Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie

Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux

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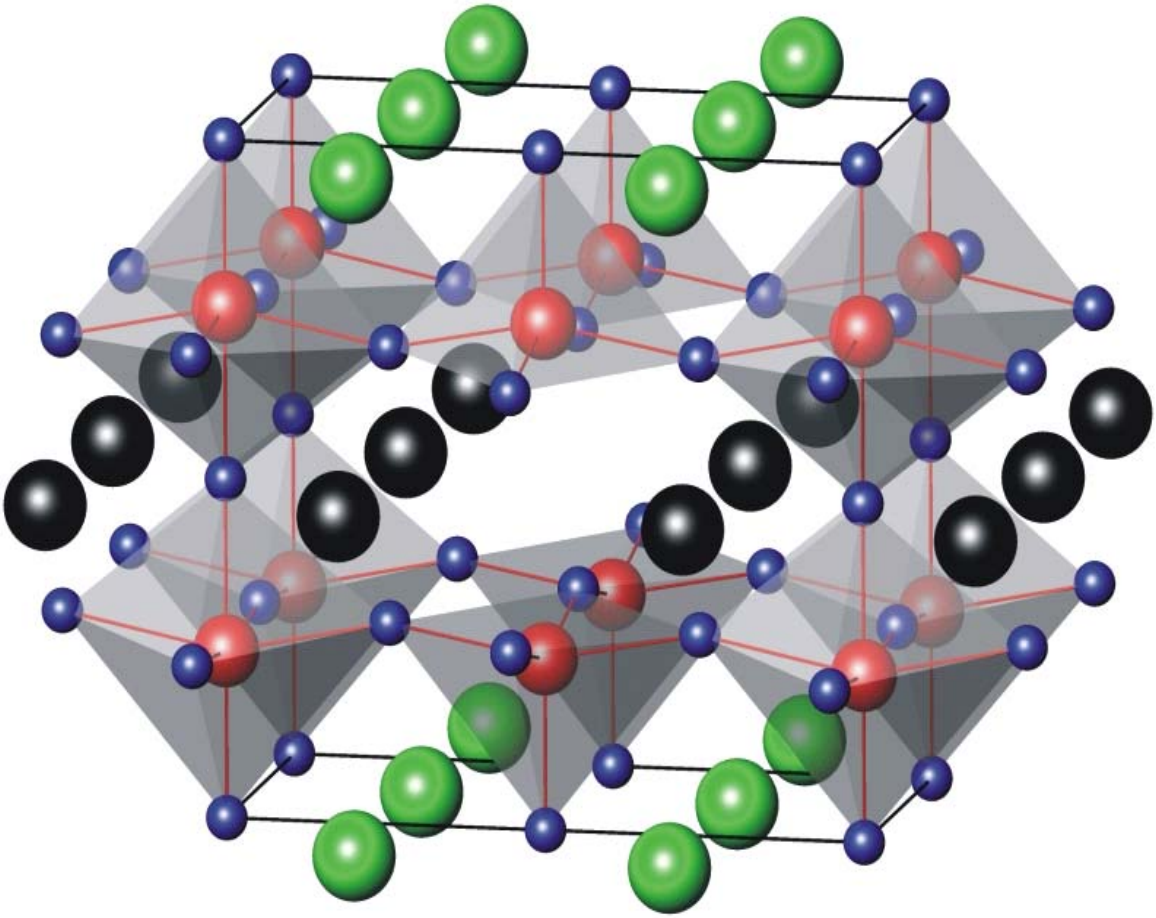

No. 68

SGK/SSCr NEWSLETTER July 2006

On the Cover:

Great controversy has been arisen regarding the issue of the Co spin state and the explanation of numerous physical properties (magnetic and transport transitions, charge and orbital ordering) of compounds from a **layered perovskite $RBaCo_2O_{5+\delta}$ family** (R = rare earth element). Diffraction measurements of the crystal structure across the MI transition in $HoBaCo_2O_{5.5}$ were, therefore, performed. Neutron powder diffraction measurements were carried out at the high-resolution HRPT diffractometer at SINQ neutron spallation source (PSI, Switzerland). Details are given in the scientific contribution on page 9.

SGK/SSCr Newsletter No. 68

In Memoriam of Fritz Laves

by Dieter Schwarzenbach, Lausanne (dieter.schwarzenbach@epfl.ch)

This year, we commemorate Fritz Laves who was born 100 years ago, on 27 February 1906, in Hannover. The *Deutsche Gesellschaft für Kristallographie* has organized at its annual meeting in Freiburg (Breisgau) a memorial session on April 3, 2006 where two of his former students and associates, W. Hoffmann and D. Schwarzenbach, presented their recollections of the times when Laves headed one of the most influential research institutes of crystallography at ETH-Zürich. It seems to be fitting to remember him also in Switzerland.

Fritz Laves was the scion of a respectable Hannover family. Although his father had some reservations concerning the choice of his son to engage in an unprofitable science, Laves studied mineralogy, at Innsbruck (1924), Göttingen (1924-1926) and Zürich (1926-1929) where he earned his doctorate under the supervision of the great Paul Niggli with a thesis on the classification of crystal structures using topological concepts ("Wirkungsbereiche"). He then accepted an invitation from V.M. Goldschmidt at the University of Göttingen where he remained until 1943. Particularly noteworthy during this period is the determination of the structure of gallium, and of the alloy structures which are known as *Laves phases* ($MgCu_2$, $MgZn_2$, $MgNi_2$). He became *Privatdozent* already in 1932, but promotions to higher academic positions were slow to come, no doubt because of his critical attitude towards the German regime. After short-lived appointments as professor in Halle (1943-1945) and Marburg (1945-1948), he became professor at the Geology Department of the University of Chicago in 1948. There, in close collaboration with J.R. Goldsmith, he developed another research topic he became famous for, on order-disorder in silicates and in particular in feldspars. He continued this work with notable success in Zurich where in 1954 he accepted the succession of Paul Niggli at the University and the ETH.

