, giving XPS exquisite surface sensitivity [2]. Especially by using tunable synchrotron radiation the surface sensitivity can be enhanced to a maximum.

For measurements under elevated pressures it has to be considered that photoelectrons are strongly scattered by gas molecules, which complicates the application of XPS at this conditions. For instance, the inelastic mean free path of electrons with 100 eV kinetic energy in 1 mbar water vapor is about 1 mm [3]. This is much shorter than the typical working distance between sample and analyzer. The attenuation of photoelectrons by gas molecules can be overcome by the use of differentially pumped analyzer lens systems and a special geometry between X-ray source, sample and analyzer.

The proposed talk will focus on the method of synchrotron based XPS for obtaining detailed geometric and electronic surface structure on different materials. With the use of tunable synchrotron radiation a 3-dimensional picture of the near surface region can be obtained via depth profiling. Additionally the principles of XPS at elevated pressures (AP-XPS) and the needed advanced experimental equipment will be highlighted. On the example of selected research topics the possibilities of this spectroscopic method will be demonstrated. In particular how correlations between the electronic and geometric structure and the chemical reactivity of model systems can be obtained.

Multiscale tomography and diffraction for stress measurements and damage characterization in cast components

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The increasing demand on light weight and efficiency of modern combustion engines requires the implementation of light alloys with improved high temperature strength and creep resistance. Particularly, the cylinder head must be able to withstand multiple thermo-mechanical loads that can lead to stress-induced crack formation under operation conditions. Thus, new cast AlSi alloys are developed for structural parts to increase their long term stability in an engine. In cast components with complex shapes and composite-like microstructures, as it is the case of cast AlSi alloys, a superimposed macro-micro stress state influences crack formation and damage evolution. Models have been developed to simulate macroscopic stresses generated during casting and predict failure initiation in heterogeneous cast alloys on the microscopic scale. Although some effort has been made to validate these models experimentally, several unsolved physical matters have so far restricted their success of non-destructive internal stress analysis.

The grain structure of shape-ready produced components is coarse compared to small test specimens due to the slowly cooling rates after casting. Conventional non-destructive stress analysis like X-ray diffraction is limited by low grain statistics in a small gauge volume. Neutrons, which provide the highest penetration depth in metals, allow stress analysis deep inside bulk components with improved grain statistics in large gauge volumes. The alignment of samples with complex geometries is critical to avoid the gauge only being partially flooded by the beam, causing unpredictable surface effects. In the present work, X-ray tomography (XCT) was applied to image the internal structure of a cylinder head component of AlSi7MgCu for diffraction alignment. The real sample geometry and simulated stress results were overlapped three-dimensionally to allow in-axis strain mapping into the calculated principal stress directions using a robot sample positioning system at the STRESS-SPEC strain scanner at the high flux neutron source FRMII, Munich.

The heterogeneous microstructure of cast AlSi alloys causes local stress gradients by a combined effect of load partitioning between α-Al and Si phase and the CTE mismatch during changing temperatures. In-situ neutron diffraction during tensile testing was applied on StressSpec at FRMII for phase sensitive stress analysis in AlSi7MgCu. The results reveal the elasto-plastic deformation behavior between α-Al and Si. Complementary high resolution synchrotron tomography was applied on ID19 at ESRF on the same tensile test specimens as used for micro stress analysis to qualify the stress-induced damage mechanism in AlSi7MgCu. The results obtained in each set of experiments allow analyzing the influence of macro stresses on micro stress distributions and internal architecture of cast AlSi alloys on damage formation in cast engine components. Two examples of CT techniques are shown on different length scales complementary to non-destructive stress analysis by neutron diffraction. A new procedure for determination of elasto-plastic deformation in cast components will be proposed, with promising capabilities for industrial applications.
Neutron scattering – from phonons to magnetic excitations

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Neutron scattering is being broadly used to characterize solids. In many cases, it provides key information that advances the understanding of the material's physical properties substantially. In the talk, I will demonstrate this with two examples: (1) Intermetallic clathrates show extremely low lattice thermal conductivities and as such are promising materials for thermoelectric applications. To clarify the mechanism thereof, inelastic neutron scattering experiments on single crystals were used to determine the phonon dispersion relations [1]. (2) Strongly correlated intermetallic compounds are a topic of great fundamental interest. They typically contain rare earth elements like Ce or Yb which interact with the conduction electrons in the system, giving rise to complex magnetic properties. Of interest here are, e.g., the determination of the energies of the ground state 4f multiplets split by crystal electric fields, of magnetic structures, and of quantum critical fluctuations [2]. All experiments were done at European facilities.


Today non-destructive techniques are favorably applied for the investigation of invaluable artworks or objects of the Cultural Heritage, because “damage” to the original by taking – even very small – samples can be avoided. At the same time more accurate information on the manufacturing technique or composition of objects is asked for by scholars and restorers, so high sophisticated modern instrumental methods need to be applied for answering certain questions.

In special cases neutron, synchrotron and other ion beam techniques can help to answer some of the questions asked by archaeologists, art historians, numismatists and restorers in a non-destructive way.

The presentation gives an overview of selected examples of the application of neutron, synchrotron, and PIXE techniques to study coins of different origins to answer a variety of questions within projects performed at the Academy of Fine Arts Vienna and the Kunsthistorisches Museum Vienna during the last 10 years.

The studies include the investigation of ancient Greek bronze coins by neutron diffraction and neutron tomography for a better understanding of their composition and severe corrosion supporting their preservation. Also neutron diffraction phase and texture analysis on 16th century “Ferdinand-Taler” were used to distinguish genuine and fake coins. Furthermore, a series of Ottoman silver coins from the Hoard of Beçin was studied for the composition of their base alloys and origin and provenance of the minted metal using synchrotron X-ray fluorescence analysis (SRXRF) in combination with other analytical methods, e.g. Proton Induced X-ray Emission (PIXE).
In-situ Synchrotron Multi-Reflection X-ray Line Profile Analysis of Semicrystalline Polymers

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To date polymers and particularly semicrystalline polymers have gained considerable importance for structural applications in industries because of their relatively high strength and good processability. However, the changes in microstructure during plastic deformation are still not fully understood, due to their complexity in scales and phases. Within the crystalline phase of semicrystalline polymers, two mechanisms are likely to occur, i.e. (i) adiabatic melting and subsequent recrystallization, and (ii) crystallographic slip. Using the method of Multi-Reflection X-ray Bragg Profile Analysis (MXPA) [1], it was proven in some polymer systems [2, 3] that dislocations play a major role in process (ii). Making use of their characteristic strain field, MXPA [3] revealed to be capable of investigating the presence, density and character of dislocations [4].

We present results of several in-situ annealing and deformation experiments during X-ray diffraction carried out at the Austrian SAXS Beamline at Elettra. Careful MXPA evaluation gave a significant dislocation density of $1 \times 10^{15} \text{m}^{-2}$ for $\alpha$-isotactic polypropylene ($\alpha$-iPP), with a marked increase during deformation which, however, has not been observed for the $\gamma$-phase [4]. The latter combines with the very high strength of $\gamma$-iPP reported in literature suggesting a mechanism operating without dislocations.

Biodegradable poly(3-hydroxybutyrate) (P3HB) showed grown-in dislocations but no deformation induced ones leading to an increase of their density [6]. Here, microcracking and/or shear banding in the amorphous phase seem to be the predominant deformation mechanisms which is supported by the fact that only weak changes in texture are observed.

Also the annealing of deformation induced dislocations in $\alpha$-iPP has been studied by in-situ synchrotron X-ray diffraction. Samples have been cold rolled to high plastic strains - in order to introduce high densities of dislocations - and immediately stored in liquid nitrogen to prohibit any undesired relaxation or even losses of the defects introduced. MXPA evaluation of the in-situ annealing experiments reveals a continuous annihilation of dislocations up to the glass transition, followed by recrystallization and increase of lamellar thickness.

X-ray Nanodiffraction Characterization of Residual Stresses and Microstructure in Thin Films

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The aim of this contribution is to demonstrate our recent activities in the field of position-resolved X-ray nano-beam characterization of local microstructure and residual stresses in nano-crystalline thin films. Nano-crystalline thin films usually exhibit pronounced microstructure and residual stress depth gradients which predefine their physical and functional properties. Using a monochromatic beam of 100 nm, depth profiles of crystallographic texture, strain, composition and grain morphology were determined in nano-crystalline thin films using cross-sectional scanning wide-angle X-ray diffraction performed in transmission geometry at the nano-focus extension of the ID13 beamline. The new approach opens the possibility to map the structural properties of thin films on the sub-micron scale and, in the combination with finite-element modeling, allows assessing the residual stress gradients across compositionally graded nanostructures. Finally, the new approach opens a unique opportunity to correlate thin films performance and actual nanostructural design.
Neutron optics using holographic gratings

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All neutron-optical phenomena are governed by the neutron-optical potential or, equivalently, the neutron refractive-index. Thus, an important task in the design of neutron-optical elements is patterning the neutron refractive-index of materials in an efficient way. For this purpose we employ materials that are sensitive to light and use a holographic technique to produce diffractive optics for cold and very cold neutrons. We will discuss recent neutron-optic experiments with holographic gratings in which we have demonstrated that two- and three-port beam-splitters as well as free-standing film mirrors for cold and very-cold neutrons are feasible by exploiting the Pendellösung interference effect well known in dynamical diffraction theory [1-6]. Perspectives on novel optical devices for cold and very cold neutrons will be given.


In collaboration with: I. Drevensek-Olenik, S. Gyergyek (both J. Stefan Institute, Ljubljana, Slovenia), J. Kohlbrecher (ETH Zurich & PSI, Switzerland), P. Geltenbort (ILL, France)
Particle Physics at the high-precision/low-energy frontier with Ultracold Neutrons at the Institut Laue-Langevin in Grenoble

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Due to their outstanding property to be storable and hence observable for long periods of time (several hundreds of seconds) in suitable material or magnetic traps, ultra-cold neutrons (UCN) with energies around 100 neV are an unique tool to study fundamental properties of the free neutron, like its beta-decay lifetime, its electric dipole moment and its wave properties.

The search for the electric dipole moment (EDM) of the neutron plays a prominent role in particle physics because of its direct bearing on CP and T violation: a non-zero value of the neutron EDM would be evidence of CP and T violation.

Precision measurements of the neutron lifetime provide stringent tests of the standard electroweak model as well as crucial inputs for tests of Big-Bang nucleosynthesis. Neutron lifetime can be related to CKM Matrix unitarity. Neutron lifetime also dominates the uncertainty in theoretical calculation of primordial $^4$He.

After the observation of quantum states of UCN in the gravitational potential of the Earth, a new powerful resonance spectroscopy technique has been established. It allows precision experiments as tests of the equivalence principle and Newton’s gravity law at the micrometre scale.

In this talk, current ILL experiments linked to these fundamental questions are presented and a brief outlook is given.
Inelastic Neutron Scattering and Neutron Diffraction of Nitric Acid Hydrates

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The IPCC report 2007 underlines the particular importance of aerosol particles for the water cycle and the radiation balance, and thus for the global climate.[1] The contribution of aerosols and clouds to radiative forcing might be comparable to the most important greenhouse gases like CO₂ but is much less understood. Nitric acid hydrates are important constituents of solid cloud particles in the lower polar stratosphere (Polar Stratospheric Clouds) and the upper troposphere (Cirrus Clouds). The exact phase composition of these particles is still a matter of controversy.[2] Especially, metastable modifications have, as recent measurements show, a particular relevance for the atmosphere, which have been ignored up to now.[3] Spectroscopic data for their detection are urgently needed and can be gathered with laboratory models. Only recently we have recorded the FTIR and Raman spectra of all nitric acid hydrates, stable and metastable.[4,5] These data have been corroborated by X-ray diffraction measurements.[6] However, when interpreting the spectroscopic data it became evident that not all bands could be explained reasonably. Here, DFT calculations were extremely helpful [7], but still the translational and librational bands were not fully understood. Hence, inelastic neutron scattering was employed in order to investigate this region.

For neutron scattering and neutron diffraction, samples were prepared ex-situ in an amorphous state and were transferred into a cryostat, where the sample has been annealed. Characteristic changes have been observed and have been correlated with the respective phase transitions. The structure of an unknown nitric acid hydrate has been discovered and solved and has in turn allowed the calculation of its vibrational spectra.

