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Swiss Society for Crystallography

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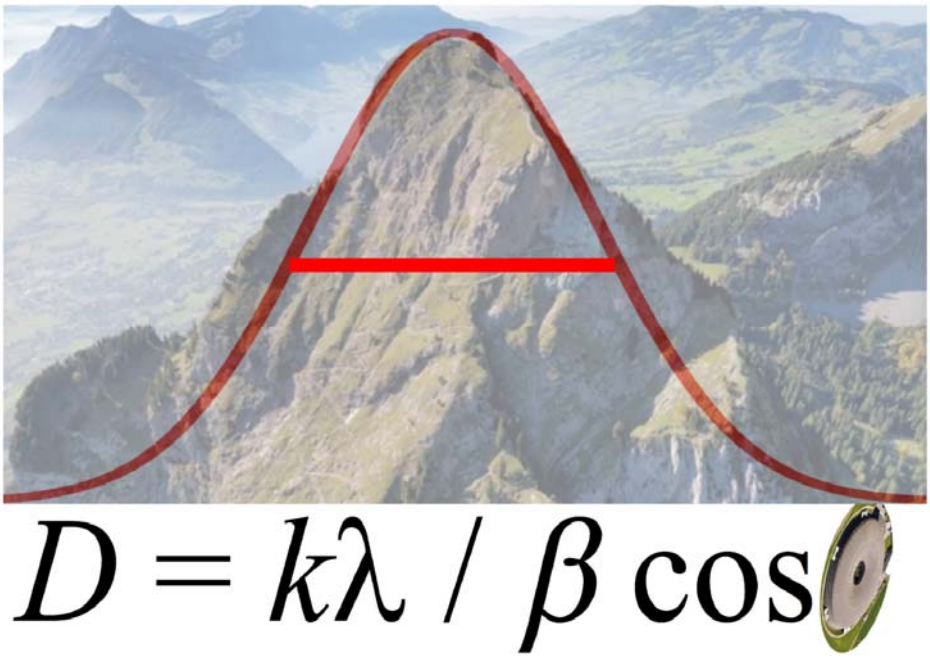
Annual Meeting of the Swiss Society for Crystallography

Paul Scherrer Institute, Villigen, 12 Sept. 2018

The Breadth of Crystallography



In this issue:

On the Cover:
Announcement and Program for the Annual Meeting of the Swiss Society for Crystallography at the Paul Scherrer Institute , VILLIGEN on 12 Sept. 2018

SGK / SSCr Newsletter No. 100

The President's Page

Dear Member of the Swiss Society of Crystallography,

By rephrasing William Wordsworth, "Three years have past; three summers, with the length / Of three long winters! and again I hear / These waters, rolling from their mountain-springs / With a soft inland murmur".
Yes, three years have passed since I started my office as president of the Swiss Crystallographic Association and now my mandate is almost over. A new president of the society will elected at the annual meeting, organized by Nicola Casati and Antonio Cervellino at the Paul Scherer Institute on September 12.
Therefore, my last "page of the president" is mainly a report about these three years of activity.
No doubt that the most hectic event during this period has been the organization of European Crystallographic Meeting in Basel in 2016, which was possible thanks to a seamlessly efficient synergy between various Swiss groups, coordinated by my two predecessors in the office of SGK president, namely Katharina Fromm and Jürg Schefer. ECM30 has been a wonderful opportunity to exhibit the research in Crystallography in Switzerland.
Swiss crystallographers have contributed to scientific meetings also after ECM30. At the meeting of the International Union of Crystallography in Hyderabad (August 2017), Switzerland was the 10th most represented country. Swiss scientists are members of many commissions of the IUCr and this is certainly sign of a well-recognized role in the international community. Moreover, the society has continued to organize internationally reckoned schools on single crystal x-ray diffraction, powder diffraction and on crystal growth.
During this triennium, SGK has launched new activities. The prize for the best PhD thesis in crystallography (first edition in fact took place in Neuchatel in 2015). It has rapidly emerged as a very good opportunity for younger researcher and the two prize-winner have been very talented young scientists who will certainly bring prestige to the society who awarded them.
Another new activity launched in this period is the crystallographic lecture cycles, named after Howard Flack. Apart from being an excellent way to remember an extraordinary colleague who left us prematurely, these lecture cycles (inaugurated in 2018 with the visit of Prof. Omar Yaghi from Berkeley) represent an exceptional occasion to advertise crystallography to our colleagues of other scientific disciplines and show the outcome of the research in our fields.
Another goal at the beginning of my mandate was that of expanding the society. This is certainly difficult, given that crystallography is suffering in many universities. However, apart from the above-mentioned initiatives, we could resurge the section of crystal growth, especially thank to the board member Enrico Giannini, who was able to organize meetings in collaboration with other societies (like the German Crystal Growth Association) and has contributed to revitalize the field in Switzerland as well. More work is necessary in this direction, in particular with colleagues of physics, materials science and structural biology.
I wish to thank all the current board members for their invaluable support during these three years. In particular, Antonia Neels, who has been vice-president and treasurer, and Michael Wörle, who has been extremely active as secretary and editor of the newsletter.

The board of the society has proposed Antonia as new President, and I hope that the assembly will approve this decision, given that she is extremely well aware of the Swiss scientific community and has very good connections with the international community as well. The board has also proposed to confirm Michael as secretary and nominate Anthony Linden as future vice-president and Enrico Giannini as treasurer. Again, I hope that the assembly will accept these nominations because this team has successfully worked together for the last three years.
I hope to meet you at the annual meeting on September 12 at the Paul Scherer Institute and of course, I wish “LLAP” to the Swiss Society of Crystallography.

Piero Macchi
(President of the SGK-SSCr)

Important Notice concerning the Newsletter

Dear members of the Swiss Society for Crystallography,

As many associations already do, we **distribute our newsletter from this issue on (no. 100/2018) preferentially via email in pdf-format.** This will drastically reduce the number of printed copies and therewith contribute to an economic and sustainable policy.

For those of you who might still prefer to receive the printed copies, we offer this option too:

For receiving hardcopies of the SSCr-newsletters in the future, please return the coupon below to the secretary of the SSCr:

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PROGRAM Swiss Society Annual Meeting 2018, PSI Villigen

Wednesday , 12th September 2018

09:30 – 09:50		***Registration & Welcome Coffee***
09:50 – 10:00	*P. Macchi (U Bern)* *A. Cervellino (PSI)*	***Welcome Address***
10:00 – 11:50	***Session 1***	***Chair: A. Cervellino***
10:00 – 11:00	*Dr. Ing. Hans Scheel, (General Protection Engineering GmbH)*	Invited Lecture #1 "Crystal Growth and Crystal Technology"
11:00 – 11:25	*Prof. Hans Grimmer (PSI)*	Oral contribution #1 "DFT Calculations of Twin Boundaries in KLiSO4"
11:25 – 12:15		***Lunch – Poster Session***
12:15 – 14:00		***General Assembly of the SGK-SSCr***
14:00 – 15:50	***Session 2***	***Chair: N. Casati***
14:00 – 15:00	*Prof. Wendy Lee Queen (EPFL Valais)*	Invited Lecture #2 TBA
15:00 – 15:25	*Prof. Radovan Cerny (U Geneva)*	Oral contribution #3 "Metal Hydro-Borates for Li- and Na-ion Batteries"
15:25 – 15:50	*Dr. Amin Sadeghpour (EMPA)*	Oral contribution #4 "The Semi-crystalline Structural Features Revealed by Diffractions at Small Angle Regime"
15:50 – 16:10		***Coffee Break – Poster Session***
16:10 – 18:15	***Session 3***	***Chair: R. Sibille***
16:10 – 17:10	*Prof. Johan Chang (U Zurich)*	Invited Lecture #3 TBA
17:10 – 17:35	*Dr. Sumit Maity (PSI)*	Oral contribution #5 "Neutron diffraction studies of oxygen disorder in Nd2NiO4+d"
17:35 – 18:00	*Dr. Zoltan Balogh-Michels (EMPA)*	Oral contribution #6 "Crystallinity and crystallite size determination of recrystallized nanocellulose"
18:00 – 18:15		Poster prize ceremony & Farewell

Abstracts

Plenary lectures

Crystal Growth and Crystal Technology

Hans J. Scheel

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The invention of the germanium transistor in 1947 and subsequently the silicon transistor in 1954 initiated the solid-state electronics revolution based synthetic crystal and epitaxial layer (epilayer) production including crystal machining (sawing, polishing etc.). This crystal technology allowed the development of all aspects of modern communication, global commerce, medical technology and energy production.

In connection with the discovery of new materials, for instance ferroelectric materials at ETH Zurich with Paul Scherrer and Georg Busch who, in 1935, discovered ferroelectric KDP, crystals of high quality were required for research. Also, ferromagnetic, laser, superconducting materials and compound semiconductors were of interest, and phase transitions in general developed as a topical research field with the need for crystals. Not only universities, but also industrial research laboratories and national and military research laboratories established crystal growth facilities in the 1960s.

Initial crystal growers often kept their process secret. A problem with many crystal growers was, and still is, that often they apply a crystal growth method which is not optimum leading to unsatisfactory results with respect to size and quality of crystals. Only with high-quality crystals and their sufficient characterization can reproducible physical properties be achieved.

The science of crystal growth developed slowly and was assisted by the Journal of Crystal Growth and by national and international conferences. The first ICCG met in Boston in 1966 and the second in Birmingham, UK in 1968. National and international crystal growth societies were formed, in Switzerland as a joint Society of Crystallography and Crystal Growth 1969 with initiators Nowacki in Berne, Laves and Kaldis in Zurich, and Hans Schmid in Geneva. In 1970 the first International Conference on Vapor Growth and Epitaxy was organized by E. Kaldis, myself and others at a time when at least 12 crystal growth laboratories already existed in Switzerland. The first European Conference on Crystal Growth in 1976 was again organized by Kaldis and myself, when I introduced poster sessions for the first time which were then widely accepted. After 1980, short-term profits in industry became dominant so that, unfortunately, most crystal growth laboratories with their long-term developments were terminated.

The industrial production of crystals of silicon, GaAs, InP, SiC, sapphire/ruby, quartz, Li-niobate, CdTe, garnets etc. developed slowly because there had been, and still is, no education of crystal technologists. Companies had to hire a chemist, physicist, or materials engineer and train him for up to 10 years to become an independent crystal producer/engineer working without supervision. Most companies would be happy if they could hire crystal technologists. How much faster could silicon technology have been developed if there had been well-educated crystal technologists?