Paul Niggli's *Institut für Mineralogie und Petrographie* had been devoted essentially to the Earth Sciences, notwithstanding the phenomenal contributions of Niggli to mathematical and physical crystallography. Laves developed from this basis an interdisciplinary institute comprising scientists with extremely diverse interests ranging through all the natural sciences from mathematics to petrology, with the exception of biology, whose unifying topic was *crystallography*. The external sign of this new orientation was the modification of the name of the institute to *Institut für Kristallographie und Petrographie* (IKPETH). But what is *crystallography*? For Laves, a possible definition might have been "geometry and patterns: the spatial arrangements of atoms in all types of matter", determination, description, classification, implications of atomic patterns. Crystallography was thus the centre of all natural science, including mathematics, physics and chemistry. X-ray diffraction using all sorts of cameras from Precession to high-resolution powder methods and early hand-operated diffractometers, was of course an important tool of investigation in the IKPETH. Neutron diffraction and electron microscopy figured prominently. The first computer-driven 4-circle X-ray diffractometer was installed in the late 1960s. But spectroscopic methods such as IR, ESR, NMR-NQR were also employed. Electron

microprobe analysis was an important tool very early on. In addition, there were ovens and pressure vessels for crystal synthesis. However, structure determination for chemical analysis, which serves today as a more narrow definition of crystallography, did not play an important role; the field of chemical crystallography was developed by Jack Dunitz in the Laboratory for Organic Chemistry of ETH, and became important at the IKPETH only in the early 1970s. Graduate students like myself who graduated in the mid-1960s did not know how to determine crystal structures. Interestingly, this was hardly a disadvantage in their careers as crystallographers.

The IKPETH functioned in the spirit of classical academic freedom. Laves did not systematically control the work of his students and collaborators. They were supposed to work on their own incentive and initiative. They were always welcome, but not required, to ask for direction and help. They could follow courses or read the literature without anybody breathing down their neck to inquire about the newest publishable material. They could work whenever they liked, also at night, much to the dislike of the syndicated administrator (janitor is too lowly a word) of the building. But despite the loose reins, Laves was the uncontested master who dominated his institute with his personality and broad culture. He was a very humane and just boss, and very tactful and forgiving when confronted with blunders or incorrect behavior of his subordinates. He maintained a wonderfully humane atmosphere. Also, he worked a great deal and was in his office from early morning to late evening. The so-called support personnel was of excellent quality and contributed greatly to the success of the institute. The IKPETH of the mid-1960s was a tolerant society with remarkably little quarrel and strife. Most members assembled for the afternoon tea, and had animated discussions on about any subject. There were excursions, not only scientific ones, and parties. Surely, freedom and a good working climate can lead to at least as convincing results as increased pressure on the collaborators.

The IKPETH had a profound influence on the development of crystallography, particularly in Germany. It has been said that professorial appointments of former associates of Laves marked a wide cross over the Bundesrepublik: Bochum, Freiburg, Hannover, Karlsruhe, Konstanz, Mainz, Marburg, Munich, Münster, Regensburg. Several Laves associates made their career at ETH-Zurich and some obtained positions outside the German-speaking world. Others went to administrative or industrial jobs.

The IKPETH of the 1970s had grown to considerable size with about 100 members. There were three full professors of crystallography, a professor of petrology (before this field was separated into an independent institute) and three professors for radiometric age determination, all of them assorted with high-level permanent positions. ETH, too, had grown from a relatively small institution into a large complex organism. The evolution to the modern academic enterprise with its competition and insecure employments was well under way. Laves retired 30 years ago, and died on 12 August 1978 in his beloved house at Laiguelia. Crystallography appears to have become an endangered branch of science. A reason for this apparent decline might be the modern definition of crystallography as nearly exclusively structure determination. The legacy of Laves, however, lives on and is still of great

importance, albeit not necessarily under the name of crystallography. In this sense it is fitting that the successor institute of the IKPETH is now part of Material Science.

For more information and a list of publications of Fritz Laves, see:
H. Jagodzinski, *Z. Krist.* **133**, 2-6 (1971); E. Hellner, *Z. Krist.* **151**, 1-20 (1980).

Rückblick des ehemaligen Newsletter-Redaktors

von Hans Grimmer, Villigen (hans.grimmer@psi.ch)

Während 8 Jahren, von 1998 bis 2005, habe ich den SGK/SSCr Newsletter herausgegeben. Dabei sind die Hefte 44 bis 66 enstanden. Neben den Vereinsnachrichten erschienen wissenschaftliche Beiträge, wurden 21 Dissertationen vorgestellt, auf Kongresse und Workshops aufmerksam gemacht, sowie über deren Ergebnisse berichtet. Die Termine für Strahlzeitanträge an den Swiss-Norwegian Beamlines (SNBL) in Grenoble und den Einrichtungen am Paul Scherrer Institut (PSI) wurden in Erinnerung gerufen. Die von Helen Stöckli-Evans initiierte Reihe von Berichten über Kristallographielabors wurde ergänzt durch Beiträge über Nesper's Labor an der ETH, Bürgi's Labor in Bern, die Pharmaforschung in Basel und die Kristallzucht am PSI. Auch über neue Experimentiermöglichkeiten an SNBL, SINQ und SLS wurde regelmässig orientiert. Allen Autoren möchte ich für ihre wertvollen Beiträge nochmals bestens danken.

Anstelle der vorangegangenen Umschläge in wechselnden Farben, wählte ich hellgelb, bis mich ein Titelbild, das ohne Farben nicht zur Geltung gekommen wäre, zur Umstellung auf farbige Titelbilder veranlasste. Bei deren Auswahl versuchte ich alle kristallographischen Zentren der Schweiz im Laufe der Zeit zu berücksichtigen.

Die Mitgliederzahl betrug 1998 etwa 190, sank dann auf 155 und stabilisierte sich seit 2000 bei etwa 165 Personen. Ein Grund für die anfängliche Abnahme war der Beschluss des Vorstands, säumige Zahler auf ihre ausstehenden Jahresbeiträge aufmerksam zu machen. Es ergaben sich aber auch Umschichtungen: Am PSI z.B. verdoppelte sich die Mitgliederzahl von 8 auf 16. Das hat damit zu tun, dass das PSI für Kristallographen wichtige experimentelle Einrichtungen seit 1998 stark erweiterte: Zur Neutronenquelle SINQ kam insbesondere die neue Synchrotronstrahlungsquelle SLS hinzu.