Poster contributions
Simultaneous Small and Wide Angle X-ray Scattering (SWAXS) is considered in the meanwhile as standard tool for the structural characterization of nanostructures in all states of matter: solution, solid, surfaces and gas phase. The key factor of success is its versatile applicability and its high precision in structure analysis for tackling specific questions. By combining it with results from other complementary methods like e.g. electron microscopy detailed structural information (from atomic lattice to supramolecular envelope) can be obtained by performing simple and fast experiments under in situ conditions.

Although in the beginning the main focus of the beamline was devoted to time-resolved experiments down to the µs regime [1], in the meanwhile also a considerable fraction of work is done in the grazing incidence scattering geometry.

Some latest scientific highlights are presented covering biology and material science, such as phase transitions in biological relevant lipids, ultra-fast nucleation and growth, or (evaporation induced) self-assembly of mesoporous materials on surfaces and in the gas phase. Special attention will be given to the combination with other techniques (i.e. IR, UV-Vis, DSC).

X-ray Absorption Near Edge Structure Spectroscopy to Resolve the in Vivo Chemistry of the Redox-Active Indazolium trans-[Tetrachlorobis(1H-indazole)ruthenate(III)] (KP1019)

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Indazolium trans-[tetrachlorobis(1H-indazole)ruthenate(III)] (1, KP1019) and its analogue sodium trans-[tetrachlorobis(1H-indazole)ruthenate(III)] (2, KP1339) (Fig. 1) are promising redox-active anticancer drug candidates that were investigated with X-ray absorption near edge structure spectroscopy. The analysis was based on the concept of the coordination charge and ruthenium model compounds representing possible coordinations and oxidation states in vivo. 1 was investigated in citrate saline buffer (pH 3.5) and in carbonate buffer (pH 7.4) at 37°C for different time intervals. Interaction studies on 1 with glutathione in saline buffer and apo-transferrin in carbonate buffer were undertaken, and the coordination of 1 and 2 in tumor tissues was studied too. The most likely coordinations and oxidation states of the compound under the above mentioned conditions were assigned. Microprobe X-ray fluorescence of tumor thin sections showed the strong penetration of ruthenium into the tumor tissue, with the highest concentrations near blood vessels and in the edge regions of the tissue samples.

Figure 1. Molecule formulas of KP1019 (left) and KP1339 (right).

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Crystal structures of the latent and in vivo proteolytic activated aurone synthase from Coreopsis lanceolata

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Aurone synthase (AUS, EC 1.21.3.6) belongs to the family of the polyphenol oxidases (PPOs). These enzymes are type-III copper proteins, containing a dinuclear copper center, and catalyze the oxidation of monophenols to o-diphenols (monophenolase activity, EC 1.14.18.1) and the subsequent oxidation of o-diphenols to o-quinones (diphenolase activity, EC 1.10.3.1). Aurone synthase exhibits, in contrast to other PPOs, a high substrate specificity towards chalcones. These compounds are responsible for the yellow blossom coloration of several flowers, e.g. Asteracea.

Aurone synthase is expressed in its latent 64 kDa form. After proteolytic processing of the transit peptide, the C-terminus, which shields the active site of the enzyme, is proteolytically attacked, resulting in several different processed active and semi-active forms. The crystal structure of the active 42 kDa and the latent 64 kDa form will be presented to get further insights in the proteolytic activation mechanism, the enzymatic reaction mechanism and the physiological role based on aurone synthase as a specialized plant polyphenol oxidase.

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Synchrotron-based in situ XPS and XANES of CuNi-ZrO$_2$ during methane decomposition

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Ni/ZrO$_2$ is used as catalyst for methane reforming reactions, which are key processes for hydrogen production in industry and in solid oxide fuel cells. Nickel shows a good activity but is rapidly deactivated by coke formation, which is a major problem. The addition of copper and formation of a CuNi alloy are expected to reduce coke formation [1].

We have characterized zirconia based copper, nickel and bimetallic copper/nickel catalysts and explored the formation of the CuNi alloy, their catalytic properties for methane decomposition and the surface composition in the reaction atmosphere to get insights into surface processes occurring as a consequence of the reaction with methane.

The samples were prepared by impregnation of ZrO$_2$ with copper and nickel nitrate and calcined at 450 °C. The catalysts contain 5% w/w metal. For XPS an additional catalyst with 50% w/w metal was prepared.

In this contribution in situ X-Ray Absorption Near Edge Structure (XANES) and synchrotron-based in situ X-Ray Photoelectron Spectroscopy (XPS) were applied under reducing conditions and under reaction conditions in methane.

The formation of a copper-nickel alloy during reduction in hydrogen flow was observed by XANES indicated by a lower reduction temperature compared to monometallic copper and nickel catalysts.

In situ XPS of CuNi-ZrO$_2$ in 0.25 mbar methane was applied at different temperatures to allow for the quantification of the Cu:Ni ratio in the surface-near region. In the Cu 2p region it could be shown, that the amount of alloyed Cu on the surface increased with temperature. Copper carbonates formed at around 450 °C accompanied by strongly increasing hydrogen production at these conditions. At the same time a decrease of surface nickel carbonates was observed in the Ni 2p region with increasing temperature. The amount of coke formed on CuNi-ZrO$_2$ was much lower compared to Ni-ZrO$_2$.

Investigation of Hierarchical Mesostructured Silica Synthesized in the Gas Phase

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The spray-drying of aerosol droplets is an economically attractive method to obtain mesostructured nanoparticles.

Understanding the self-assembly process during the precursor’s condensation is the key to control the size and the architecture of the nanoparticles, which can be subsequently used for many different applications, i.e. as hollow delivery vehicles for drugs, or for catalysis.

In this communication the in-situ characterization with SAXS of the formation and organization of mesostructured silica nanoparticles synthesized in the gas phase will be presented.

Different precursor’s solutions were tested and the effect of increasing temperatures and humidity conditions during the evaporation process will be shown.
Deep X-ray Lithography for Biology and Material Science

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The integration of micro and nano-fabrication techniques with bottom-up and top-down processing of materials is fundamental, as the recent miniaturization of chemical and biological assays requires a careful selection of the fabrication methods and the development of tailored materials for specific applications. To produce functional integrated components there is need of techniques that achieve high aspect-ratio, patterning of thick layers, high resolution, and complex shapes. Deep X-ray Lithography (DXRL) is a very promising candidate both for the fabrication of microdevices and for top-down patterning. In this communication we will present an overview of our research on the application of DXRL dedicated to biology and material science. The activity was conducted at the DXRL beamline at Elettra synchrotron (Italy) where Graz University of Technology has a partnership. First, we will discuss microdevices fabricated for time resolved experiments of fast reactions [1], or for the study of confinement on crystal growth [2]. Then, we will present some examples of radiation assisted material synthesis and processing: micro patterning of mesoporous materials and simultaneous nucleation of metal nanoparticles [3], micro fabrication of mesoporous silica encapsulated enzymes for bio sensing [4], efficient functionalization of large quantities of carbon nanotubes [5], fabrication of micro channels with enhanced transport properties using a polymer whose micro porosity is tunable with the X-ray dose [6].

DXRL can really open new routes both in materials science and in the fabrication of micro-nano devices based on functionalized materials.

We present observations of transitions between quantum states of gravitationally bound neutrons using a three-part Rabi resonance spectroscopy setup.

In our experiments, ultra-cold neutrons are trapped in the gravitational field of the Earth. Quantum interferences between different states are observed by inducing transitions by mechanical vibration. The latest improvement, omitting the upper confining mirror, allows the shift from a frequency reference to a frequency standard, where the transition frequency depends solely on the neutrons mass, Planck’s constant and Earth’s gravity.

This tests Newton’s Inverse Square Law of Gravity in the micrometer range, which is sensitive to hypothetical Fifth Forces, the origin of the cosmological constant, as well as potential large extra dimensions of submillimetre size of space-time. Our experimental results agrees with Newton’s Inverse Square Law at the present sensitivity of $\Delta E = 10^{-14}$ eV.
Will batteries with tin nanocrystals work in winter?

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It is well known for several hundreds of years that tin based materials can undergo a phase transition when cooled below 13°C. Already Napoleons army might have been stopped by this phase transition on their invasion of Russia in the 17th century \cite{1}. The process of the phase transition is also called tin pest and limits that use of tin based materials in electronics \cite{2}.

In detail the process behind the tin pest is a crystallographic phase transformation of tin, which at normal conditions is stable in a tetragonal crystal structure (white tin, beta-form) and below 13°C is transformed to the diamond structure (gray tin, alpha-form). Along with this transformation also the material properties of tin change severely \cite{3}, while white tin is a metal needed for the application in electronic devices such as batteries, grey tin is a semiconductor.

We show that in tin nanocrystals with a thin oxide shell the transformation can not be found also in quite wintery conditions. By synchrotron powder diffraction measurements we monitor the crystal structure of the tin nanocrystals in-situ while cooling from room-temperature to -100°C and thereby confirm that the nanocrystals are stable in the beta-form. Our results show that for battery electrodes made from tin nanocrystals \cite{4} degradation during cold periods is not problematic.

\cite{1} http://en.wikipedia.org/wiki/Tin_pest
\cite{3} http://youtu.be/sXB83Heh3_c
Crystal structures of legumain reveal an open sesame activation mechanism

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The cysteine protease legumain plays important functions in immunity and cancer at different cellular locations, some of which appeared conflicting with its proteolytic activity and stability. Here we report crystal structures of legumain in the zymogenic and fully activated form in complex with different substrate-analogues [1]. We show that the eponymous Asparagine-specific EndoPeptidase activity (AEP) is electrostatically generated by pH-shift. Completely unexpectedly, the structure points towards a hidden carboxypeptidase activity that develops upon proteolytic activation with the release of an activation peptide. These activation routes reconcile the enigmatic pH-stability of legumain, e.g. lysosomal, nuclear and extracellular activities in immunology and cancer. A dual pH dependence tightly regulates substrate access and turnover by selective protonation of the S1 pocket (KM) and the catalytic nucleophile (kcat), respectively. The multi-branched and context-dependent activation process of legumain illustrates how proteases can act not only as signal transducers but also as decision makers.

Observing the Unobservable: Imaging the Wave Functions of Adsorbed Molecules

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In quantum mechanics, the electrons in a molecule are described by a mathematical object termed the wave function or molecular orbital. This function determines the chemical and physical properties of matter and consequently there has been much interest in measuring orbitals, despite the fact that strictly speaking they are not quantum mechanical observables. With results for prototypical organic molecules adsorbed on metal surfaces, we present a procedure for analysing angle-resolved photoemission data obtained at the Synchrotron Radiation Facility BESSY II, Helmholtz Center Berlin. This allows the recovery of both the spatial distribution and phase of molecular orbitals in excellent agreement with wave functions from ab-initio calculations. The technique requires no a priori knowledge of the orbitals and unlike other techniques to measure orbitals, such as laser tomography or STM, our approach enables orbital imaging for complex molecules and nanostructures and is applicable to more strongly interacting molecule-substrate systems. With the large angular accepting electron analysers now commercially available in combination with state of the art synchrotron radiation facilities, we foresee the technique to find many applications in chemical, physical and materials related sciences.

Confinement Effects of Li and Na in Nanoporous Glasses

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Effects of confinement on Li and Na in nanoporous systems (Vycor and Gelsil) are studied during in situ heating and cooling experiments. Porous silica matrices are loaded with metal using a vacuum vaporization method. Diffraction experiments using X-rays and synchrotron radiation show that, at ambient temperature, the metal inside the pores exhibits no more its bulk BCC structure but forms a mixture of several close-packed phases similar to the bulk low-temperature phase. On heating, the observed room temperature phases of Li and Na remain stable in crystalline form up to several hundred degrees above their bulk melting points.

X-ray diffraction patterns of Lithium in porous Vycor glass (pore size ~10 nm) during in-situ heating and cooling (closeup for small scattering angles).

While melting of bulk bcc Lithium occurs at 180°C various modifications of solid crystalline Lithium are observed up to at least 650°C in confinement. Chemical reaction with the glass matrix is found to set in only at still higher temperatures.

