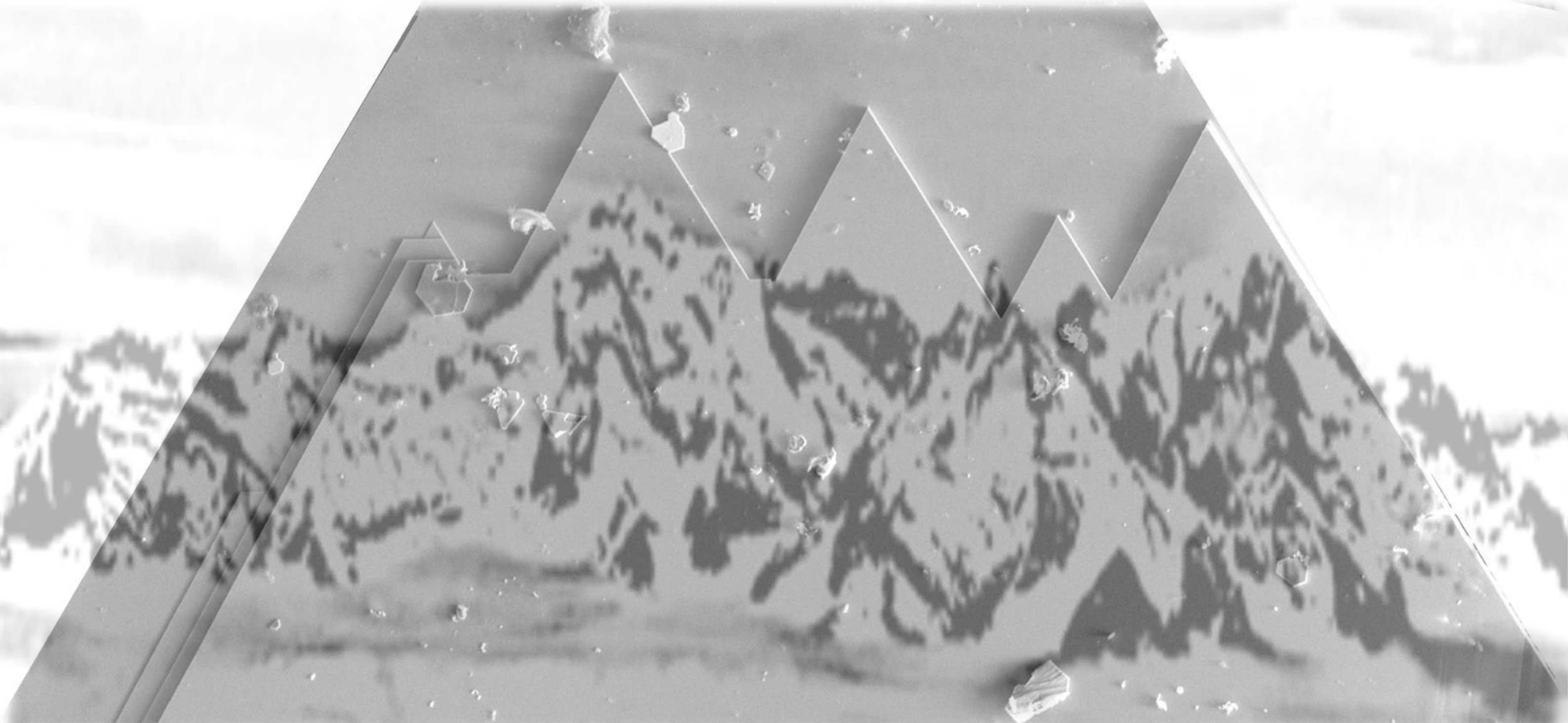
26th – 27th August 2024
Paul Scherrer Institute
Villigen, Switzerland

Workshop on Tips and Tricks for the Crystal Growth of Inorganic Materials



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Overview

Welcome Address

We are pleased to welcome you at the Paul Scherrer Institute (PSI) to the workshop on Tips and Tricks for the Crystal Growth of Inorganic Materials.

The event takes places over the course of two days at the PSI and provides a scientific forum to share the accomplished progress and perspectives for future developments in the synthesis and crystal growth of materials with novel and interesting physical properties.

The exciting scientific programme of the workshop covers topics from the main growth techniques used to prepare crystals of inorganic compounds, without neglecting the connection between processing aspects and physical properties, practical applications of the materials, as well as theoretical predictions. Relevant materials comprise, but are not limited to, oxides, intermetallics, borides, chalcogenides, pnictides and halides. The materials investigated could exhibit a broad range of exciting properties, such as multiferroicity, superconductivity, frustrated magnetism, high spin polarization, magnetic anisotropy, high entropy, first order phases transitions, strong spin-orbit coupling, nontrivial topology, and many more.

The main goals of the event are to bring together experts from the Solid State Chemistry and Condensed Matter Physics communities and to enable scientific exchanges between crystal growth and physics specialists. The workshop on Tips and Tricks for the Crystal Growth of Inorganic Materials aims to emphasize the value of the synthesis and crystal growth work carried out in the field of Solid State Chemistry for the areas of Condensed Matter Physics and Materials Science, an aspect which is often neglected at large, international conferences.

We hope that you enjoy the workshop and look forward to hearing about your research work.

Organisation

The workshop is held at the PSI, the largest research institute for natural and enigneering sciences in Switzerland, and home of the Swiss Light Source SLS, the Swiss X-ray free-electron laser SwissFEL, the Swiss Spallation Neutron Source SINQ, the Swiss Muon Source SμS and the Swiss Research InfraStructure for Particle physics CHRISP. A visit of the Swiss Spallation Neutron Source SINQ is planned on Tuesday, 27th of August, in the afternoon.

The **lectures** will be held in the **PSI Auditorium**, in the WHGA building. The event includes a series of **keynote talks** (30 minutes + 10 minutes discussion) and **contributed talks** (20 minutes + 5 minutes discussion).

There are numerous opportunities for networking over coffee, poster session and Apéro.

The **coffee breaks, poster session and Apéro** will take place in the foyer of the WHGA building. The **poster session** will be held on Monday evening, however, we encourage presenters to display the posters throughout the entire duration of the workshop to stimulate discussions during the coffee breaks.

The **workshop dinner** will be held at the **PSI OASE Restaurant**, on Monday evening. Please bring and display your name tags during the dinner, the proof of payment for the dinner is marked on the name tags.

Sponsors

We are extremely grateful for the support and generous contributions made by the Swiss National Science Foundation (SNSF), Paul Scherrer Institute (PSI), MaNEP Switzerland Network, Swiss Society for Crystallography (SGK/SSCr) and Swiss Neutron Scattering Society (SGN/SSDN).

We also thank PSI for hosting the Workshop on Tips and Tricks for the Crystal Growth of Inorganic Materials.

Swiss National
Science Foundation

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NETWORK

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Swiss Society for Crystallography

SSSN
SGN

Organising Committee

Dr. Monica Ciomaga Hatnean	Paul Scherrer Institute, Switzerland
Dr. Dariusz Jakub Gawryluk	Paul Scherrer Institute, Switzerland
Dr. Enrico Giannini	University of Geneva, Switzerland
Dr. Ekaterina Pomjakushina	Paul Scherrer Institute, Switzerland

Scientific Committee

Prof. Ana Akrap	University of Zagreb, Croatia
Dr. Monica Ciomaga Hatnean	Paul Scherrer Institute, Switzerland
Dr. Dariusz Jakub Gawryluk	Paul Scherrer Institute, Switzerland
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Dr. Romain Franck Sibille	Paul Scherrer Institute, Switzerland
Prof. Arkadiy Simonov	ETH Zürich, Switzerland

Secretariat

Mrs. Sabine Pfeifer	Paul Scherrer Institute, Switzerland

Scientific Programme

KT: Keynote Talk, CT: Contributed Talk.

Monday, 26th of August

08:00 - 08:55	**Registration**	
08:55 - 09:00	**Welcome remarks**	
Crystal growth using the Czochralski and Bridgman methods (Chair: Prof. Kazimierz Conder, PSI)		
09:00 - 09:40	KT	**Dr. Christo Guguschev** Leibniz Institute for Crystal Growth, Germany *Bulk growth of oxide single crystals using the Czochralski (Cz), top-seeded solution growth (TSSG) and edge-defined film-fed growth (EFG) techniques*
09:40 - 10:20	KT	**Dr. Karl Krämer** University of Bern, Switzerland *Bridgman crystal growth of rare earth halides*
Crystal growth using the floating zone method (Chair: Dr. Ekaterina Pomjakushina, PSI)		
10:20 – 10:45	CT	**Dr. Monica Ceretti** Institute Charles Gerhardt Montpellier, University of Montpellier, France *Growth and characterisation of high quality single crystals of some Ruddlesden–Popper phases by floating zone method*
10:45 – 11:15	**Coffee break**	
11:15 – 11:55	KT	**Prof. Geetha Balakrishnan** University of Warwick, United Kingdom *Use of the optical floating zone method for crystals of quantum materials*
11:55 - 12:20	CT	**Dr. Arnau Romaguera Camps** Paul Scherrer Institute, Switzerland *Effect of floating-zone growth conditions on the structural and magnetic properties of the YBaCuFeO$_5$ high-T_c spiral multiferroic*
12:20 – 12:45	CT	**Dr. Yong Liu** EPFL, Switzerland *Laser floating-zone growth of single-crystal YTiO$_3$*
12:45 – 14:00	**Lunch break**	
14:00 – 14:25	CT	**Dr. Dorota Pulmannova** Leibniz Institute for Crystal Growth, Germany *Optical floating zone growth of a new high-temperature polymorph of Sr$_2$TiO$_4$ with tetrahedral Ti-coordination*
Synthesis and crystal growth in extreme conditions (Chair: Dr. Enrico Giannini, UNIGE)		
14:25 – 15:05	KT	**Dr. Pascal Puphal** Max Planck Institute for Solid State Research, Germany *Synthesis and crystal growth in extreme conditions: around perovskite and Ruddlesden-Popper nickelates*
15:05 – 15:30	CT	**Dr. Igor Plokhikh** Paul Scherrer Institute, Switzerland *Mechanochemical reaction for synthesis of quantum materials: case study of magnetic clathrate-like compound EuNi$_2$P$_4$ and skyrmion host MnGe*
15:30 – 16:00	**Coffee break**	
Crystal growth using the chemical vapour transport method (Chair: Dr. Dariusz Jakub Gawryluk, PSI)		
16:00 – 16:40	KT	**Prof. Anna Böhmer** Ruhr University Bochum, Germany *Synthesis with volatile and reactive elements: chalcogenides and alkali-based materials*
16:40 – 17:05	CT	**Anastasiia Lukovkina** University of Geneva, Switzerland *The vapor growth of van der Waals multiferroic crystals Co$_{1-x}$Ni$_x$I$_2$ with tunable magnetic properties*
17:05 – 17:30	CT	**Dr. Ashutosh Wadge** Institute of Physics, Polish Academy of Sciences, Poland *Topological semimetals: Chemical Vapor Transport*
17:45 – 19:15	**Poster session and Apéro**	
19:30 – 21:30	**Workshop dinner**	

Tuesday, 27th of August

Crystal growth using the flux method (Chair: Dr. Monica Ciomaga Hatnean, PSI)		
08:30 – 09:10	KT	**Prof. Tomasz Klimczuk** Gdańsk University of Technology, Poland *Single crystals growth from metallic fluxes - technical details and case studies*
09:10 – 09:35	CT	**Lea Richter** Max Planck Institute for Chemical Physics of Solids, Germany *Single-crystal growth of perovskite molybdates in controlled oxygen partial pressure*
09:35 – 10:00	CT	**Kai Daniel Röseler** University of Geneva, Switzerland *Acid assisted synthesis of large* $CrTe_2$ *crystals*
10:00 – 10:30		**Coffee break**
Perspectives on materials science: from prediction to realisation (Chair: Dr. Enrico Giannini, UNIGE)		
10:30 – 11:10	KT	**Prof. Nicola Marzari** EPFL, Switzerland *The powerful synergies of computational materials discovery and experimental synthesis and characterization*
11:10 - 11:35	CT	**Dr. Jonathan Schmidt** ETH Zürich, Switzerland *Machine-Learning-enabled ab initio study of quantum phase transitions in* $SrTiO_3$
11:35 – 12:00	CT	**Timo Reents** Paul Scherrer Institute, Switzerland *Thermodynamic stability of the materials in the Materials Cloud three-dimensional crystals database (MC3D)*
Overview of Tips and Tricks for the Crystal Growth of Inorganic Materials (Moderator: Dr. Romain Franck Sibille, PSI)		
12:00 – 12:45		**Round table discussions**
12:45 – 12:50		**Closing remarks**
12:50 – 14:00		**Lunch break**
14:00 – 15:30		**Visit to SINQ**

Poster Session

P1	**Edan Bainglass** *Automating experimental workflows with AiiDA: from battery cycling to thin film growth*	Paul Scherrer Institute, Switzerland
P2	**Aditya Bhardwaj** *Growth of Bi-based halide single crystals for X-ray detection application*	ETH Zürich, Switzerland
P3	**Petr Čermák** *Bright future: automated sample preparation*	Charles University, Czech Republic
P4	**Vasile Cristian Ciomaga Hatnean** *Progress in the growth of rare earth silicate crystals*	Alexandru Ioan Cuza University of Iasi, Romania
P5	**Ross Colman** *Optimising the growth of incongruently melting materials by floating zone methods with the aid of finite element modelling*	Charles University, Czech Republic
P6	**Pia Maria Düring** *Ultrathin Fe on* $SrTiO_3$*: interplay of redox reaction and band alignment*	University of Konstanz, Germany
P7	**Maria Herz** *Design of high-temperature syntheses in* $(Bi_{2x}A_{1-3x})[PtBi_6I_{12}]$ *compounds with* A *= Pb, Sn, Mn, Fe*	University of Geneva, Switzerland
P8	**Thomas Hicken** *The versatile general purpose surface-muon instrument (GPS) for* μ*SR at the Swiss Muon Source*	Paul Scherrer Institute, Switzerland
P9	**Andrii Kanak** *Single crystal growth of* $CsPbBr_3$ *by Bridgman method*	ETH Zürich, Switzerland
P10	**Jonas Andreas Krieger** *The FLexible Advanced MuSR Environment (FLAME)*	Paul Scherrer Institute, Switzerland
P11	**Frank Lichtenberg** *Special approaches and systems at the floating zone method: Preparation and use of rectangular rods, an image and data recording, processing, and visualization system, and the synthesis of reduced Carpy-Galy phases of the Schückel-Müller-Buschbaum type such as* $Sr_{17}Ca_2Nb_{19}WO_{64}$ *by melting and solidifying the fully oxidized composition under Ar +* H_2	ETH Zürich, Switzerland
P12	**Marisa Medarde** *Design of multiferroic spiral magnets with ordering temperatures far beyond 300 K*	Paul Scherrer Institute, Switzerland
P13	**Samuel Harrison Moody** *Updates and capabilities of the Cold Neutron Diffractometer at PSI*	Paul Scherrer Institute, Switzerland
P14	**Jana Pásztorová** *New path of the* Ba_2MgWO_6 *single crystal growth using* $BaCl_2$*-*$MgCl_2$ *flux*	Heinz Maier-Leibnitz Zentrum, Germany
P15	**Nataliya Paulish** *Automated prediction of Fermi surfaces from first principles*	Paul Scherrer Institute, Switzerland
P16	**Vladimir Pomjakushin** *High Resolution neutron Powder Diffractometer HRPT at Swiss neutron spallation source SINQ*	Paul Scherrer Institute, Switzerland
P17	**Jiří Pospíšil** *MGML – open access infrastructure for single crystal growth*	Charles University, Czech Republic
P18	**Soohyeon Shin** *Kondo-controlled topological phases in the antiferromagnetic Weyl semimetal CeAlGe*	Paul Scherrer Institute, Switzerland
P19	**Toni Shiroka** *The multi-purpose surface-muon instrument at PSI: a versatile tool for studying novel materials*	Paul Scherrer Institute, Switzerland
P20	**Romain Franck Sibille** *The upgraded neutron single-crystal diffractometer Zebra at SINQ*	Paul Scherrer Institute, Switzerland
P21	**David Sviták** *Proof of concept: automatic coalignment of flux-grown crystals*	Charles University, Czech Republic
P22	**Yvonne Tomm** *Single crystals of novel chalcogenides, grown by chemical vapor transport*	Helmholtz-Zentrum Berlin, Germany
P23	**Fatih Uzun** *Eigenstrain tomography*	University of Oxford, United Kingdom
P24	**Olesia Voloshyna** *Investigation of* Li_3N *crystallization by FZ technique under high nitrogen pressure*	Leibniz Institute for Solid State and Materials Research Dresden, Germany
P25	**Dorota Walicka** *Synthesis and characterization of rare-earth halides*	Paul Scherrer Institute, Switzerland

P26	**Felix Wirth** Institute of Physics II, University of Cologne, Germany *Challenging growth of doped* Sr_2RuO_4 *using the floating zone method*
P27	**Hasan Yilmaz** University of Stuttgart, Germany *Synthesis and optical properties of Re:* $LaSrGaO_4$ *(Re =* Eu^{+3}, Sm^{+3} *and* Ho^{+3}*) single crystal via optical float zone method*
P28	**Hasan Yilmaz** University of Stuttgart, Germany *Synthesis and optical properties of Re:* $Gd_3In_2Ga_3O_{12}$ *(Re =* Nd^{+3}, Ho^{+3} *and* Lu^{+3}*) single crystal via optical float zone method*

List of Abstracts – Talks

Monday, 26th of August

KT Bulk growth of oxide single crystals using the Czochralski (Cz), top-seeded solution growth (TSSG) and edge-defined film-fed growth (EFG) techniques

Christo Guguschev[1], ***Mario Brützam***[1], ***Ramazan Koc***[1], ***Michael Schulze***[1], ***Roberts Blukis***[1], ***Christian Rhode***[1], ***Carsten Richter***[1], ***Julia Köpp***[1], ***Darrell Schlom***[1,2,3], ***Matthias Bickermann***[1]

[1]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany; [2]Department of Materials Science and Engineering, Cornell University, Ithaca, USA; [3]Kavli Institute at Cornell for Nanoscale Science, Ithaca, USA

This contribution will give an overview about the growth and characterization of selected oxides with perovskite, pyrochlore or magnetoplumbite structure and with melting points the range between 1500 °C and 2200 °C. As substrates, such crystals serve as the literal foundation for the preparation of epitaxially grown oxide thin films with interesting ferroelectric, superconducting, ferromagnetic, piezoelectric, multiferroic, or electron transport properties. Some of the bulk crystals are attractive for optical applications as well, e.g. as scintillators, Faraday rotators or solid-state lasers.