The problem of educating crystal engineers is multi-disciplinary. It involves, besides crystal growth mechanisms and crystal technology, chemical and materials engineering/thermodynamics, mechanics, including hydrodynamics and aerodynamics, aspects of crystallography and of solid-state physics, machine and process engineering, and of course computer simulation and informatics, of the latter fields the basics so that the crystal technologists can discuss and collaborate (details

in WHITE PAPER in Project 16 of the homepage). This education would prevent the application of ten or more different methods to produce silicon solar cells instead of one optimum technology with respect to crystal quality and cell performance, economics, efficiency of process, and ecology. Similar arguments can be applied to laboratory crystal growth for research samples, and to epitaxial deposition processes.

Understanding the structure-derived function of metal-organic frameworks and their application in separations

Prof. Wendy Lee Queen

EPFL Valais, Wallis campus, Sion

Title to be announced

Prof. Johan Chang, Department of Physics

University of Zurich

Oral contributions

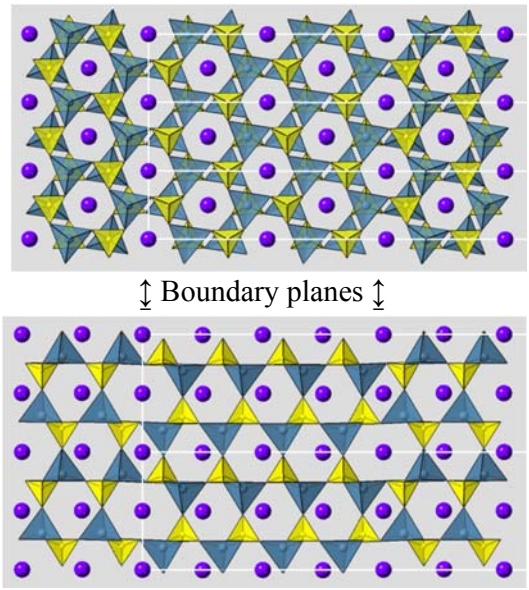
DFT Calculations of Twin Boundaries in $KLiSO_4$

Hans Grimmer and Bernard Delley

Paul Scherrer Institut, Research with Neutrons and Muons, 5232 Villigen PSI, Switzerland

The room temperature phase of $KLiSO_4$ has the tetartohedral hexagonal space group $P6_3$. It follows that three merohedric twin laws are possible: mirror reflection twins with $m \parallel [001]$, rotation twins with $2 \perp [001]$ and their combination, inversion twins. Structural models for these three laws have been proposed in [1] for boundary plane $(1\ 0\ \bar{1}\ 0)$, and, in the case of mirror reflection twins, also for boundary plane $(0\ 0\ 0\ 1)$.

The energies of these twins are studied here for the first time. For this purpose, density functional theory calculations have been carried out using the DMol^3 code with the functional PBEsol [2]. Polysynthetic twins with constant lamellae thickness have been considered for thicknesses 1 to 4 times the minimum value that is possible for structural reasons. The energies rapidly converge with increasing lamellae thickness.



Relaxed inversion twin with boundary planes $(1\ 0\ \bar{1}\ 0)$ *and lamellae thickness four times minimum, viewed parallel and perpendicular to the 6-fold axis of* $KLiSO_4$

O at the edges of the tetrahedra,

S inside the yellow tetrahedra

Li inside the blue-green tetrahedra

K violet balls

Most common is the mirror reflection twin with boundary plane (0001). In this case, the polysynthetic twins have energy 0.001 eV per unit cell independent of lamellae thickness. For maximum lamellae thickness, the energies per unit cell found for the polysynthetic twins with boundary plane $(1\ 0\ \bar{1}\ 0)$ were 0.09 eV for the inversion twin, 0.55 eV for the rotation twin and 0.58 eV for the mirror reflection twin. The first case was frequently observed in growth twins doped with Cr, the second was never observed and the third only rarely.

[1] H. Klapper, Th. Hahn & S.J. Chung, *"Optical, Pyroelectric and X-ray Topographic Studies of Twin Domains and Twin Boundaries in $KLiSO_4$"*, Acta Cryst. B**43** (1987) 147-159.

[2] B. Delley, *"From molecules to solids with the DMol^3 approach"*, J. Chem. Phys. **113** (2000) 7756-7764.

Neutron diffraction studies of oxygen disorder in Nd_2NiO_{4+d}

S. Maity[1, 2], J. Schefer[1], L. Keller[1], M. Ceretti[3], W. Paulus[3]

1) Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen, Switzerland.
2) University of Geneva, Department of Quantum Matter Physics (DQMP) 24, Quai Ernest Ansermet CH-1211 Genève 4, Switzerland
3) Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France

Better understanding of oxygen diffusion mechanism in non-stoichiometric oxides becomes essential for further development of intermediate temperature solid oxide fuel cells. In this prospect, rare earth nickelates ($R_2NiO_{4+\delta}$) emerged as promising materials in which oxygen could be intercalated with electrochemical methods at room temperature. The crystal structure consists of $RNiO_3$ perovskite layers sandwiched between R_2O_2-type rock salt layers and extra oxygens are intercalated in tetrahedral sites inside the rock salt layer. Oxygen diffusion, in these materials, is highly anisotropic and described by interstitialcy hopping mechanism [1] at high temperature (≈800˚C) in which excess oxygens diffuse via apical site inside the rack salt layer. However, close to room temperature, oxygen diffusion is non-Aarhenius type rather a phonon assisted process [2].

In this talk, I will address neutron diffraction studies which were recently performed on powder and single crystal $Nd_2NiO_{4+\delta}$ compounds (with δ=0.25; S1 and 0.1; S2) as a function of temperature to obtain usefull insights on phonon assisted diffusion mechanism. Superstructure reflections related to 3d-ordering of excess oxygens were found below 823 K in S1, confirming the pinning of excess oxygens to the crystal lattice and incommensurate crystal structure while the average structure is orthorhmbic F*mmm*. Incommensurate oxygen superstructure reflections start to drop intensity around 400 K and loss of 3d-oxygen ordering occurs arround 823 K accompanied by F*mmm* to F4/*mmm* structural transition. In comparion, the crystal structure of S2 sample is tetragonal commensurate $P4_2$/ncm and shows no evidence of long range ordering of excess oxygens in the investigated temperature range. Least square refinements of neutron diffraction data of both samples show unusually high anisotropic thermal displacement factors both for equatorial and apical oxygen atoms showing amplitudes toward [001] and [110] direction respectively *w.r.t.* the F-symmetry cell, which are getting amplified in the high temperature phase. Maximum entropy recostruction of neutron data shows additional anharmonic displacement of apical oxygen atoms toward nearest interstitial site due to steric chemical pressure from excess oxygen atoms. We show that such displacement pattern of apical oxygens, largely depends on amount of intercalated oxygen atoms and also reported previoulsy with ab-initio calculations [3] on $Nd_2NiO_{4+\delta}$ compounds, are important pre-requisite for oxygen diffusion close to room temperature.

[1] Chroneos. A. et.al. J. Mater. Chem., (2010) 20, 266 [2] Ceretti M. et.al. (2015) J. Mater. Chem. A 3, 21140
[3] Perrichon. A. et. al. (2015) J. Phys. Chem. C 119, 1557

Metal Hydro-Borates for Li- and Na-ion Batteries

R. Černý, M. Brighi, E. Didelot, Y. Sadikin, F. Murgia, P. Schouwink
DQMP, Laboratory of Crystallography, University of Geneva

Complex hydrides based on light hydro-borate anions such as borohydride BH_4^- or *closo*-borate anion $B_{12}H_{12}^{2-}$ find their place as solid stores for hydrogen, and since recently, also as solid electrolytes in Li- and Na-ion batteries. The mobility of the cations depends on the pathways available in the anion packing, chemical interaction of cations with anions and on the anion thermal motion such as tumbling or rotation. While the latter two require important experimental and theoretical effort, the first parameter can be easily analysed and quantified from the crystal structure data obtained by X-ray diffraction.

Improving $Na_2B_{12}H_{12}$, promising Na-ion solid electrolyte, by anion modification and anion mixing will be shown (Figure 1). [1-3] Novel synthetic way completed by *ab inito* structural characterization and *ab initio* calculation allowed discovery of several 3*d* transition metal *closo*-borates - potentially battery electrodes (Figure 2).[4]

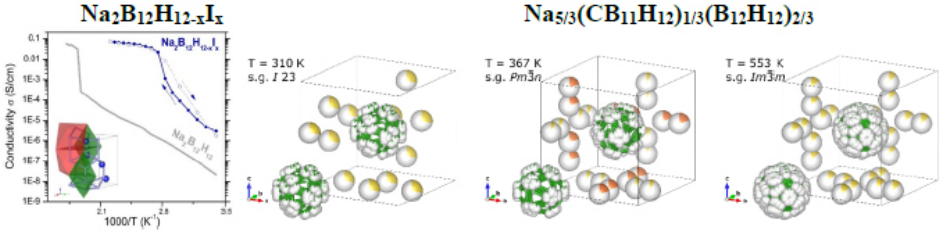


Figure 1: **(left)** Ionic conductivity of a sample containing 52 wt% $Na_2B_{12}H_{12-x}I_x$ and 48 wt% NaI. The conductivity of the precursor $Na_2B_{12}H_{12}$ is shown for comparison. Na-ion conduction channels in *hcp* sublattice with face-sharing T and O interstices sites in *h*-$Na_2B_{12}H_{12-x}I_x$. In blue the static Na positions as optimized by DFT. **(right)** Evolution of anionic and cationic disorder in $Na_{5/3}(CB_{11}H_{12})_{1/3}(B_{12}H_{12})_{2/3}$. Green and yellow spheres represent boron and sodium atoms respectively. Orange spheres indicates a different Wyckoff site for Na (only in *Pm*-3*n*). The colour partial filling indicates the partial site occupation.

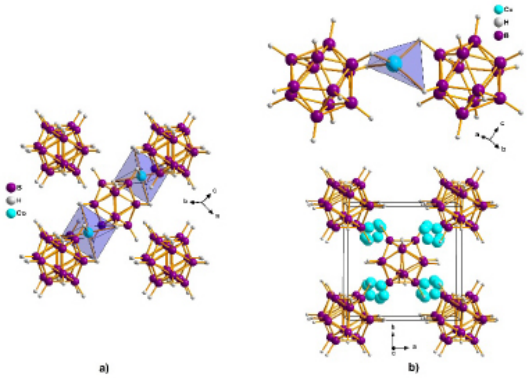


Figure 2: **a)** Crystal structure of anhydrous $M(B_{12}H_{12})$ for bivalent M (Co, Ni) as optimized by DFT. A part of the trigonal structure (*R*-3) corresponding to the *bcc* unit cell is shown. **b)** Experimental structure of anhydrous *c*-$Cu_2(B_{12}H_{12})$. The metal is disordered around a position bridging two *closo*-borates. Local coordination as optimized by DFT is shown above.