In addition, crystallization of the amorphous quartz matrix takes place on heating followed by the formation and crystallization of elemental silicon. Powder lines arising from the sample environment have been removed.
Neutron diffraction study of lattice damage induced by tritium decay in palladium tritide

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Tritium is an isotope which, for safety reasons, is usually stored in metals such as palladium where a metal hydride (tritide) with low equilibrium pressure is formed. Due to the radioactive beta decay of tritium (half-life 12.3 years) He-3 atoms are generated which are retained within the metal up to a concentration of about He/Pd = 0.33. However, various defects are gradually induced such as He bubbles, self-interstitial atoms, dislocations and dislocation loops entailing an increasing level of lattice damage with aging time. This process is studied by neutron scattering techniques both in single crystals and polycrystalline samples. The hydrogen charging process, generally, also induces lattice defects leading to diffuse scattering and, therefore, was studied in a deuterated sample.

Fig. 1: Diffuse intensity patterns around the (200) Bragg peak shown for a deuterated crystal (PdD, left) and two crystals charged with tritium and aged for 15 days and 1 year, respectively (PdT, center and right). The scattering patterns are plotted on a logarithmic scale (the numbers at the isointensity curves represent the log-10 logarithms of the intensity).

Comparison shows that the distortions arising from helium are much more significant than those due to deuterium charging. Quantitative analysis shows that the diffuse scattering in the aged samples is more strongly developed on the high-Q side in agreement with the presence of compressive strains such as created by the helium bubbles.
Exploring Fundamental Interactions via Neutron Decay

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The Standard Model (SM) of particle physics is a theory that describes all interactions of subatomic particles, except those due to gravity. Although the SM explains a wide variety of experimental results, it falls short of being a complete theory of fundamental interactions. Extensions of the SM are needed to explain its deficiencies.

Precision measurements of the parameters describing the beta decay of free neutrons address important questions in nuclear and particle physics, astrophysics, and cosmology \[1, 2\]. Our main emphasis is on the search for evidence of possible extensions of the SM and on searches for new symmetry concepts. In high energy physics with colliders, one directly searches for new particles, complementary to low energy physics with neutrons, where we indirectly probe their existence.

Together with scientists from the Universities of Heidelberg and Mainz, the TU München (all Germany), the Institut Laue-Langevin (ILL) in Grenoble (France), and the TU Wien, we propose to perform next generation high-precision measurements with the new instrument PERC (Proton and Electron Radiation Channel) \[3\]. In the search for new symmetries, measurements of correlation coefficients, inter alia $a$, $A$, $B$, $C$, and the Fierz interference term $b$, are of uttermost importance: unitarity of the CKM matrix, left-right symmetry, leptoquarks, supersymmetry, etc. With the new facility PERC, several symmetry tests based on neutron beta decay data become competitive \[4\].

PERC is under development by an international collaboration \[5\]. Until PERC is built and installed at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz in Garching (Germany), we perform precision measurements of neutron decay observables with the existing aSPECT \[6\] and PERKEO III \[7\] experiments at ILL.

A series of resonant magnetic x-ray scattering experiments have been performed on the magnetoelectric multiferroic DyMn$_2$O$_5$, with measurements in both the hard and soft x-ray regimes. Using resonant magnetic x-ray scattering, the magnetic structure of DyMn$_2$O$_5$ has been determined in the ferroelectric phase. The ferroelectric phase of DyMn$_2$O$_5$ was previously shown to have the largest polarization of all of the members of the R$_2$Mn$_2$O$_5$ (where R is a rare earth, Y or Bi ion) series of manganites [1]. The magnetic structure observed is similar in character to that discovered in other members of the series, but differs in the direction of the ordered moments. In DyMn$_2$O$_5$ the Dy and Mn moments are approximately aligned with the b-axis, whereas in the other members of the series, the magnetic rare earth and Mn moments are approximately aligned with the a-axis.

Pyroxene-type compounds have a rich magneto- and crystal chemistry. Especially the Li-bearing silicates Li(M\textsuperscript{3+})Si\textsubscript{2}O\textsubscript{6} with M = Fe, Ga, Sc, V show crystallographic phase transitions from a low temperature \(P2_1/c\) to a high temperature \(C2/c\) structure between 230 and 340 K [1]. We also have found that the analogue germanates exhibit similar phase transitions; however \(T_{Tr}\) is shifted towards higher temperatures by \(\sim 600\) K. On a polycrystalline sample of LiCrGe\textsubscript{2}O\textsubscript{6} we have done the in-situ low (0.3 K - 300K) and high temperature (300 K – 1473 K) neutron diffraction experiments to determine lattice parameter variation and the thermal expansion tensor and found the \(P2_1/c \leftrightarrow C2/c\) phase transition occurring between 1130 K and 1170 K. Similar to LiFeGe\textsubscript{2}O\textsubscript{6} the phase transition is accompanied by a large volume increase of 1.9 %. The variation of lattice parameters is linear over a wide temperature range. Towards low temperature, however there are some non-linear changes – as an example the \(a\)- and \(b\)-axes are shown – which are due to magneto-elastic couplings of the lattice. The strong changes above 1150 K are due to the \(P21/c \rightarrow C2/c\) phase transition. From neutron data also variation of structural parameters could be extracted with good precision. Especially the Li-O bonds show a distinct increase with both temperature and phase transition.

Magnetic ordering is observed below 6 K in the neutron diffraction data, this is somewhat higher than reported in the literature so far (\(\sim 3\) K.) Data could be indexed with \(k = (0 \ 0 \ 0)\) in space group \(P2_1/c\). Among the four possible irreducible representations only one gives satisfactorily description of the experimental data. This model of the magnetic structure has a pure antiferromagnetic arrangement of spins, both within and between the M1 chains, as displayed below. The spins are within the \(a-c\) plane with a neglecting component along the \(b\) – axis.

Nuclear and incommensurate magnetic structure of NaFeGe$_2$O$_6$ between 5K and 298K

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Pyroxene-type compounds are well known and studied in geo-science for decades. They are important constituents of the upper mantle and have a rich crystal chemistry, displaying several structural phase transitions as a function of temperature, pressure and chemical composition. However, they also possess interesting magnetic properties due to their low-dimensional structural characteristics with infinite chains of transition metal bearing M1-octahedra; the geometry of M1-octahedra and the interplay of magnetic moments within and between these chains is determining the magnetic spin structure. Among the members of the pyroxenes, one can find compounds with spin-gaps, pure ferromagnets and pure antiferromagnets and even multiferroics. In the last few years, we have studied in great detail the low temperature magnetic properties of the pyroxenes, among them CaM(Si,Ge)$_2$O$_6$ with M = Fe$^{2+}$, Ni$^{2+}$, Co$^{2+}$ and Mn$^{3+}$, LiFe$^{3+}$(Si,Ge)$_2$O$_6$, LiCrGe$_2$O$_6$, FeGeO$_3$, MnGeO$_3$ or CoGeO$_3$ [1] and references therein). In the present contribution we present results on the synthetic germanate-pyroxene NaFeGe$_2$O$_6$ and compare the results with the analogue silicate, also known as the fancy mineral aegirine.

The compound NaFeGe$_2$O$_6$ was grown synthetically as polycrystalline powder and as large single-crystals suitable for X-ray and neutron diffraction experiments to clarify the low temperature evolution of secondary structural parameters and to determine the low temperature magnetic spins structure. NaFeGe$_2$O$_6$ is isotypic to the clinopyroxene-type compound aegirine and adopts the typical HT-C2/c clinopyroxene structure down to 2.5 K. The Na-bearing M2 polyhedra were identified to show the largest volume expansion between 2.5 K and room temperature, while the GeO$_4$ tetrahedra behave as stiff units and tend to shrink with increasing temperature. Magnetic susceptibility measurements show a broad maximum around 33 K, which marks the onset of low-dimensional magnetic ordering. Below 12 K NaFeGe$_2$O$_6$ transforms to an incommensurately modulated magnetic spin state, with k = [0.323, 1.0, 0.080] and a helical order of spins within the M1-chains of FeO$_6$ octahedra. This is determined by neutron diffraction experiments on a single-crystal. Comparison of NaFeGe$_2$O$_6$ with NaFeSi$_2$O$_6$ is given and it is shown that the magnetic ordering in the latter compound, aegirine, also is complex and best is described by two different spin states, a commensurate one with C2/c' symmetry and an incommensurate one, best being described by a spin density wave, oriented within the (1 0 1) plane.

X-ray micro tomography can describe the three dimensional internal microstructure of materials also under the effect of external thermal/mechanical/thermo-mechanical loads [1]. This technique is applied to study the microstructural evolution of A206 (AlCu4.5Mg0.3) and AlCu7 alloys as function of solution treatment (ST) time: 1h, 4h and 16h at 530°C. All samples were overaged 100h at 250°C.

![Figure 1](image)

Figure 1 shows the evolution of the volume fraction (Vf) and interconnectivity (volume of biggest aluminide/total aluminide volume) of the aluminides. It was observed that there is a partial dissolution of the phases segregated during casting that stabilizes at <4h ST and the interconnectivity remains over 80% for both alloys. In situ synchrotron tomography is carried during tensile deformation out to characterize the damage mechanisms and evolution. Damage initiation seems to be more likely in the aluminides with a large surface or eutectic areas perpendicular to the loading direction. Cracks propagate along the aluminide network while shrinkage pores ~ (100 µm)³ play a minor role either for initiation or propagation. This confirms that the interconnectivity of the aluminides network plays a decisive role in the crack propagation process. The alloy after 4 h ST shows an ultimate tensile strength ~ 50 % higher than in as-cast condition as well as an increase of ductility by a factor of ~ 3. The Vf of voids created in the plastic region up to the UTS for the A206 (AC and 4h) is the same, although this is reached at a higher strain after 4 h of ST. This indicates that the microstructure is able to accommodate the same amount of damage in AC and 4 h ST conditions. The fact that the ST alloy shows an increase of strength together with an increase of ductility is a result of the homogenization of rigid phases that retards the damage formation in the highly interconnected alumide network.

Phase transformation kinetics during continuous heating of a \(\beta\)-quenched Ti\(_{10}\)V\(_2\)Fe\(_3\)Al alloy

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The effect of heating rate on the phase transformation kinetics of a Ti-10V-2Fe-3Al metastable \(\beta\) titanium alloy quenched from the \(\beta\) field is investigated by fast in situ high energy synchrotron X-ray diffraction and differential scanning calorimetry. The initial microstructure is formed by \(\alpha''\) martensite distributed decorating grain boundaries of the retained \(\beta\)-phase matrix and dispersed \(\omega\) particles.

At low temperatures (~ 170 – 315 °C) a \(\alpha'' \rightarrow \beta\) reversion associated to a one-way shape memory effect takes place. The degree of transformation increases with the heating rate and a full reversion of \(\alpha''\) into \(\beta\) is achieved at 50 K/min. Precipitation and growth of the \(\omega\) phase is observed for 5 and 20 K/min heating rates during the shape memory effect, while at higher temperatures (~ 250 – 400 °C) stabilization and growth of solute depleted \(\alpha''\) occurs. An example of this sequence is illustrated in Fig. 1a), where the intensity fall of the \(\alpha''\) reflections at around 300 °C coincides with the appearance of small diffraction peaks corresponding to \(\omega\). For the 50 K/min heating rate reflections similar to those expected for \(\alpha''\) suddenly grow at ~ 450 °C from \(\beta\).

Between ~ 420 – 650 °C \(\alpha\) forms through three different paths: a) as an evolution of the orthorhombic structure transformed from the \(\alpha\) phase (\(\alpha \rightarrow \alpha'' \rightarrow \alpha\)), b) from the orthorhombic \(\alpha''\) martensite (\(\alpha'' \rightarrow \alpha\)) and c) from the \(\beta\) phase (\(\beta \rightarrow \alpha\)). These transformations can be observed in Fig. 1b) for the 5 K/min condition.