Depending on the requirements on microstructural quality, chemical homogeneity, purity and crystal volume the crystals were grown by various methods and techniques like Czochralski, top-seeded solution growth and edge-defined film-fed growth. A selection of grown single crystals is exemplary shown in Fig. 1.

The talk is intended to point out the advantages and disadvantages of these techniques and to provide guidance on which crucible-based crystal pulling techniques are useful and effective depending on the temperature-dependent material properties such as infrared transmissivity and thermal conductivity of various complex oxides.

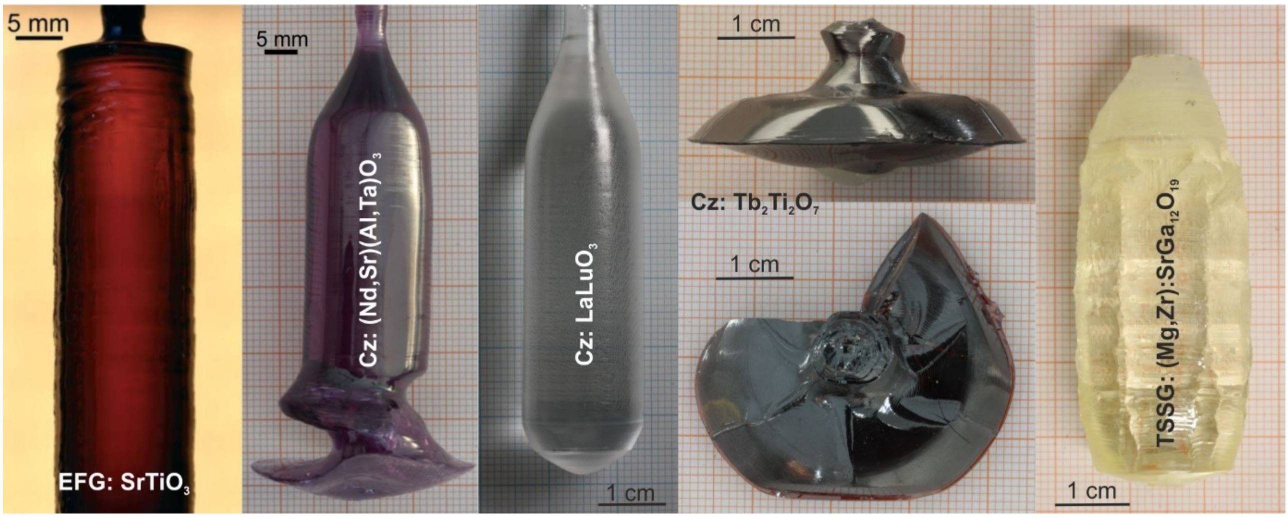

Figure 1: Examples of single crystals with perovskite, pyrochlore or magnetoplumbite structure grown by various crystal growth methods/techniques.

KT Bridgman crystal growth of rare earth halides

Karl Krämer

Department of Chemistry, Biochemistry, and Pharmaceutical Sciences, University of Bern, Bern, Switzerland

The Bridgman crystal growth technique is presented and illustrated on examples of rare earth halide crystals. The Bridgman technique is especially suited for:

- chemically sensitive materials (e.g. hygroscopic, oxidation sensitive);
- small sample batches (lab scale);
- expensive materials (e.g. isotope pure);
- high quality crystals due to slow cooling rates.

Starting materials are handled in a glove box, filled into silica ampoules with a special design to initiate single crystal growth, and sealed under diffusion pump vacuum ($p < 10^{-5}$ mbar). Crystals can be grown by a moving furnace or moving ampoule technique. The moving furnace technique is discussed in detail, e.g. furnace design, temperature distribution, growth speed. After the growth crystals are removed from the silica ampoule in a glove box, cleaved or cut with a diamond saw, and oriented under a microscope between crossed polarizers.

Congruently and incongruently melting materials are discussed and the basics of a phase diagram are reviewed. For incongruently melting materials the composition of the starting materials has to be adjusted and part of the product is lost as eutectic mixture.

The Bridgman technique is compared to the Czochralski technique, which is often used in industrial crystal growth.

CT Growth and characterisation of high quality single crystals of some Ruddlesden–Popper phases by floating zone method

***Monica Ceretti*, Werner Paulus**

Institute Charles Gerhardt Montpellier, University of Montpellier, France

Complex transition metal-based perovskite-related oxides provide fascinating examples of systems where the presence of strong interactions between crystal structure, electronic, and magnetic degrees of freedom leading to a rich variety of intriguing physical phenomena, such as high-Tc superconductivity, metal-to-insulator transitions, non-Fermi-liquid states, (zig-zag)-antiferromagnetism, spin glass states, intermediate valence states etc. The Ruddlesden-Popper oxygen-rich $RE_2MO_{4+\delta}$ compounds, with layered K_2NiF_4 structure, appear particularly interesting because, in addition to their electronic complexity, they exhibit enhanced oxygen conduction already at moderate temperatures. Their crystal structure consists of alternating perovskite and rock-salt layers along the stacking axis. The extra oxygen atoms ($0 < \delta < 0.25$), occupying the interstitial lattice remain mobile close to room temperature, leading to complex ordering scenarios depending on δ and T. The only phases known so far in this range of non-stoichiometry are $La_2CoO_{4+\delta}$, $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$, providing a unique opportunity to study the interplay between the dimensionality, lattice, charge, spin and orbital momentum degree of freedom by tuning the metal valence state via oxygen doping.

Ordering phenomena and their interplay are generally difficult to explore related to weak satellite intensities and thus the availability of high purity single crystals is mandatory. Therefore, we report here on the growth by floating zone method and characterization of high quality, centimeter sized $La_2CoO_{4.25+\delta}$, $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$, single crystals, suitable for neutron scattering experiments.

For $La_2CoO_{4+\delta}$, the main problem to overcome for crystal growth was related to the incongruent melting and associated difficult nucleation and growth behavior. Instead of separately preparing a pre-enriched CoO seed rod as it is usually the case [1], a stable melt zone was obtained here using stoichiometric feed and seed rods. In this case, the molten zone regulates itself with the solidification of La_2O_3, thus continuously enriching the quantity of Co in the traveling solvent. The optimized growth parameters allowed obtaining large and homogeneous crystals, as confirmed by diffraction measurements (X-rays and neutrons) as well as scanning electron microscopy coupled with elemental analysis (EDS). Post synthesis annealing at 500 °C in oxygen flux yielded phase pure $La_2CoO_{4.25}$, showing a complex structure with a 2D modulation vector related to oxygen ordering as revealed by single crystal X-ray and neutron powder diffraction studies [2]. In particular, X-ray single crystal diffraction revealed in addition to the main reflections, a huge amount of satellite reflections. Their intensities are nevertheless significant, suggesting strong structural modulations induced by oxygen ordering, as confirmed by neutron diffraction, but also charge ordering of Co^{2+}/Co^{3+}.

For the nickelates $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$, the primary challenge in crystal growth was achieving the precise cation stoichiometry in the final crystal, to compensate the NiO evaporation. Even minor deviations from the ideal cation ratio can result in the segregation of NiO or the formation of intergrowth phases, such as $Pr_4Ni_3O_{10-x}$, in both systems. Additionally, too much of an excess of the rare earth (RE) metal leads to the formation of RE_xO_y intergrowth phases, causing the crystals to rapidly disintegrate under ambient conditions in air. Thus, a subtle compromise has been found in adding a NiO over-stoichiometry in the feed rod to obtain large, high-quality single crystals avoiding disintegration, although this inevitably leads to epitaxially grown intergrowth phases [3]. The as-grown single crystals were characterized by neutron and X-ray diffraction as well as by electron microscopy (SEM/EDS), revealing their excellent quality in terms of composition, homogeneity and crystallinity. For each crystal, the oxygen content was determined by thermogravimetric analysis in a reductive atmosphere. Single crystal synchrotron diffraction highlighted a complex incommensurate structure with a 2D modulation vector related to oxygen ordering up to the sub-mesoscale, together with fast ordering kinetics [4-7].

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KT Use of the optical floating zone method for crystals of quantum materials

Geetha Balakrishnan

Department of Physics, University of Warwick, Coventry CV4 7AL, UK

To make headway in understanding the physics of quantum materials, high quality single crystals are absolutely essential. One of the best techniques used very widely to obtain large, high purity and high quality single crystals is the floating zone technique, employing either optical or radio-frequency heating. In this talk, I will present an overview of the crystal growth of various important quantum materials by the floating zone technique using the optical furnaces at Warwick. I will describe the single crystal growth of materials which have especially high melting points such as refractory oxides, borides, and also intermetallic materials using a high powered optical floating zone furnace. New methods to produce single crystals of some topological insulators using the floating zone technique will also be explored.

CT Effect of floating-zone growth conditions on the structural and magnetic properties of the YBaCuFeO_5 high-T$_C$ spiral multiferroic

Arnau Romaguera Camps[1,2], **Elia Razzoli**[1], **Hiroki Ueda**[1], **Marisa Medarde**[2], **Monica Ciomaga Hatnean**[2,3]

[1]Laboratory for Advanced Spectroscopy and X-ray sources, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland; [2]Laboratory for Multiscale Materials Experiments, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland; [3]Materials Discovery Laboratory, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

The search for novel magnetoelectric (ME) multiferroic (MF) materials, where magnetic order combines with ferroelectricity (FE) and both are mutually coupled, is a topic of high interest in condensed matter physics and the development of spin-related communication technologies. Spiral multiferroics naturally exhibit robust ME coupling, yet the inherent presence of frustrated spin networks often leads to low magnetic transition temperatures, typically below 100 K. Despite their huge potential for advanced applications, this presents a critical challenge to their practical use in spintronics, ultra-low-power data storage, and electronic devices at ambient temperature.

Among the limited array of spin-induced multiferroics, YBaCuFeO_5 (YBCFO) stands out for its incommensurate (ICM) spiral magnetic order at unexpectedly high temperatures [1-4]. The spin-orbit coupling associated with the cycloidal component of this spiral structure induces spontaneous ferroelectric polarization via the Dzyaloshinskii-Moriya (DM) interaction [5,6]. Although this compound lacks geometric frustration, the presence of a spiral phase can be explained by a non-conventional mechanism ("spiral order by disorder"), theoretically developed by Scaramucci *et al.*, where frustration arises from randomly distributed Fe-Fe dimers with strong antiferromagnetic (AFM) coupling [4,7].

Leveraging this mechanism, recent efforts have effectively focused on extending the stability range well beyond room temperature through various manipulation routes of the YBCFO layered structure, including modifying the Cu/Fe chemical disorder in bipyramids and applying chemical pressure via selective cation substitutions [1-3]. Despite the progress made with polycrystalline samples, gaining deeper insights into the microscopic mechanisms underlying the existence and nature of the spiral state in YBCFO requires conducting sophisticated experiments on single crystals utilizing quantum-beam techniques. However, such studies are still lacking in part due to the difficulty of obtaining high-quality specimens in single crystal form. Moreover, the final magnetic properties of YBCFO are highly sensitive to subtle variations in structural parameters and cation ordering. While polycrystalline synthesis allows controlled modifications to tailor these properties, the complexity of growing single crystals via solvent-based Floating Zone methods poses significant challenges. In particular, B-site cation distribution, and consequently the final magnetic properties of as-grown single crystals, are difficult to control precisely due to their strong dependence on the number of parameters involved in the growth process. This often results in samples where the incommensurate magnetic spiral ($\mathbf{k}_\mathrm{s}$ = [0.5, 0.5, 0.5 $\pm\ \delta$]) is replaced by a commensurate magnetic order ($\mathbf{k}_\mathrm{c}$ = [0.5, 0.5, 0]).

This presentation focuses on the development and characterization of YBCFO single crystals. It will cover: (i) the efforts to grow samples of this non-congruently melting oxide using complex Traveling Solvent Floating Zone (TSFZ) techniques, with both laser and infrared-based Optical Floating Zone furnaces, and (ii) the characterization of the grown single crystals using in-house physical property characterization techniques, synchrotron x-ray spectroscopies, and both unpolarized and polarized neutron beams.

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CT Laser Floating-zone growth of single-crystal $YTiO_3$

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YTiO3, which possesses a $GdFeO_3$-type crystal structure, belongs to $R$$TiO_3$ family, where $R =$ La to Tm, including Y. The magnetism of $R$$TiO_3$ series changes with varying rare earth R ions, transitioning from antiferromagnetic ordering for $R =$ La, Ce, and Pr, to paramagnetism when $R =$ Nd, to finally to ferromagnetism (for $R =$ Y, with a Curie temperature $T_\mathrm{C} \approx$ 30 K) or ferrimagnetism (for R ranging from Gd to Tm) [1]. In this study, we report the growth of $YTiO_3$ single crystals under different atmospheres by using the laser floating zone growth technique: (i) 97% Ar/ 3% H_2; (ii) Ar; (iii) forming gas (97% N2/ 3% H_2). This study aims to adjust the oxygen content δ in $YTiO_{3+\delta}$ during the crystal growth, instead of during the post annealing. Our results suggest that the optimal growth condition is a fast growth at a traveling speed of 10 mm/h under the mixture of Ar and H_2. However, we find that the chamber must be well sealed and evacuated before the growth. The remnant air in the chamber or weak leakage of air will produce Y_2TiO_5 and TiN impurities in the final product. In case of forming gas, a golden layer of TiN was formed in the surface of rod. The magnetic property drastically depends on the growth atmosphere. Under Ar/H_2 mixture and Ar, $YTiO_3$ crystals show a ferromagnetic transition at $T_\mathrm{C} \approx$ 30!K, whereas the ferromagnetic transition is almost suppressed under N_2/H_2 mixture.

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CT Optical floating zone growth of a new high-temperature polymorph of Sr_2TiO_4 with tetrahedral Ti-coordination

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Sr_2TiO_4, first member of the Ruddlesden-Popper series $Sr_{n+1}Ti_nO_{3n+1}$, has been long known to undergo a phase transition at 1550 °C. This transition makes the growth of single crystals of this material highly challenging, because it usually breaks the crystal into a periodic array of uneven lamellae. While the low temperature tetragonal phase is widely studied due to its close connection to the famous perovskite $SrTiO_3$, there is little information about the high temperature α-phase, except for an unindexed powder pattern by Drys & Trzebiatowski [1].