Der Höhepunkt meiner Redaktionsjahre (und meiner drei Jahre als Präsident der SGK) war der 19. IUCr Kongress, der 2002 in Genf stattfand und von zwei Satellitenkonferenzen in der Schweiz begleitet wurde: Auf dem Rigi-Kulm war Kristallphysik das Thema, am PSI Streuexperimente mit Neutronen und Synchrotronstrahlung.

Die Herausgabe des Newsletters hat mir Spass bereitet. Ich danke für die aufmunternden Kommentare, die ich erhalten habe, und bitte um Nachsicht für die Fehler, die mir unterlaufen sind. Besonders gefreut hat mich, dass mein Kollege Jürg Schefer sich spontan bereit erklärt hat, meine Nachfolge zu übernehmen. Das vorliegende Heft ist bereits das zweite, das er mit viel Elan und neuen Ideen gestaltet hat.

Es ist mir ein Anliegen, dem PSI zu danken, das Herausgabe und Versand des Newsletters stets grosszügig unterstützt hat.

Mein Wunsch an die Leserschaft, den ich im 50. Heft äusserte, gilt weiterhin: Ich hoffe, dass Sie den Redaktor auch in Zukunft mit interessanten Beiträgen unterstützen, so dass der Newsletter ein gern gelesenes Bindeglied unter den Mitgliedern unserer Gesellschaft bleibt.

PS: Hans Grimmer geht per Ende Monat in Pension, wird aber sicherlich auch in Zukunft noch aktiv in unserem Feld weiterarbeiten. Ich möchte mich hier ganz herzlich bei ihm bedanken, im Namen der Gesellschaft und sicher auch der Mitglieder. Die offizielle Verabschiedung findet am 20. Oktober in Bern statt (siehe Seite 22). /J.S.

Section for Crystal Growth Technology (SKT)

Presently, 24 members of the SGK/SSCr have registered as members of this subsection.
It is headed by Dr. Hans J. Scheel. The finances are managed by Prof. Dr. Katharina Fromm. One of the major activities is the organization of the international Beatenberg workshops. The successful workshop 2005 was presented in our last issue.

Financial Report 2005 (Credit Suisse Account)

Status 31.12.2004	4906.30
Credits:	
SGK/SSCr contribution	600.00
Interest (minus fees)	20.65
Total Income	**620.65**
Debits:	
Artwork GmbH	350.00
Total Expenses	**350.00**
Status 31.12.2005	5176.95

High resolution neutron diffraction study of the metal-insulator transition in layered cobaltites

Published in Phys. Rev. B **73**, 1143105 (2006)

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Great controversy has arisen regarding the issue of the Co spin state and the explanation of numerous physical properties (spin state and magnetic field induced transitions [1], charge and orbital ordering) of compounds from a layered perovskite RBaCo$_2$O$_{5+\delta}$ family (R = rare earth element). All the compounds are oxygen non-stoichiometric ($0 < \delta < 1$) and the cobalt cations can adopt different oxidation and spin states. In the RBaCo$_2$O$_{5.5}$ structure cobalt cations exist in two coordination environments – pyramidal CoO$_5$ (Co2) and octahedral CoO$_6$ (Co1) in both having oxidation state 3+ (see Fig.1). Cobalt electron configuration $3d^6$ leads to a Jahn-Teller distortion of the oxygen octahedra (Pmmm space group). Compounds with $\delta \sim 0.5$ display a metal-insulator transition (MIT) accompanied by structural changes. The driving force of this transition is closely related to the Co spin state and the corresponding electronic structure.

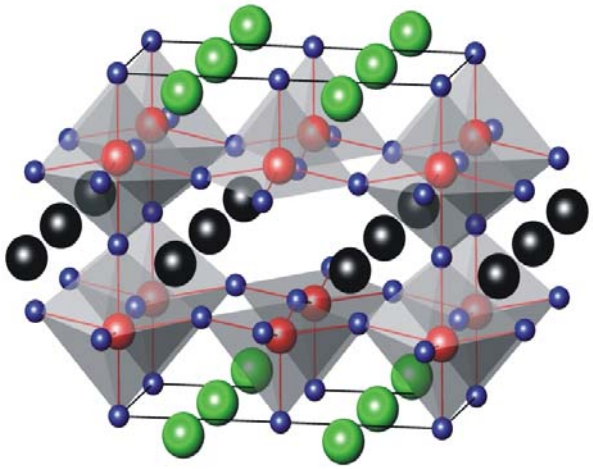

Figure 1. The crystal structure of RBaCo$_2$O$_{5.5}$ (see also cover page).

On the basis of measurements of effective magnetic moments in RBaCo$_2$O$_{5.5}$, Maignan *et al* [2] proposed a low-spin ordering (LS, S=0) in octahedral Co1 and an intermediate-spin (IS, S=1) in pyramidal Co2, below the metal-insulator transition temperature, T_{MI}. Above T_{MI} both spin states evolve towards a high-spin (HS, S=2) order. Morimoto *et al* [3] suggested for TbBaCo$_2$O$_{5.5}$, on the basis of structural investigations, that the MIT is induced by a spin state transition from $3x^2 - r^2/3y^2 - r^2$ orbital-ordered IS state below T_{MI} to the HS state above T_{MI}. Frontera *et al* [4] ruled out orbital ordering and indicated that the MIT is driven by a sudden electron excitation in the octahedral Co1 ions from LS to the HS states, while the pyramidal Co2 ions remain in the IS state. The lattice anomaly at T_{MI} was attributed to the Co1

LS-HS transition. Another model was proposed by Hua Wu [5] on the basis of electron-correlation-corrected density functional calculations for $GdBaCo_2O_{5.5}$. It has been found that the *pdσ* hole delocalisation in the 'almost high-spin' state is responsible for the MIT in $LnBaCo_2O_{5.5}$ (Ln=Sm, Eu, Gd, Tb, Dy, Y), and that the simultaneous [octahedral Co1 $3z^2 - r^2/3x^2 - y^2$ (pyramidal Co2 x^2-y^2) $\rightarrow$ Co1 (Co2) *yz*] electron transfer gives rise to the lattice anomaly at T_{MI}. Thus, a key aspect of layered cobalt perovskites, namely the spin-states of Co ions, which determine magnetic and transport properties, is not yet understood.