Fig.1. a) Example of the evolution of the diffraction patterns and b) cell parameters obtained during a 5K/min continuous heating.
3D Damage characterisation during sequential tensile loading of a multidirectional carbon fibre reinforced epoxy laminate

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Damage of carbon fibre reinforced polymer matrix composite laminates subjected to tensile stress is characterised by intra-laminar cracks, delamination between plies, fibre pull-out and fibre fracture [1]. The aim of this work is to follow in-situ the formation and evolution of damage as well as the change in fibre orientation in a multidirectional carbon fibre reinforced laminate during tensile loading. The laminate was manufactured by hot pressing. Six prepreg-layers with a nominal thickness of 0.19 mm were stacked with a [+45/-45/+45]s lay-up. Synchrotron micro tomography was carried out in-situ during tensile deformation of a notched sample with a notch radius of 1 mm and a cross section of ~1 mm² at the ID15A beamline of the European Synchrotron Radiation Facility. The first tomographic scan was performed using a preload of ~5 MPa. Then, the sample was deformed stepwise using constant steps with a strain rate of 5 µm/s. Nine tomographic scans were carried out at each deformation step until fracture. Volumes of 1017x1017x800 voxels with a voxel size of (1.4 µm)³ were obtained after reconstruction. Only one manufacturing pore was found within one of the plies, whose size 0.4·10⁶ µm³ represents 0.05 vol.%. Pre-existing cracks within plies dominate damage progression over manufacturing porosity. The change of orientation of the carbon fibres during tensile deformation was investigated for each ply. Fibres rotate about 2° aligning in the loading direction independently of the position of the ply within the laminate.

Residual stresses in continuously cast steel slabs

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Steel slabs produced by continuous casting allow fast processing. The molten metal is poured into a channel through a nozzle and bent by rolling while solidification takes place. The partly solidified slab suffers a combination of internal stresses by thermal gradients, phase transformation and externally applied deformation. A complex superimposed stress situation is responsible for crack formation during cooling and further manufacturing. The current simulation models take into account thermal stress calculations, which deliver the starting stress condition to predict crack formation and failure. The experimental proof of this initial stress state in steel slabs is still missing.

Non-destructive neutron diffraction was applied in-situ on a large continuously cast steel slab, with an initial thermal gradient to simulate solid state cooling during the casting process. Neutrons were chosen as probe particles due to their high penetration depth in metals to enable diffraction on coarse grained cast structures under extreme conditions. In-situ strain scanning was performed to determine the temperature dependent strains as a function of depth in the slab during cooling. Additional stress mapping at room temperature in segments of a steel slab revealed the 3D macro stress state after casting.

The stresses originating from the austenite (f.c.c.) to ferrite (b.c.c.) phase transformation dominate the stress state, during and after cooling. The volume increase of ~ 1% by phase transformation produces high macro stress gradients which superimpose to the thermal stresses. The phase sensitive strain analysis of the in-situ experiment during cooling, while passing the transformation temperature, was correlated to the final 3D stress state measured in the as cast condition at room temperature. Compared to the thermal model, an overall inverse stress situation was observed, as a consequence of transformation gradients during cooling.
Load partitioning and microstructural evolution in Ti-alloys during hot tensile tests

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Synchrotron X-Ray Diffraction (SXRD) has become an essential tool to study either the averaged internal stresses in the bulk or the microstructural changes with time of multiphase materials. Its high penetration, high flux and short acquisition times in comparison with laboratory X-ray diffraction allow to characterize the phase evolution in short time tests. The present work shows in situ investigations using this technique to follow the evolution of both internal strains and microstructure during tensile tests of Ti\(_6\)Al\(_6\)V\(_2\)Sn (Ti662) at different temperatures in argon atmosphere. A monochromatic beam with a 2D-Detector was used for this purpose. Ti662 alloys were produced by means of two different processing routes, i.e., powder metalurgy (PM) and ingot (ING). PM material exhibits lamellar microstructure and the ING material has globular microstructure provoked by the pre-forging process. Analyzing the different crystallographic planes in the load direction, strains in \(\alpha\)-phase are always higher compared with those in the \(\beta\)-phase. For the PM material, \(\alpha\)-phase shows maximum strains at the maximum tensile stress and subsequently softens due to damage in the samples, while the ING material exhibits plastification once the maximum tensile stress is reached. The orthogonal direction exhibits the Poisson’s effect with negative strain values for all the materials and tests. The evolution of the microstructure is analyzed by processing the Debye Scherrer rings for different crystallographic planes of the \(\alpha\)- and \(\beta\)-phases. The PM material exhibits subgrain formation in the \(\beta\)-phase, observed as a spreading of the spots. Rotation of \(\alpha\)-phase can be determined by a splitting of the spots. In ING samples this effect is not observable due to the fine microstructure. Electron BackScatter Diffraction (EBSD) before and after the tensile tests confirm these microstructural changes showing the subgrain formation in the \(\beta\)-phase and the lattice rotation of \(\alpha\) grains with increasing strain.
Innsbruckite, Mn$_{33}$(Si$_2$O$_5$)$_{14}$(OH)$_{38}$: a new manganese phyllosilicate mineral from the Tyrol

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The mineral was discovered in a Mn-rich carbonate layer sandwiched between a serpentinite body and cherts at the locality Staffelsee, Geier in the innermost Wattener Lizum (Tyrol, Austria). Geologically these rocks belong to an Austroalpine nappe called the Tarntal mesozoic. The serpentinite belongs to the Reckner complex and the cherts are part of the Ruhpolding formation. The sample was collected during the diploma thesis of Klier [1].

Small fragments of crystals have been extracted from a thin-section, and investigated using single-crystal synchrotron diffraction experiments at the X06DA beamline at the Swiss Light Source (Paul Scherrer Institute, Villigen, Switzerland). The crystal structure was solved and refined in space group Cm ($a = 17.2760(19)$, $b = 35.957(5)$, $c = 7.2560(8)$ Å, $\beta = 91.359(7)^\circ$ and $Z = 2$). The structure can be described as a 1:1 single layer silicate (monophyllosilicate), which exhibits a new layer topology. The layers are built from 8-, 6-, 5-, and 4-membered rings in a ratio of 2:9:2:1, respectively (Fig. 1). The unbranched fundamental chain has a periodicity of 7. According to the nomenclature of Liebau, the silicate sheets are siebener single layers with the symbol $\{uB,7,12\infty\}$ representing the silicate anion. To our best knowledge no other minerals or synthetic structures with siebener single layers are known. The free apices of the silicate layer connect to both neighbouring MnO$_6$ octahedral layers. The hydro-gen atoms are bonded to the free oxygen atoms (the ones not bridging between tetrahedra and octahedra) at the surface of the octahedral layers.

![Figure 1: The $\{uB,7,12\infty\}$ silicate layer of Mn$_{33}$(Si$_2$O$_5$)$_{14}$(OH)$_{38}$. The fundamental siebener chain is parallel to $a$ (numbered tetrahedra 1-7).](image)

Temperature-induced phase transitions in KMnPO₄

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KMnPO₄ is a representative from the large class of ABW-type zeolite compounds with threedimensional tetrahedral framework structures [¹]. At room temperature it has the lowest possible space group symmetry (P -1) of all members of this family [²]. Own studies revealed the existence of several phase transformations of this compound. DTA experiments showed a sequence of six reversible phase transitions between RT and 500°C at temperatures of 169, 340, 354, 359, 365, 385°C (Fig. 1). However, by X-ray powder diffraction analysis using a lab diffractometer we were able to detect only one phase transition at 400°C. Given the low symmetry of KMnPO₄ (P -1), fast kinetics and small changes in the crystal structure, time resolved high temperature in-situ synchrotron powder diffraction experiments with extremely fast data acquisition were performed at the X04SA beamline at the Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland, using radiation of 0.775Å and the latest generation Mythen II detector. The diffraction data show rich detail in the temperature region above the pronounced transition at 340°C (Fig. 2). The expected results of the ongoing data evaluation will be fundamental for the understanding of temperature induced phase transformation mechanisms of zeolite ABW-type materials and for the general knowledge of the crystal chemistry of inorganic three-dimensional tetrahedral framework structures under non-ambient conditions.

Figure 1: DTA signals of a series of phase transitions at ca. 340, 354, 359, 365 and 385°C.

Figure 2: Temperature-dependent powder diffraction data of KMnPO₄. Δ T=0 corresponds to the pronounced transition at ca. 340°C (see Fig. 1).

Using synchrotron based XPS to characterize ZrO₂ ultrathin film grown on Pt₃Zr

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ZrO₂ is widely used in the field of heterogeneous catalysis, and is known as an excellent support and catalysts material itself [1]. However, microscopic mechanisms of the functions of ZrO₂ and of the oxide-metal interactions need to be better understood. In order to conduct fundamental studies on ZrO₂ via a surface science approach, thin film model catalysts have been prepared and characterized.

In this study, a previously described route was followed to obtain well-ordered and ultra-thin zirconia film [2]: A cleaned Pt₃Zr (0001) alloy substrate was oxidized at 673 K, followed by post-annealing at 1023 K. The chemical composition of the film is investigated by high resolution X-ray Photoelectron Spectroscopy (XPS) based on synchrotron radiation. The structure of the film is characterized by Scanning Tunneling Microscopy (STM).

Besides a signal for metallic zirconium from the substrate (Zr-substrate), XPS showed two distinctive oxidic species (Zr₁st and Zr₂nd) upon oxidation at 673 K and post-annealing at 1023 K. With increasing photon energy, the ratio between Zr₂nd and Zr₁st increased, indicating that Zr₂nd are located in a deeper layer than Zr₁st. After post-annealing of the oxide at 923 K, STM detected many small clusters with a height of about 1nm, in addition to the film terraces. Increasing the annealing temperature to 1023 K led to the disappearance of a considerable amount of the small clusters, accompanied by the significant decrease of the intensities of Zr₂nd shown by XPS. Therefore, Zr₁st and Zr₂nd could be assigned to Zr oxide species within the trilayer thin film and Zr oxide specie in the clusters, respectively.

In situ HP-XPS during methanol decomposition and oxidation on Pd(111)

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Pd alloys have recently raised great interest as catalysts for hydrogen production via methanol steam reforming (MSR). In this work we could show that instead of the formation of a selective palladium-carbon phase at elevated temperature, the Pd(111) catalyst was significantly covered (poisoned) by laydown of carbonaceous species during methanol decomposition. Graphitic carbon is the dominant species in pure MeOH atmosphere, most pronounced at 330 °C due to intensive formation of carbonaceous species (CH<sub>x</sub>) via C-O bond cleavage. These carbonaceous species effectively block the Pd surface. The amount of poisoning could be drastically removed upon adding O<sub>2</sub> to the reaction feed. At 330 °C the surface was actually completely free from carbon.

Figure 1: Methanol decomposition on Pd(111): 0.5 mbar CH<sub>3</sub>OH + 0.1 mbar O<sub>2</sub> at various temperatures.

Like presented in Figure 1, we could demonstrate that ambient pressure XPS is a valuable tool to study a catalytic reactions, e.g. it allows to follow the presence/absence of species depending on reaction conditions, their quantification and depth profiling via photon energy variation.
Following \textit{in situ} Regeneration and Ordering in Amorphous Cellulose Thin Films via GISAXS

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Despite more than 150 years of intense research on cellulose, the interaction between water and cellulose is still not understood although this has strong implications on the industrial applicability and materials properties of cellulosic materials. One reason for this lack in knowledge is the inhomogeneity of the samples under investigation (e.g. fibers and pulps are highly inhomogeneous in terms of composition, crystallinity and surface morphology). A more convenient way for the investigation of structure-property relationships in cellulosic materials is the use of amorphous cellulose model films.\textsuperscript{1} These films have a defined surface morphology, composition and degree of crystallinity.\textsuperscript{2} As starting material trimethylsilylcellulose (TMSC), a cellulosic derivate which is highly soluble in organic solvents due to the presence of hydrophobic side chains, is used to prepare model films in the sub nanometer range. Uniform and homogeneous thin films are prepared via spin coating with a low overall RMS roughness.\textsuperscript{3} In acidic vapor the trimethylsilyl groups are cleaved off and a pure cellulose film remains. This process is better known under the term regeneration. The morphology, crystallinity and surface energetics are studied using atomic force microscopy (AFM), grazing incidence x-ray diffraction (GIXD) and contact angle measurements, respectively.\textsuperscript{2,4} The regeneration was followed using \textit{in situ} synchrotron grazing incidence small angle x-ray scattering (GISAXS) at the Austrian SAXS beamline at the ELETTRA synchrotron in Trieste (IT). Further the structural dependent changes upon heat treatment and relative humidity changes are investigated.