We stabilized the high-temperature α-Sr_2TiO_4 single crystals by rapid cooling of the grown crystal from above the transition temperature. The α-phase crystallizes in the orthorhombic $Pna2_1$ group with lattice parameters a = 14.2901(5) Å, b = 5.8729(2) Å, c = 10.0872(3) Åand is isostructural to the orthorhombic forms of Sr_2VO_4 and Sr_2CrO_4 (which belong to the β-K_2SO_4 structure type). Its structure is formed by a complicated framework of large SrO_x polyhedra with tetrahedral cavities occupied by the transition metal. The tetrahedral coordination of Ti^{IV} makes the α-Sr_2TiO_4 quite a rare case among titanate compounds, the only other known example being the barium orthotitanate Ba_2TiO_4 [2].

However, whereas in Ba_2TiO_4 the coordination is tetrahedral in both high- and low-temperature polymorphs and the topotactic relation between the two is known, in the case of Sr_2TiO_4 a transition occurs to the layered Ruddlesden-Popper structure with octahedral titanium coordination.

In this work, we report for the first time the crystal structure of the high-temperature α-phase of Sr_2TiO_4. We elucidate the structural differences between the related compounds and discuss possible mechanism driving the structural transition.

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KT Synthesis and crystal growth in extreme conditions: Around perovskite and Ruddlesden-Popper Nickelates

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High Tc superconductivity remains one of the main focuses in condensed matter research, in which, rare-earth nickel oxides have emerged as a new class with potential for unconventional superconducting behavior. Here, two types of structures have drawn particular interest:

The first are nickelates with the infinite-layer crystal structure, such as $\mathrm{Nd_{0.8}Sr_{0.2}NiO_2}$, with superconducting transition temperatures up to 20 K.

The second type was found in Ruddlesden-Popper (RP) phase nickelates, such as $\mathrm{La_3Ni_2O_7}$, which under hydrostatic pressure realize a remarkably high T_C of 80 K.

Many details of these systems are not yet fully understood especially as for the first type only thin films show superconductivity up to now. In my talk I will show the challenges of optimal doping perovskite single crystals in high oxygen pressures, and show the advancements we have done in obtaining optimal reduced crystals as well as the effects of intercalation on these single crystals.

Furthermore, I present our findings on $\mathrm{La_4Ni_3O_{10}}$, $\mathrm{La_3Ni_2O_7}$, where sizable single crystals can be readily grown using the optical floating zone. Here, we recently observed that these crystals exhibit multiple crystallographic phases and a pronounced sensitivity to oxygen stoichiometry, affecting their physical properties and fascinating pressure dependence as will be highlighted in the talk. Finally, I will present a sub-family of nickelates and discuss their relevance to the existing RP.

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CT Mechanochemical reaction for synthesis of quantum materials: case study of magnetic clathrate-like compound $EuNi_2P_4$ and skyrmion host MnGe

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Not all intriguing quantum materials are straightforward to produce, whether in single-crystalline form or as powders. New materials predicted through chemical analogies or theoretical modeling often face significant challenges due to chemical obstacles. When the reactivity of starting reagents is low or the stability of the target phase is poor, conventional solid-state synthesis falls short, necessitating more sophisticated techniques. Among these, mechanochemical reactions, involving ball milling at high speed, stand out for their efficacy. Unlike high-pressure methods, mechanochemical reactions are more scalable and require less expensive equipment. Additionally, unlike soft-chemistry approaches, they are not restricted to materials that are stable in air and moisture.

In this work, I present two examples of materials synthesized using mechanochemically-assisted reactions: the clathrate-like magnetic compound $EuNi_2P_4$ [1] and MnGe [2], an analog of the prototypic skyrmion host MnSi. The first material, $EuNi_2P_4$, was predicted based on crystal-chemical analogies between Sr^{2+} and Eu^{2+}, considering the existence of $SrNi_2P_4$. A distinguishing feature of its structure is the presence of Eu^{2+} cations with a coordination number of 24, located in the voids of the framework formed by Ni and P atoms. This unique geometry drives several physical phenomena, including low thermal conductivity, characteristic of clathrates, and magnetic frustrations that result in a complex magnetic phase diagram at low temperatures. The preparation of large MnGe samples enabled the establishment of its magnetic structure using (3+N)D magnetic crystallography approaches.

In the talk, besides discussing the power of mechanochemical reactions, I will present the results of comprehensive characterization for the title materials. This will include detailed structural and physical properties analyses, showcasing the effectiveness of mechanochemical synthesis in producing high-quality quantum materials with desirable properties.

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KT Synthesis with volatile and reactive elements: Chalcogenides and alkali-based materials

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Transition-metal dichalcogenides with orthorhombic marcasite structure have been extensively studied for their applications in various fields. Lately, this structure type has also gained interest as a candidate for the newly-discovered altermagnetic order. We study transition-metal diantimonides and transition-metal diselenides using a two-step synthesis of granular films, comprised of combinatorial deposition and subsequent selenization/antimonization at different temperatures. The technique allows to efficiently and quickly explore the possible ranges of substitution within the marcasite structure type. In particular, we investigate the formation and crystal structures of the $\mathrm{(Fe,Ni)Sb_2}$, $\mathrm{(Fe,Cr)Sb_2}$ and $\mathrm{(Fe,Co)Se_2}$ substitution series. We find a clear region of phase separation between a Ni-rich $\mathrm{Ni}_{1-z}\mathrm{Fe}_z\mathrm{Sb}_2$-phase and $\mathrm{Fe}_{0.5}\mathrm{Ni}_{0.5}\mathrm{Sb}_2$ beyond 50% average Ni content, although both phases are of the same marcasite structure type. Cr-substituted $\mathrm{FeSb_2}$, in contrast, shows a much more subtle phase separation if synthesized to 500 $^\circ$C. At a slightly higher synthesis temperature of 540 $^\circ$C the continuous substitution of $\mathrm{FeSb_2}$ with Cr is possible. Finally, we find that $\mathrm{Fe}_{1-y}\mathrm{Co}_y\mathrm{Se}_2$ can be synthesized in the marcasite structure over the entire substitution range only at a very low synthesis temperature of 250 $^\circ$C. For higher synthesis temperatures, a Co-rich phase with the cubic pyrite structure forms instead, such that an apparent "miscibility gap" closes at low temperatures - likely due to kinetic effects. This work represents an example for the agility of combinatorial deposition of granular thin films in exploring the phase diagrams of transition-metal dichalcogenides as a unique tool to study this broad material family [1].

Alkali metals are another highly reactive and volatile element. We report on the development of a convenient sealing method for alkali-containing melts, with high vapor pressure and reactivity. Our newly designed container made of high-temperature resistant steel can be sealed manually and reliably without any air exposure of the containing material. The closed container may be heated in air up to at least 1150 °C. The containers were applied for the development and optimization of a high-temperature self-flux growth of $\mathrm{KFe}_{1-x}\mathrm{Ag}_{1+y}Ch_2$ (Ch = Se, Te) single crystals. The successful growths of these air-sensitive materials out of a reactive self-flux confirm the reliability of the container [2]. Such containers also enable extending the combinatorial synthesis of chalcogenide materials towards of co-substitutions.

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CT The Vapor Growth of van der Waals Multiferroic Crystals $Co_{1-x}Ni_xI_2$ with Tunable Magnetic Properties

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In the growing family of magnetic van der Waals materials multiferroic compounds CoI_2 and NiI_2 have drawn significant attention lately due to the multiferroicity down to the monolayer and frustrated cycloid ground state caused by Kitaev interactions, respectively [1,2]. Despite prior investigations of these materials, the evolution of magnetic ground states within the solid solution between them remains unresolved. Investigation of these new materials requires the development of a pathway for growing crystals of uniform compositions.

Processing sizeable and pure crystals of the solid solution $Co_{1-x}Ni_xI_2$ for physical measurements is challenging in this system. We find that physical vapor transport (PVT) growth leads to phase separation despite the adjusting synthesis conditions, probably caused by the differing vapor pressures of CoI_2 and NiI_2. In the PVT growth experiments, we systematically observed that crystals could grow at both the cold and hot ends of the reactor. This observation suggested that another less-spread vapor-based growth process could be successful, namely the self-selecting vapor growth (SSVG) [3,4].

Here, we have employed the SSVG technique for the crystal growth of the $Co_{1-x}Ni_xI_2$ solid solution and developed the necessary synthesis conditions according to the composition. We have successfully grown large homogeneous crystals of the whole solid solution. Furthermore, the crystal size for the compositions with $x > 0.2$ is only limited by the initial amount of employed chemicals and the diameter of the reaction vessel, as all the starting material is converted into one or a few large crystals. We suggest that this technique may be a successful pathway for the crystal growth of solid solutions for transition metals halides.

Both the lattice parameters and the magnetic properties of the solid solution evolve continuously and smoothly from one end member to the other, showing that they can be finely chemically tuned. We also observe that the Ni substitution for Co affects the metamagnetic transition typical for CoI_2. In particular, we find the existence of a range of compositions of $Co_{1-x}Ni_xI_2$ ($0.2 \leq x \leq 0.3$), which host magnetic order with metamagnetic transition similar to that for CoI_2 in the NiI_2 crystal structure. Based on magnetic and structural measurements we construct the phase diagram of the $Co_{1-x}Ni_xI_2$ system, which shows that physical properties can be finely chemically tuned by composition.

Bulk crystals of the solid solution $Co_{1-x}Ni_xI_2$ hold a possibility to be exfoliated into two-dimensional (2D) thin flakes and are expected to have thickness-dependent magnetic behavior down to a monolayer. This may open a pathway for fabricating 2D magnetic devices with new magnetic properties.

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CT Topological semimetals: Chemical Vapor Transport

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The single crystals growth of topological materials, focusing on $TaAs_2$, NbP, and $ZrAs_2$ is discussed. These materials hold significant promise for exploring novel physical phenomena such as extremely large magnetoresistance, chiral magnetic effects, band crossings robust to spin orbit coupling, etc. owing to their unique topological properties. The chemical vapor transport (CVT) technique was employed for the growth of high quality, relatively large single crystals, suitable for studies by various experimental methods. The CVT method facilitates the synthesis of these materials by leveraging heterogeneous reactions with a transport agent, iodine, to achieve volatilization and subsequent crystallization [1].

$TaAs_2$, a promising Dirac semimetal, was grown using a one-step process initially, followed by a two-step method. Polycrystalline $TaAs_2$ was synthesized by heating tantalum foil and arsenic within a quartz ampoule, yielding shiny long crystals upon cooling [2]. NbP, topological Weyl semimetal, was synthesized by loading compressed Nb pellets and red phosphorus into an evacuated ampoule with iodine as the transport agent. Shiny double trapezoidal-shaped crystals were obtained through controlled temperature gradients [3]. $ZrAs_2$, a nodal line semimetal, was synthesized similarly, yielding needle-like crystals after 21 days of growth [4].

Characterization techniques including X-ray diffraction (XRD) and energy-dispersive X-ray spectroscopy (EDX) confirmed the crystal structures and stoichiometry of the synthesized materials. These findings lay the groundwork for further exploration of the unique electronic and topological properties of $TaAs_2$, NbP, and $ZrAs_2$ [2-4].

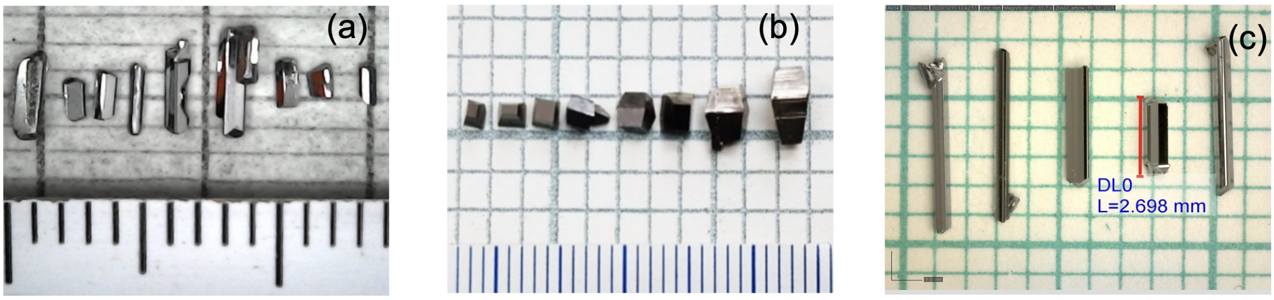

Figure 1: Single crystals of (a) $TaAs_2$, (b) NbP and (c) $ZrAs_2$.

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Tuesday, 27th of August

KT Single crystals growth from metallic fluxes - technical details and case studies

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The lecture will focus on the technical aspects of the metal flux crystal growth technique.

I will start with choice of the ampoule and crucible materials, then discuss the details of experimental design, and conclude with the centrifugation process. Along the way, I will discuss what I consider to be the most important, critical features of metal flux crystal growth experiments. I will present the tricks we have used to successfully – sometimes unintentionally – grow of $CaBi_2$, LiBi, $U_3Bi_4Rh_3$ and $U_3Bi_4Ni_3$, $(Yb_{0.24}Sn_{0.76})Ru$, $RE_3Ni_5Al_{19}$, REV_2Al_{20}, $CoAl_9$, Ba,$SrCo_2Al_9$, $EuAg_4Sb_2$, etc.

CT Single-Crystal Growth of Perovskite Molybdates in controlled Oxygen partial pressure

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Molybdates in the perovskite and related structures promise an exciting platform to study physics in the intermediately correlated regime accessible by 4d oxides. Two compounds have attracted particular attention. Ultra-low resistivity at room temperature has been reported for single crystals of $SrMoO_3$ [1]. The material is believed to be Pauli-paramagnetic down to lowest temperature [2], in contrast to its ferromagnetic structural analogue $SrRuO_3$ [3]. Secondly, the single-layer member in the Ruddlesden-Popper series, Sr_2MoO_4 is proposed to be the particle-hole counterpart of the unconventional superconductor Sr_2RuO_4 with the profound difference that the Fermi energy is further from a van-Hove singularity for the Molybdate [4]. Single crystals of Sr_2MoO_4 would thus enable studying the latter's influence on electronic correlations.

In-depth study of members in the Molybdate family has been hampered by the challenge of synthesizing phase pure powders and single crystals [5]. $SrMoO_3$ is the only material for which the growth of single crystals has been reported [1]. However, subsequent studies on synthesis and detailed characterization have not been widely carried out. This is mainly because stabilization of Molybdates in d^2 configuration necessitates precise control of the oxygen partial pressure during crystal growth [5].

In this work, we discuss different methods for controlling the oxygen partial pressure, which is crucial to growing $SrMoO_3$ reproducibly. From this understanding, we establish a successful protocol for the controlled growth of $SrMoO_3$ single crystals. The protocol is versatile and likely to enable the growth of various members in the Molybdate family. Our work showcases how consideration of thermodynamic data can be harnessed to choose an appropriate growth method, enabling optimization of growth conditions for oxides with extremely narrow stability windows at the growth temperature.

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CT Acid assisted synthesis of large $\mathrm{CrTe_2}$ crystals

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$\mathrm{CrTe_2}$ is a metastable room-temperature ferromagnetic van der Waals material with a Curie temperature of $T_\mathrm{C} \sim$ 320 K, which was first mentioned by Freitas *et al.* in 2015 [1]. We have recently discovered a novel synthesis route using diluted acids to deintercalate flux-grown $\mathrm{LiCrTe_2}$ [2] yielding big, x-ray pure single crystals of this intriguing quantum material. Deintercalation of $\mathrm{LiCrTe_2}$ using iodine, previously reported for the deintercalation of $\mathrm{KCrTe_2}$ [1,3-5], was significantly slower and yielded partially deintercalated crystals. The crystal structure previously reported based on powder data was confirmed using single-crystal diffraction experiments. We found the Curie temperature of this ferromagnetic van der Waals material to be precisely $T =$ 318 K using an Arrott plot. Combined DSC, DTA and diffraction experiments were used to determine the thermal transition of 1T-$\mathrm{CrTe_2}$ due to loss of Te. Our findings expand the synthesis methods for 1T-$\mathrm{CrTe_2}$ crystals having the potential to be integrated into spintronic devices [6].

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KT The powerful synergies of computational materials discovery and experimental synthesis and characterization

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The well-being and sustainability of 8 billion+ people are the defining challenges of our times. At the core of our human footprint lie materials: they enable the technologies that power our economy and, for better or for worse, support our society. It's the discovery of the catalyst that can convert air into ammonia and then fertilizers that has saved 1 billion people from starvation (while killing a fair percentage thanks to all the explosives produced). And novel materials can provide alternatives in our quest for efficiency, sustainability, and development: from energy harvesting, storage, conversion, and efficiency, to environmental protection and reparation, to the materials that support the high-tech high-value industries of modern economies – with the added task of finding earth-abundant and recyclable solutions.