We have undertaken diffraction measurements of the crystal structure across the MI transition in $HoBaCo_2O_{5.5}$ [6]. Neutron powder diffraction measurements were carried out at the high-resolution HRPT diffractometer [7] at SINQ neutron spallation source (PSI, Switzerland). The high intensity mode of HRPT was used with the neutron wavelength λ=1.49 Å. The refinements of the crystal structure parameters were performed using the FULLPROF program [8].

Whereas the observed crystal symmetry was orthorhombic (*Pmmm*) in the whole investigated temperature range (250 – 400 K), the lattice constants undergo dramatic changes. With an increase in temperature both *b* and *c* parameters show sharp positive jumps of +0.7% and +0.3%, respectively at T_{MI}=305 K, at the same temperature *a* parameter drops by −0.3% and the crystal unit cell volume shows an abrupt negative drop (−0.15%) at T_{MI} (see Fig2).

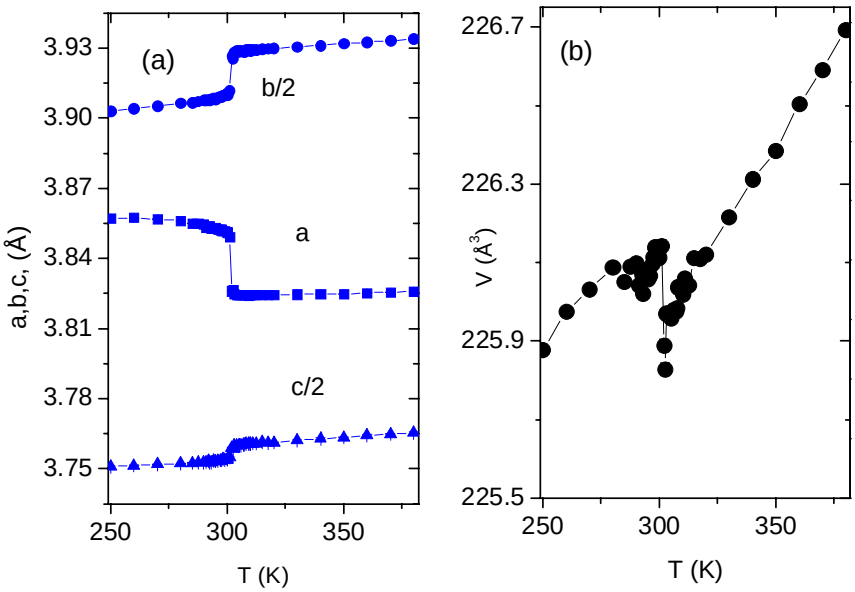

Figure 2. Temperature dependence of (a) crystal lattice constants, (b) unit cell volume.

In a narrow temperature interval (2 K) in the vicinity of T_{MI}, a coexistence of the low- and high-temperature structures has been clearly observed in the diffraction data, providing evidence for the first-order type of transition. A contraction of the unit cell volume at the insulator to metal transition is a usual feature in manganites and cobaltates, reflecting the delocalization of the charge carriers.
The temperature dependence of the bond lengths in CoO_5 pyramids is shown in Figs. 3. In the high-temperature phase all the Co2-O bond distances become equal, and

consequently the CoO_5 pyramids are regular above the transition. In contrast, in the CoO_6 octahedra the bond distances along the *c* direction become different in the high- temperature phase, whereas in-plane bond lengths are almost unaffected by the transition. These results suggest an orbital ordering (OO) in the *ab*-plane below T_{MI}. The bond lengths in the *ab* plane are significantly different, implying that the $d_{3x^2-r^2}$ orbitals are ordered similarly, as has been proposed [3]. The OO expands over all Co ions in both octahedral (Co1) and pyramidal (Co2) surroundings, i.e., the longest bond length Co1-O6 matches the shortest Co2-O6. Above T_{MI} the OO in the pyramids completely disappears. The OO transition can originate from the delocalization of the electrons on the pseudocubic e_g orbitals in the one dimensional Co2 pyramid network. Both angles φ (between octahedra Co1-O5-Co1 and between pyramids Co2-O4-Co2) are increased at the transition temperature (Fig.4), implying that the electron transfer integral through Co-O-Co, which is proportional to $cos(\pi-\varphi)$, has a step like increase, suggesting that the electron delocalization occurs in all directions. The results of our studies qualitatively support the models in which the observed MI transition is associated to charge delocalization rather than the spin-state transition of the Co2 ions in pyramids.