[1] Sadikin Y., Brighi M., Schouwink P., Černý R., *Adv. Energy Mater.* **2015**, 1501016
[2] Sadikin Y., Schouwink P., Brighi M., Łodziana Z., Černý R, *Inorg. Chem.* **2017**, *56*, 5006-5016
[3] Brighi M., Murgia F., Łodziana Z., Schouwink P., Wolczyk A., Černý R., submitted.
[4] Sadikin Y., Didelot E., Łodziana Z., Černý R., *Dalton Trans.* **2018**, *47*, 5843-5849

Zoltán Balogh-Michels, Jean Buffiere, Marc Borrega, Thomas Geiger, Herbert Sixta, Tanja Zimmermann Antonia Neels

Empa, Swiss Federal Institute for Materials Science and Technology
Aalto University, School of Chemical Engineering
VTT Technical Research Centre of Finland

Cellulose is a versatile and abundant biopolymer, which is already used in many applications. Nanocelluse, either in the form of cellulose nanofibrils or cellulose nanocrystals has extended these applications in bio-nanocomposites and hybrid functional materials [1].

In this work we are going to present X-ray diffraction investigation of nanocellulose produced by recrystallization of microcrystalline cellulose (MCC) through hydrothermal (HTC) and microfluidic methods (MFC) [2].

The microfluidic treatment did not change the β-I crystalline structure of the microcrystalline cellulose (Fig. 1). The hydrothermal treatment however resulted in a cellulose material which is dominantly β-II. The crystallinity ratio was about 80% for all the MCC, HTC and MFC independently of the estimation method. The crystallite size was determined by the Scherrer-equation. For the MCC and MFC materials the domain size was 7 nm, while a growth to about 12 nm was observed for the HTC material.

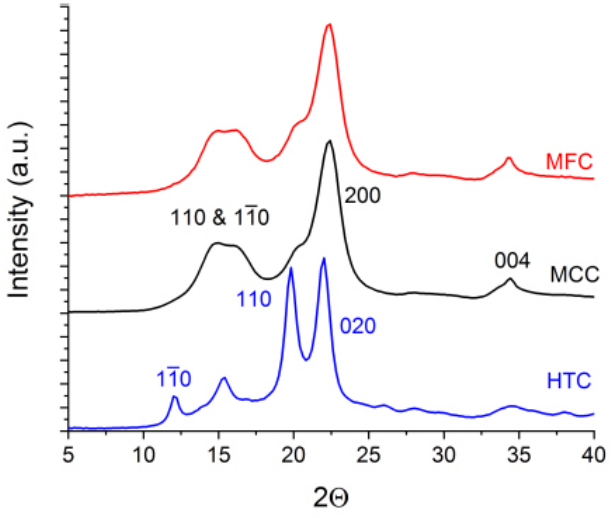


Fig. 1: the XRD spectra of the MCC, MFC and HTC materials, and the peaks of the β-I and β-II cellulose respectively.

[1] T. Abitol et al., Curr. Opin. Biotech., 39 (2016) 76-88.
[2] J. Buffiere et al., Carbohyd. Polym., 178 (2017) 48-56.

The Semi-crystalline Structural Features Revealed by Diffractions at Small Angle Regime

Amin Sadeghpour[1,2,3], Alex Dommann[1,4], Antonia Neels[1]
[1]*Empa, Swiss Federal Laboratories for Materials Science and Technology, Center for X-Ray Analytics, Dübendorf, Switzerland*
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[3]*Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory of Biointerfaces, St. Gallen, Switzerland*
[4]*Cellular and Biomedical Sciences, Faculty of Medicine, University of Bern, Switzerland*

Mesophases are the structures that are neither fully crystalline nor isotropic fluids, but an intermediate state of matter. These thermodynamically stable structures normally form upon self-assembly of molecules in which the building-blocks are partially correlated within a few nanometre range scale. Various macroscopic properties like particular shear viscosity behaviour or their environmental responses are highly dependent to their nanostructures. Detailed understanding of the nanostructural features provides new possibilities for steering the functionality of mesophases, particularly in the field of biomedicine and pharmaceutics and food science.
At the Center for X-ray Analytics at Empa we are positioned at the intersection of forefront research in materials science towards biomedical applications. The materials include self-assemblies in solution, macromolecules at bio-interfaces and the polymer-based biomimetic membranes for wound dressing. In this contribution, we demonstrate our recent advances in analysis of total scattering at small angle regime from examples of such partially ordered systems. The combined scattering and diffraction signal analysis provides a comprehensive understanding about the multiphase systems. In addition, we will highlight combined small and wide angle scattering approaches to achieve structural characterisation within a wide length-scale.

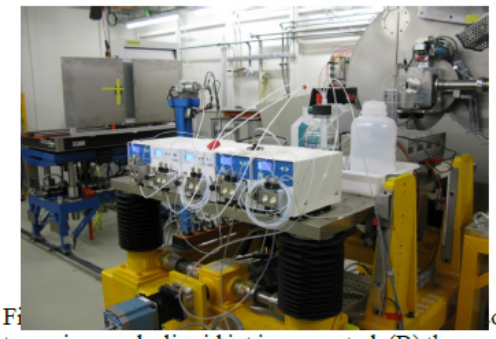
Poster contributions

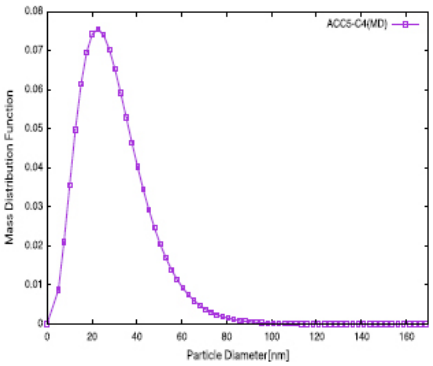
In situ synchrotron scattering studies on ACC colloidal suspension objects in solution

Ahmed S. A. Mohammed, A. Cervellino, A. Testino, A. Carino, M. R. Andalibi

Paul Scherrer Institute (PSI)

The nature of entities present in suspension solutions at the early stage of the precipitation pathway of calcium carbonate is largely debated in literatures. Despite the great scientific relevance of calcium carbonate in different areas of science, little is known about the early stage of its formation. Classical scattering methods such as Wide-Angle X-ray Scattering (WAXS) and Small-Angle X-ray Scattering (SAXS) techniques were employed for the investigations of amorphous calcium carbonate (ACC) entities formed from supersaturated solutions. SAXS, in particular, is important for detecting the entities and investigating their size and shape. SAXS experiments were conducted at the material science beamline (MS – X04SA) of SLS at PSI. We specially designed contactless devices for the measurements, generating liquid jets from supersaturated solution. Four HPLC pumps were delivering diluted solutions (e.g., NaOH, $CaCl_2$, $NaHCO_3$, H_2O) in order to obtain a desirable *pH* and saturation (figure 1a). Supersaturation was controlled by mixing four diluted solutions at constant *T* and *pH* and the scattering data were collected using Mythen II detector. The data were modeled using parametric statistical models providing insight about the size and shape distribution of denser matter in the liquid jet. A representative example for the mass distribution of the investigated entities is shown below (figure 1b).





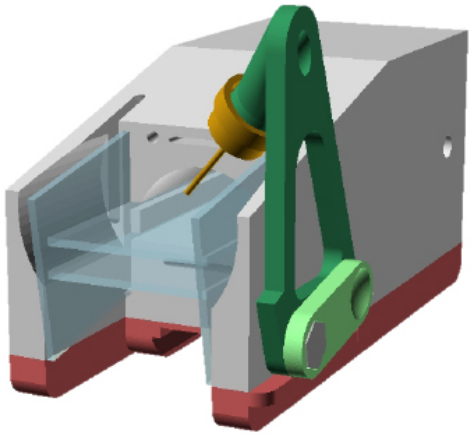
Fi or solutions to a mixer and a liquid jet is generated. (B) the mass distribution obtained for one of the supersaturation levels (S =1.46).

Low-Cost Portable Devices for Inert Low-Temperature Sample Manipulation

Nils Trapp*, Michael Solar and Michael Wörle
Small Molecule Crystallography Center, ETH Zürich, Zürich, Switzerland

Sample cooling has become widely implemented in crystal structure determination, due to the broad array of advantages it offers (Goeta & Howard, 2004). In particular, measurement at reduced temperatures can severely improve data accuracy and resolution for small molecule crystals, due to reduced and more isotropic atomic vibration (Brock & Dunitz, 1990). In addition, it can reduce radiation damage in protein crystals, enable variable temperature or phase transition studies and allow measurements of samples that are not stable or solid under ambient conditions. Low temperature can also prevent crystal damage due to the escape of co-crystallized solvent, which often retains a relatively high vapor pressure. Because the cooling medium used in open-flow sample cryostats is either nitrogen or helium gas, air-sensitive and even pyrophoric crystals can be measured using standard equipment. However, transferring sensitive samples from storage vessel to diffractometer, without compromising crystal and data quality, remains a challenge in many cases.

A straightforward procedure for preparing and mounting crystals under inert conditions is demonstrated, using a specialized apparatus (μCHILL). The technique is extremely flexible, requiring only a single operator, little practice and almost no preparation time. The device enables a wide temperature range (at least –60 °C to room temperature), providing temperature control and very stable conditions with no ice formation over extended time periods. The flexible, modular and low-cost design is based on 3D printed parts and readily available standard components, potentially making the device available to a wide range of users and applications not limited to single crystal studies.



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Brock, C. P. & Dunitz, J. D. (1990). *Acta Cryst. B. 46*, 795–806.