With this aim, computational design and discovery of novel materials provides an unprecedented accelerator to our innovation pipeline, that can become very poweful when partned with experimental synthesis and characterization. I'll illustrate this model: the capabilities and challenges that we have in predicting accurately properties and performance from first principles, and the power of a paradigm shift where experimental research and discovery becomes driven or inspired by simulations and AI. Some examples will cover materials for energy (Li-ion cathodes and solid-state conductors) and materials for information-and-communication technologies (from low-dimensional materials to superconductors).

CT Machine-Learning-enabled ab initio study of quantum phase transitions in $SrTiO_3$

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Understanding phase transitions in $SrTiO_3$ (STO) from an ab-initio perspective presents significant theoretical challenges. By integrating the self-consistent harmonic approximation (SSCHA) with machine learning force-fields we revisit the isotope effect in STO - specifically, the transition to a ferroelectric phase when 16O is replaced by 18O. We study the behaviour of the ferroelectric soft mode as a function of volume, lattice shape and temperature for STO-16 and STO-18, finding a limited phase space where STO-16 shows quantum paraelectric behaviour, while STO-18 becomes ferroelectric. These results demonstrate that ab-initio methods can explain the isotope effect in STO as a purely displacive phase transition.

We also analyse the effects of different levels of electronic correlation and convergence of SSCHA calculations on the phase diagram.

While machine learning force-fields allow us to scale to temperature dependent simulations that include quantum and anharmonic phonon effects, a quantitative prediction of phase diagrams remains challenging.

CT Thermodynamic stability of the materials in the Materials Cloud three-dimensional crystals database (MC3D)

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High-throughput studies based on ab initio methods such as Density Functional Theory (DFT) are the framework of choice when studying the physical properties of a broad chemical space, aiming to facilitate the interpretation of experimental results. Here, we present the Materials Cloud three-dimensional crystals database (MC3D)[1], a DFT optimized and curated structural database of inorganic crystals. The MC3D is fully based on initial experimental structures available in the databases MPDS [2], ICSD [3], and COD [4]. All calculations are managed and driven by the AiiDA [5,6] workflow engine, allowing to browse the full provenance graph and to share the results in the Materials Cloud. In this work, we focus on the thermodynamic stability of the materials in the MC3D by calculating the formation energies and inspecting their energies above the convex hull. In this way, we can identify stable compounds that are expected to be more likely to exist and be synthesizable under experimental conditions. To improve the agreement between the theoretical and experimental thermodynamic stability, we apply empirical [7] and machine-learning [8] based corrections, and improve upon them, discussing the agreement with experimental data on stability. We expect that our MC3D database becomes a reference resource for experimentalists interested in the materials properties of inorganic materials and, thanks to our recent additions, also facilitates the estimation of materials stability.

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List of Abstracts – Posters

P1 Automating experimental workflows with AiiDA: from battery cycling to thin film growth

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Scientific discovery via experimentation alone can be cumbersome and costly. Thanks to theoretical and computational advances, simulations can be quantitatively predictive and provide insight at a fraction of the cost. Simulation-assisted analysis of experimental observations can thus further accelerate scientific discovery. Automated high-throughput simulations carried out by modern workflow management systems (WFMSs) have been a go-to approach in recent years, particularly in materials science. The AiiDA (https://www.aiida.net) WFMS has historically managed complex simulation workflows, storing all the steps (provenance), thus ensuring reproducibility. Recently, AiiDA has been shown equally successful in automating experimental workflows [1], providing an additional avenue for discovery. We present here the use-case of battery cycling experiments driven by the AiiDA ecosystem and discuss future directions towards end-of-life battery optimization as an example of further integration with autonomous loops, driven by AI/ML, for future autonomous/self-driving labs, for materials discovery and characterization. A similar approach is presently considered for an internal PSI collaboration on thin-film growth automation via growth parameters optimization. We discuss the complexities of managing open research data (ORD) from mixed experimental/simulation workflows across research data management (RDM) platforms in a FAIR manner and highlight the efforts of the PREMISE (https://ord-premise.org) Establish project (of the ETH Board ORD program) towards facilitating interoperability of open and FAIR research data.

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P2 Growth of Bi-based halide single crystals for X-ray detection application

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The Metal halides perovskites such as $CsPbBr_3$ and $MAPbI_3$ have gained significant attention for X-ray detection application over a decade. Recently Pb-free alternatives, particularly Bi-based metal halide family has been considered as environmentally greener alternatives to CdTe and $CsPbBr_3$. In this study, we synthesized various class of Bi-based halides using conventional supersaturated solution cooling, Inverse Temperature Crystallization (ITC), Vapor Transport and Bridgman growth. We further characterized these materials using PXRD, rocking curve XRD, SEM-EDS, Raman, Absorption and PL measurements. Finally, we fabricated and tested single channel X-ray detectors using these crystals as X-ray sensor. Our studies reveal that among all the material, the highest X-ray photocurrent and sensitivity was obtained by double Perovskite namely $Cs_2AgBiBr_6$ that holds promise as good X-ray detector.

P3 Bright Future: Automated Sample Preparation

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Charles University, Prague, Czech Republic

Automated sample preparation is revolutionizing research in chemistry [1] and biology [2], enhancing precision, reproducibility, and efficiency in experimental workflows. Recent studies have demonstrated significant advancements in automated liquid handling and sample analysis, driving discoveries at an unprecedented pace. This automation trend is also poised to transform crystal growth, with recent developments in condensed matter physics showcasing automated systems for synthesizing and characterizing crystalline materials. Notably, recent progress highlighted by Szymanski *et al.* [3] in the field of solid-state chemistry illustrates the potential for automated methodologies to streamline and accelerate research in this field, promising a bright future for automated sample preparation across scientific disciplines.

The automation of more advanced crystal growth techniques requires state-of-the-art robotic systems taking advantage of computer vision and machine learning. The integration of robots and automation processes, familiar in large-scale factories, into sample preparation not only makes the entire process more efficient and faster but also renders the sample preparation process (especially for monocrystals) fully reproducible through precise measurement of hundreds of parameters.

We will be also mentioning the Automatic Laue Sample Aligner (ALSA) prototype [4], which fully automates the process of arranging monocrystals using X-ray Laue diffraction, robotic manipulators, real-time camera recognition, and specialized artificial intelligence-based software for analyzing crystal placement. The ALSA device represents a revolutionary change in the field of sample preparation, as it drastically speeds up the process and significantly increases the precision of arrangement, specifically for inelastic neutron scattering, for example at SINQ@PSI.

Technical details of the ALSA and also proof of concept experiment will be presented in a separate contribution [5].

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P4 Progress in the growth of rare earth silicate crystals

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Rare earth silicates are an interesting class of materials owing their potential for optical (laser diodes, scintillators) and environmental barrier coating (EBC) applications. One of the major difficulties encountered in the synthesis and study of these systems is due to the existence of a relatively large number of chemical phases (e.g. $R_2\mathrm{SiO}_5$, $R_2\mathrm{Si}_2\mathrm{O}_7$, $R_{4.67}(\mathrm{SiO}_4)_3\mathrm{O}$ and polymorphism possible at ambient pressure, i.e. depending on the nature of the lanthanide ion and temperature, $R_2\mathrm{SiO}_5$ crystallizes in 2 crystal-types, whereas $R_2\mathrm{Si}_2\mathrm{O}_7$ forms 7 crystal structures. Moreover, there is an overlap of the thermodynamic stability ranges of the different polymorphs and/or chemical phases, thus hindering the synthesis of pure phase ceramic materials by conventional solid state reaction. To overcome these drawbacks and study the intrinsic properties of these systems, one can attempt to prepare these materials in crystal form.

Some members of the $R_2\mathrm{Si}_2\mathrm{O}_7$ family were previously grown by the floating zone method using conventional halogen-lamp-heated furnaces. Nevertheless, the boules obtained were comprised of multi grains, had thermally generated cracks and the single crystals isolated from the boule were too small to study extensively these materials. The growth of some members of the $R_2\mathrm{SiO}_5$ family has recently seen a renewed interested due to advances in the floating zone method with the development of laser-diode-heated floating zone furnaces. However, some of the crystals obtained were comprised of multi grains, opaque and had thermally generated cracks.

Here, we present the results of our investigations to optimize the synthesis and crystal growth conditions of $R_2\mathrm{SiO}_5$ (R = Dy, Ho and Er), and discuss the properties of these materials [1]. Our study proves the complementarity to the conventional halogen-lamp-heated and laser-diode-heated floating zone furnaces. Our attempts to grow members of the $R_2\mathrm{SiO}_5$ series using conventional halogen-lamp-heated furnaces failed to yield any crystals, i.e. the desired chemical phase appears to melt incongruently, and the melt was found to be composed of other chemical phases than the desired one. Alternatively using a laser-diode-heated furnace we successfully prepared large, high quality, crack-free and pure phase single crystals of $R_2\mathrm{SiO}_5$. Our results show that the different thermal profile of the heated zone compared with conventional halogen heated floating zone furnace is crucial in the stabilisation of the $R_2\mathrm{SiO}_5$ phase and our findings could be extended to other families of rare earth silicates. This progress is crucial for the study of the intrinsic structural, chemical and physical properties of these materials which will open the route for improving the properties of these materials for applications.

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P5 Optimising the growth of incongruently melting materials by floating zone methods with the aid of finite element modelling

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Incongruently melting materials can be troublesome to prepare using standard melt-crystallisation techniques. Depending on the system of interest, utilising floating zone techniques can overcome some of these difficulties due to segregation of components at the crystallisation surface that change the composition of the molten zone until a steady state is reached, with crystallisation of the target incongruently melting material may be realised [1].

The expected compositional segregation behaviour during a growth can be naively approximated using a modified Scheill-Gulliver equation, but several assumptions in the derivation of these equations make them not directly applicable to a typical floating zone experiment.

Heusler alloys within the Ni-Mn-Ga system are of industrial interesting due to their magnetic-shape-memory alloy properties, but to utilise these properties single crystals are needed, and very stringent compositional controls are required due to rapid changes in material properties with only minor compositional changes [2,3].

We have recently been using COMSOL Multiphysics software to perform finite element modelling of the crystallisation process within our floating zone furnace (Fig. 1). Accurately following the heat flow and phase changes during the crystal growth allows us to accurately predict and follow the compositional variation (Fig. 2).

In this contribution I will discuss the difficulties and assumptions necessary for the modelling process as well as our successes in accurately modelling the compositional segregation within the floating zone crystallisation of Ni-Mn-Ga crystals.

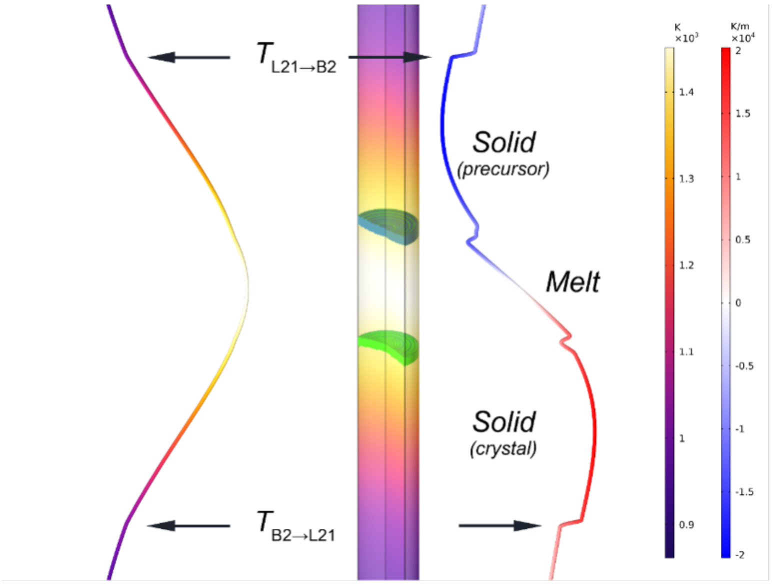

Figure 1: A time-snapshot of the calculated growth process using COMSOL Multiphysics. Left deformed tube graph shows the radially averaged temperature distribution, $T(z)$, along the ingot. The central 3D figure shows the ingot model with overlayed temperature distribution and highlighted melting (blue) and solidification (green) interfaces. Deformed tube graph on the right shows the temperature gradient along the ingot, $dT/dz(z)$. Anomalies in the temperature derivative are seen at the structural transformations of B2$\rightarrow$L21 type, as well as at the melting and solidification interfaces.

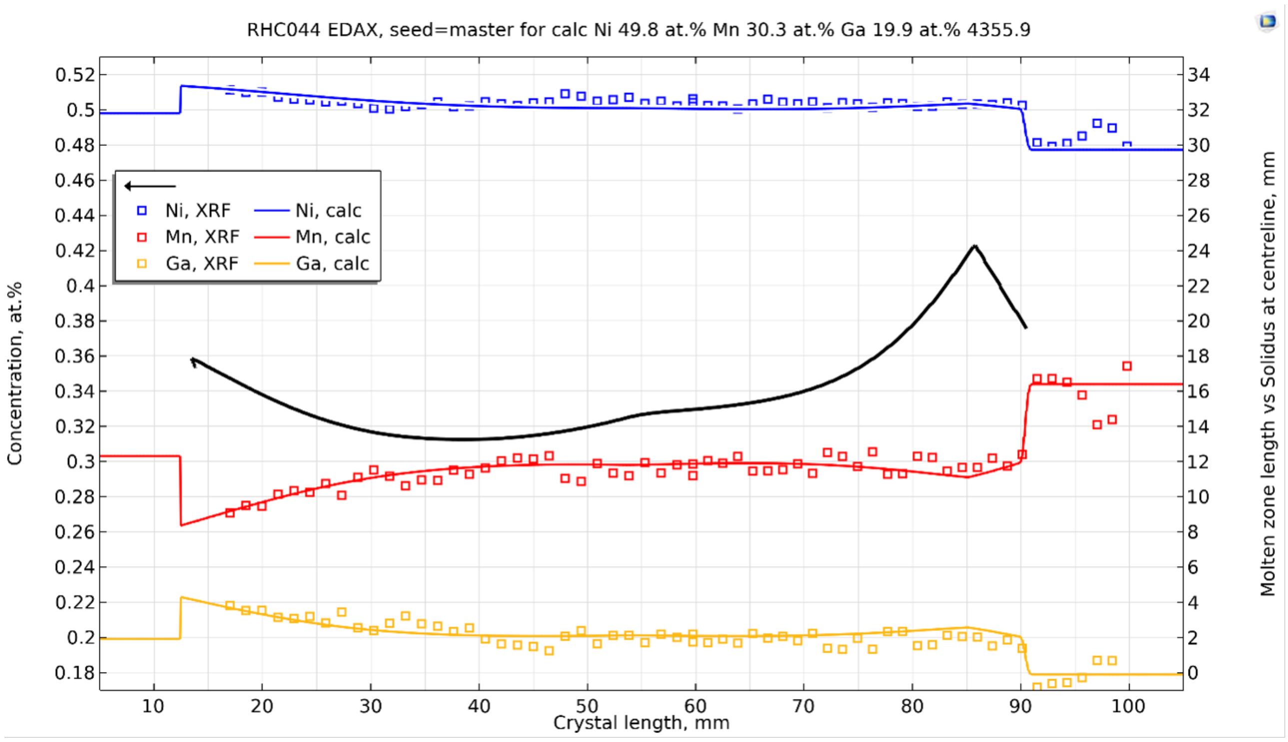

Figure 2: Experimental macroscopic composition variation along a prepared single crystal ingot (points) compared to calculated composition distribution after the recrystallisation (lines). Black line shows the length of the molten zone at a given position of the solidification interface during the calculation.

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P6 Ultrathin Fe on $SrTiO_3$: Interplay of redox reaction and band alignment

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Oxide electronics provide key concepts for enhancing silicon-based semiconductor technologies with novel functionalities. In a recent paper, we provide evidence for individually emerging hole- and electron-type 2D band dispersions at Fe-$SrTiO_3$ heterostructures [1]. Theoretical calculations suggest that the emergence of p- or n-type bands is closely linked to the Fe oxidation state which enables the possibility to tune the interface properties to set or even switch between negatively (n) charged electrons or positively (p) charged holes. One of the main processes that controls the interface properties is the oxygen exchange between the film and the substrate: We find an unexpected oxygen vacancy characteristic for the hole-type interfaces, which as of yet had been exclusively assigned to 2D electron gases. The tunability of the oxygen transfer through various growth parameters opens up the possibility of specifically adjusting electronic properties.