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In-Situ SAXS and Microfocus XRD of Hierarchical Materials

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Modern European Synchrotron Facilities are state of the art research tools providing possibilities far beyond laboratory X-ray equipment. The focusing techniques and a very high brilliance allow experiments with high spatial resolution and allow studying time dependent processes in-situ with high accuracy.

In our poster four examples for measurements at the Synchrotron Facilities of Elettra – Trieste, BESSY – Berlin, and ESRF – Grenoble are given:

- The formation of a mesoporous networks from water soluble bridged phenylene ethylene glycol-modified silane was studied in real time in dependence of the solvent concentration at ID 2 at ESRF, Grenoble.
- The structural development of polystyrol cross-linked with a different amount of a multifunctional zirconium oxo- cluster was followed in-situ during tensile tests at the Austrian SAXS beamline at Elettra, Trieste.
- The structural change of different types of single carbon fibers due to creep at high temperatures and loads was investigated in-situ at the µ-Spot beamline at BESSY, Berlin.
- A complete image of the helical arrangement of cellulose fibrils in the S2 layer of wood cells was obtained by application of position-resolved synchrotron X-ray micro diffraction at ID13 at ESRF, Grenoble.

All examples show new and valuable information only accessible with Synchrotron Facilities – the results have been published in highly acknowledged journals.
Experiments with Si perfect-crystal neutron interferometers have been established as one of the most ideal method to study foundations of quantum mechanics [1]. In particular, the beam line S18 at the Institut Laue Langevin (ILL) has been serving the most powerful neutron interferometer setup in the world. The present setup at S18 is a multi-purpose instrument for neutron interferometry and Ultra Small Angle Neutron Scattering (USANS) spectroscopy with wide range tunability of wavelength. Many experiments have been carried out, like measurement of Bell-like inequalities and a lot of topics are on the list of future investigations at S18, such as quantum weakness experiments and Aharonov’s quantum Cheshire cat. Since these experiments demand high stability in phase and therefore in temperature. Such a high stability can only be achieved by proper thermal insulation and regulation: this should be done not only around the interferometer but also in the monochromator-crystal region, i.e. of the whole optical bench. This is due to the fact that, according to our estimation, instable temperature around the monochromator-crystal by 0.1°C as well as that around the interferometer by 0.01°C already gives phase drift by 1° of the interferogram. In parallel, the reduction of temperature gradients is crucial for higher contrasts. We are planning an upgrade of the S18 beamline.

Figure 1: Neutron interferometer (left) and Ultra small angular scattering (USANS) spectrometer (right).

Crystallization kinetics in hydrogen bonded pseudo-block copolymers measured by in-situ SAXS

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The kinetics of structure formation in novel “pseudo block copolymers” has been determined by in-situ Small Angle X-ray Scattering (SAXS). The competition between microphase separation and crystallization at the nanoscale, has been investigated in polymeric samples consisting of PCL (poly(ɛ-caprolactone)) and PIB (poly(isobutylene)) blocks.

The blocks are not covalently bonded, as it is usual in block copolymers, but are weakly connected by hydrogen – bonds appearing between the thymine and 2,6-diamino triazine groups, linked to the individual blocks. These hydrogen-bonds lead to a so called supramolecular interaction between the blocks.

The melting point of PCL is around 55°C. After fast cooling the material below the melting point, crystallization of nanometer sized building blocks starts and occurs the faster the lower the temperature is. Thus, high time resolution is required to follow the formation of the structure.

The intensities obtained from the SAXS patterns allow the application of Avrami theory. Measurements at different temperatures make the determination of the activation energy of the crystallization process possible. In order to realize the in-situ experiment, an X-ray transparent Peltier device was developed, which can be built into either the vacuum chamber of the laboratory SAXS equipment or can be transported to synchrotron radiation sources for fast quenching experiments with extremely high time resolution.
Preparing a Measurement of the Charge of the free Neutron within qBounce

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With a new Gravity Resonance Spectroscopy technique we plan to probe the electric neutrality of the neutron. This is possible by using Ramsey’s Method of separated oscillating fields. The approach has the potential to improve the 25 years old existing limit [1] [2]. Our project is related to the question of the quantisation of the electric charge, which is a well established experimental observation. Since charge quantisation in the Standard Model of Particle Physics requires an additional free parameter that must be determined experimentally a charge measurement is a promising way to refine the theoretical framework. Further it has consequences for various topics i.e. neutron-antineutron oscillations or the search for a Grand Unified Theory.

PERC: The future neutron beta decay facility

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High precision experiments in neutron beta decay can solve open questions in particle physics and cosmology [1, 2]. Main emphasis lies on the search for evidence of possible extensions of the Standard Model (e.g., SUSY, right handed currents, etc.). The new user facility 'Proton and Electron Radiation Channel' (PERC) is designed to provide a high intensity beam of charged neutron decay products. The phase space of the particle beams can be precisely selected by the adjustable instrument setup. That way, we can measure energy spectra and angular correlation coefficients of the decay products with unprecedented precision [3] and determine unmeasured parameters, e.g., the Fierz interference term.

PERC is under development by an international collaboration and will be installed at the FRM II in Munich, Germany. The Vienna group focuses on the PERC instrument design as well as energy and momentum spectroscopy of the decay products in the analyzing area. The completed magnetic field design and design proposals for post-spectrometers will be presented on this poster.

We present a novel type of neutron spin resonator for precise wavelength selection and definition of the time structure of thermal, cold and even very cold polarised neutron beams [1]. This device exploits the fact that upon passage of neutrons through a spatially alternating transverse static magnetic field each neutron in its rest frame experiences an alternating field with a frequency depending on the neutron velocity and the spatial period of the resonator. If this frequency equals the Larmor precession frequency a resonant spin flip will take place [2]. Furthermore, the tailoring of the time structure of this neutron beam is completely decoupled from the adjustment of the wavelength resolution and allows for almost arbitrarily shaped neutron pulses by purely electronic means.

To demonstrate the feasibility of this technique, we designed and engineered two prototypes consisting of individually ultra-fast switchable aluminum stages for the generation of neutron pulses in the microsecond regime [3]. These resonators were installed at a polarised neutron beamline at the 250 kW TRIGA reactor of the Vienna University of Technology. Driven by the promising results of these test measurements, a new resonator, for the application at very cold neutron (VCN) beamlines, has been developed. Here, we present results which demonstrate the successful operation of this device [4].

These developments are connected to the PERC project which searches for new physics beyond the Standard Model of particle physics via the beta-decay of free neutrons [2]. The related high precision measurements demand perfect knowledge of the key beam parameters, like wavelength distribution, degree of polarisation and time structure. Another direction is the implementation of our device as integrated monochromator and chopper for advanced neutron time-of-flight spectroscopy. In this context a novel Ramsey-type setup was introduced and experimentally tested [5].

Ultra-small-angle polarized neutron scattering (USANSPO) allows for the study of magnetic structure in condensed matter in the micrometer range [1]. This technique takes advantage from the narrow angular width of the Bragg reflection by perfect crystals and is employed in a double-crystal configuration of perfect silicon crystals. Angular-correlated polarisation of the neutron beam is obtained by placing magnetic prisms between the monochromator and the analyser crystal [2]. Then, samples are placed between the polariser prisms and the analyser crystal. The scattering of spin-up and spin-down neutrons is recorded in a single measurement and identified by an angular shift of their respective scattering curves [3].

We have developed a special sample environment and handling system by which anisotropic samples may be aligned in different orientations and be subjected to varying external magnetic fields and mechanical stresses [4, 5]. Here, we present experimental results on a variety of magnetic ribbons which represent both novel technologically relevant complex materials which are currently developed for use as magnetic sensors and actuators as well as illustrative examples for methodic development of the USANSPO technique.

Experiments were carried out under various environmental conditions, including zero-field environment, the influence of external magnetic field, mechanically induced stress, or a combination of both effects, and in magnetically saturated state. Corresponding measurement results allow us to assess the native sample state and thereby also to characterise the manufacturing process which may create form anisotropies. Recording of the scattered neutron intensity under different sample orientations is essential for non-isotropic structures [5]. The evolution of the magnetic structure from this starting point is seen from experiments with applied external magnetic field and/or mechanical stress of varying strength and can be followed up to the angular resolution limit of the technique which corresponds to structure sizes of the order of a few ten micrometers. At the upper end of the internal length scale, we observe the sample under saturation conditions from which we may distinguish crystalline and amorphous states on a microstructure level with considerable implications on the applicability of the materials under investigation.

Semiconductor nanowires are interesting for devices for several reasons. Compared to planar layers, elastic relaxation allows for larger lattice mismatch in heteroepitaxy, without introducing defects into the wires. This is interesting for instance to realize multi-junction solar cells. Besides quantum confinement due to heterojunctions, for band structure engineering also strain plays an important role. While external strain can only be realized within strict limits in bulk devices, nanowires can withstand more strain than planar layers or nanoscale objects fabricated by etching processes.

We report x-ray diffraction studies of tensile strain in Ge and Si nanowire devices with additional external strain. The strain state is determined using x-ray diffraction from single wires, employing nanofocused x-ray beams. The experiments have been performed at the European Synchrotron Radiation Facility.

Figure 1: FEM modeling of the strain distribution in a single Ge nanowire with a tapered shape.

In situ spectroscopy of gas and liquid phase reactions on Pd-bimetallic surfaces: structure and mechanistic insights

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In this contribution the structure, surface chemistry and reactivity of oxide-supported Pd-based bimetallic nanoparticles have been investigated by combining in situ/operando FTIR and X-ray absorption spectroscopy (XAS). Two case studies will be discussed: (i) Pd-Ga/Ga₂O₃ catalysts applied in methanol steam reforming (MSR), and (ii) Pd-Cu/Al₂O₃ catalysts employed for the catalytic reduction of nitrates in aqueous solution. Changes in the metallic state (oxidation state, alloy formation) and the evolution of surface species during the catalytic reaction were connected to establish structure-performance relationships.

Methanol is of interest for chemical storage of hydrogen, which is converted to H₂ by steam reforming. While metallic Pd is completely unselective in this reaction, Pd/Ga₂O₃ is highly selective to MSR after high temperature reduction, which was attributed to Pd-Ga intermetallic formation [1]. By in situ XAS we followed in detail the formation process of the Pd-Ga intermetallic compound and identified Pd₂Ga as the phase that is most likely formed under reaction conditions [2]. Mechanistic aspects of the MSR reaction are still highly debated. In order to identify differences in the evolution of surface-adsorbed species over Pd₂Ga/Ga₂O₃ vs. Pd/Ga₂O₃ that result in the pronounced differences in catalytic properties, the conversion of methanol over both systems was studied by in situ steady state and concentration modulation FTIR measurements. Based on the obtained structural and mechanistic information, a detailed reaction scheme for selective MSR was established [3, 4].

The selective hydrogenation of nitrates in drinking water to nitrogen was studied over PdCu and PtCu bimetallic catalysts. The nature of the active sites is highly debated. The oxidation state of Cu was determined by in situ high energy resolution XAS. It was demonstrated that Cu undergoes a redox cycle, in which it gets oxidized (inactive state) when it converts nitrates to nitrites and is subsequently regenerated to the metallic state by active hydrogen spillover from the noble metal [5]. Differences were observed of PdCu compared to PtCu catalysts, probably related with the Pd-hydride phase, which could lead to differences in the regeneration step of the oxidized copper.

Morphology effect of $\text{Co}_3\text{O}_4$ nanostructures on the reducibility and catalytic performance for CO oxidation

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Due to the limited availability of noble metals, increasing attention in recent years has been paid to transition metal oxides as catalysts for CO oxidation. Among these oxides especially cobalt oxides with defined nanoshapes (e.g. rods) have turned out to be perspective catalysts for CO oxidation [1]. However, the origin of this extreme structure dependence is entirely unexplained, and the active sites, reaction mechanism for CO oxidation, as well as influence of pretreatment are still under debate. Therefore, in the present work we have studied the effect of the morphology of $\text{Co}_3\text{O}_4$ nanostructures and pretreatment conditions on the catalytic activity in CO oxidation by employing in situ X-ray absorption spectroscopy (XAS).