"NEMS for sensing applications: structural understanding by combining X-ray nano-diffraction and micro-Raman methods"

Simone Dolabella[a*], Zuhal Tasdemir[c], Oliver Braun[a], Yusuf Leblebici[b], Erdem Alaça[c], Gilbert Chahine[d], Michel Calame[a], Alex Dommann[a], Antonia Neels[a]

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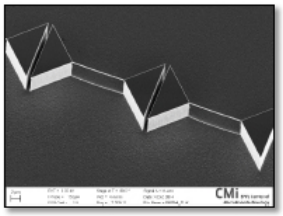
* *simone.dolabella@empa.ch*



In the last decades the wide field of applications of electronic devices and the miniaturization of materials brought us to study and develop devices such as MEMS and NEMS especially due to the increase in demand from the medical and aerospace sectors. The applicability of Nanoelectromechanical systems (NEMS) is based on their ability to operate reliability over time under service conditions. The purpose is to link atomic structure and physical properties for silicon NEMS. The object under investigation - the nanowire system - is shown in *figure*. A monolithic fabrication has been performed. Structural analysis such as High Resolution X-ray Diffraction (HRXRD) for defect and strain analysis has been applied and performed using the nano-beamline ID01 at the ESRF. HRXRD is used as a non-destructive method to gather more structural information on the inner part of the material framework[1]. The performed experiments show us that the intensity of the diffracted X-ray beam of the Si-nanowire can be probed on the given setup. The Y and Z scanning of the shows that the Si-pillars and nanowires exhibit inhomogeneous strain, defect and tilt states. The reciprocal space map (RSM) shows the 2D and 3D diffraction peaks of the substrate and for the Si-nanowires superposed with the Si-pillars.

In addition, the use of micro-Raman spectroscopy will support the discussion about local strain[3] within the nanowires. These methods are also combined with FEM simulations in order to evaluate diffraction patterns with respect to material parameters such as Poisson's ratio, Young's modulus etc.. This approach allows us to go one step further in understanding mechanical, electrical or thermal behaviors of this class of nanowires.

[1] Schifferle A., Dommann A. and Neels A. *Science and Technology of Advanced Materials,* 2017, 12, 1.
[2] Tasdemir Z., Wollschläger N., Österle W., Leblebici Y. and B Erdem Alaca. *Nanotechnology,* 2016, 2, 8.
[3] Yazji S., Hoffman E. A., Ercolani D., Rossella F., Pitanti A., Cavalli A., Roddaro S., Abstreiter G., Sorba L. and Zardo. *Nano Research,* 2015, 9, 28.

Keywords: silicon nanowires, HRXRD, micro-Raman

Effect of shock peening on residual stresses in Selective Laser Melting

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3 Rutherford Appleton Laboratory, Harwell Campus, Oxfordshire OX11 0QX, United Kingdom

Keywords: Selective Laser Melting, Laser, Shock peening, residual stress, XRD

Selective Laser Melting (SLM) processing of metals results in high residual stresses, that limit the mechanical properties of the fabricated material, which can directly affect the industrial applicability of the process. Laser shock peening (LSP) is a potential technology to engineer such stresses, in order to render them beneficial towards the mechanical stability of the material. This work investigates the influence of overlapping laser shocks and water confinement on the surface microstructure and the related surface residual stress profiles of 316L stainless steel (SS316L). The near-surface stress state was measured using X-Ray Diffraction (XRD) measurements through the $\sin^2\Psi$ method, measured in four ϕ directions (0°, 45°, 90°, 135°). Based on these data, the principal stresses σ_{11} and σ_{22} are calculated. The residual stress state was also measured as a function of depth beneath the SLM- and LSP-treated top surface using the incremental centre-hole drilling (ICHD) technique.

LSP of SLM-processed SS316L without water confinement results in strong tensile residual stresses at the immediate surface of the samples and imparts no beneficial compressive stress state at the surface. On the other hand, LSP of SLM-processed SS316L with a water confinement increases the magnitude and depth of compressive residual stress. Laser peening at 2.8GWcm^{-2} with dual shocks and 50% overlap, resulted in a maximum compressive stress of -200MPa, with the compressive stress state extending down to 500µm beneath the treated surface.

Since the use of water during the SLM build process is not feasible, the possibility of developing a hybrid additive manufacturing build process with in-line LSP will require an alternative solution to water confinement. The results of this study enable process optimisation to open new opportunities in post-processing and hybrid manufacturing of high-quality SLM-parts in combination with laser shock peening.

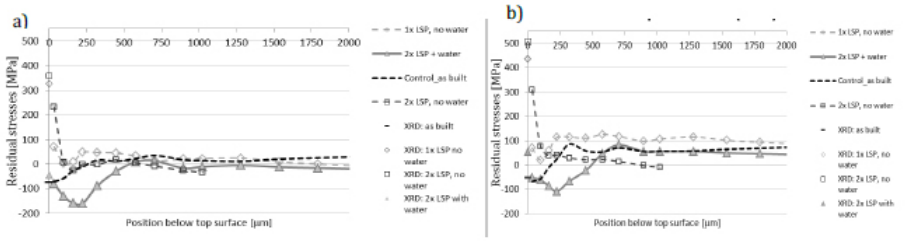

Image 1: a) Minimal and b) maximal principal residual stress profiles for different LSP conditions when compared to the as-built condition. The near surface (at position 0) values are obtained from XRD analyses.

Pure gyrotropic phase transitions in the arcanite related materials $PbMGeO_4$ (M = Ba, Sr)

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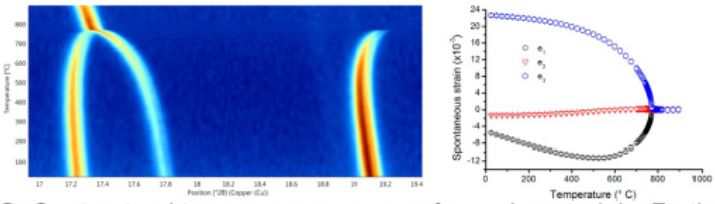
Gyrotropic phase transitions are characterized by the appearance of a spontaneous optical activity [1]. The appearance of such activity is very common in ferroelectric materials. In such materials, the optical activity is a secondary order parameter and is coupled to the primary order parameter which is the electrical polarization. However, only very rare examples are known of a pure gyrotropic phase transition. Among those, one can cite $BiFeO_3$ under strain [2] or $(C_{2n}H_{2n+1}NH_3)_2ZnCl_4$ as function of temperature [3]. In both cases, the transition exhibits a change from Pnma to $P2_12_12_1$ symmetry.

In this contribution, we have investigated 2 materials belonging to the $BaNdGaO_4$ structural type, namely $PbBaGeO_4$ and $PbSrGeO_4$ using powder X-ray diffraction as function of temperature. While $PbBaGeO_4$ exhibits a first order phase transition from $P2_12_12_1$ to Pnma symmetry, $PbSrGeO_4$ exhibits a second order phase transition.

Not only, $PbBaGeO_4$ exhibits a first order phase transition but especially show a phase coexistence and competition over a wide temperature range of about 200°C. On the contrary, $PbSrGeO_4$ shows a phase transition towards a Pnma structure with nearly metrically hexagonal cell.



This work demonstrates that both materials are purely gyrotropic and identify $BaNdGaO_4$ structural type as a new source for such materials. Furthermore, those phase transitions seem unusual in light of the complex behavior reported here for these 2 compounds.

[1] C. Konak, V. Kopsky, F. Smutny; *J. Phys. C: Solid State Physics*,1978, 11, 2493

[2] S. Prosandeev, I. A. Kornev, L. Bellaiche; *Phys. Rev. Lett.* , 2011, 107, 117602

[3] A. Gomez Cuevas, J. M. Perez-Mato, M. J. Tello, G. Madariaga, J. Fernandez, L. Echarri, F. J. Zuniga, G. Chapuis; *Phys. Rev. B* , 1984, 29, 2655

Keywords: gyrotropic materials, phase transitions, spontaneous strain

Study the effect of nanofiber fabrication processes into the modification of internal structure at nanoscale

A. K. Maurya[1,4], A. Sadeghpour[1,2], L. Weidenbacher[2], F. Spano[2], G. Fortunato[2], R. Rossi[2], M. Frenz[3], A. Dommann[1,4], A. Neels[1]*

[1]Center for X-Ray Analytics, Empa, St Gallen, Switzerland, [2]Laboratory for Biomimetic membranes and Textiles, Empa, St. Gallen, Switzerland, [3]Institute of Applied Physics, University of Bern, Switzerland, [4]Cellular and Biomedical Sciences, Faculty of Medicine, University of Bern, Switzerland

Electrospinning has been developed as a technique to produce nano to micron-sized fibers. It is well understood that the internal structure of these fibers highly depends on the polymer type, the spinning solution properties and the spinning parameters [1]. In our recent studies, we have investigated the structure of electrospun Poly(vinylidene fluoride-co-hexafluoropropylene), PVDFhfp, based fiber membranes for non-aligned and aligned (using a high speed rotating drum) samples by SAXS and WAXS techniques. We demonstrate that high operational speed of a rotating drum collector used for nanofiber fabrication modify the degree of alignment of the nanofibers without modifying the internal structure of the nanofibers. Furthermore, there is a possibility to modify the internal structures at nanoscale length at extremely high speed of the rotating drum along with the degree of alignment.

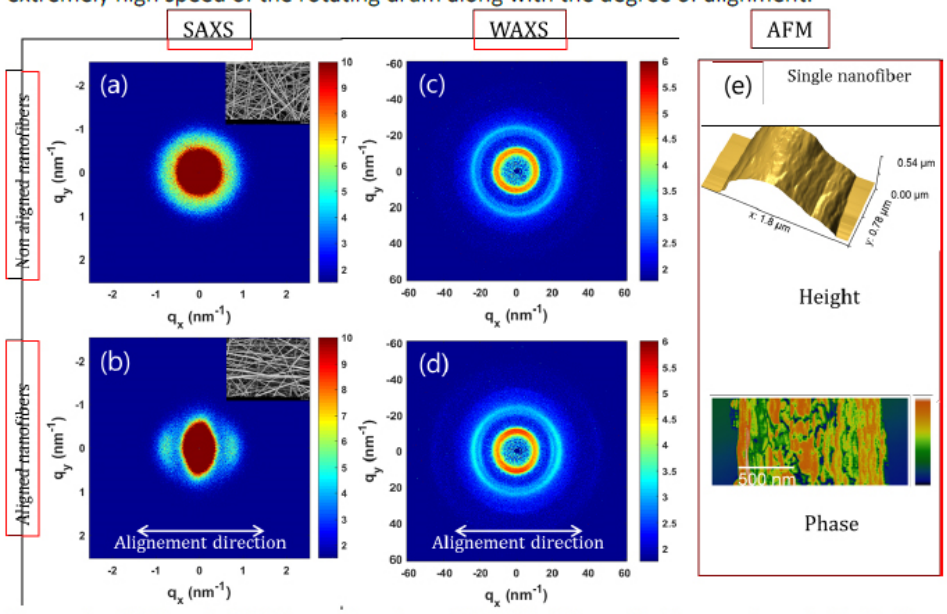


Figure 1. SAXS and WAXS profiles from PVDFhfp fibers; (a,c) non-aligned, (b,d) aligned samples, and their corresponding SEM image in the inset. (e) AFM of single fiber, height (top) and phase image (bottom).