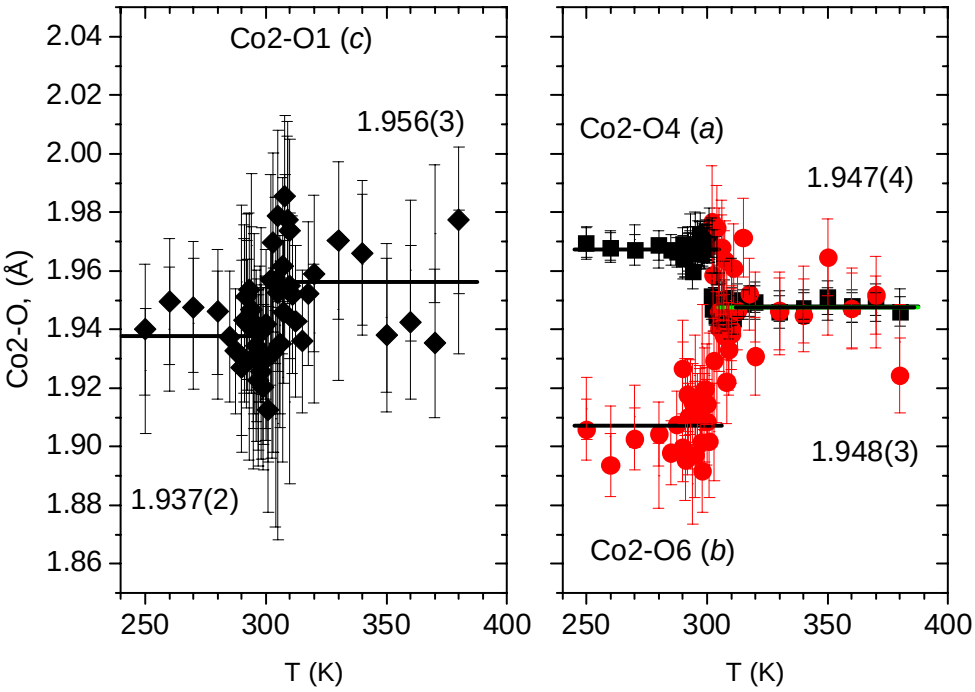

Figure 3. Temperature dependence of Co2-O bond lengths in CoO5 pyramids: Co2-O1 (*c*), Co2-O4 (*a*), Co2-O6 (*b*). The letters *a*,*b*,*c* indicate the approximate direction of the bonds with respect to the crystal axes. Lines are the linear fits above and below the transition with the refined values of the bond lengths indicated.

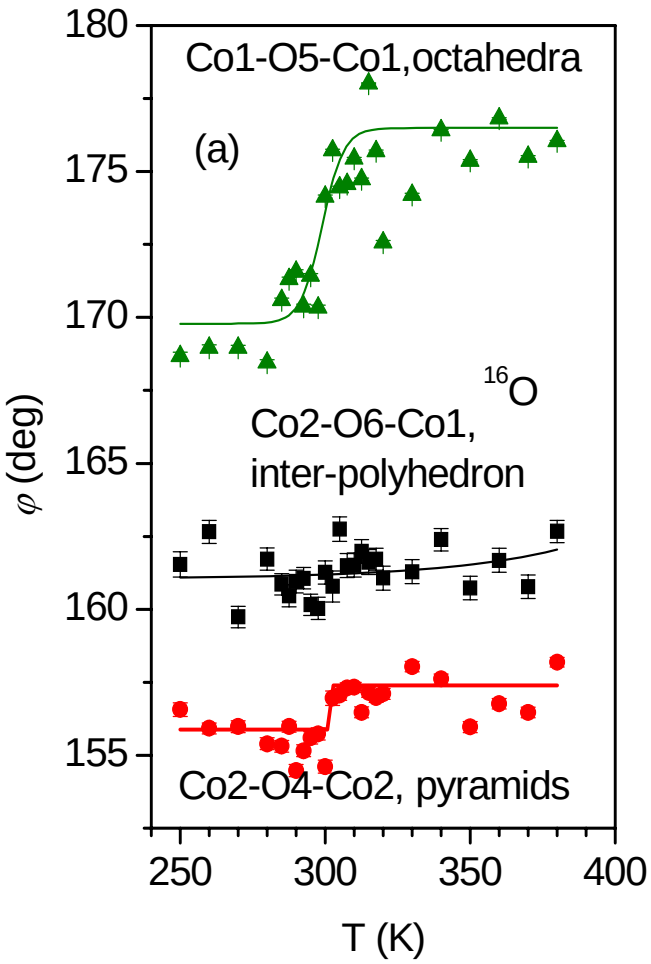

Figure 4. Temperature dependence of the angles φ between octahedral (Co1-O5-Co1), pyramids (Co2-O4-Co2), and interpolyhedron (Co2-O6-Co1).

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New PhD Thesis Work

We present here summaries of recent thesis work, which has been accepted in the area of crystallography.

Sergiy Katrych

Laboratory for Crystallography, ETH Zurich, PhD Thesis No. 16559

X-ray diffraction study of quasicrystals and related phases in the systems Al–Co–Ni and Al–Ir–Os.

Quasicrystals are the most complex intermetallic phases known. They are constituted of clusters that are packed in a quasiperiodic way. Even after more than twenty years of research little is known about the factors governing their formation and stability. To improve our understanding, still much more information on phase relations of quasicrystals and periodic crystals is needed. Besides thermodynamic information, i.e. the study of mostly ternary phase diagrams, information on atomic scale is needed. This means, structure and structural ordering of quasicrystals has to be investigated as function of chemical composition, temperature and pressure. Approximants, periodic crystals with structures constituted of similar clusters as the quasicrystals with similar chemical composition, can give the key to the understanding of the quasiperiodic structures.

In the present thesis, the focus is on two systems that contain decagonal phases, i.e. quasicrystals with diffraction symmetry 10/*mmm*. The first system, Al-Co-Ni is the model system *par excellence*. Its decagonal phase has very broad stability range with numerous different modifications as function of the Co/Ni ratio. There are also several approximants known in this system. The second system, Al-Ir-Os, has been largely unknown. Due to the existence of approximants in the binary systems, Al-Ir and Al-Os, the ternary system should be studied around to the stability field of the expected decagonal phase. The main interest was finding a quasicrystal with high melting temperature.

The first part of the thesis presents the results of the x-ray diffraction study of decagonal **Al–Co–Ni (D-phase)** as a function of chemical composition, temperature and pressure. It reports also structural investigations of two ternary phases, the X- and the W-phase, coexisting with the D-phase in equilibrium.

In an extended single-crystal x-ray diffraction investigation samples of decagonal Al–Co–Ni, annealed at 900ºC, were studied in its stability range with steps of 0.5 at. % Co/Ni ($Al_{71.5}Co_{28.5-x}Ni_x$ ($8 \leq x \leq 20$). The substitution of Co by Ni causes complex structural ordering phenomena. At 900ºC five distinct ordering states have been identified, the basic Co-rich and the basic Ni-rich phase, the superstructure type I (S1 + S2) and (S1) as well as the superstructure type II. The detailed composition dependence, $a(x_{Ni})$, of the (quasi)lattice parameters of decagonal Al–Co–Ni across its stability field has been evaluated. It can be described by the linear function $a\,(x_{Ni}) =$

3.8435 – 0.406x_{Ni} Å. The parabolic composition dependence along the tenfold axis, $d(x_{Ni})$, follows a polynomial of second order $d(x_{Ni}) = 3.9943 + 1.113x_{Ni} – 3.2773x_{Ni}^2$ Å.