Using our UHV-MBE system, we grow high-quality ultrathin Fe films on $SrTiO_3$ substrates by systematically varying the growth parameters, e.g. (i) growth temperature, (ii) substrate annealing, and (iii) Fe film thickness. Performing in situ X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction enables the analysis of the electronic properties and crystalline structure of ultrathin Fe films directly after the growth without any atmospheric contamination.

The present work discusses the effect of different growth temperatures, substrate annealing procedures, and film thicknesses of the Fe films on the interfacial properties like oxygen vacancies. The oxidation state of Fe as well as the concentration of defects in $SrTiO_3$ strongly influences the valence band alignment between electron and hole band bending. We find that by tuning such growth parameters it is possible to control the 2D interface properties.

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P7 Design of High-Temperature Syntheses in (Bi$_{2x}A_{1-3x}$)[PtBi$_6$I$_{12}$] Compounds with A = Pb, Sn, Mn, Fe

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During the search for novel topological insulators [1], we discovered new pseudo one-dimensional compounds. The reactions of stoichiometric amounts of Bi with Pt, BiI$_3$ and A (A = Pb[2], Sn[3], Fe, Mn) above 300 °C yielded shiny, black, air insensitive crystals of the subiodides (Bi$_{2x}A_{1-3x}$)[PtBi$_6$I$_{12}$], with $0 \leq x \leq 1/3$. Based on extensive investigations into the synthetic pathways and growth mechanisms with the help of differential scanning calorimetry, compounds with various x could be isolated and synthesized reproducibly by growing the crystals from their respective melts and through extensive annealing. The rhombohedral crystal struc¬tures consist of alternating cuboctahedral [PtBi$_6$I$_{12}$]^{2ˇ} cluster anions that are connected by A^{2+} or Bi^{3+} cations, which are in an octahedral coordination between the opposite trigonal faces. Depending on the cation charge, this concatenation results in infinite cluster strands A[PtBi$_6$I$_{12}$] or in finite chains, such as Bi$_2$[PtBi$_6$I$_{12}$]$_3$ [4]. The cube-shaped morphology of the crystals originates from Bi···I inter-cluster bridges and with this ad¬ditional connectivity the structures can be seen as defect variants of the NaCl structure type. The heavy elements show strong spin-orbit coupling, which if it exceeds the width of the chemical band gap of the compound, could lead to a non-trivial topology.

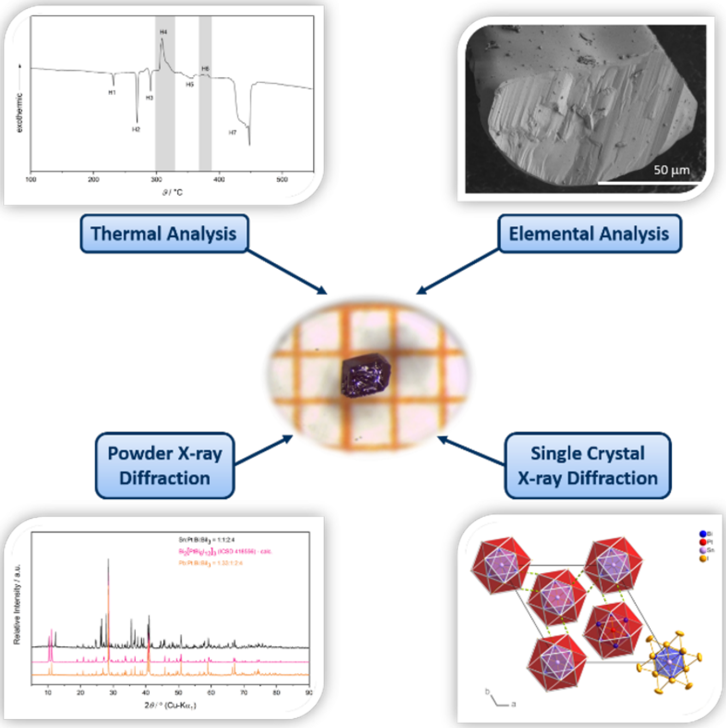

Figure 1: The different analytical methods involved in the design of the synthetic pathways for the new phases.

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P8 The versatile general purpose surface-muon instrument (GPS) for μSR at the Swiss Muon Source

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We present on the design and operation of a versatile spectrometer for muon-spin relaxation/rotation studies installed at the Swiss Muon Source (SμS) of the Paul Scherrer Institute (PSI, Switzerland). This instrument, the general-purpose surface-muon (GPS) instrument, has long been the workhorse of the μSR user facility at PSI. By making use of muon and positron detectors made of plastic scintillators read out by silicon photomultipliers, a time resolution of the complete instrument of about 160 ps (standard deviation) is achieved. In addition, the absence of light guides, which are needed in traditionally built μSR instruments to deliver the scintillation light to photomultiplier tubes located outside applied magnetic fields, allowed us to design a compact instrument with a detector set covering an increased solid angle compared with older designs. The result is an instrument that can be used for almost all areas in which μSR is useful, with fast temperature operation from 1.4 K up to 475 K, and magnetic fields from nearly zero (< 30mG) up to 0.8 T.

P9 Single Crystal Growth of $CsPbBr_3$ by Bridgman method

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Cesium Lead bromide has recently attracted increased attention among researchers due to its excellent optoelectronic properties. It is a very promising material for X- and γ-ray detectors because it consists of heavy elements (high atomic numbers), has a suitable high density (4.85 g/cm^3), and a wide bandgap (2.24 eV). One of the fundamental technological advantages of $CsPbBr_3$ is its capability to be obtained in the form of large bulk single crystals (SC). Among the two main methods used for that (solution growth and growth from the melt - Bridgman technique), the Bridgman growth has several advantages, as it can provide uniform, high-quality centimeter-size crystals. Additionally, this technique can prevent contamination by solvent molecules that the crystal matrix can trap during crystallization from the solution.

Although the Bridgman method has long been widely used to obtain bulk crystals of various semiconductors, its use for acquiring $CsPbBr_3$ SC still has many aspects and problems that must be considered during the crystal growth process. One of these issues is the tendency of the melt to supercool, resulting in crystallization below the melting point. The degree of supercooling can be as high as 30 °C below the melting point [1]. It could be even higher during the actual growth process (Fig. 1a). Crystallization with supercooling occurs rapidly, resulting in the formation of polycrystalline ingots with low quality, making them unsuitable for use as detectors (Fig. 1b).

In order to improve the quality of $CsPbBr_3$ crystals, we conducted an optimization process of the growth conditions. This involved adjusting the temperature profile within the crystallization range of 520-580 °C inside the Bridgman furnace. In this way, a sharper temperature gradient is achieved, which leads to a faster temperature change from the tip to the top of the ingot. We reduced the tip region of the ingot, which reaches the supercooling temperature range and crystallizes below the melting point. This helps to minimize the ingot's lower polycrystalline part (0.5-1 cm) and increase its single-crystalline upper part volume (Fig. 1c). As a result, we were able to obtain larger single-crystals with good transparency and crystal quality.

Even though several issues, such as cracks and twins, still need to be resolved to obtain high-quality single crystals, eliminating the effect of supercooling is a significant step on this path.

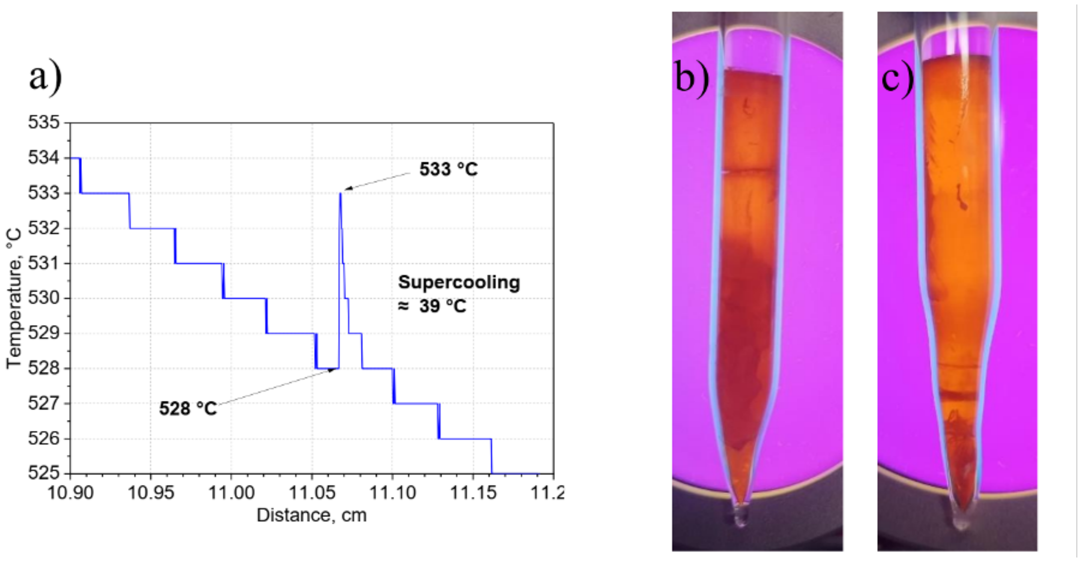

Figure 1: a) Temperature of the ampoule tip in the furnace passing through the crystallization region of $CsPbBr_3$. The detected peak corresponds to the exothermic crystallization effect with supercooling of 39 °C; Photos of $CsPbBr_3$ ingots with large - b) (strong effect of supercooling) and reduced - c) polycrystalline parts.

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P10 The FLexible Advanced MuSR Environment (FLAME)

Jonas Andreas Krieger[1]***, Thomas James Hicken***[1]***, Christopher Baines***[1]***, Marek Bartkowiak***[2]***, Matthias Elender***[1]***, Alexey Stoykov***[1]***, Hansueli Walther***[1]***, Markus Zolliker***[2]***, Alex Amato***[1]***, Hubertus Luetkens***[1]

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Muon spin spectroscopy (μSR) at ultra-low temperatures and in high magnetic fields has important applications in the study of unconventional superconductivity, quantum phase transitions, hydrogen-like states in semiconductors, and frustrated magnetic systems. Here we report on the design, technical realisation, and characterisation of a new μSR spectrometer, with moniker FLAME, at the Swiss Muon Source (SμS) of the Paul Scherrer Institute (PSI, Switzerland). This new instrument replaces the low temperature facility (LTF) instrument at the πM3.3 beamline. The sample environment allows operation in a temperature range from sub-30 mK up to room temperature and in magnetic fields up to 3.5 T, with low background and a time resolution better than 200 ps. The instrument is optimised for a high sample throughput and allows users to simultaneously mount two samples with a short changeover time of less than $\sim$ 8 h between subsequent base temperature measurements. We will illustrate the capabilities of the new instrument with some initial research examples.

P11 Special approaches and systems at the floating zone method: Preparation and use of rectangular rods, an image and data recording, processing, and visualization system, and the synthesis of reduced Carpy-Galy phases of the Schückel-Müller-Buschbaum type such as $Sr_{17}Ca_2Nb_{19}WO_{64}$ by melting and solidifying the fully oxidized composition under $Ar + H_2$

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The most common shape of polycrystalline and sintered compositions which is prepared for the floating zone method is a cylindrical rod. Another shape and its preparation by particular pressing dies, made of magnesia-stabilized zirconia or quartz glass, and special associated components will be presented, namely rectangular rods which are used at the Cyberstar mirror furnace at the ETH Zürich [1]. That furnace is equipped with a custom-made image and data recording, processing, and visualization system [2]. It allows the creation of a fast-mode video of an overall mirror furnace run or a real time video of a short section. The created video displays in one and the same video frame the progression of the image, power of the left and right lamp, speed of the upper and lower shaft, and other quantities versus time. Examples will be presented.

Carpy-Galy phases $A_nB_nO_{3n+2} \triangleq ABO_x$ represent a homologous series of perovskite-related layered oxides which exist for B = Ti, Nb, Ta. Along the c-axis the layers consist of [110]-oriented perovskite type slabs which are n BO_6 octahedra thick. For $n = \infty$ the non-layered perovskite structure ABO_3 is realized. Carpy-Galy phases are interesting for several reasons such as (see Refs. [3-6] and references therein):

- In contrast to most other layered materials the Carpy-Galy phases are significantly anisotropic not only with respect to the ab-plane versus c-axis but are also pronounced anisotropic with respect to the a-axis versus b-axis.
- The Carpy-Galy phases comprise the highest-T_C ferroelectrics which are $n = 4$ types such as $La_4Ti_4O_{14} \triangleq La_2Ti_2O_7 \triangleq LaTiO_{3.5}$ and $Sr_4Nb_4O_{14} \triangleq Sr_2Nb_2O_7 \triangleq SrNbO_{3.5}$ and their T_C's are in the range from 1615 K to 1850 K.
- The Carpy-Galy phases comprise quasi-1D metals such as the $n = 5$ type Sr5$Nb_5O_{17} \triangleq SrNbO_{3.4}$ in which the delocalized electrons are embedded in a ferroelectric-like environment and some of them are potentially polar or ferroelectric quasi-1D metals.
- The quasi-1D metals $SrNbO_{3.45}$ ($n = 4.5$) and $Sr_{0.95}NbO_{3.37}$ (Sr- and O-deficient $n = 5$) were studied by special optical techniques which revealed the presence of photoinduced metastable dd-exciton-driven metal-to-insulator transitions.
- The Sr- and O-deficient $n = 5$ type quasi-1D metal $Sr_{0.95}NbO_{3.37}$ was studied by resonant soft x-ray scattering which revealed the presence of two distinct and simultaneous charge density waves along the non-metallic c-axis.
- Carpy-Galy phases might have the potential to create superconductors / multiferroics.
- Many Carpy-Galy phases can be prepared via the melt by using the floating zone method.

Another interesting item are Carpy-Galy phases of the Schückel-Müller-Buschbaum type [3]. In a paper from 1985, K. Schückel and Hk. Müller-Buschbaum report that a small amount of crystals with the composition $Sr_5Nb_5O_{16}$ were obtained by a special synthesis experiment which involves the use of a H_2 / H plasma [7]. The crystal structure of $Sr_5Nb_5O_{16}$ was determined by single crystal x-ray diffraction [7]. Physical properties of $Sr_5Nb_5O_{16}$ are not reported. Later, in a paper from 2008, F. Lichtenberg *et al.* present the realization that the non-centrosymmetric $Sr_5Nb_5O_{16}$ can be considered as an oxygen-deficient variant of the centrosymmetric $n = 5$ type quasi-1D metal $Sr_5Nb_5O_{17}$ with fully ordered oxygen vacancies [6,8]. That leads to several interesting questions and comments which are presented on pages 225 – 227 in part 6.7 of Ref. [3]. The crystal structure of $Sr_5Nb_5O_{16}$ appears unusual and interesting and it seems to be worthwhile to study its physical properties. However, in a paper from 2008 it is reported that an attempt to prepare $Sr_{20}Nb_{20}O_{64} \triangleq Sr_5Nb_5O_{16} \triangleq SrNbO_{3.2}$ by melting and solidifying polycrystalline sintered rods with the reduced composition $Sr_{20}Nb_{20}O_{64}$ under argon was not successful and resulted in a multiphase material [6]. Meanwhile, however, in a paper from 2020 a special approach is presented which allows the melt-grown synthesis of related, reduced, and Sr-deficient $n = 5$ type Carpy-Galy phases of the Schückel-Müller-Buschbaum type such as $Sr_{17}Ca_2Nb_{19}WO_{64}$ [3]. They were prepared by melting and solidifying polycrystalline sintered rods with a fully oxidized Nb^{5+} and W^{6+} composition such as $Sr_{17}Ca_2Nb_{19}WO_{69.5}$ under flowing 95 % Ar + 5 % H_2. Pictures and videos from synthesis experiments and their results will be presented. The magnetic susceptibility $\chi(T)$ of $Sr_{17}Ca_2Nb_{19}WO_{64}$ suggests it is a quasi-1D metal like the related $Sr_{20}Nb_{20}O_{68} \triangleq$

$Sr_5Nb_5O_{17} \triangleq SrNbO_{3.4}$ [3]. The existence of $Sr_{17}Ca_2Nb_{19}WO_{64}$ and related materials leads to several interesting questions and comments, see part 6.9.8 of Ref. [3].

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P12 Design of multiferroic spiral magnets with ordering temperatures far beyond 300 K

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In the past years, magnetism-driven ferroelectricity and gigantic magnetoelectric effects have been reported for a number of frustrated magnets with spiral magnetic orders [1]. Such materials are of high current interest due to their potential for spintronics and low-power magnetoelectric devices. However, their low magnetic order temperatures (typically <50 K) greatly restrict their fields of application [2].