[1] D. Kolbuk, P. Sajkiewicz, K. Maniura-Weber, G. Fortunato, *European Polymer Journal,* **2013**, 49 2052.

Novel quantitative method based on small angle X-ray scattering for in-situ understanding of nanoparticles agglomeration kinetics

Neda Iranpour Anaraki*[1, 2, 3], Anjani Maurya[1], Claudio Toncelli[4], Peter Wick[2], Alex Domann[1], Amin Sadeghpour[1], Antonia Neels[1, 3]

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[2]*Laboratory of Particles-Biology Interactions, Empa, St. Gallen, Switzerland*

[3]*Department of Chemistry, University of Fribourg, Fribourg, Switzerland*

[4]*Laboratory of Biomimetic Membranes and Textiles, Empa, St. Gallen, Switzerland*

Abstract:

Colloidal stability of nanoparticles in biological media is a crucial issue in bio-medical application since the change in the size distribution could change the nanoparticles behavior and cause some undesired effects. An experimental method for in-situ quantitative observation of nanoparticles agglomeration in biological media would provide detailed understanding about the influence of effective parameters at nano-bio interfaces. For biomedical applications, the agglomeration kinetics of nanoparticles at different environments are not concretely determined yet. Here we develop an in-situ method based on small angle X-ray scattering and microfluidics to measure the agglomeration rate constant and the mean agglomeration number of nanoparticles. By using this method, the influence of various buffer systems, ionic strength, pH, temperature, and competing biomolecules such as proteins on nanoparticles agglomeration can be studied. In addition, a comparative analysis by dynamic light scattering (DLS) has been carried out which demonstrates a good agreement with SAXS data.

Effects of crystallization on electronic and optical properties of SnO_2 transparent conducting oxide thin films

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Abstract

Intrinsically doped SnO_2 films were grown by sputtering at 60°C in order to study the effects of crystallization upon annealing on electronic and optical properties of the films for applications as transparent conductive electrodes. Post-deposition annealing of as-grown films above 350°C leads to a decrease of charge carrier concentration and mobility. By performing in-situ high-temperature XRD analysis we have demonstrated that this degradation of electrical properties occurs due to formation of grain boundaries and reduction of the donor defect concentration as a result of crystallization of the amorphous as-grown films. Post-deposition annealing has, however, a positive effect on the optical properties of the films. Annealed crystallized samples exhibit lower absorptance in the visible and near-UV wavelength range due to a blue shift of the absorption edge, which results from the decrease of sub-bandgap states associated to point defects. Obtained results indicate that in order to achieve the best combination of electronic and optical properties of SnO_2 films for applications as transparent conductive electrodes the post-processing annealing temperature shall not exceed 350°C at which the films start to crystallize.

Applications of PDF Analysis to Organic Molecular Compounds

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** pamela.whitfield@excels.us*

Total scattering methods have been used for many years to study short-range behaviour in liquids and glasses. The Pair Distribution Function (PDF) methodology gained popularity when nanomaterials became a popular area for study, and continued when local-range effects in inorganic functional materials were recognized as important factors.
The application of the technique to organic molecular systems has traditionally been a more modest area of study but is growing in importance as the use of amorphous materials in pharmaceuticals has grown rapidly. Where structural and quantitative phase analysis using reciprocal space data has become a routine tool for crystalline materials and formulations, PDF may provide some of the same information for nanoscale, amorphous and mixed formulations. The more limited potential information available in a PDF versus a Bragg dataset increases the tendency to over-parameterization and challenges the analyst to become more imaginative with respect to the possible physically and chemically-reasonable restraints and constraints that may be applied.
The study of organic molecular systems via PDF present some additional problems over and above the more familiar systems. The reduced scattering power of the samples means accurate corrections for background, multiple scattering and Compton scattering are increasingly important compared to many semiconductors and oxides for instance. The non-spherical shape of many of the molecules makes r-dependent corrections for factors such as U_{iso} less useful than for other systems due to the significant overlap in r between intra- and inter-molecular interactions. The approach published by Prill ***et al*** [1] offers a work-around to better fit this troublesome region. Amorphous materials become even more problematic with truncation of small angle scattering and an uncertain shape function among the issues that may become apparent. Extracting information about the intermolecular interactions in an amorphous system ideally requires stripping out the single molecule contribution to the reduced PDF. Benmore ***et al*** [2] fitted S(Q) in the high Q region to extract the single molecule U_{iso} to more accurately model the single-molecule peak widths in the G(r).
Examples will be given highlighting some of the problems that may be encountered, current approaches that may be used to overcome them, and where further developments may be required to fully realize the technique's potential.

[1] Prill D., Juhás P., Schmidt M.U., Billinge S.J.L. ***Acta Cryst.,*** 2016, A72, 62.
[1] Benmore C.J., Weber J.K.R., Tailor A.M., Cherry B.R., Yarger J.L., Mou Q., Weber W., Neuefeind J., Byrn S.R. ***J. Pharm. Sci.,*** 2013, 102, 1290.

Keywords: PDF, molecular systems, pharmaceuticals

Formation of hybrid organic-inorganic guanidinium lead(II) iodides from mechanochemical reactions

M. Wilke, N. Casati
Swiss Light Source, Material Science Beamline, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Mechanochemistry is increasingly used for solid state reactions because of its advantages like high yields, high conversion rates, the easy handling, the small produce of waste and the good energy consumption, for which it belongs to green chemistry. [1-3] Metal organic frameworks and cocrystals are the most studied materials. Nevertheless, the mechanisms behind mechanochemical reactions are still under investigation. Recently, setups were developed for monitoring mechanochemical reactions *in situ* using X-ray diffraction[4], Raman spectroscopy[5] or both combined.[6] In all setups the originally steel made milling jar is replaced by a plastic jar.

Here we present the *in situ* investigation of the formation of a series of organic-inorganic hybrid materials from mechanochemical synthesis. The compounds are constructed by guanidinium-, lead(II)- and iodide-ions, with the formula $(C(NH_2)_3)_nPbI_{2+n}$. For the *in situ* investigations a new setup, developed at the MS beamline is used.[7] Due to the gained high quality data an automatic quantitative analyses of the time-resolved powder patterns was possible and revealed intermediate formations, solid-solid phase transitions and reactions between the guanidinium lead(II) iodides during the syntheses.

[1] S. L. James et al., *Chem. Soc. Rev*. **41**, 413 (2012).
[2] A. A. L. Michalchuk et al. C*rystengcomm* **15**, 6403 (2013).
[3] L. Tröbs et al. *Faraday Discuss.* **170**, 109 (2014).
[4] T. Friscic et al., *Nat. Chem*. **5**, 66 (2013).
[5] D. Gracin et al., *Angew. Chem. Int. Ed.* **53**, 6193 (2014).
[6] L. Batzdorf et al., *Angew. Chem. Int. Ed.* **54** 1799 (2015).
[7] V. Ban et al., *Anal. Chem.***89**, 13176, (2017).

Mesquik, a mail-in service for synchrotron powder diffraction at SLS

Dr. Nicola Casati
Paul Scherrer Institute

The Material Science beamline at the SLS offers different types of diffraction experiments to its users via an external-review proposal system.[1] A faster access proposal system for powder diffraction, named Mesquik, is also in place. It consists of a permanently-open, fast-tracked and externally-reviewed system for simple powder diffraction data collections. It provides for accepted proposals synchrotron data delivered to a mailbox within 10 weeks from the proposal submission. The limitations and characteristics of the service will be presented, including general guidelines on how to plan its usage.

Total Scattering at the X04SA beamline of SLS

Antonio Cervellino (Photon Science Division, Paul Scherrer Institute, Villigen, Switzerland)

Ruggero Frison (Department of Chemistry, University of Zurich, Switzerland & Excelsus Structural Solutions (Swiss AG), PARK innovAARE, Switzerland, Zurich, Switzerland)

email: antonio.cervellino@psi.ch (mailto:antonio.cervellino@psi.ch)

The X04SA Powder Di!raction beamline [1] has been developed with Total Scattering (TS) experiments at the forefront. The requirements for TS are perfectly compatible with maintaining the best capabilities for classical synchrotron XRPD, as the main TS requirement is – top data quality. The energy "exibility of the beamline (5 – 30 keV with high photon "ux and su#cient detection e#ciency) and the excellent detectors installed (a 2D Pilatus 6M and a large 1-D Mythen II) make up the rest, allowing for the required momentum transfer especially with the Mythen II [1]. In fact, collecting data to 140 deg with the Mythen, the Qmax can reach > 28 Å-1, su#cient for most materials, while especial emphasis is given to reciprocal space TS (modelling the data directly from atomic coordinates via the Debye Scattering Equation, as per the DFA method [2]), where the absence of a direct Fourier transform of the data makes the need for high Qmax less stringent whilst the data quality must be even higher in all respects. Increasing data quality is a process that involves the hardware – whereas all forms of parasitic scattering and all instrumental and intrinsic distortions (inelastic scattering, absorption,..) can be minimised and/or corrected whilst maximizing the sample scattering signal. The software plays also a critical role, inasmuch the information content of the data is fully preserved and the raw data are processed, corrected and subtracted [2] to yield precisely the desired part – the sample's elastic scattering pattern and its absolute scale sharpened counterpart S(Q) or the latter's direct space Fourier equivalent interatomic distance pair distribution function G(r). The hardware (rotating capillary, liquid jet and suspended droplet) enhancements will be presented, together with the state-of-the-art, never before presented procedures and algorithms for calibrating the detector (pixel-wise positional and e#ciency corrections [2]) together with the most e!ective and still partly unpublished algorithms and methods for data processing, merging, subtraction and correction – including a novel lossless smoothing-denoising [2] that permits to acquire high-quality low-noise background patterns in a fraction of the time previously required. Furthermore, subsequent processing [2] to obtain the absolute scale sharpened S(Q) and the G(r) functions in a reliable and automated way are presented and compared with existing dedicated softwares like (GudrunX [3], PdfGetX3 [3]. As an outlook, simultaneous Quantitative Phase Analysis in Q and r spaces – thus made independent from the crystallinity of components - is envisaged.