An *in-situ* high-temperature (at 860ºC and 975 ºC) single-crystal x-ray diffraction data study of basic Co-rich decagonal Al–Co–Ni shows the transition of its modification into another ordering state. The Bragg-like sharp diffuse layers of the basic Co-rich quasicrystal become more diffuse at 975 ºC. This means that the correlation length of the columnar clusters building decagonal Al–Co–Ni decreases with increasing temperature. Dilatometric measurements were performed in the range from 50ºC to 600 ºC on single D-phase samples with compositions $Al_{71.5}Co_{15}Ni_{13.5}$ and $Al_{71.5}Co_{14}Ni_{14.5}$. At 315ºC, the almost linear dilatometer curve slightly changes its slope indicating a structural reordering.

An *in-situ* high-pressure x-ray diffraction study of decagonal basic Ni-rich Al–Co–Ni at 8.51, 16.0 and 20.85 GPa has been performed using diamond anvil cell and synchrotron radiation. No significant variations of the diffraction patterns with pressure were observed indicating a high stability of this quasiperiodic structure in the investigated pressure range.

The stability range of the ternary W-phase in the Al–Co–Ni system was studied at 900ºC and 1000ºC by x-ray diffraction, DTA and metallography. It is found quite narrow at 900ºC, $Al_{72}Co_{19-20}Ni_{7-8}$. At 1000ºC, the stability field of the W-phase becomes larger, $Al_{71-72}Co_{19.8-20.5}Ni_{7.5-8.7}$. Isothermal sections at 800ºC, 900ºC and 1000ºC close to the stability field of the W-phase were constructed. It resulted that at 900ºC and 1000ºC the W-phase is in equilibrium with three neighboring phases, decagonal Al–Co–Ni, X-phase and $Al_5(Co, Ni)_2$. The high-temperature W-phase is not found below 800ºC. It forms at ~900ºC by the ternary eutectoidal reaction

$$X + D + (Co,Ni)_2Al_5 <=> W$$

A structure analysis of the W-phase was performed based on single crystal x-ray diffraction data. Its symmetry can be described by the monoclinic space group *Cm* (No. 8) with lattice parameters a = 39.668(8) Å, b = 8.1580(16) Å, c = 23.393(5) Å, β = 90.10(3)º, Pearson symbol *mS*534-24. Its four-layer structure is closely related to the four-layer structure of basic Co-rich decagonal Al–Co–Ni.

The structure of the previously unknown ternary X-phase, $Al_9(Co,Ni)_4$, was solved. It is representative of a new structure type with Pearson symbol *mS*26, lattice parameters a = 12.146(2) Å, b = 4.0702(5) Å, c = 7.652(1) Å, β= 105.88(1) º, V = 363.83(9) Å^3, and space group *C*2/*m* (No.12). This phase may be considered as a continuation of the two-layer decagonal phase at its lowest possible Al concentration towards lower Ni contents.

The second part of the thesis is devoted to the phase relations in the ternary **Al–Ir–Os system** as well as to the structure analyses of the newly discovered **decagonal phase** and one of its approximants.

A new binary phase, Ir_9Al_{28} phase was discovered and its complex crystal structure determined by single-crystal x-ray diffraction. It is the first representative of a new structure type with Pearson symbol *hP*236-14, a = b = 12.2864(4) Å, c = 27.341(1)

Å, γ = 120 º, space group *P*31*c* (No. 159). The crystal structure can be described likewise as stacking of eight puckered and flat layers with sequence ...$P^0PFpp^0p^jF^jP^j$...along [0 0 1], as a six-layer stacking sequence along [1 0 0], or as packing of pseudo-Mackay icosahedra.

The new decagonal quasicrystal with composition ~$Al_{73}Ir_{14.5}Os_{12.5}$ has been found stable up to a temperature of at least 1283 ºC. At 800ºC, it grew in equilibrium with Al-rich melt. A first structure model of decagonal Al–Ir–Os (with 16.819(4) Å translation period along the 10-fold rotations) was obtained by two different methods, the pseudo-approximant method and the 5D charge-flipping method. The pseudo-approximant method applies a linear phason strain to the 5D reciprocal space of the decagonal phase in order to obtain a rational approximant. The approximant structure then is solved by conventional crystallographic techniques such as direct methods. The 5D charge-flipping method assigns random phases to the experimentally observed structure amplitudes. Then they are Fourier transformed and the negative electron densities flipped to positive ones. New structure factors are obtained by Fourier transformation and the whole procedure is repeated again and again. Both techniques gave the same results for the local cluster. Its structure can be described as a periodic stacking of eight almost equidistant atomic layers *ABCDA'B'C'D'* with an average interlayer distance of ~2.1 Å.

The phase relations of the ternary Al–Ir–Os system were studied for the first time. The solidification pathway of Al(Ir,Os)–Ir–Os alloys indicate the β-phase, (Ir) and (Os) as primary. The isothermal section at 1400ºC of the Al(Ir,Os)–Ir–Os system shows a large mutual solid solubility of the components: ~ 18.5 at.% Al and ~40 at.% Ir in (Os), ~ 28 at.% Al and ~22 at.% Os in (Ir), ~ 48 at.% Al in the continuous β-solid solution. The isothermal section at 1250ºC in the β–Al_2Os–$Al_{2.7}Ir$ phase field also illustrates the large solid solubility of the third components in the β, Al_2Os and $Al_{2.7}Ir$ phases: ~ 54 at. % Al, ~ 8 at.% Ir, ~10.5 - 14 at.% Os respectively.

The thesis starts with an introduction into the field of quasicrystals. The following two parts, on the systems Al-Co-Ni and Al-Ir-Os, respectively, contain two publications each. Additional information is given in appendices to each publication.