The $\text{Co}_3\text{O}_4$ nanorods and nanoparticles were synthesized according to a procedure described in the literature [1]. The catalysts were characterized by X-ray powder diffraction, N$_2$ adsorption, Transmission Electron Microscopy (TEM) and CO temperature programmed reduction (CO-TPR), activity and stability in CO oxidation reaction. Before the reaction the catalysts were pretreated either in synthetic air or in 5 vol.% H$_2$ in N$_2$ at 400 °C for 30 min. In situ XAS at the Co K edge (7709 eV) was carried out in the transmission mode at the SuperXAS beamline at the Swiss Light Source in Villigen, Switzerland. The catalyst (2 mg) was diluted with BN and placed in a quartz plug flow reactor supported by quartz wool. X-ray absorption data were analyzed using the IFEFFIT software package.

Synthesis of $\text{Co}_3\text{O}_4$ at 160 °C followed by calcination in air at 450 °C leads to the formation of nanorods with a width of 8-10 nm and length of 20-40 nm, as revealed by TEM, while $\text{Co}_3\text{O}_4$ synthesis at room temperature (RT) results in nanoparticles with diameters around 15-20 nm. The pretreatment conditions and consequently the Co oxidation state have a strong influence on the catalytic activity in CO oxidation. After oxidation pretreatment nanorods show full conversion of CO to CO$_2$ already at RT. However, after 6 h the catalyst completely lost its activity. On the contrary, for $\text{Co}_3\text{O}_4$ nanoparticles the CO conversion decreased rapidly and after 2 h no CO$_2$ was produced anymore. After reduction both nanostructures do not show any conversion of CO to CO$_2$ at RT and reach full conversion of CO only at 150 °C for nanorods and at 210 °C for nanoparticles when the catalyst was reoxidised to $\text{Co}_3\text{O}_4$, as revealed by in situ XAS. The reducibility of the materials was studied by TPR and in situ XAS analysis in H$_2$ and CO. The CO-TPR experiment shows that $\text{Co}_3\text{O}_4$ nanoparticles have two narrow reduction peaks at 255 °C and 300 °C. In contrast, the nanorods exhibited two rather broad reduction peaks at 240 °C and 325 °C. From the XANES spectra it was evident that for the nanoparticles the $\text{Co}_3\text{O}_4$ phase was reduced to metallic Co at 400 °C, while for nanorods about 50 % of the cobalt was in CoO phase additionally to metallic Co after H$_2$-TPR, and no metallic Co was observed after CO-TPR according to linear combination fitting of the spectra. The different reduction profile of nanorods compared to nanoparticles at temperatures higher than 300 °C might be attributed to a higher fraction of surface Co$^{3+}$.

Structural Characterization of Substrate Binding in Monoglyceride Lipase

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Monoacylglycerol lipases (MGLs) play an important role in lipid catabolism across all kingdoms of life by catalyzing the release of free fatty acids from monoacylglycerols. The three-dimensional structures of human and a bacterial MGL were determined only recently as the first members of this lipase family. In addition to the α/β hydrolase core, they showed unexpected structural similarities even in the cap region. Nevertheless, the structural basis for substrate binding and conformational changes of MGLs is poorly understood. Here we present a comprehensive study of five crystal structures of MGL from Bacillus sp. H257 in its free form and in complex with different substrate analogues and the natural substrate 1-lauroyl glycerol (1-LG). The occurrence of different conformations reveals a high degree of conformational plasticity of the cap region. We identify a specific residue, Ile145 that might act as a gate keeper restricting access to the binding site. Site directed mutagenesis of Ile145 leads to significantly reduced hydrolase activity. Bacterial MGL in complex with 1-LG, myristoyl-, palmitoyl- and stearoyl-substrate analogues enable identification of the binding sites for the alkyl chain and the glycerol moiety of the natural ligand. They also provide snapshots of the hydrolytic reaction of bMGL at different stages. The alkyl chains are buried in a hydrophobic tunnel in an extended conformation. Binding of the glycerol moiety is mediated via Glu156 and water molecules. Analysis of the structural features responsible for cap plasticity and the binding modes of the ligands suggest conservation of these features also in human MGL.
Despite the fact that glasses have been studied for many decades, they stay enigmatic at the atomic level and refuse to reveal their underlying dynamics to a satisfactory level. Many of these materials like fast ionic conducting glasses are relevant both on the theoretical and on the technological level. With the availability of synchrotron sources like the ESRF, the well established technique of Photon Correlation Spectroscopy (PCS) could be expanded to the X-ray regime (XPCS). We extended this method to the sub-nanometer range, obtaining insight into dynamics on atomic length scales (aXPCS) [1]. We subsequently proved that our method performs in very good agreement with other measurement techniques for different types of crystals [2].

After successfully utilizing this powerful tool for observing atomic dynamics in crystal model systems, we aim at gaining deeper insight into the dynamics of the physically interesting case of non-crystalline materials. One of physics’ unsettled questions are the dynamic properties of these amorphous materials. We selected lead-silicate glass systems as good candidates for studying diffusion in glasses with aXPCS, where both components can act as network formers. Our recent study in metallic glass [3] at temperatures around the glass transition revealed highly non-equilibrium atomic mobility which was independently confirmed by another group [4, 5]. We further investigated into the low-temperature dynamics of alkali borate ionic conducting glasses, where the network structure influences the way ions diffuse and thus the conductivity of the material. These materials are well known for their fast diffusive motion and thus also promising for pushing the limits of the accessible range for aXPCS. With our analysis we can draw conclusions on physical properties like the mean distance of ionic motion and thus shed light on the processes which govern glassy dynamics. I will give an overview on our recent results obtained from synchrotron measurements and show the consequences for our picture of the atomic dynamics in glasses.

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Structural and functional studies of a ClpC-MecA unfoldase

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Throughout evolution, adenosine triphosphate (ATP)-dependent proteolysis (i.e. the degradation of proteins in a process utilising the chemical energy in the form of ATP) is required for both the general protein turnover and the controlled removal of regulatory proteins. It is thus a critical process involved in a variety of functions on both the cellular (e.g. cell cycle) and organismal level (e.g. adaptive immunity), and implicated in many pathological states (e.g. the neurodegenerative diseases, cancer). The process is carried out by compartmentalised proteases such as the core particle of the eukaryotic proteasome or the prokaryotic protease ClpP. The access to the degradation chamber being restricted by a narrow gate, unfolding and translocation of substrate proteins is first required. This is in turn effected by a hexameric, ATP-dependent AAA-family unfoldase, as exemplified by the regulatory particle of the eukaryotic proteasome or the bacterial unfoldases ClpA, ClpC and ClpX. The ClpCP-MecA complex involved in the heat shock response in *Bacillus subtilis* is a simple example of an unfoldase-protease complex and thus a useful model of the eukaryotic proteasome. ClpC comprises two ATPase domains per monomer, each containing conserved loops which line the central pore, contact the substrate and transmit onto it the energy derived from ATP hydrolysis, thus leading to its unfolding and translocation. MecA is an adaptor and is additionally required for the functional hexamerisation. In our structural and biochemical studies, conducted partially at the ESRF, Grenoble, we are probing into the unfoldase activity of the ClpC-MecA complex, aiming at providing answers to the general questions concerning the cooperativity within AAA unfoldase rings, the symmetry thereof and the coupling between the ATP hydrolysis and the movement of the pore loops. This can shed light on the mechanism of ATP-dependent proteolysis in particular and the transformation of chemical energy into mechanical force in biological systems in general.
InAs$_{1-x}$P$_x$ segment in an InAs nanowire: A characterization with nano-focused X-ray diffraction

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For the fabrication of future electronic, and photoelectronic devices new materials as well as new designs are crucial. Such devices must have enhanced physical properties in comparison with the current state of the art. This can be achieved by precisely tailoring semiconductor nanostructures from different kind of materials, which means a detailed understanding of the fabrication of such nanostructures is mandatory [1,2]. Here we will demonstrate a small InAs$_{1-x}$P$_x$ segment in an InAs NW. Figure 1 a) illustrates the fabricated structure, which was grown by a self-seeded method, using a special switching sequence of gas precursors in metal-organic vapor phase epitaxy.

Characterization of a single segment in a NW was done using a nano-focused synchrotron radiation beam. This method fills the need for destruction-free 3D strain evaluation of buried nano structures, avoiding ensemble-averaging effects. The experiment was performed at beamline ID01 at the ESRF in Grenoble, and allowed us to record the scattering pattern due to the strain inside the segment and the NW around the dot region, by illuminating just the segment region of a single NW. We performed finite element method simulations of the strain inside a heterostructured NW with the outer dimensions obtained by scanning electron microscopy. By using this results we simulated the diffraction pattern of a single dot inside a NW as well as the diffraction pattern of an ensemble of NWs. Figure 1 b) shows the recorded diffraction intensity of the single dot inside a NW with the simulated intensity giving the highest agreement between measurement and simulation.

The obtained inhomogeneous strain distribution is the prerequisite for simulations and hence understanding of the electronic and optical properties of such nanowire heterostructures.

Studies of atomic-scale diffusion by x-ray photon correlation spectroscopy

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In the last decades certain experimental techniques, like for example Quasielastic Neutron Scattering (QNS) or Quasielastic Mößbauer Spectroscopy (QMS) have proven successful in investigating diffusive dynamics at the atomic level. However the limits for the diffusion coefficients accessible with these techniques are relatively low and they favor certain atoms, like iron in the case of QMS or hydrogen and lithium in the case of QNS. Whilst this second limitation quite obviously restricts these methods to certain systems, the first limitation, on a closer look, limits them to measurements in the vicinity of the melting transition. In solid state systems this means that extrapolating down to lower temperatures means projecting a theory onto a system with possibly very different ordering parameters. The goal of our studies in the last years was to develop a new method to study atomic motion at the fundamental level which would overcome both limitations. This method should work at low as well as at high system temperatures and expand the range of accessible systems.

We successfully achieved this goal by extending the relatively new technique of x-ray photon correlation spectroscopy to work on the atomic scale. Atomic x-ray photon correlation spectroscopy (aXPCS) relies on a number of time series of x-ray scattering patterns recorded under different scattering angles to measure chemical fluctuations. It is therefore not subject to the limitations mentioned above. Towards fast dynamics, the time resolution is only limited by the readout time of the detector and intensity of the x-ray beam. A limitation towards slower dynamics is only given by the stability and the duration of the experiment. This new technique therefore allows to investigate atomic scale diffusion in the temperature range of intermetallic phases or to study dynamics of glasses well below glass transition temperatures. Due to today’s technical limitations at synchrotron sources there is a constraint to systems with a high contrast in the scattering length of the system under investigation at the moment. However, there is no systematical or theoretical restriction to certain elements and with the ongoing improvement of modern synchrotron sources more and more systems become available to aXPCS.

Our group carried out the first successful aXPCS experiment only few years ago [1]. This poster will show what we achieved experimentally since then. It gives an overview of what an aXPCS experiment looks like and present some of the results we obtained, in particular on a Ni-Pt solid solution with jump frequencies in the order of $\tau^{-1} \sim 10^{-3}$ s$^{-1}$ [2] and an Fe-Al intermetallic alloy.

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State-of-the art X-ray line profile analysis (XPA) using synchrotron radiation allows for in-situ investigation of the evolution of several microstructural parameters during elastic and plastic deformation. These include the size distribution of the Coherently-Scattering-Domains (CSD), the density and arrangement of dislocations, and the frequency of planar defects.

In the present case, thin films of nanocrystalline palladium produced by pulsed magnetron sputtering on a Kapton foil were subjected to tensile deformation [1]. High resolution X-ray profiles were recorded in-situ at the MS-Powder diffraction beamline of the Swiss Light Source SLS, Villigen (Switzerland). The average CSD-size of the initial Pd film was found to be of the order of 30nm.

Samples were deformed to $\varepsilon \sim 0.02$ and unloaded in a first cycle, immediately followed by a second one deforming the sample to $\varepsilon \sim 0.04$, and unloading. Several hundreds of X-ray profiles were recorded during each cycle and subsequently evaluated using the CMWP-fit program [2] together with own software [3]. The asymmetry of the (220) peak, and the changes of the background-to-peak ratio with increasing deformation were also determined which implies the deformation induced evolution of the residual internal stresses and diffuse scattering, respectively.