References:

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[2] Cervellino A. et al., J. Appl. Cryst. 2015, 48, 2026-2032; J. Comput. Chem. 2006, 27, 995-1008; J. Appl. Cryst. 2014, 47, 1755-1761; Cervellino A., Frison R. (2018), unpublished

[3] Soper Alan K. and Barney Emma R., (2011). J. Appl. Cryst., 44, 714-726; Juhàs, P. and Davis, T. and Farrow, C. L. and Billinge, S J.L., (2013). J. Appl. Cryst. 46, 560-556

Keywords: Synchrotron XRPD, Total Scattering, Data processing

Swiss Crystallographic Association SGK / SSCr

General Assembly 2018

Tuesday, September 12, 2018, 12:15-14:00
Paul Scherrer Institute, 5232 Villigen
Auditorium WHGA/001,

Agenda of the General Assembly 2018

The minutes of our last General Assembly (Geneva, Tuesday, September 12, 2017) are published on page 36-42 of the SGK/SSCr newsletter No. 100, August 2018 (this issue), which is also available electronically at http://www.sgk-sscr.ch/newsletter/

1) Determination of the quorum according to Art. 12/by-laws

2) Proposition for acceptance of the minutes of the General Assembly 2017, Geneva

3) a) Annual report/Jahresbericht / le rapport annuel

   b) Annual financial statement /Jahresrechnung / les comptes annuels

   c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivante

   Elections / Wahlen / Élections

4) a) definition of a chairperson for the elections

   b) confirmation of the present board members.

   c) elections of 2 new board members
   (replacement for P. Macchi and C. Besnard).
   Already available candidates are: Dr. Dubravka Sisak (Dectris) and Dr. Pascal Schouwink (EPFL). Further nominations should be communicated to the president prior to the meeting.
   Candidates are asked for a short 1-2 minute oral presentation.

   d) assigment of new treasurer, secretary, president and vice president

   e) election/confirmation of the auditors

5) 2019 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!

6) Anträge von Mitgliedern
   other motions of members

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06)	3	4
2017 (as of 17.07)	10	4
2018 (as of 18.08.)	8	19*

* in 2015 and 2018, a large number of SGK/SSCr members (18 and 19, resp.) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and could not be contacted.

Quorum for final decisions (Art.12, by-laws):
As of 18.08.2018, we have 195 records in our database.
They are grouped as:
- 7 of these are companies (or corporate members),
- 30 are “libraries” (incl. some “quasi-personal” members, from whom we don’t expect any fees, but to whom we are regularly sending our Newsletters);
- 158 are personal members (full: 124, students: 30, honorary: 4)

I.e. for the quorum to be able to make decisions, we should have **10%** out of **165** corporate and personal members, i.e. at least **17** people.

Board Members:
see last page of this newsletter

Delegates

ECA:	A. Linden (Zurich), K. Fromm (Fribourg)
IOCG:	E. Giannini (Fribourg)
ScNat:	P. Macchi (automatically assigned to the acting president)
Steering Comm. SNBL	G. Chapuis (Lausanne), R. Cerny (Geneva)

Revisorenbericht für die Jahresrechnung 2017 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS	UBS	279-C0291110.0
Credit Suisse	CS	913652-00

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2017 bis 31. Dez. 2017. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2017 ist der Stand der Konten und der Kasse:

UBS	SFr.	30'798.60
CS	SFr.	18'340.47
Kasse	SFr.	542.10
Summe SGK	SFr.	**49'681.17**

Die Unterzeichneten beantragen von der Versammlung die Entlastung des Kassierers und der Revisoren für die geprüfte Periode.

Ort / Datum
BERN, 8 Februar 2018

Unterschriften

B. Spingler
(Universität Zürich)

K. Schenk
(EPF Lausanne)

Summary SGK Finances

	CHF
Total 31.12.2016	**34'538.83**
UBS account	30'798.60
CS account	18'340.47
Cash on hand	542.10
Total 31.12.2017	**49'681.17**
Balance	**15'142.34**

SGK Financial Report 2017
UBS Account

	CHF
UBS Balance 31.12.2016	**15'669.24**
Income:	
Membership dues	
full members (various amounts due to debts)	
88x40 +2x30 +3x50 +1x60	3'790.00
Students 13x10	130.00
Companies 7x130 +1x142	1'052.00
SCNAT support	12'074.00
ECM30 reimbursement, 2016	27'908.90
SGK Annual Meeting 2017 reimbursement	1'262.70
Interest	3.25
Total Income	**46'220.85**
Expenses:	
Membership dues to SANW (170 members)	1'148.00
SCNAT reimbursement from ECM30, 2016	9'435.00
ECA reimbursement from ECA, 2016	8'304.50
SGK Annual Meeting 2017 at the University of Geneva	3'000.00
ECA member fees 2016 and 2017	406.73
ZH Crystallography School	2'000.00
PhD Price 2017: Dr. Stef Smeets	2'393.00
Travel support for students: Michelle Ernst, Afshin Abrishamkar & Rebecca Scatena	2'000.00
Travel support for Delegates to the IUCr Meeting in Hyderabad, India, 2017 for Tony Linden and Piero Macchi	2'000.00
General expenses (switch)	8.90
Bank and Post expenses	395.36
Total Expenses	**31'091.49**
Income – Expenses	**15'129.36**
Starting Balance + Income – Expenses	**30'798.60**
UBS Balance 31.12.2017	**30'798.60**

Cash on Hand - 2016

	CHF
Status 31.12.2015	**542.10**
Total Income	0.00
Total Expenses	0.00
Balance (Income – Expenses)	0.00
Starting Balance + Income – Expenses	542.10
Cash on Hand 31.12.2016	**542.10**

Credit Suisse (savings account)

	CHF
Status 01.01.2017	**18'327.49**
Interest (0.10% or 0.05%, resp.)	12.98
Withholding Tax*	-.-
Balance 31.12.2017	**18'340.47**

*(only applicable when amount of interest exceeds CHF 200)

SGK Budget 2019
To be proposed at the SGK assembly 12.09.2018

Credits:	**Budgeted**
Membership dues	5'000.00
SANW reimbursement for ECM delegates (ECM32 in Vienna, Austria)	2'000.00
SANW contribution for SGK annual meeting including poster prize	3'000.00
SANW contribution for Zurich School of Crystallography	2'000.00
SANW PhD / master students travel grants	2'000.00
SANW contribution for PhD Thesis prize	1'000.00
SANW Crystallographic Lectures: Howard Flack Series	3'000.00
SANW ECA membership	300.00
Total Income	**18'300.00**

Debits:	
Membership dues to SANW	2'000.00
Annual meeting + poster prize	3'000.00
Travel Grants to Young Scientists	2'000.00
SGK support for Zurich School of Crystallography	2'000.00
SGK support for 'Symposium Max Perutz' in April 2019	2'000.00
PhD Thesis prize	2'000.00
Crystallographic Lectures: Howard Flack Series	4'000.00
ECM delegates (ECM32, Vienna, Austria)	2'000.00
ECA national membership dues 2019	300.00
Bank charges	250.00
Total Expenses	**19'550.00**
Income – Expenses	**-1'250.00**

Minutes of General Assembly 2017

Tuesday, September 12, 2017
Faculty of Science - University of Geneva, 30, quai Ernest-Ansermet – Geneva
12:50-13:50
Schweizerische Gesellschaft für Kristallographie

Agenda:

1) Determination of the quorum according to Art. 12/by-laws

2) Proposition for acceptance of the minutes of the General Assembly 2015, Neuchâtel

3) a) Annual report/Jahresbericht / le rapport annuel

   b) Annual financial statement /Jahresrechnung / les comptes annuels

   c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivante

   Elections / Wahlen / Élections

4) a) definition of a chairperson for the elections

   b) confirmation of the present board members

   c) confirmation of the delegates for the Swiss Steering Committee of SNBL:

   d) election/confirmation of the auditors, the ECA-delegates and the delegate for the IO for Crystal Growth

5) 2018 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!

6) PhD Prize 2019 (rules, amount)

7) Other motions of members

Minutes:

The president P. Macchi has sent the agenda via email on 06.09.2017 with detailed comments to the members, in order to keep discussions short.
Formalities:

The General Assembly was chaired by Piero Macchi, President, and started at 13.05 h
The Agenda has been published in the Newsletter 98 on 25. July 2017 (Art. 11)
As keeper of the minutes the secretary Michael Wörle, ETH, was elected unanimously, no abstentions.

Ad 1.
With 25 members being present at this assembly, the necessary quorum of 10% (18) is reached to constitute a quorum (Art. 12).
As of 17.07.2017, we have 206 records in our database.
They are grouped as:
- 9 of these are companies (or corporate members),
- 30 are “libraries” (incl. some “quasi-personal” members, from whom we don’t expect any fees, but to whom we are regularly sending our newsletters);
- 167 are personal members (full: 131, students: 32, honorary: 4)
10% out of 176 corporate and personal members, i.e. at least 18 people. Two corporate members present are Dubravka Sisak and Eric Hovestreydt (named according to Art. 14 of the bylaws)

Ad 2.
The minutes of the General Assembly 2016 on 31/08/2016 in Basel, reported in newsletter 98, have been approved unanimously, no abstentions.

Ad 3 a)
The president expresses thanks to Katharina Fromm and Jürg Schefer for organizing the ECM-30. Piero called a moment of silence for our dear colleague Howard Flack, who died in 2017. After ECM30, the main activities concern the organization of a joint meeting with the German Society of Crystal Growth (co-organized by Enrico Giannini), the support for the Zurich School of Crystallography (organized by Tony Linden and Hans-Beat Bürgi), the participation to the general assembly of the IUCr in Hyderabad (Tony Linden, Piero Macchi), the support of young students for participation to schools and workshops, the second edition of the PhD prize (to be awarded in Geneva).
Enrico Giannini reports on joint meeting with the German Society of Crystal Growth: There were about 100 participants, 20-25 from Switzerland. One of the main topics has been protein crystallography. Prof. Hans Scheel was awarded the DGKK-Prize 2017. The President reported on the General Assembly 2017 of the IUCr in Hyderabad: the new president of the IUCr is Sven Lidin. The upcoming meetings will take place in Prague 2020 and Melbourne 2023.
The support for students; CHF 500.- for poster and CHF 750.- for oral contributions
In October 2018 there will be a celebration at PSI on the occasion of 100th anniversary of the death of Paul Scherrer.

Ad 3 b)
The president Piero Macchi gives the financial report for 2016.