News for and from Members

We welcome the following new members of the SGK/SSCr:

Dr. Denis Cheptiakov (Laboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institut, WHGA-133, CH-5232 Villigen PSI)

Dr. Dmitry Chernyshov (Swiss Norwegian Beam Lines, SNBL at the ESRF, FR 38043 Grenoble Cedex, France)

Nouar Bensemma (Nuclear Techniques Application Institution, Nuclear Research Center of Birine, Djelfa, Algeria)

Travel Grants for Young SGK/SSCr Members

The committee will award the grants according to the following rules:

- Preference is given to PhD students
- Proof has to be given that there are no grants available covering the expenses
- A supporting letter by the supervisor of the applicant is necessary

If you whish to apply for a travel grant, please send the above mentioned documents to the president of the SGK/SSCr anytime.

At the last board meeting, such a grant was provided to Jean-Nöel Chotard from the university of Geneva to support his participation at the MH2006 – International Symposium on Metal-Hydrogen Systems - in Hawaii. A report of his conference contribution will follow in the next issue of our newsletter.

Missing Addresses of SGK/SSCr Members

We have problems to contact the following members (last known affiliation in brackets):

Dr. O. Crottaz (1227 Carouge)
Dr. Petra Simoncic (Bern)
J.D . Bochud (Comadur Ltd. , 1784 Courtepin)

If the new address is known to you, please send an E-mail or FAX to the editor.

New Books

Arthur Schoenflies: Mathematiker und Kristallforscher. Eine Biographie mit Aufstieg und Zerstreuung einer jüdischen Familie

by Thomas Kaemmel
ISBN: 3866341091, Publishing date: June 2006, Language: German, 159 pages

Arthur Schoenflies lived from 1853 to 1928 and has shaped the development of mathematics of his time. He stimulated it's practical implementation in engineers training. His mathematical systematisation of all possible symmetries of crystal forms opened the way for a breakthrough in the research and application of crystals and molecules in geo- and material sciences after Laue's discovery of x-ray interferences 1912.
In the book it becomes apparent how strongly he was integrated into the scientific and social networks of his time. The inclusion of the history of his Jewish family since 1700, from which also Walter Benjamin and Gertrud Kolmar have descended, conveys a naturalistic insight into the many challenges and tragic fates of the family that was scattered over the whole world. Schoenflies is appreciated as a teacher, researcher and manager of science. Especially his achievements in crystallography and mineralogy are emphasised. A very comprehensive list of literature and many original documents complete the book.

(contribution of Wilko Müller, DE-Halle, wilkomueller@web.de)

Used Diffraction Equipment

We are offering here old equipment which may be of interest for our community. If you have X-ray or neutron diffraction related equipment in a reasonable condition which is preferably in operating condition or at least may be used as spare parts, please send a note with all the relevant information to the editor.

Equipment	Offered by	Contact
Presently, no equipment is advertised here.	--	--

EPDIC-10, September 1-4, 2006, Geneva

The **European Powder Diffraction Conference (EPDIC)** is the only European conference completely dedicated to all aspects of the analysis of polycrystalline materials by diffraction methods. Started in Munich in 1991, **EPDIC**s have rapidly become reference points for all researchers in the field, and are now ideal places for the presentation and diffusion of new developments in powder diffraction instrumentation, analysis, and applications

Invited Speakers
Simon Billinge, *Michigan University*
Olivier Thomas, *Université Paul Cezanne*
Andreas Leineweber, *MPI Stuttgart*
Irene Margiolaki, *ESRF*
Vitalij K. Pecharsky, *AMES*
Winfried Kockelmann, *ISIS*

Contact
Radovan Cerny
Phone : [+[41] 22] 37 964 50
University of Geneva
Radovan.Cerny@cryst.unige.ch

Workshops (August 31 – September 1)
Powder Diffraction Software Workshop 'Under the Bonnet'
Pharmaceutical Applications of Powder Diffraction
Nano-materials and Powder Diffraction
ICDD Workshop

Methods, techniques

- structure solution and refinement
- indexing powder patterns
- line profile analysis
- stress, strain and texture
- phase analysis
- instrumentation
- non-ambient conditions
- phase transitions
- fiber diffraction
- software, databases
- hard X-rays, neutrons, electrons
- reflectivity, grazing incidence
- small-angle scattering

Applications in

- materials science
- biology
- pharmaceutical research
- chemistry
- physics
- industry

Materials

- organic materials
- polymers
- inorganic materials
- minerals
- disordered structures
- thin films and multilayers
- metals and alloys
- intermetallic compounds
- magnetic materials
- ferroelectric materials
- energy storage materials
- ionic conductors
- nano-materials
- composites
- ceramics
- catalysts
- amorphous materials, glasses

EPDIC-10 Microsymposia

MS 1 TOTAL SCATTERING ANALYSIS
Chairpersons : Thomas Proffen (LANL Los Alamos), Simon Billinge (Uni Michigan)

MS 2 STRUCTURE DETERMINATION FROM A SINGLE POWDER DIFFRACTION PATTERN
Chairpersons : Arnt Kern (Bruker AXS), Anton Meden (Uni Ljubljana)

MS 3 POWDER DIFFRACTION AND BIO-MATERIALS
Chairpersons : Bob von Dreele (Argonne National Laboratory), Marc Schiltz (EPFL)

MS 4 COMBINING POWDER DIFFRACTION WITH OTHER METHODS
Chairpersons : Lynne McCusker (ETHZ), Christian Baerlocher (ETHZ)

MS 5 ENERGY STORAGE MATERIALS
Chairpersons : Klaus Yvon (Uni Geneva), Torbjorn Gustaffson (Uni Uppsala)

MS 6 INSTRUMENTATION
Chairpersons : Andrea Lausi (ELETTRA), Steve Hull (ISIS)

MS 7 STRESS AND TEXTURE ANALYSIS
Chairpersons : Udo Welzel (Max Planck Institute Stuttgart), Matteo Leoni (Uni Trento)

MS 8 STRUCTURE DETERMINATION FROM MULTIPLE POWDER DIFFRACTION PATTERNS
Chairpersons : Bill David (ISIS), Jordi Rius (CSIC Barcelona)