Here, I show that chemical disorder is a powerful tool that can be used to stabilize magnetic spiral phases at higher temperatures. As example of this novel mechanism I present our recent investigations on AA'CuFeO_5 layered perovskites, where a controlled manipulation of the Cu/Fe chemical disorder and some interatomic distances was successfully used to increase the spiral order temperature from 154 K to nearly 400 K [3-5]. The observation of a gigantic, positive impact of the Fe/Cu disorder in the stability of the spiral magnetic order was extremely puzzling and seemed at odds with traditional frustration mechanisms. Interestingly, both observations could be rationalized in terms of a novel, disorder-based frustration mechanism based on the gigantic impact of a few Fe-Fe “defects” occupying the bipyramidal units of the layered perovskite structure, which host majoritarily Cu-Fe pairs [6-7]. On the basis of these findings, we propose a general set of rules for designing magnetic spirals in layered perovskites using external pressure, chemical substitutions, and/or epitaxial strain, which should guide future efforts to engineer magnetic spiral phases with ordering temperatures suitable for technological applications [8-10].

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P13 Updates and Capabilities of the Cold Neutron Diffractometer at PSI

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The cold neutron diffractometer (DMC) at the Paul Scherrer Institute (PSI) has been recently updated to enhance its capabilities in crystallographic studies. With the replacement of the cold neutron guide and the integration of a large, high-performance neutron detector featuring two-dimensional readout, DMC offers improved efficiency and precision for diffraction experiments.

DMC's flexible design allows for a wide range of experimental setups, making it suitable for studying various aspects of crystal growth, including the determination of magnetic structures, analysis of crystallographic phase transitions, and reciprocal space mapping in single crystals. The instrument's oscillating radial collimator system effectively reduces background interference, ensuring high-quality data acquisition.

Operated by the Laboratory for Neutron Scattering and Imaging (LNS), DMC serves as a valuable resource for researchers in the field of condensed matter physics. By providing a platform for in-depth analysis of material properties, DMC facilitates collaboration and fosters advancements in crystal growth techniques. As crystal growth continues to play a crucial role in the development of novel materials with unique physical properties, DMC remains committed to supporting research in this important area.

P14 New path of the Ba_2MgWO_6 single crystal growth using $BaCl_2$-$MgCl_2$ flux

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Double perovskites are capturing the attention of scientific community for several reasons. Fundamental – such as investigation of intriguing multipolar ordering in $5d^1$ double perovskites [1-3] – as well as practical applied use in photovoltaics, electro- and photocatalysis [4].

In order to understand the complex phenomena present in double perovskites, with a vast variety of electric, magnetic and optical properties, our goal was to synthesize single crystals of non-magnetic Ba_2MgWO_6. Difficulties to grow single crystals of a size suitable for macroscopic material property measurements caused the majority of characterization being published on polycrystalline samples [5] and ceramics [6,7]. We present a new method of Ba_2MgWO_6 single crystal synthesis that allows to grow mm-sized crystals using a $BaCl_2$ and $MgCl_2$ flux [8]. The single crystal diffraction and energy dispersive X-ray analysis confirmed high quality of synthesized samples. Heat capacity measurements from 300 K to 2 K do not show any phase transitions. However, Raman spectra measured down to 77 K contain additional weak peaks at all temperatures probed, which is in a contrast with only 4 Raman active modes expected from the crystal structure with the space group $Fm\bar{3}m$.

This calls for a more detailed study of potential symmetry breaking that might have an impact on the electric properties of the material.

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P15 Automated prediction of Fermi surfaces from first principles

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Knowing the shape of the Fermi surface (FS) and the energy dispersion in its vicinity is crucial to understand the electronic properties of materials and identify materials relevant for applications. Experimental methods to measure FSs, including angle-resolved photoemission spectroscopy (ARPES), Shubnikov-de Haas (SdH) and de Haas-van Alphen (dHvA) techniques, are very expensive and time-consuming, and accurate theoretical predictions would help to get deeper insights from the experimental data. Direct first-principles calculations of the FS require very dense sampling in reciprocal space, and are thus limited by the computational cost. To accelerate the calculations, we use interpolation with Maximally Localized Wannier Functions [1] (MLWFs), powered by a new method developed in the group that allows users to perform fully automated calculations of MLWFs [2]. We first validate the numerical approach by comparing our simulation results with literature data for de Haas-van Alphen (dHvA) oscillation frequencies and investigate the main sources of numerical errors. Then we use our high-throughput setup, with our code implemented as an AiiDA [3] workflow, to perform simulations for all non-magnetic inorganic metals from Materials Cloud 3D crystals database [4] (MC3D) - a curated set of experiment-based three-dimensional inorganic crystal structures complemented with density functional theory (DFT) simulations. The resulting database of Fermi surfaces and dHvA oscillation frequencies will be made available online openly as an extension to MC3D, together with the other materials properties predicted by DFT simulations and available in MC3D. The goal is to provide a curated database of materials properties that can guide experiments, and help in identifying materials with outstanding properties that might deserve being synthesized and experimentally measured.

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P16 High Resolution neutron Powder Diffractometer HRPT at Swiss neutron spallation source SINQ

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There are four main diffraction instruments at the Swiss spallation neutron source SINQ: the high resolution neutron powder diffractometer HRPT, the cold neutron powder diffractometer DMC, the neutron single crystal diffractometer ZEBRA, and a small-angle neutron scattering instrument SANS-I. An in-house single-crystal alignment instrument ORION is available as well.

The multidetector diffractometer HRPT is designed as flexible instrument for efficient neutron powder (and optionally single crystal) diffraction studies - also for small sample sizes. High resolution ($\delta d/d < 0.001$) is achieved by thermal neutrons of 0.84 Å to 2.45 Å, high scattering angles of the monochromator and of the sample (up to 165°). Complementary to synchrotron X-ray powder diffraction studies, the applications of HRPT are high-resolution refinements of chemical and magnetic structures as well as phase analysis of novel materials. Because of the generally weak absorption, neutrons yield information on bulk properties (average over large sample volumes) and permit in a non-destructive way the detection of lattice distortions, defects and internal microstrains. Also, real-time (in-situ) investigations of chemical or structural changes and of magnetic phase transitions in crystalline, quasicrystalline, amorphous, and liquid samples including technically interesting new materials are possible.

P17 MGML – open access infrastructure for single crystal growth

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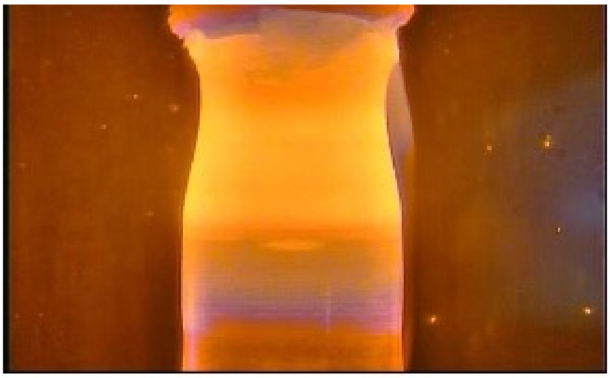
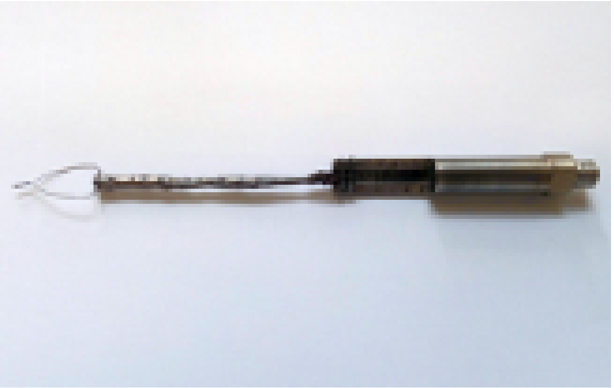
Materials Growth & Measurement Laboratory (MGML) (see mgml.eu or use QR code) is the Czech open access scientific infrastructure located in Prague. The leading host institution is Faculty of Mathematics and Physics of Charles University (FMP CU) and the partner host institution is Institute of Physics of Czech Academy of Sciences (IoP CAS). MGML offers for external users the instrument suite dedicated to measurements of a rich spectrum of physical properties of materials in a wide range of temperatures, magnetic and electrical fields, and hydrostatic uniaxial pressures. The MGML technology facilities also enable controlled preparation and characterization of high-quality single crystals of materials of various types which is available to users who do have not their own well-characterized samples needed for measurements in MGML as well as in anywhere scientific facility. The access to the infrastructure is via the User Portal through the proposals. During more than two decades of development, the MGML offers a variety of single crystal growth techniques suitable for the growth of single crystals of all classes of materials and properties respecting the hot scientific subjects in condensed matter physics. Nowadays, MGML provides users with these options:

- **Czochralski method** (triarc furnace);
- **Bridgman method** (induction furnace on closed sealed ampoules);
- **Floating zone method** (four-mirror and modern five-laser furnace);
- **Flux method** (flexible conditions-crucibles, solvents, temperature);
- **Hydrothermal synthesis** (bombs for aqueous solution up to 250 °C);
- **CVT method** (quartz ampoules operated in gradient furnaces).

The MGML laboratory is also equipped with a series of characterization techniques for the validation of the single crystal quality and orientation (Laue method with robotics arm for automatic arrangement of multiple sample targets), crystal structure (powder and single crystal X-ray diffraction in wide temperature interval 1000 °C - He temperature), composition (EDX and EXRF analysis), and followed by further machining to appropriate shape and size of single crystal sample (precise belt and wire saws, polishers, optical and electron microscopes…). The MGML provides top-quality input materials purified by two installed Solid-State-Electrotransport (SSE) apparatus which is an essential condition for the production of the top-quality single crystals. The thermal treatment of the grown single crystals can be performed in various conditions including UHV SSE treatment. The MGML also provides a unique offer to grow single crystals of actinide materials. See the recent examples of single-crystal production in MGML (in agreement with the crystal growers in MGML):

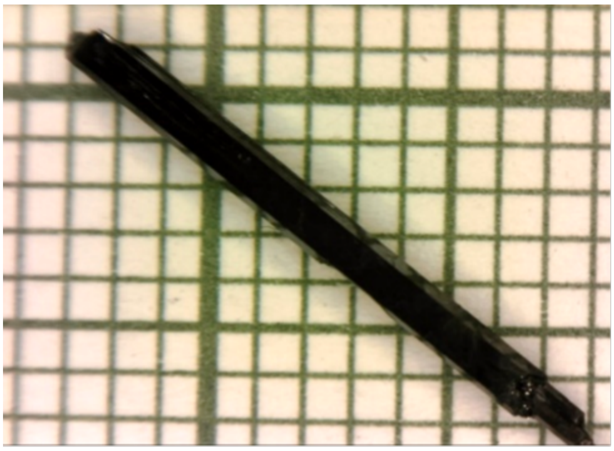


Single crystal growth process of solid state laser material Nd:YAG in laser furnace [1].

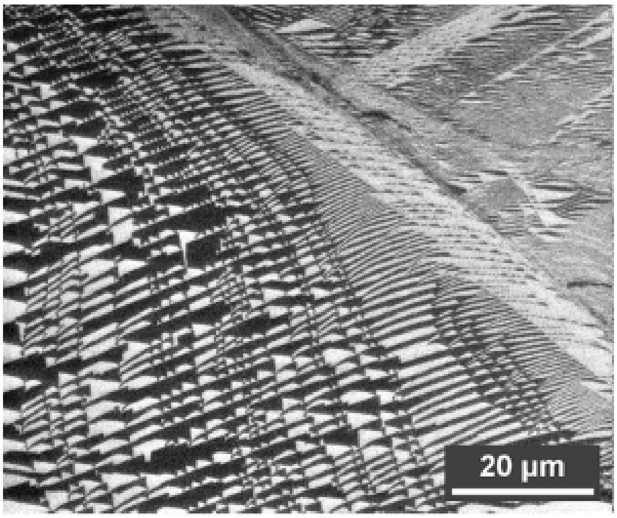


UNi$_4$^{11}B, actinide isotope single crystal with magnetic toroidal order [2].

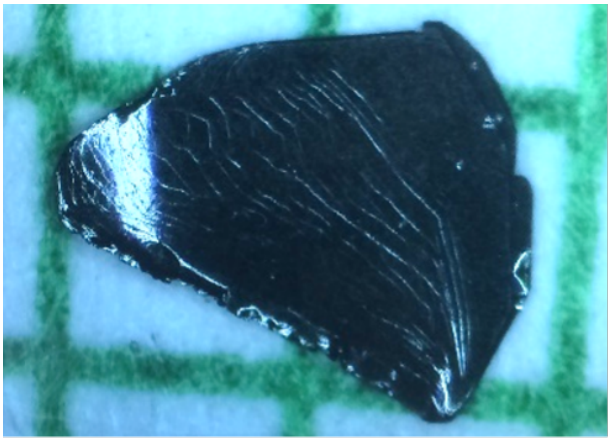
MnTe, first altermagnet with the documented lifting of Kramers spin degeneracy [3].



UTe_2 single crystal grown by Molten Salt Flux method used to observe quantum oscillations [4].



$(PbS)_{11}VS_2$, first misfit layer bulk sliding ferroelectric material (SEM image of a cleaved crystal) [5].



VI_3, vdW ferromagnet with large intrinsic orbital magnetic moment [6].

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P18 Kondo-controlled topological phases in the antiferromagnetic Weyl semimetal CeAlGe

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The magnetic Weyl semimetal CeAlGe is a model system for investigating the relationship between electronic and magnetic topologies. CeAlGe crystalises in tetragonal structure $I4_1md$, where the spatial-inversion symmetry is broken, and exhibits Weyl fermions near a Fermi surface that becomes more stable by broken time-reversal symmetry [1,2]. It has been known that the magnetic ground state and relevant topological properties of CeAlGe depend on the crystal synthesis methods. For example, CeAlGe grown by the flux method exhibits a commensurate antiferromagnetic (AF) order below T = 5.1 K [3], whereas the crystal grown by floating-zone methods with high pressure of Ar gas (p = 30 bar) exhibits an incommensurate AF order below T = 4.4 K in which topological Hall effects are induced by external magnetic fields applied along the c-axis [4]. In order to understand the relationship between electronic and magnetic topologies in CeAlGe, it is necessary to reveal the microscopic mechanism of the topological magnetism, which has yet to be investigated. In this presentation, we show the experimental results of newly synthesised CeAlGe using the same floating-zone method but with lower Ar pressure of p = 5 bar. The lower pressure of the synthesis environment slightly changes the crystal unit cell parameters and the stoichiometry, by which the Kondo coupling strength can be modified, thereby the suppressed magnetic ordering temperature to T = 4.1 K. Our neutron diffraction and electrical Hall transport experiments revealed that the topological magnetism is still stabilised with shorter periodicity. Given all experimental results of flux-grown and two floating-zone-grown CeAlGe, we will discuss the relevant factors in stabilising topological magnetism and a possible way to tune the Kondo coupling strength to unveil the relationship of two topological phases.

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P19

The multi-purpose surface-muon instrument at PSI: A versatile tool for studying novel materials

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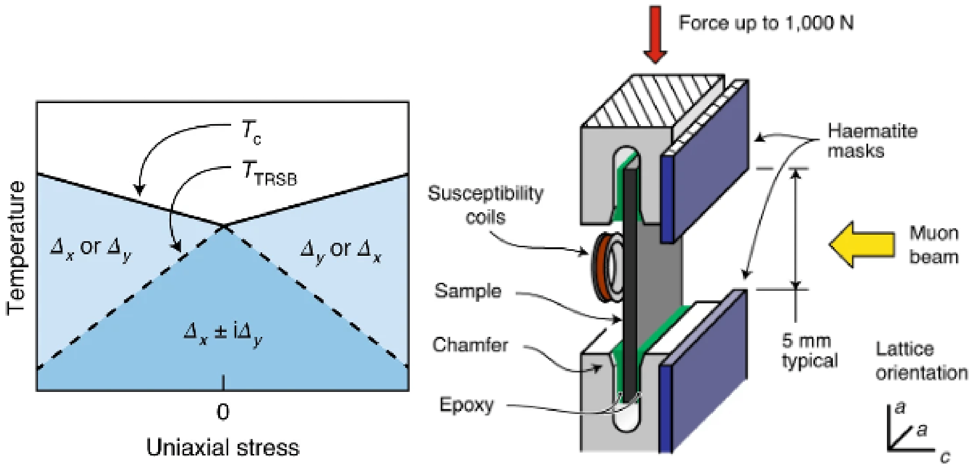
As local probes, muons have long been used to study a wide range of materials. Their high sensitivity to internal magnetic fields is due to their availability as fully polarized beams and the high correlation between the muon spin direction and that of the decaying positrons. Over the years, muon-spin relaxation/rotation (μSR) has become the technique of choice to study unconventional superconductivity, exotic magnetic order, time-reversal symmetry breaking, etc.