Summary SGK Finances

Total 31.12.2015	**34'713.46**
UBS account	15'669.24
CS account	18'327.49
Cash on hand	542.10
Total 31.12.2016	**34'538.83**
Balance	-174.63

SGK Financial Report 2016
UBS Account

	CHF
UBS Balance 31.12.2015	**15'892.54**
Income:	
Membership dues	
full members (various amounts due to debts)	
82x40 +7x30 +5x70 +9x50 +1x53.85 +1x37 +1x35.50	4'416.35
Students 14x10	140.00
Companies 4x130 +1x390 + 1x390 (for 2017-2019) +1x118 +1x194	1'612.00
Reimbursement ScNat 2015	8'000.00
Interest	2.20
Total Income	**14'170.55**
Expenses:	
Membership dues to SANW (170 members)	1'190.00
ECM 2016 (Poster prizes)	511.00
Promotion ECM 2016 (Congrex invoice)	9'299.90
ECM Satellite Meeting in Nancy	1'000.00
Powder Diffraction School: PSI Villigen	2'000.00
Travel costs for ECA board meeting, Parma, IT (Fromm)	274.00
General expenses (switch)	8.90
Bank and Post expenses	110.05
Total Expenses	**14'393.85**
Income – Expenses	-223.30
Starting Balance + Income – Expenses	15'669.24
UBS Balance 31.12.2016	**15'669.24**

Cash on Hand - 2016

	CHF
Status 31.12.2015	**542.10**
Total Income	0.00
Total Expenses	0.00
Balance (Income – Expenses)	0.00
Starting Balance + Income – Expenses	**542.10**
Cash on Hand 31.12.2016	542.10

Credit Suisse (savings account)

	CHF
Status 01.01.2016	**18'278.82**
Interest (0.385% or 0.100%, resp.)	48.67
Withholding Tax*	-.-
Balance 31.12.2016	**18'327.49**

*(only applicable when amount of interest exceeds CHF 200)

- The budget 2016 has been approved by the auditors Kurt Schenk and Bernhard Spingler (Bern, 21.02.2017)

- The budget 2016 was approved unanimously by the delegates, no abstentions.

Ad 3 c)
Budget 2018:

Credits:	**Budgeted**
Membership dues	5'000.00
SANW reimbursement for IUCr delegate	1'500.00
SANW master students travel grants	2'000.00
SANW contribution for SGK annual meeting	3'000.00
SANW contribution for PSI School	2'000.00
SANW contribution for PhD prize	1'000.00
Interest (est.)	100.00
Total Income	**14'600.00**
Debits:	
Membership dues to SANW	2'000.00
Annual meeting + poster prize	3'000.00
Travel Grants to Young Scientists	2'000.00
SGK support for PSI School	2'000.00
PhD poster prize	1'500.00
IUCr delegates	2'000.00
ECA national membership dues 2018	250.00
Bank charges	250.00
Total Expenses	**13'000.00**
Income – Expenses	**1'600.00**

The budget 2018 was approved unanimously by the members

For the year 2017, the treasurer reports on a surplus generated by ECM30 and transferred to SGK in 2017. The president asked for ideas on how to invest this surplus (27'908.90 CHF). The general purpose is an investment for the visibility of Crystallography in Switzerland, at various levels (within the science community as well as within the society). So far, the board meeting has elaborated a proposal to establish a series of crystallographic lectures at Swiss Universities, supporting the costs of an invited internationally reckoned crystallographer per semester for a tour in 4-5 Swiss institutions. Estimated costs are ca. 3'000 CHF per person.
On a long term scale, this support may be limited to costs of international flights, leaving each group paying the costs for accommodation. In this way the project may become sustainable with the ordinary budget.
We received also suggestion from a member (Hans-Beat Bürgi). One of the suggestion is basically coinciding with the lecture program described above, the other is the institution of a fund to support retired scientists for participation to meetings.
Lively discussion of two proposals;

1. Lecture series in Switzerland, invited prof should travel, second half of 2018.
2. Several lectures at 1 site
   (Proposed name: Howard Flack lecture series)

Votation: 11 for first proposal, 7 for second proposal.
The board will consider both proposals.

Elections:

Ad 4 a)
Chairperson for the election is Piero Macchi (approved unanimously by the delegates, no abstentions)

Ad 4 b)
Confirmation of the present board members:
No member has to leave the board in 2017 because of exceeding the nine year term.
The president proposes to confirm all board members until 2018.
All present board members are confirmed unanimously:
Piero Macchi (president)
Antonia Neels (vice-president and treasurer)
Michael Wörle (secretary)
Antony Linden
Olha Sereda
Enrico Giannini
Céline Besnard (website manager)

Ad 4 c)
Confirmation of the delegates for the Swiss Steering Committee of SNBL:
At meeting in Basel, it was discussed the participation of SGK to the Swiss steering committee of the Swiss Norwegian Beamline at SNBL, led by the PSI (in response to the request of the minister of research). The committee was established in March 2017 and the board has temporarily proposed Gervais Chapuis and Radovan Cerny (as previous members of SNX foundation). The president asks the assembly to confirm these names for a period of 3 years, as requested by the Swiss steering committee.
Gervais Chapuis and Radovan Cerny are accepted unanimously by a collective election (no abstentions).

Ad 4 d)
Election/confirmation of the auditors:
The president asks that Bernhard Spingler and Kurt Schenk be confirmed as auditors until 2018. Moreover, the president asks that since 2018, the auditors be nominated for a period of 3 years, coinciding with the mandate of the president and the treasurer.
Both auditors were reelected unanimously with no abstentions: Bernhard Spingler and Kurt Schenk

Both ECA delegates were reelected unanimously with no abstentions:
Antony Linden
Katharina Fromm

Delegate for the International Organization for Crystal Growth:
Enrico Giannini (replaces Katharina Fromm)
Enrico was confirmed unanimously

Ad 5)
Next annual meeting:
Candidate: PSI Villingen. As organizers Nicola Casati and Antonio Cervellino.
Proposal was unanimously accepted.

Ad 6)
PhD prize 2019

Given the success of the second edition (5 candidates, with high qualification), the president proposes to establish the third edition of the PhD prize in 2019, with the same rules as for 2017: a) thesis discussed within the previous two years; b) thesis discussed by a Swiss citizen in any university or by a foreign citizen at a Swiss university; c) a prize of 2'000 CHF and an invited lecture at the SGK meeting.

Conditions:
Finished between March 2016 and March 2019
Submission deadline: May 31, 2019
Decision; June 30. 2019

Votation for overlap: 3 years period: 10 members, against 9 members, abstentions 3 members

Proposal from Hans-Beat Bürgi: The name of the prize winner should be announced in the program for the respective meeting.

Ad 7)
Other motions of members:
Establishing funds for retired members (Proposal of Hans-Beat Bürgi).
Under the conditions that none of the young crystallographers should suffer
That there is an active contribution and it is compatible with the overall budget.

Votable proposal at the general assembly 2019

Meeting ends at 14:09

Minutes written by the Secretary
Michael Wörle, 17.08.2018

Approved by the President
Piero Macchi

Swiss Society for Crystallography PhD prize

The Swiss Society for Crystallography establishes a prize for the best PhD thesis in crystallography.

Requirements:
The prize is open to

a) Students, of any nationality, who earned a PhD title from a Swiss University
b) Students, of any nationality, who earned a PhD title from a University abroad, but carried out significant amount of work for the PhD title at a Swiss Research Institution, like EMPA, PSI or SNBL.
c) Students of Swiss nationality who earned a PhD title from any University worldwide.

The student must have earned the title between **March 31st 2016 and March 31st 2019**.
The subject of the thesis can be in any area of crystallography (structural biology, chemical crystallography, solid-state physics, crystallography of materials, etc.). The implications of the obtained results for crystallography should be evident.

Application:
The application for the prize should be submitted before **31st May 2019** by the student himself or by the thesis supervisor. The applicant should submit: a) a pdf copy of the thesis; b) a letter of the supervisor approving his/her candidature; c) pdf copies of the articles published from the results obtained during the thesis; d) a pdf scan of the PhD diploma; e) a short CV of the candidate. Applications for this SGK Thesis Prize are accepted only once per applicant.
The application should be sent to the secretary of the Swiss Society of Crystallography (info@sgk-sscr.ch)

The award
The winner will be selected by a commission, based on the quality of the research, the quality of the publications, and the effective contribution of the candidate to the scientific work. The commission may decide not to assign the prize if none of the candidates fit the minimal prerequisites concerning the topic, the quality of the thesis, the papers published from it and the approval of the supervisor.
The winner will be announced before the annual meeting and will be invited to give a short talk of the results of his/her thesis.
The Swiss Society of Crystallography will award the winner with a diploma and will reimburse the participation of the student to the annual meeting.
The award is endowed with CHF 2000.-

Meetings, Conferences, Workshops, Schools, Courses

Annual SGK/SSCr-Meeting at PSI Villigen

Swiss Society for Crystallography
SGK / SSCr
Annual meeting 2018

Wednesday, September 12, 2018
Main Auditorium – PSI Villigen
WHGA/001 – 5232 Villigen PSI

Meeting Title:
"The Breadth of Crystallography"

The 2018 annual meeting of the SGK/SSCr will take place at the **PSI in Villigen** on **Wednesday 12th of September 2018**.

Meeting registration
From 1st May 2018 on http://indico.psi.ch/event/SGK-SSCr/annualmeeting2018

Abstract submission
Until 8th July 2018 by email to sgk-sscr_meeting2018@psi.ch
Please indicate your preference for poster or oral communication

The detailed program can be found here:
http://indico.psi.ch/event/SGK-SSCr/annualmeeting2018

Local organization and contact
On behalf of the Swiss Society for Crystallography: Antonio Cervellino, Nicola Casati

Symposium on the occasion of the „Chemical Landmark 2019“

Advance notice:
The award of the «Chemical Landmark 2019» to the High Altitude Research Station Jungfraujoch given by the Swiss Academy of Sciences will be occasion for a one-day Symposium in **Bern**, which is planned for the **25. April 2019**. The Symposium will highlight the historical and current role of this Research Station in an international context. Since Max Perutz (Nobel Prize in Chemistry, 1962) had been conducting studies at the Jungfraujoch Research Station in the 1930s, the Symposium will be of interest for the crystallographic community as well. Consequently, the Swiss Society for Crystallography will together with the Swiss Chemical Society co-organize this event. More details will follow.

Contact person: Prof. Silvio Decurtins, President of the International Foundation for the High Altitude Research Stations Jungfraujoch and Gornergrat.

ECM31 in Oviedo

The **31st European Crystallographic Meeting**, ECM31, will take place in the Palace of Exhibition and Congresses (PEC) in Oviedo, Spain, from 22-27 August 2018.

ECM31 is setting up an attractive programme covering the latest advances in crystallography and related sciences to attract young and senior scientists as well as companies and general public.

One extensive agenda for accompanying people will be offered, with special attention to babies and children, with a specific programme of baby-care and children activities during the conference. Asturias, and the city of Oviedo in particular, is a cultural, active and organized region of open minded, hospitable and altruist citizens. Asturias may be easily reached by air, train or car.