In the present case, the large number of physical parameters accessible by XPA – CSD size distribution, density and arrangement of dislocations, frequency of planar defects as well as the residual internal stresses and the diffuse scattering – combined with synchrotron radiation, allowing to observe these parameters in-situ, during the deformation, gives a very detailed picture of the changes of the microstructure due to the deformation (see for example figures 2 and 3). Evidence for both dislocation and grain boundary slip is found and the findings fit well to results from TEM and numerical simulations [4].

Humidity Driven Pore Lattice Deformation of Ordered Mesoporous Thin Films

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Adsorption induced deformation of mesoporous powders \([1, 2]\) and thin films \([3]\) can provide valuable information about their mechanical properties. For instance, one can extract a stiffness parameter by in-situ X-ray scattering using synchrotron radiation.

Two types of films were prepared by dip- and spin-coating silicon substrates with a sol made of TEOS and triblock copolymer (P123) in acidic solution, followed by evaporation induced self-assembly and subsequent calcination at 400°C. GISAXS measurements revealed ordered mesoporous films with 2D hexagonal structure with a macroscopic alignment of the pore axis within the plane of the substrate. In-situ GISAXS was applied to determine the pore-lattice deformation due to adsorption of water in a relative humidity range of RH=5% to RH=95%. As a major feature, both films showed a reversible out-of-plane contraction due to the condensation of water in the pores. Strain isotherms (i.e. pore lattice strain vs. RH) showed clear differences between the two types of samples.

If the porous film is grown on a thin substrate, humidity changes can cause a bending of the whole system, thus representing a simple actuator driven by humidity. This was demonstrated by depositing a mesoporous film on an AFM cantilever by dip coating and exposing it to the humidity changes. The readout system of an AFM was used to quantify the cantilever bending as a function of RH.

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Shape Retrieval from Colloidal Nanocrystals by SAXS

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Chemically synthesized nanocrystals (NCs) show a great potential for novel applications in magneto-electronic or bio-medical systems [1]. Many technical applications will require, however, micrometer scaled NC assemblies [1]. For instance, nearly monodisperse In-NCs are used recently for nanoelectrodes [2] and Bi NCs for 3D ordered colloidal crystals [3]. Not only the size, but also the shape of the NCs influences the self-assembled colloidal crystal formation [1]. One reason for the deviation of the spherical shape is the crystallographic facet formation on the NC surface. These facets are more pronounced for large NCs as can be seen e.g. for individual Bi-NCs with 22 nm diameter in the TEM image shown as inset in Fig. 1. The recently achieved control of the synthesis process [2, 3] of these NCs results in size distributions below 5%. This nearly monodispersity allows to retrieve the mean shape of a large ensemble of inorganic NCs by synchrotron SAXS analysis.

In this work, we revealed that the 22 nm Bi NCs are nearly monodisperse, but deviates significantly from a spherical shape. A good correspondence between SAXS data and fit was found for an elliptical shape with two main axes with 18 and 22 nm (see Fig. 1), which could not be detected in the previous TEM studies. A nearly perfect fit was achieved by using the ATSAS software package developed originally for shape retrieval of monodisperse protein structures [4]. The obtained mean shape clearly reveals the faceted NC surface (see Fig. 1). In future we will test in detail the reliability of the retrieved shape and we will implement also the small but finite size distribution using an alternative new software package (2D-GIFT) [5].

Fig. 1: SAXS pattern (red spheres) together with the fits assuming a spherical (green line), elliptical (blue line) shape of the Bi NCs shown in the lower inset. The best fit (black line) is achieved, however, for the retrieved faceted shape using dummy atoms (beads) of around 1 nm as shown in the upper inset. (measured at the Austro-SAXS beamline at ELETTRA)

Hierarchical biotemplating in nanometer scale

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To create bio inspired functional materials one method is the direct conversion of a biological material to an inorganic phase in a process known as biotemplating. The way to such a material can include thermal or chemical pretreatment of the template, introduction of a material precursor in liquid or gas form and removal of the template by thermal or chemical means. The structure of the obtained material can feature several or all levels of hierarchical structure of the original template. The goal to receive the hierarchical structure from the meter- down to the nanometer scale leads to a processing challenge [1]. Using silica as either the final phase or a coupling layer leads to replica that mimics the natural material particularly well with regard to its original surface- and structuring [2–4]. When wood is used as the natural template, the obtained hierarchical structured material shows an anisotropic helical porosity, aerogel-like specific surface areas, and the prospect of serving as a chiral substrate. Small-angle X-ray scattering (SAXS) experiments prove the hierarchical structure of the wood templated replica generated by the main processing steps i) selective template component removal and optional functionalization, ii) deposition of silicon alkoxides and iii) simultaneous thermal removal of the organic phases and condensation of the alkoxide (calcination) [2,3]. By a series of tests, it was verified that the steps were indeed necessary to obtain this degree of structural replication [5].

The thermal development of the hierarchical structure of the finally obtained material was assessed by a series of small-angle X-ray scattering investigations [6]. From samples treated at different temperatures, it could be shown that indeed the cellulose elementary fibrils with diameters from 2-4 nm were replicated possibly as pores. Based on the evaluation of the scattering data, a structural model was developed. It matched the structure expected from the assumed deposition sites of the silica precursor. Further, the structural transition from a silica/wood composite material to a purely ceramic nanoscale replica and the retention of the original structuring could be shown from in-situ X-ray scattering and heating experiments.

Further, the observation of the scattering patterns during the adsorption of n-pentane vapour confirmed the previously suggested porosities and high specific surface areas of the materials. With the measurements of isotherms and in-situ SAXS experiments the shape and the accessibility of the pores could be shown and led to a new model of the replica structure. Also the influence on the structure of heating and cooling rates during the calcination was received [5].

References
Violation of Heisenberg's Error-Disturbance Uncertainty Relation in Neutron Spin Measurements

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It is an ineluctable feature of quantum mechanics that simultaneous measurements of certain pairs of observables are impossible. This is reflected in the famous Heisenberg uncertainty principle, published in 1927 [1], which is without any doubt one of the cornerstones of quantum physics. In its original formulation, illustrated by Heisenberg’s famous gamma-microscope gedankenexperiment (which is solely based on the Compton effect), it gives a rather heuristic estimate for the product of the inaccuracy (error) of a position measurement and the disturbance induced on the particles momentum. Shortly after, the uncertainty relation was reformulated in terms of standard deviations of position and momentum, focusing only on the limitation of preparing a quantum system without taking the accuracy of the measurement device into account [2]. Robertson generalized this relation between standard deviations to arbitrary pairs of observables \( A \) and \( B \) [3]. The corresponding generalized form of Heisenberg’s original error-disturbance uncertainty relation for arbitrary observables however has been proven to be formally incorrect [4].

A correct formulation of the error-disturbance uncertainty relation, including the unavoidable recoil of the measuring apparatus, was given by M. Ozawa in 2003 [5]. In a neutron optical experiment, where the error of a spin-component measurement and the disturbance caused on another spin-measurement are recorded, the validity of the new uncertainty relation is demonstrated. Our results clearly confirm that both error and disturbance obey this new (universally valid) uncertainty relation but violate the original one in a wide range of experimental parameters [6, 7]. In addition, our data reveal a counterintuitive behavior of the error-disturbance relation, namely that increasing error does not always lead to decreasing disturbance and vice versa in spin measurements. Such a reciprocal behavior occurs only in certain experimental configurations [7].

Determination and speciation of Rh in cancer cells by TXRF and K-edge SR TXRF XANES


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Dinuclear metal-metal-bonded complexes have attracted great attention because of their chemical reactivity, high catalytic activity in many reactions. These complexes, mainly rhodium (Rh), ruthenium (Ru) and rhenium (Re) are also known for their cytostatic properties since the 1970s and are among the most promising non-platinum anticancer complexes. It was shown that dirhodium tetra acetate exhibits appreciable cytostatic activity against a variety of cell lines, including L1210 tumor, sarcoma 180, Ehrlich ascites, P388 lymphocytic leukaemia, etc. Among the recognized non-platinum antitumor agents are dinuclear carboxylates species of Rh, Re; and Ru. Some years ago, it was elucidated that Rh(II)-Rh(II) carboxylate can interact with DNA giving a biologically active metal-metal-bonded system, which is the primary target in the design of replacements for platinum anticancer agents. To elucidate the possible binding modes of DNA to the dirhodium core Rh-Rh, interactions with nucleobases, nucleotides, dinucleotides were studied. Total reflection X-ray fluorescence (TXRF) spectrometry and X-ray absorption near edge spectroscopy (XANES) are suitable for quantitative determination and elemental speciation of cellular samples treated with Rh complexes, respectively. Human colon cancer cell lines (HT-29 cells) were cultured to 80% confluency, harvested by trypsin, washed twice with isotonic NaCl solution and centrifuged at 7,000 rpm. The treatments with different rhodium compounds (dinuclear carboxylates species of Rh) were carried out for 4 hours. After the second centrifugation, the cells were re-suspended in 100 μL of an isotonic NaCl solution and 5 μL of cell suspension was pipetted onto quartz carrier plates for XANES analysis (HASYLAB at DESY) and cells were digested for TXRF measurements (Atomika 8030C). The K-edge XANES measurements in fluorescence mode and grazing incidence geometry were carried out using the setup at the beamline L at the Hamburger Synchrotronstrahlungs labor (HASYLAB) at DESY. All measurements were performed in vacuum. A Si(311) double crystal monochromator was used for selecting the energy of the exciting beam from the continuous X-ray spectrum emitted by the 1.2 T bending magnet at beamline L. The primary beam was collimated horizontally and vertically by a cross-slit system. The incident X-ray intensity was monitored with an ionization chamber. During the measurements, the excitation energy was tuned in varying steps (10-0.5 eV) across the K-edge of Rh at 23220 eV. At each energy a fluorescence spectrum was recorded using a 50 mm² silicon drift detector (SDD). For each specimen not less than three consecutive scans were performed. The SR-TXRF setup – a vacuum chamber with an 8 stage sample changer - installed at Beamline L was used for the experiments. The TXRF results show a clear correlation between the toxicity and the intracellular concentration of the applied Rh complexes. Moreover, the effective complex can be detected in the DNA fraction of the samples. Evaluation of data collected at HASYLAB Beamline L shows the feasibility of SR-TXRF-XANES analysis for Rh in cell lines. The evaluation of the XANES spectra was performed as a fingerprint method by comparing the spectra of the unknown samples to those of prepared standards. Different types of dirhodium complexes and RhCl₃ were used as standards. Our measurements show a clear difference between the XANES spectra of effective and ineffective Rh complexes (both of them with high intracellular concentration). In the cellular samples, the XANES spectra of effective type complex are similar to those of the RhCl₃ standard, while the spectra of the ineffective type complex show a similar pattern to those of the dinuclear Rh standards.

These results show the intracellular accumulation of the applied Rh complexes into the cells. In the case of the effective dirhodium complex, the geometry of the resulting Rh form would be similar to RhCl₃ due to the dinuclear Rh bond cleavage. The above-mentioned phenomenon was observed when using cellular samples or the nuclear phase of the cells for the XANES measurements. It is necessary to emphasize that a very limited number of samples could be analyzed by XANES.
The Differential accumulation of S, Ca, Fe and Zn in human osteosarcoma tissue


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Typically occurring during the adolescent growth spur, Osteosarcoma is the most common primary bone malignancy [1]. It is characterized by the production of tumour osteoid and immature bone matrix by malignant cells [2]. With today’s combination of chemotherapy and surgery long-term survival rates of more than 70% have been reported. In recent years, dramatic changes in minor and trace elements (e.g. Zn, Cu) were found in various different cancer types - e.g. breast cancer, prostatic carcinoma [3], [4], [5]. These metals bind to proteins - so called metalloproteins - that perform different biological and physiological functions [4]. However, very little is known about trace element levels and accumulations in osteosarcoma.