Extending these capabilities to the study of novel quantum materials requires continuous development efforts, including access to low and ultra-low temperatures, exact zero magnetic field, or the application of uniaxial (tensile and compressive) strain. The reward is new insights into topological nodal lines [1] and Weyl-Kondo semimetals [2], quantum criticality, phase diagrams of unconventional superconductors [3-5], etc. Given the importance of anisotropy and rotational symmetry breaking, these efforts should be accompanied by new developments in the growth of high-quality single-crystal and 2D materials. Such joint efforts will enable the future study and exploitation of these new materials of both fundamental and technological importance.



Split superconducting and time-reversal symmetry-breaking transitions under uniaxial stress [3]. Stress-temperature phase diagram for chiral superconductivity in Sr$_2$RuO$_4$. Here Δ_x stands for either p_x or d_{xz}. Schematic sample setup for μSR measurements under uniaxial stress. Coils are used for in-situ Tc measurements.

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P20 The upgraded neutron single-crystal diffractometer Zebra at SINQ

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The single-crystal neutron diffractometer Zebra at the Swiss Spallation Neutron Source SINQ, Paul Scherrer Institut (PSI), Switzerland, has been commissioned in 2016 after construction at the beamport of the former TriCS instrument. Zebra has an optimized neutron delivery system and a non-magnetic high-precision sample table compatible with extreme sample environments. Three detectors are available: a ^{3}He point detector with collimation capabilities, an area detector with $14^\circ \times 14^\circ$ angular coverage equipped with a non-magnetic radial oscillating collimator, and a 2-inches ^{3}He point detector equipped with a graphite analyzer. All detectors can be lifted out-of-plane ($\pm 15^\circ$) when sample environment requires. A set of motorized slits contributes to achieve a high peak-to-background ratio. The python-based software package ‘pyzebra’, tailored specifically for the needs of the instrument, is available. We present examples of typical experiments, showcasing examples for small samples and other weak signals, and discuss present limits and possible upgrades.

P21 Proof of concept: Automatic coalignment of flux-grown crystals

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Inelastic neutron scattering is very useful experimental method used across all scientific fields. It is mainly used for uncovering the dynamics and excitations in single crystals. Although it is very powerful method, inelastic neutron scattering suffers from the low flux scattered from sample. This can be improved by increasing the mass of the sample, which becomes limiting for samples only incongruently growing using flux-growth.

Traditionally, experimental physicists are co-aligning hundreds of single crystals together to increase weak inelastic scattering flux [1]. This process is very time consuming and often not very precise [2]. We have developed a state-of-the-art robotic machine ALSA: Automatic Laue Sample Aligner, which will automatize sample coalignment process while increasing the precision of the coalignement. We will present technical details of the prototype, including hardware solutions for calibrating computer vision cameras with robotic arm, automatic glue dispenser and Laue X-Ray diffractometer with focusing optics. In addition, we present software algorithms for automatic sample picking, automatic Laue pattern solving as well as automatic sample placing.

Lastly, we prove the quality of the first automatically coaligned crystal assembly by inelastic neutron experiment. We have prepared triangular lattice antiferromagnet Na$_2$BaMn(PO$_4$)$_2$ by the flux growth method. Grown crystals are typically 1-4 mm plates with well-defined hexagonal c-axis, but a and b-axis are not possible to determine by eye, rising needs for using Laue diffractometer. ALSA robotic machine successfully coaligned over 300 crystals with mass 3.1!g and overall mosaicity spread below 2°. The quality of coalignment was checked by scanning the plates using X-Ray Laue and using neutrons on OrientExpress and IN12 at ILL. Coaligned assembly was later used for investigation of the spin excitations in this triangular lattice antiferromagnet.

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P22 Single crystals of novel chalcogenides, grown by chemical vapor transport

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Chalcogenides are becoming increasingly important materials that combine ideal properties as solar absorbers with earth-abundant and low-toxic components. In particular, adamantine-type compounds, including kesterites, are currently the most promising material for fully inorganic thin-film photovoltaic technology that is free of critical raw materials and thus offers sustainable solutions. These compounds also include Cu-Sn-S compounds, e.g., Cu_2SnS_3 (Mohite) and Cu_2CuSnS_4 (Kuramite), as well as defect-adamantines like $CuGaSnS_4$. In parallel, other chalcogenides, e.g. of the ABS_3 type such as $BaZrS_3$, as well as binary chalcogenides, e.g. Sb_2S_3, play an important role in the search for new materials.

The ternary $A^{I}B^{III}X_2^{VI}$ chalcopyrite compound family, which includes the compound semiconductor $Cu(In,Ga)Se_2$ - used as an absorber layer in high-efficiency thin-film solar cells - can be transformed into quaternary adamantines by chemical substitutions by obeying the valence octet rule. Due to added chemical and structural freedom, these quaternary compounds have some novel and exciting properties. One possible substitution would be $A^{I} + B^{III} \leftrightarrow C^{IV} + \square$, resulting in the quaternary semiconductors $A^{I}\square B^{III}C^{IV}X_4^{VI}$ (the symbol $\square$ indicates cation vacancies, i.e., empty cation sites in the crystal structure). These compounds are referred to as defect adamantines [1] and can be considered as potential absorber materials for thin-film solar cell applications.

$A^{I}\square B^{III}C^{IV}X_4^{VI}$ defect adamantines are formed from ternary chalcopyrite-type compounds ($A^{I}B^{III}X_2^{VI}$) by doubling the entire formula unit and replacing one A^{1+} and one B^{3+} cation with one C^{4+} cation. This results in a balanced valency but an unbalanced cation - anion ratio (with respect to the ratio of cation and anion sites in the chalcopyrite-type structure). Accordingly, the structure must be compensated by vacancies ($A^{I} + B^{III} \leftrightarrow$ vacancy + C^{IV}). With band gap energies ranging from 1.42 eV for $CuGaSnSe_4$ [2] to 2.34 eV for $CuAlGeSe_4$ [2], these defect adamantines, in particular are potentially very interesting materials for photovoltaic applications.

Perovskite chalcogenide materials have gained increasing interest as potentially stable materials with promising optoelectronic properties owing to their structure type. These materials have the general formula of AMX_3 with A being a group II cation (i.e., Ca^{2+}, Sr^{2+}, or Ba^{2+}), M a group IV transition metal (i.e., Ti^{4+}, Zr^{4+}, or Hf^{4+}), and X a chalcogen anion (S^{2-} or Se^{2-}). These materials have been known for a long time and attempts to prepare them have been made in many ways. Single crystals of this group of materials were prepared by the flux method. However, most of the data regarding structure and optoelectronic properties were determined on polycrystalline thin films [3, 4].

$BaZrS_3$ as a representative of this class of materials crystallizes in the orthorhombic perovskite-type structure. For thin films of $BaZrS_3$ a band gap energy of 1.95 eV [5] and 1.99 eV [4], respectively, has been determined.

Figure 1: Single crystal of $CuGaGeS_4$.

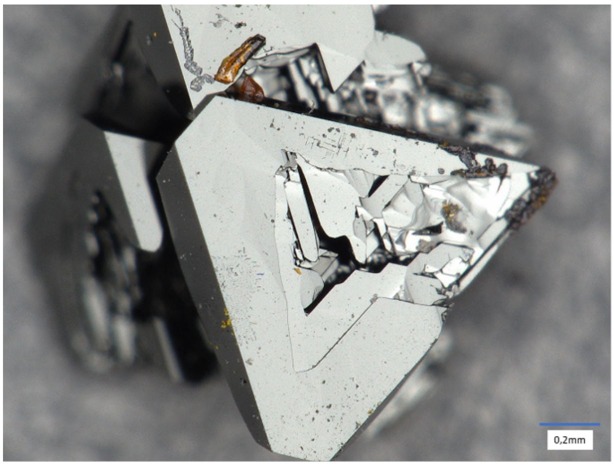

Figure 2: Single crystal of $CuAlSnS_4$.

The most suitable method for growing chalcogenide single crystals considering the phase diagrams would be chemical vapor transport (as introduced by Nitsche [6]). With chemical vapor transport enhanced by halogens, crystals can be grown below critical temperatures. Such crystals grow near the thermodynamic equilibrium. For single crystal growth,

growth conditions such as source temperature, temperature gradient, and transport agent concentration are important. The main challenge is to control the composition of the gas phase and to optimize the temperature field during growth.

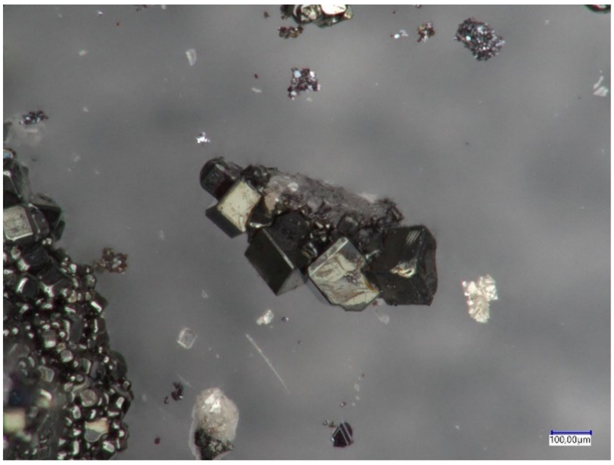

Figure 3: Single crystals of $BaZrS_3$.

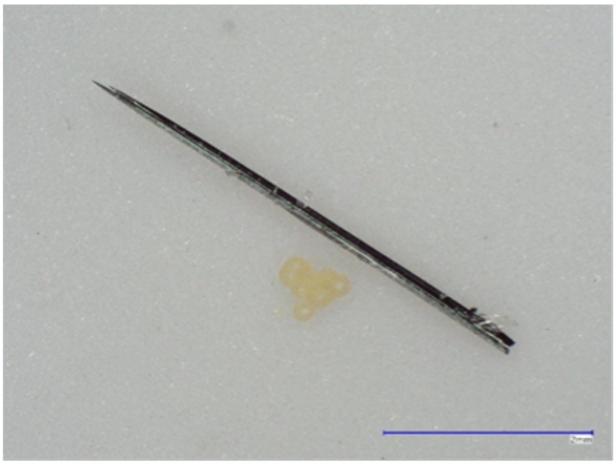

Figure 4: Single crystal of $BaZrS_3$.

The resulting material and grown crystals were characterized by powder X-ray diffraction (XRD) and LeBail analysis of the diffraction pattern, as well as by single-crystal X-ray diffraction. The chemical composition of the crystals was determined by X-ray fluorescence. The band gap energy was determined from the diffuse reflectance measured by UV-VIS spectroscopy.

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P23 Eigenstrain Tomography

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Residual stresses, originating from various mechanical, thermal, metallurgical, and environmental factors, significantly influence material performance in engineering applications. Understanding and managing these stresses are crucial for ensuring structural integrity and reliability. This paper introduces Eigenstrain Tomography, a pioneering approach in polycrystalline X-ray diffraction, for comprehensive residual stress reconstruction. Unlike traditional methods, Eigenstrain Tomography directly measures residual stress fields across specimens, enabling detailed analyses of stress distributions. Numerical experiments validate the method's accuracy, demonstrating its effectiveness in reconstructing intricate stress patterns with discontinuous processing properties. Eigenstrain Tomography offers a potent tool for non-destructive evaluation of residual stresses, enhancing our understanding of material behavior and aiding in process optimization across various industries.

P24 Investigation of Li_3N crystallization by FZ technique under high nitrogen pressure

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Lithium nitride (Li_3N) with hexagonal layered structure ($P6/mmm$) possesses the highest conductivity among all inorganic lithium salts and is a perspective ion conductor [1,2]. But only a few papers, dealing with the single crystal growth of the Li_3N can be found in the literature.

The Czochralski growth of Li_3N had shown, that Li_3N melt intensively interacts with crucible materials, such as iron, vitreous carbon and molybdenum [3].

The FZ growth of Li_3N was realized in N_2 atmosphere with pressure up to 2 bar [4]. During the growth the following effects were observed: (i) a decomposition of the Li_3N melt, resulting in a metallic luster of the surface of the molten zone (MZ) and both seed- and feed-rods; (ii) the evaporation of the Li_3N from the MZ; and (iii) the deposition of the evaporated from the MZ Li_3N as needle-like crystals on the feed-rod slightly above the MZ. All these effects together negatively influenced on the growth run stability, in particular, on the maintenance of the optimal MZ size and shape, and on the quality of obtained crystals. Thus, for the successful realization of the FZ growth of Li_3N the solution on how to suppress all these negative effects should be found.

Recently the chromium nitride (Cr_2N) single crystals have been grown by FZ method under nitrogen pressures up to 10 bars [5]. It was shown that with increase of the nitrogen pressure from 1 bar (0.1 MPa) to 10 bar (1 MPa) the stoichiometry and the quality of obtained crystals have been improved significantly. For instance, in crystals grown at nitrogen pressures lower than 10 bars a metallic chromium phase segregated as inclusions in a parent Cr_2N phase have been detected. While for crystals grown at nitrogen pressure 10 bar only pure chromium nitride phase with stoichiometry $Cr_2N_{0.9}$ has been found. Thus, the increase of the nitrogen pressure during the FZ growth may significantly suppress the decomposition of the nitride melt, leading to the change of the quality of a growing crystal. Besides, increased pressure of the growth atmosphere can lead to reduction of the evaporation from the melt [6].

In the present work the crystallization of the Li_3N by FZ technique under the high nitrogen pressure has been studied for the first time. Application of high nitrogen pressure significantly changes the optimal growth parameters: with rise of the pressure rotation rate for seed- and feed-rods decrease from 15 rpm to 5 rpm and from 20 rpm to 10 rpm, respectively, while growth rate increases from 6 mm/h to 16 mm/h. Crystalline samples with sizes of dia. 8 mm and length up to 40 mm have been obtained and characterized.

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P25 Synthesis and characterization of rare-earth halides

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Binary rare-earth halides MX_3, with X = Cl-I, are a rich family of compounds that crystallize in the UCl_3, $PuBr_3$, and BiI_3 structures with space groups $P6_3/m$, $Ccmm$, and $R\bar{3}$, respectively. Their structures vary from 2D with honeycomb or distorted triangular layers to 3D with edge and face sharing polyhedra. These compounds are of interest as candidate quantum frustrated magnets and were studied by neutron experiments at low temperatures. For instance, single crystal neutron scattering data on $ErBr_3$ have shown a magnetic phase transition to a continuously degenerate non-collinear 2D state at T = 280 mK [1], while $YbBr_3$ does not show ordering down to 100 mK [2]. Here, we present an overview of the rich family of binary rare-earth halides, the Bridgman technique as a suitable method for the growth of high-quality single crystals that are required for neutron scattering studies, as well as results of some magnetic studies.

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P26 Challenging Growth of Doped Sr_2RuO_4 using the Floating Zone Method

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The family of the Ruddlesden-Popper ruthenates exhibits a wide variety of different and interesting physics. Significant attention has been drawn to the single-layer Sr_2RuO_4 showing unconventional superconductivity below 1.5 K [1]. Isostructural to the High-Tc Cuprades and flanking the ferromagnetic infinite layered $SrRuO_3$ the pairing symmetry was proposed to be of p-wave type driven by ferromagnetic fluctuations [2,3]. This idea was shattered when a drop in the spin susceptibility was demonstrated by a revisited NMR experiment [3]. Besides this, a competing and dominant antiferromagnetic fluctuation was found in Sr_2RuO_4, which could be stabilized to a spin-density wave by doping a low amount of Ca and Ti [4-6].

The superconducting state in Sr_2RuO_4 is very fragile and can be suppressed rapidly by impurities which can enter during the growth process [8]. Therefore, only pure single crystals are suitable for experiments focused on the superconducting phase, setting a high standard for the crystal growth. In contrast, intentional doping of ruthenates often leads to fascinating magnetic behaviors. However, achieving phase-pure, high-quality single crystals during doping is challenging, as sister compounds such as $SrRuO_3$, $Sr_3Ru_2O_7$, or $Sr_4Ru_3O_{10}$ tend to grow parallel to Sr_2RuO_4 if optimal growth parameters are not met. Another inconvenient side effect of doping is that even small changes in the amount of dopants can shift the optimal growth parameters to new and unknown settings. These conditions, coupled with the fact that ruthenates are oxide compounds, suggest the use of the floating zone method. This method allows crucible-free growth under a controlled atmosphere and enables quick iterative refinement of the growth quality.