The PEC has a spectacular urban design and offers a modern, functional and versatile infrastructure with all facilities.For all these reasons, ECM31 will be an effervescent and fruitful scientific, social and commercial meeting with many learning opportunities in every current aspect of crystallography.

http://ecm31.ecanews.org

http://ecm31.ecanews.org/en/

2018

Swiss Workshop on Materials with Novel Electronic Properties

Basic research and applications

MaNEP
SWITZERLAND
NETWORK

August
29th - 31st

Les Diablerets

Workshop topics

- Quantum and mesoscopic magnetism
- Superconductivity, materials and mechanisms
- Oxide interface physics
- Ferroic & multiferroic materials
- 2D van der Waals materials
- Topological phases of matter
- Cold atoms
- Surfaces and interfaces
- Novel probes
- Applications

Program committee

Chair : Felix Baumberger UNIGE, Dmitry Abanin UNIGE, Christian Bernhard UNIFR, Johan Chang UNIZH, Thierry Giamarchi UNIGE, Marta Gibert UNIZH, Dirk Grundler EPFL, Martin Kroner ETHZ, Patrick Maletinsky UNIBAS, Marisa Medarde PSI, Alberto Morpurgo UNIGE, Markus Müller PSI, Titus Neupert UNIZH, Nick Plumb PSI, Christoph Renner UNIGE, Henrik Ronnow EPFL, Urs Staub PSI, Philipp Werner UNIFR, Jonathan White PSI

Organizing committee, contact address

Alberto Morpurgo, Felix Baumberger, Adriana Bonito Aleman, Pierre Bouillot, Pascal Cugni, Ivan Maggio-Aprile, Greg Manfrini, Christophe Schwarz, Natacha Triscone
24 Quai Ernest-Ansermet, CH-1211 Genève 4
Phone : +41 22 379 65 78 - E-mail : swm@manep.ch

The deadline for registration and abstract submission is :
May 11th 2018
swm18.manep.ch

Invited speakers

Leon Balents
KITP UC Santa Barbara

Kamran Behnia
ESPCI Paris

Eva Benckiser
MPA Stuttgart

Manuel Bibes
CNRS/Thales Paris

Andrea Cavalleri
MPI Hamburg

David Cobden
University of Washington Seattle

Josep Fontcuberta
ICMAB Barcelona

Vincent Jacques
University of Montpellier & CNRS

Thomas Jungwirth
Czech Academy of Sciences Prague

Philipp Moll
MPI Dresden

Virginie Simonet
Institut Néel, CNRS Grenoble

Bernhard Urbaszek
CNRS INSA Toulouse

The 6th European Conference on Crystal Growth and 2nd European School on Crystal Growth

Varna, Bulgaria, September 16-20, 2018

http://escg2.eu/

ILL and ESS European Users Meeting

The neutron landscape in Europe is going through a period of dramatic change. Two major, national facilities will close by 2020. A substantial investment in a new European facility, ESS, will deliver transformative capabilities and extend the technique to new domains by the middle of the next decade, based on the highest peak flux in the world. ILL is currently executing phase one of the Endurance upgrade programme and is preparing a second, more extensive phase of Endurance that will be the basis of future operations well beyond 2023, exploiting its world-leading continuous flux.

The future of neutron scattering is bright, but both the landscape of facilities and the community of users must take a proactive and strategic approach to navigating and managing these changes in a holistic way, in order to ensure the sustainability and vitality of this important research technique. ILL and ESS therefore feel that it is timely to review recent achievements and the current status and, above all, look forward to new scientific opportunities with neutrons for the next decade.

As the two European neutron sources, we would therefore like to invite you to the

ILL and ESS European Users Meeting

from

Wednesday, 10 October 2018

(beginning 09:00)

to

Friday, 12 October 2018

(end 12:15)

in GRENOBLE

We shall have a number of plenary speakers on future directions in neutron science, as well as reports on recent achievements and ongoing work at ILL and ESS. There will be focussed satellite meetings, in parallel with the user meeting, which will allow participants to delve deeper into specific areas of neutron science.

At this pivotal moment for neutrons in Europe, we believe that this meeting will be a unique occasion for European scientists to support and drive the opportunities for science with neutrons through the next decade.

For the time being, we should like you to put these dates in your diary. More details on the meeting will be given in a second circular and on the web site at*www.neutrons4europe.com* when this becomes active.

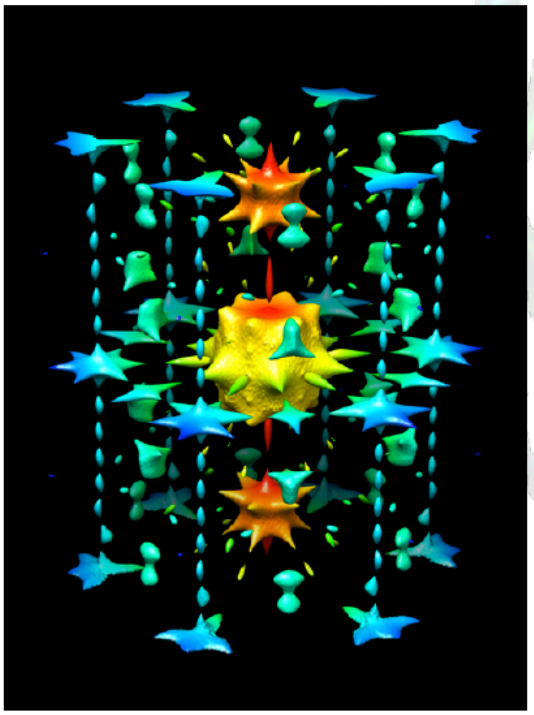
The directors of ILL and ESS

New SIG “Dynamics, Disorder, Diffuse”

Dear Crystallographers,

We are glad to invite you for the inauguration of a new Special Interest Group **SIG 14 D³ “Dynamics, Disorder, Diffuse”**. The meeting will take place **Sunday 26, from 12:00 to 13:00, room Naranco**. All scientists interested in dynamics, disorder and diffuse scattering are welcome to join SIG D³!

SIG is open to all European crystallographers active in the field of crystallography of disorder, diffuse scattering and dynamic phenomena. Participation requires ECA membership.



About new SIG

SIG D³ brings together scientists working on dynamical properties, disorder and diffuse scattering. The main objectives are to enhance the exchange of information regarding recent progress in experiment and theory, to provide a platform for discussions, to promote use of diffraction and crystallographic tools in studying the physics and chemistry of materials which display some disorder.

SIG D³ aims at achieving a coherent understanding of the various contributions to Bragg and diffuse scattering related to disorder phenomena. The disorder is taken here in a broad sense and includes structural imperfections present at different time and length scales, varying from domain walls to compositional fluctuations and fundamental excitations in non-ideal crystals. We note that this field has experienced a significant revival thanks to the advent of bright synchrotron and neutron sources, the development of new detectors, and the availability of powerful computing tools. SIG D³ also focuses on experimental techniques to probe disorder and dynamical response, and on the processing and presentation of big data sets associated with the study of diffuse scattering. SIG D³ also aims at generating a pool of software and experimental facilities best suited for studies of dynamics and disorder phenomena.

Some topics of interest

- Diffuse scattering associated with fundamental excitations
- Atomic displacements, thermal diffuse scattering and lattice dynamics
- Occupational, displacive, and orientational disorder in crystals
- Correlation analysis of diffuse scattering, 3D pair distribution functions from diffuse scattering
- Direct space modeling of disordered systems with Monte Carlo and other techniques
- Magnetic diffuse scattering
- Dynamics and disorder at extreme conditions
- Excited state crystallography
- Inelastic X-ray and neutron scattering

Feel free to come with your suggestions!

Inauguration meeting during the ECM31 in Oviedo, Sunday, Aug. 26, 12:00-13:00 in in room Naranco

Calls for proposals

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility.

Facility	Deadline(s)	Link
SLS: Swiss Light Source		
All except PX lines	15.03. and 15.09.	www.psi.ch/useroffice/
Protein crystallography beamlines (PX)	15.04. and 15.10.	
SINQ: Swiss Spallation Neutron Source		
All instruments (regular calls)	to be announced (no beam in 2019 due to guide upgrade)	www.psi.ch/useroffice/
SINQ/SLS		
Joint x+n proposals (MS/HRPT)	28.02.	www.psi.ch/useroffice/
SμS: Swiss Muon Source		
DOLLY, GPD, GPS, HAL-9500, LEM , LTF	28.02.	www.psi.ch/useroffice/
GPD, GPS, LTF, HAL-9500, LEM	not yet determined	
SwissFEL		
ARAMIS-Alvra, ARAMIS-Bernina	15.09	
ESRF: European Synchrotron		
long term proposals	15.01.2020	www.esrf.eu/
short term proposals	01.03.2020	UsersAndScience/
ILL: Institut Laue Langevin		
All instruments	17. 09. 2018	www.ill.eu/
FRM II: Heinz Maier-Leibnitz		
All instruments	28.09.2018	www.mlz-garching.de/user-office/
Rapid access program	23.08.2018	www.mlz-garching.de/user-office/
SNS Spallation Neutron Source Oak Ridge	28.09.2018	neutrons.ornl.gov

Calendar of forthcoming meetings

(Please mail the missing information on meetings of interest to woerle@inorg.chem.ethz.ch)

			Application Deadline
2018			
Sept. 12	PSI Würenlingen	Annual meeting of the SGK / SSCr	07.09.2018
Aug. 21-29	Oviedo, Spain	31th Meeting of the European Crystallographic Association http://ecm31.ecanews.org/en/index.php	20.07.2018
June 1-10	Erice, Italy	Erice International School on Quantum Crystallography	30.09.2017
July 1-4	Edinburgh, UK	16th European Powder Diffraction Conference	To be announced
2019			
Aug.	Vienna, Austria	32th Meeting of the European Crystallographic Association http://ecm32.ecanews.org/	to be announced
April, 25	Bern	Symposium on the occasion of the „Chemical Landmark 2019“	To be announced
June 16-27	Zurich	Zurich School of Crystallography - Bring Your Own Crystals	15.01.2019

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(If you would like to see your logo here, please contact our treasurer, Dr. Antonia Neels)

Become a member of SGK/SSCr

If you are working in the field of crystallography, you might be interested in becoming a member of our society. For more information as well as online registration, please go to our website (http://www.sgk-sscr.ch).
Presently, the yearly membership fee is CHF 40 (CHF 10 for students).

SGK/SSCr is a member of the Swiss Academy of Science.

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

Members of the Board of the Society for the period 2015 – 2017

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