Nine bone samples of human osteosarcomas are obtained following surgical resection at the Dept. of Orthopaedics, Medical University of Vienna, Vienna, Austria. Four samples were histologically identified as high-grade (G3) osteoblastic osteosarcomas, three as chondroblastic sarcomas and two samples were anaplastic osteosarcoma. The samples contained tumour tissue as well as adjacent normal healthy bone tissue as an internal control. The study was approved by the ethics committee at the Medical University. The undecalcified samples were examined by quantitative backscattered electron imaging (qBEI) using a pixel resolution of 1 µm. Grey-level images were generated to differentiate between healthy bone tissue and the mineralized and non-mineralized tumour tissue. Areas of interest were analyzed with synchrotron radiation induced confocal micro x-ray fluorescence analysis (SR µ-XRF) to determine the distribution of Ca, Sr, Zn, Fe in tumour tissue and healthy bone. Measurements were performed at the FLUO beamline at ANKA using a beam size of 15x12 µm² and a depth resolution of 20 µm for Au-Lα, with primary excitation energy of 17 keV. In addition measurements using the confocal low power µ-XRF setup, equipped with a vacuum chamber to enable the detection of light elements, at the Atominstitut of the Vienna University of Technology, were done in the same regions of interest, using beam size of 50x50x50 µm³ determined for Cu-Kα. Our measurements revealed significant differences between healthy bone and calcified cancerous tissue. A positive correlation of Fe and Zn and an accumulation of these elements in calcified cancerous tissue was observed. Increased Fe levels were found in both tumour types, but the degree of Fe accumulation was much higher in the chondroblastic tumour tissue. The laboratory analysis revealed increased S levels in the non mineralized cancerous matrix in case of chondroblastic sarcomas.

SR μ-XRF Imaging of Human Osteoporotic Bone


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Osteoporosis (OP) is characterized by a low bone mass and a micro architectural deterioration of bone tissue leading to increased bone fragility and fracture incidence. The general prevalence of OP raises in women rises from 5% at age of 50 years to 50% at age of 85 years. Many risk factors have been found which are associated with osteoporotic fracture, including hormonal factors, low intake of calcium and vitamin D and a history of fracture. Little is known about where Pb and other trace elements, e.g. zinc (Zn) and strontium (Sr), are incorporated within the bone tissue. Previous studies on the local distribution of Pb in bone only differentiate between cortical und trabecular bone tissues [1]. Finding new ways of treating osteoporosis and reducing the negative impacts (e.g. vertebral and non-vertebral fractures) of this disease is one of the urgent topics in medicine. Strontium ranelate (SrR) has been approved for the treatment of postmenopausal osteoporosis a couple of years ago. This agent is described to have both anabolic and antiresorptive effects in bone, but the exact mechanism of its action is not yet fully understood. Strontium (Sr) is incorporated in bone during the mineralization process. A set of five human femoral necks from patients suffered osteoporotic femoral neck fractures and five age-matched non-fractured controls (taken from a previous study [2]) have been analyzed. Additionally four femoral head samples were measured, obtained from patients undergoing a hip replacement surgery at the Trauma Centre Meidling (Hospital of the AUVA, Vienna, Austria) after suffering osteoporotic femoral neck fractures. Furthermore we had the opportunity to analyze two human bone biopsies (iliac crest, femoral neck) from patients receiving SrR therapy. The undecalcified samples were examined by quantitative Backscattered Electron Imaging (qBEI) using a pixel resolution of 1τm. Grey-level images were generated to differentiate between bone packets and osteons of different mineral content separated by cement lines. Areas of interest were analyzed with Synchrotron Radiation induced confocal micro x-ray fluorescence analysis (SR t-XRF) to determine the distribution of Ca, Sr, Zn and Pb in subchondral and cortical bone. Measurements were performed at the FLUO beamline at ANKA using a beam size of 17x12τm and a depth resolution of 19τm at Au-La, with primary excitation energy of 16.7keV. We could show that confocal micro SR t-XRF is well-suited to determine the trace element distribution in the different histological structures of subcondral and cortical bone. Pb and Sr were found to correlate positively with the Ca content among the bone packets, while Zn did not show any correlation. Furthermore an accumulation of Pb and Zn was found specifically in the cement lines (borders between bone packets), as identified in the XRF-maps by overlaying them with the corresponding qBEI. No significant differences in the elemental distributions between fractured and controls could be observed. The samples from the SrR treated patients showed high Sr accumulation in bone packests build during the therapy, which is in very good agreement with the findings of our recent study [3] analyzing samples of an experimental osteoporosis treatment model in rats [4].

X-ray strain microscopy of inhomogenously strained Ge micro-bridges

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While the SiGe semiconductor system is technologically the most important and most developed, optical emitters are still difficult to realize due to the indirect band gap. Beside efforts to overcome this limitation by very high doping [1], achieving tensile strain in Ge is a promising route. In Ge the direct band gap is predicted to be shifted below the indirect transition for strain values of a few per cent. Technical realization of such high strain values is, however, rather difficult and requires complex strain microscopy.

For this study micro bridges were investigated where strain enhancement by force field concentration in pre-strained Ge layers grown on Si was deployed: The difference in the thermal expansion coefficients results in tensile pre-strain of about 0.2% in the Ge layer after cooling to room temperature. The transfer of an electron-beam written pattern by reactive ion and anisotropic wet chemical etching techniques enhances the strain. By tuning the geometry of the structure, the strain may be enhanced to levels, which are high enough to convert the indirect band-gap of Ge to a direct one [1, 2].

The strain distribution in tensile strained Ge micro-bridges was studied by X-ray nano-diffraction which is an excellent tool to resolve the 3D displacement field spatially [3]. The strain mapping of the transition regions between the centre of the bridge and the wide feeder arms was performed at beamline ID01 of the ESRF by nano-focused X-ray diffraction experiments. A Fresnel zone plate was used to focus an 8 keV beam to a spot size of around 250 nm. Single bridges were raster-scanned in real space using a piezo stage, while the Ge Bragg peak was recorded over a certain range of scattering angles. This allowed to effectively map the full Ge Bragg peak in 3D at all raster positions with a resolution close to the beamsize [4].

The results, together with finite-element calculations, will be used to understand strain limitations of Ge and hence its lasing potential.

Phase shift measurements with a neutron interferometer close to the Bragg condition

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Our group was the first that found a theoretical description of the phase shift induced by Laue transmission in a perfect Si crystal blade in the vicinity of the Bragg condition [1]. We measured this 'Laue phase' at two wavelengths within a neutron interferometer. It reveals an extreme angular sensitivity, which allows the detection of beam deflections of the order of $10^{-6}$ s of arc.

We also searched for further influences on this phase and found a sensitive dependence on the rocking angle, monochromator function and beam divergence.

The measurements are compared with a new simulation tool, which is also presented here.

Crystal structures of the pestiviral protease Npro imply distinct roles for the catalytic water in catalysis

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Npro is a key effector protein of pestiviruses such as Bovine Viral Diarrhea Virus (BVDV) abolishing anti-viral defence mechanisms of the infected host cell. Synthesised as the N-terminal part of the ~4000 amino acid viral poly-protein, Npro fulfils this immunological function after its release from the polypeptide chain, for which Npro uses its intrinsic auto-proteolytic activity. However, the structural basis of proteolysis and its immune escape mechanisms remained unclear.

Here we present the crystal structure of Npro to 1.25 Å resolution with a two domain architecture. The geometric arrangement of the active site reveals a novel reaction mechanism involving a catalytic hydroxide ion bound to a stabilising pocket. The presentation of the substrate further explains the enigmatic latency of the protease, ensuring a single in cis cleavage. Additionally, the architecture of the TRASH motif suggests switching between a zinc-bound (reduced) and zinc-free (disulfide-linked) conformation, which may affect immunologically relevant interactions such as binding to the transcription factor IRF3. The structure impacts Npro’s use as auto-cleaving fusion protein and as pharmaceutical target.
Ultracold neutron detectors based on Boron-10 converters used in the qBounce experiments

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Newton’s Inverse Square Law of Gravity may be tested at micron distances deeply into the theoretically interesting regime by quantum interference with ultracold neutrons. Our newly developed method is based on a resonance spectroscopy technique related to Rabi spectroscopy, which has been adapted to gravitationally bound quantum systems: By coupling such a quantum system to mechanical vibrations, we observe resonant transitions, devoid of electromagnetic perturbations. The experiment is sensitive to any hypothetical short-ranged interactions, as Newtonian gravity and hypothetical Fifth Forces evolve with different phase information. One of the main challenges to achieve sufficient results is the development of dedicated detectors that are well-adapted to very low neutron fluxes of approx. 10 counts/1000s. Here, we present two detector concepts based on Boron-10 neutron converters. The first one allows measurements with a spatial resolution better than two µm and a detection efficiency of approx. 61%. The second one provides integral measurement with a total efficiency of 77% and an overall background rate of 0.65 counts/1000s.
Cu doped ZnO - X-ray Absorption Near Edge Spectroscopy (XANES) and SQUID Magnetometry studies

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Transition metal doped ZnO (TM:ZnO) as a semiconducting material system has attracted the attention of experimentalists ever since Zener’s model of ferromagnetism was used to predict dilute magnetic semiconductors $T_C > RT$ in 2000 [1]. Research in the area, though extensive, has all but converged, with different researchers reporting both the prevalence [2,3] and absence of room temperature ferromagnetism [4,5]. The case of Cu:ZnO has likewise been studied due to the primary interest in its ferromagnetic behavior and additionally from the point of view of its piezoelectric contribution in co-doped systems [6]. Though neither Cu, nor its oxides are ferromagnetic, reports of ferromagnetic Cu:ZnO can be found [7,8]. We have prepared a series of thin films on c-plane sapphire substrates by DC reactive magnetron sputter deposition with varying proportions of reactant (O$_2$) and inert (Ar) gases and have found three separate regimes in the series with a marked difference in terms of the apparent colour of the samples. In order to establish an interrelation between the observed magnetic behavior of our system with the local atomic positioning of dopant Cu atoms [9] and the valence [10], we have consequently probed the series by means of x-ray absorption spectroscopy at the Cu-K edge using linearly polarized hard x-rays. While the x-ray absorption near edge spectroscopy (XANES) spectra point to the oxidation states in the different regimes, the x-ray linear dichroism (XLD) in turn indicates the substitution of the Zn atom sites by Cu as being unfavourable. The SQUID magnetometry studies on the series have persistently revealed paramagnetic behavior irrespective of regime.

X-ray absorption spectroscopy: local structure, valence and magnetism of Co-doped ZnO

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X-ray absorption near edge spectroscopy (XANES) using linear and circular polarized light offers a powerful toolbox of element-specific probe of local structural properties, valence and magnetism. We have used XANES and in particular x-ray linear dichroism (XLD) and x-ray magnetic circular dichroism (XMCD) to study the K-edges of transition metal doped oxides. The local atomic configuration of the dopant species and its respective valence as measured using XLD is decisive in understanding the origin of the observed magnetic properties as measured with either XMCD or integral magnetometry. Hard x-rays ensure bulk sensitivity and thus buried interfaces can be studied non-destructively. We will use the example of the widely studied dilute magnetic oxide, Co-doped ZnO, where a quantitative set of XANES-based quality indicators can be introduced assuring phase pureness of the samples, i.e., Co dopant atoms substitute for Zn which is correlated with paramagnetism [1, 2]. In cases where long range magnetic order is found in the samples, it could be directly evidenced by means of XANES and XMCD that it originates from metallic Co inclusions which was corroborated by analytic transmission electron microscopy [3].

Neutron Radiography and Tomography at the Atom-institut

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Neutrons are very efficient for the non-destructive investigation of hydrogenous materials and isotope distributions, as well as the detection of defects and inhomogeneities in materials. We give an overview of recent activities using neutron imaging at the neutron radiography beam-line at the Atominstitut in Vienna.
Structure determination of Ferulic acid decarboxylase to identify the active site and catalytic mechanism

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Ferulic acid decarboxylase catalyzes the transformation of ferulic acid to 4-vinylguaiacol (4-hydroxy-3-methoxystyrene) \cite{1}. Although the non-oxidative decarboxylation of ferulic acid by ferulic acid decarboxylation can be found in fungi and yeast as well as in bacteria, its exact catalytic mechanism is largely unknown. In order to identify the active site and to elucidate the exact catalytic mechanism it is necessary to determine the crystal structure of ferulic acid decarboxylase in complex with inhibitor and/or substrate. Data for the high resolution structure determination have been collected at the ESRF, Grenoble.

\cite{1} Gu, W., et al., \textit{sp. Px6-4}. PloS one, 2011. 6(1), e16262.
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