Extensive work and effort were invested in refining the recipes and growth procedures of the ruthenates [9-12]. Due to its low vapor pressure, RuO_2 starts sublimating above 1200 °C under a standard atmosphere. Typically, temperatures necessary to melt the congruent system of SrO and RuO_2 are much higher, which causes a loss of RuO_2 during the pre-growth procedure and the growth itself. Therefore, maintaining the desired stoichiometry during growth is the main goal and essential to gain phase pure crystals.

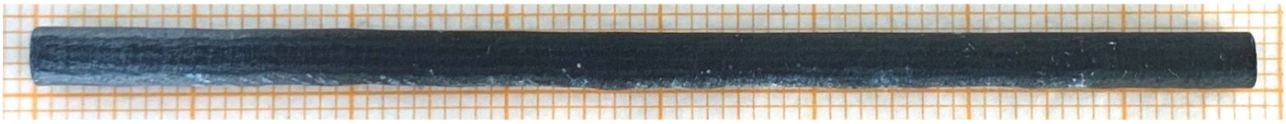

Figure 1: Large $Ca_{0.5}Sr_{1.5}RuO_4$ crystal after growth in mirror furnace.

In this contribution, our recent progress in growing Ca- (see Fig. 1), Ti- and Fe-doped single crystals of Sr_2RuO_4 using the infrared optical floating zone method will be presented. Particular attention is paid to identifying the parameters that influence the evaporation rate of RuO_2. The amount of RuO_2 in the melting zone is kept to its stoichiometric target value by the supply from the feed rod which contains an excess of RuO_2. Thus parameters like the feed and growth speed, the pressure, and the mixture of the Ar/O_2 atmosphere as well as the feed-rod diameter and the resulting diameter of the floating zone are mainly responsible for stable growth and a successful outcome.

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P27 Synthesis and Optical Properties of Re: LaSrGaO$_4$ (Re = Eu^{+3}, Sm^{+3} and Ho^{+3}) Single Crystal via Optical Float Zone Method

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Recently, there has been a growing trend to develop optical materials as an alternative to the increasing technological developments in all detectors and optical systems. These optical materials have usually been developed in single crystals since they have high optical transparency by nature [1]. This type of luminescent material usually involves a host matrix and activator ions, which are usually lanthanides or transition metals. In this case, the crystal structure and flexibility of the host matrix is also important. Because of their adjustable bandgap structure, chemical stability, charge transfer mechanism, Ruddlesden-Popper perovskites represent a promising field of research for the development of next-generation optical materials and energy applications. The versatility of this material in doping with different elements and its ability to regulate the bandgap make it an attractive prospect for researchers in this area [2, 3].

In the light of all these developments and information, to understand the scintillation mechanism of Eu^{+3}, Sm^{+3} and Ho^{+3} activator ions in the Ruddlesden-Popper type structure host, (La$_{1-x}$Re$_x$)SrGaO$_4$ (Re = Eu, Sm, Ho and x = 0; 0.05; 0.10) single crystals has been synthesized by Optical Floating Zone (OFZ) method. To analyze of single crystal quality and crystal structure, single crystal XRD measurements has been conducted as well as Rietveld refinement and their optical properties has been investigated by photoluminescence and decay time measurements. The effects on Photoluminescence and decay time profiles by using different ratios of these activators in the host structure has been focused.

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P28 Synthesis and Optical Properties of Re: $Gd_3In_2Ga_3O_{12}$ (Re = Nd^{+3}, Ho^{+3} and Lu^{+3}) Single Crystal via Optical Float Zone Method

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Single crystal garnets, in particular yttrium aluminum garnet (YAG) and gadolinium gallium garnet (GGG), exhibit superior optical transparency in the visible and near-infrared regions of the electromagnetic spectrum. This optical transparency makes these materials suitable for optical devices and systems that require high optical quality, as they can transmit light with minimal absorption or scattering [1]. Gadolinium gallium garnet (GGG) crystals are single crystal optical materials which are generally known for their high light output, fast decay time, and good energy resolution properties. Consequently, this material and its derivatives are optimally suited to the detection and measurement of ionizing radiation, including gamma rays and X-rays [2,3]. The literature contains a considerable amount of research on GAGG ($Gd_3Al_2Ga_3O_{12}$) single crystals. However, the impact of In^{+3} ions on GGG materials on optical properties has not been sufficiently investigated. Furthermore, only the B site has been studied doped with Cr^{+3} ions [4,5]. In addition, obtaining stoichiometrically single crystals was also a very challenging factor due to the volatility of In_2O_3 [6].

In this study, we achieved stoichiometrically growth GIGG ($Gd_3In_2Ga_3O_{12}$) single crystals and investigated to effect on crystal structure and optical properties in particularly photoluminescence and decay time profile of Nd^{+3}, Ho^{+3} and Lu^{+3} activators in GIGG single crystal host.

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Aditi Rajpal	University of Cambridge, United Kingdom
Sushma Lakshmi Ravi Sankar	Max Planck Institute for Chemical Physics of Solids, Germany
Timo Reents	Paul Scherrer Institute, Switzerland
Lea Richter	Max Planck Institute for Chemical Physics of Solids, Germany
Arnau Romaguera Camps	Paul Scherrer Institute, Switzerland
Kai Röseler	University of Geneva, Switzerland
Jonathan Schmidt	ETH Zürich, Switzerland
Robert Schöndube	ScIDre Scientific Instruments Dresden GmbH, Germany
Soohyeon Shin	Paul Scherrer Institute, Switzerland
Toni Shiroka	Paul Scherrer Institute, Switzerland
Romain Franck Sibille	Paul Scherrer Institute, Switzerland
Uthayakumar Sivaperumal	Royal Holloway University of London, United Kingdom
Ramūnas Skaudžius	Vilnius University, Lithuania
David Sviták	Charles University, Czech Republic
Nazanin Taheri	EPFL, Switzerland
Yvonne Tomm	Helmholtz-Zentrum Berlin, Germany
Bekir Turedi	ETH Zürich, Switzerland
Fatih Uzun	University of Oxford, United Kingdom
Olesia Voloshyna	Leibniz Institute for Solid State and Materials Research Dresden, Germany
Ashutosh Wadge	International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, Poland
Dorota Walicka	Paul Scherrer Institute, Switzerland
Felix Wirth	Institute of Physics II, University of Cologne, Germany
Hasan Yilmaz	University of Stuttgart, Germany
Mahsa Zamani	Max Planck Institute for Solid State Research, Germany

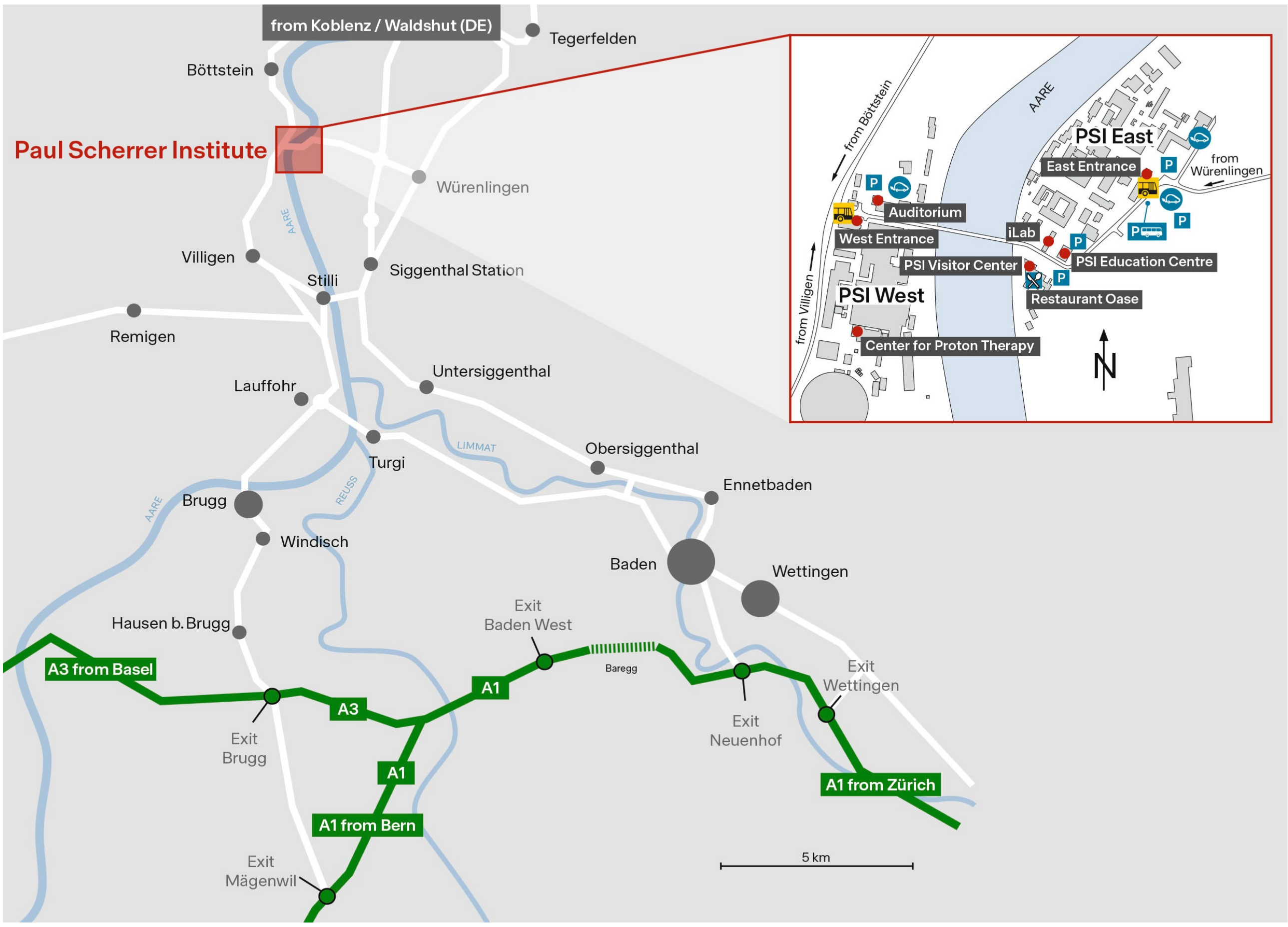
Useful Information

Below you can find a list of links that provide you with some useful information during your visit at the PSI.

For various information:	see the PSI Pocket and workshop webpage.
For WiFi:	see the WiFi provision at PSI.
For places to eat:	see food and catering at PSI and PSI gastronomy.
For shopping:	see Aarepark Würelingen and Volg Villigen.
For information about the Guest House:	see the PSI Guest House.
For public transport (timetable, prices, and tickets):	see the SBB website.
For emergency situations	see the Emergency instructions.

How to get to the Paul Scherrer Institute

PSI is located in northern Switzerland, approximately midway between Zürich and Basel. The nearest towns and railway stations are Baden and Brugg. Frequent air and train connections via Zürich or Basel are available from all major European cities.



To reach PSI from Zürich airport

There is a SBB railway station at the International Airport at Zürich-Kloten. Take the train to Brugg and a public bus (Postauto) from Brugg railway station to Villigen PSI. For the PSI Auditorium and the Guest House, use the **Villigen, PSI West** bus stop.

To reach PSI by public transport

Brugg is on the train line (Zürich–Basel, Zürich–Bern). You can take a public bus (Postauto) from Brugg railway station. Take the Brugg–PSI–Böttstein–Döttingen bus, and within 20 minutes you will arrive at PSI. For the PSI Auditorium and the Guest House, use the **Villigen, PSI West** bus stop.

To reach PSI by car

The complete address is Paul Scherrer Institute PSI, Forschungsstrasse 111, 5232 Villigen, Switzerland.

Where to eat at the Paul Scherrer Institute

On weekdays

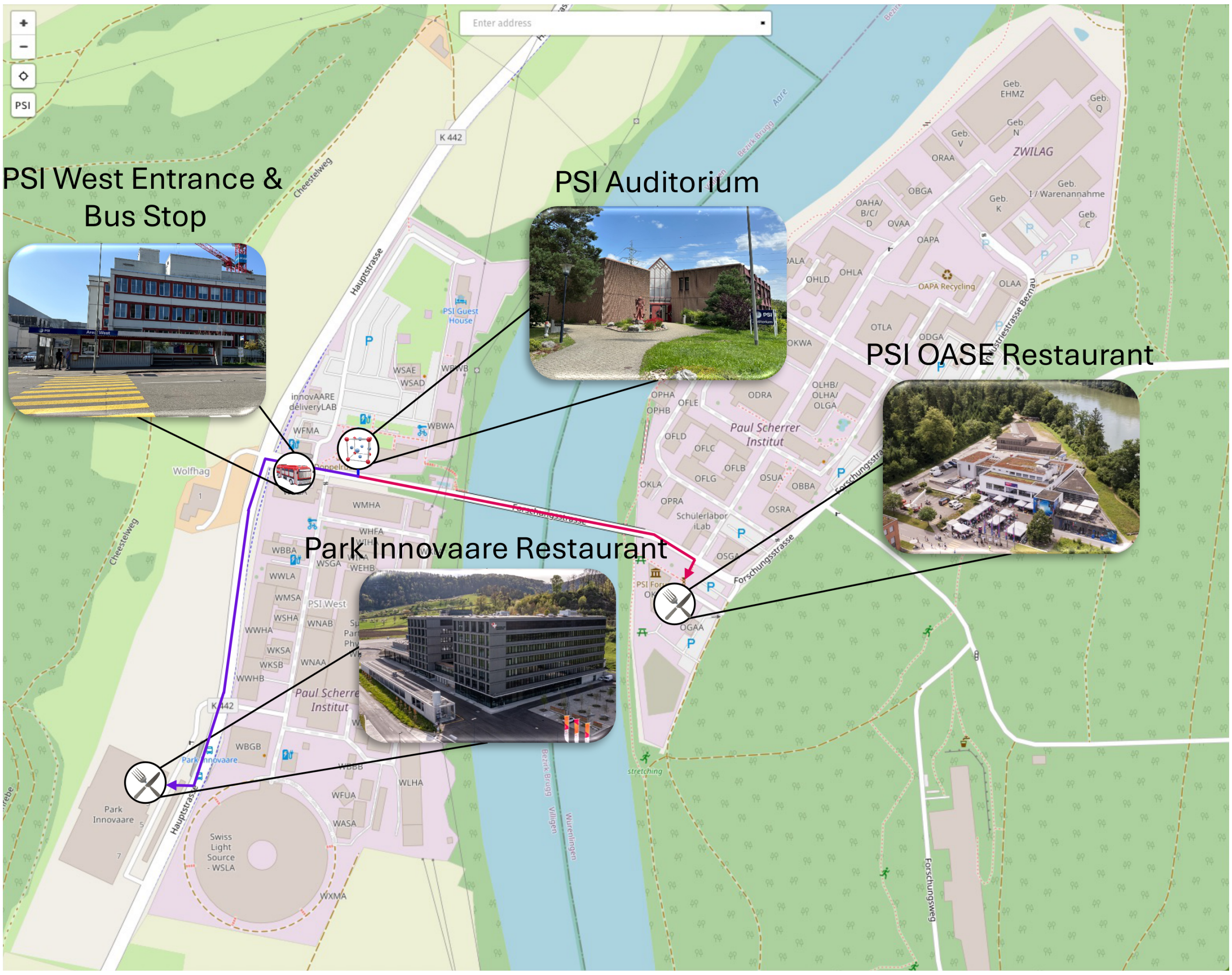
On weekdays, lunch is served at the PSI OASE Restaurant and the Park Innovaare Restaurant. Dinner is served at the the Park Innovaare Restaurant. See below the opening hours and the locations of the two restaurants in the campus. Payment methods accepted: all major credit cards and Twint (no badge) at the PSI OASE Restaurant and the Park Innovaare Restaurant, cash payments only at the PSI OASE Restaurant.

PSI OASE Restaurant

Opening hours:
Monday to Friday
Lunch 11:30 - 13:30

Park Innovaare Restaurant

Opening hours:
Monday to Friday
Lunch 11:30 - 13:30
Dinner 17:30 - 19:30 (last order)



During the weekend

During the weekend, see shopping possibilities in Useful Information. All locations can be easily reached by public transport.

Safety at the Paul Scherrer Institute

To avoid delays in case of emergency always call 3333 (or from your mobile phone: +41 56 310 3333) for expert help and assistance. For more information on how to behave in case of emergency, see the Emergency instructions.