MS 9 VALIDATING STRUCTURES
Chairpersons : Lachlan Cranswick (Canadian Neutron Beam Centre), Peter Zavalij (University of Maryland)

MS 10 ANALYSIS IN CULTURAL HERITAGE AND FORENSIC SCIENCES
Chairpersons : Eric Dooryhee (ESRF), Gilberto Artioli (Uni Milano)

MS 11 DIFFRACTION ANALYSIS OF THE MICROSTRUCTURE OF MATERIALS
Chairpersons : Paolo Scardi (Uni Trento), Nathalie Audebrand (Uni Rennes)

MS 12 NON AMBIENT CONDITIONS: PHASE TRANSITIONS/TRANSFORMATIONS
Chairpersons : Andrew Fitch (ESRF), Robert Dinnebier (Max Planck Institute Stuttgart)

MS 13 INDEXING
Chairpersons : Lachlan Cranswick (Canadian Neutron Beam Centre), Christian Lengauer (Uni Vienna)

MS 14 THIN FILMS, COATINGS AND SURFACES
Chairpersons : Radomir Kuzel (Uni Prague), René Guinebretiere (ENSCI Limoges)

MS15 NEUTRON DIFFRACTION
Chairpersons : Vladmir Pomjakushin (LNS, ETHZ&PSI, Villigen), Juan Rodriguez-Carvajal (ILL Grenoble)

MS 16 POWDER DIFFRACTION IN APPLIED RESEARCH
Chairpersons: Daniel Louër (Rennes), Rob Delhez (TU Delft)

EPDIC-10

European Powder Diffraction Conference Geneva September 1 - 4, 2006

UNIVERSITÉ DE GENÈVE

Swiss Society for Crystallography

The **European Powder Diffraction Conference (EPDIC)** is the only European conference completely dedicated to all aspects of the analysis of polycrystalline materials by diffraction methods. Started in Munich in 1991, **EPDIC**s have rapidly become reference points for all researchers in the field, and are now ideal places for the presentation and diffusion of new developments in powder diffraction instrumentation, analysis, and applications.

Invited Speakers
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Vitalij K. Pecharsky, *AMES*
Winfried Kockelmann, *ISIS*

Microsymposia
16 microsymposia on methods and applications of powder diffraction

Workshops (August 31 – September 1)
Powder Diffraction Software Workshop 'Under the Bonnet'
Pharmaceutical Applications of Powder Diffraction
Nano-materials and Powder Diffraction
ICDD Workshop

Conference venue
Uni Mail, University of Geneva

Contact
Radovan Cerny
University of Geneva
Phone : [+[41] 22] 379 6450
Radovan.Cerny@cryst.unige.ch

Methods, techniques
- structure solution and refinement
- indexing powder patterns
- line profile analysis
- stress, strain and texture
- phase analysis
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- non-ambient conditions
- phase transitions
- fibre diffraction
- software, databases
- hard X-rays, neutrons, electrons
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- small-angle scattering

Applications in
- materials science
- biology
- pharmaceutical research
- chemistry
- physics
- industry

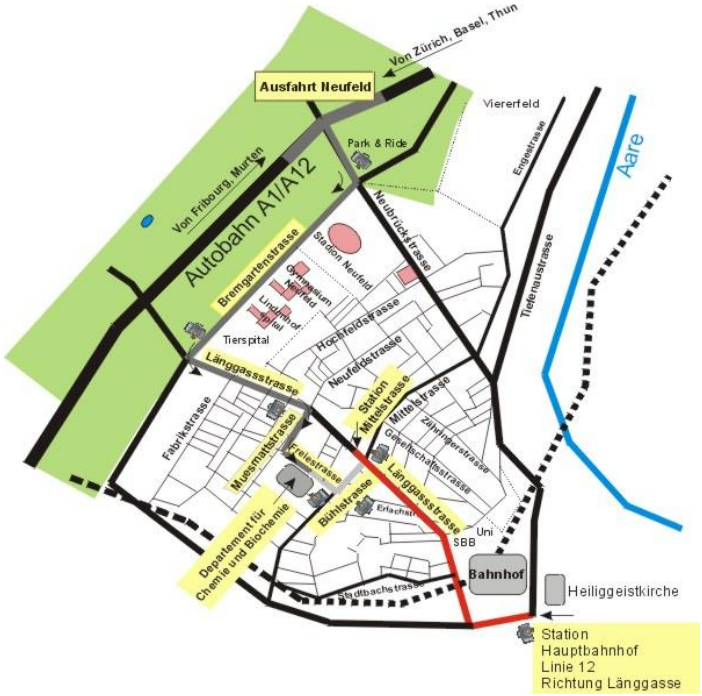
Materials
- organic materials
- polymers
- inorganic materials
- minerals
- disordered structures
- thin films and multilayers
- metals and alloys
- intermetallic compounds
- magnetic materials
- ferroelectric materials
- energy storage materials
- ionic conductors
- nano-materials
- composites
- ceramics
- catalysts
- amorphous materials, glasses

www.sgk-sscr.ch/EPDIC10

Annual Meeting of the SGK/SSCr in Berne, October 20

Topic: Expanding the boundaries
Crystallography in the gas phase, on surfaces, in picoseconds

The annual meeting 2006 will be held in Bern on the occasion of the retirement of Prof. H.-B. Bürgi, Laboratory for Chemical and Mineralogical Crystallography. The meeting will start on **October 20, 2006 at 9^{45}** at the **Departement für Chemie und Biochemie, Freiestrasse 3, 3012 Berne.**



The program is given on the next page.

A poster session will take place during the lunch break. The authors of the best four posters with **abstracts submitted before the meeting** will be invited to give five-minute **'appetizer-presentations'** immediately before the lunch break.

Deadlines:	Poster Submission:	**15.9.2006 (*)**
	Registration for participation:	no registration required
	Conference-dinner (Friday evening)	Please apply to our secretary, margrit.huegli@krist.unibe.ch

Organizing committee: hans-beat.buergi@krist.unibe.ch

(*) Posters (format A0 portrait) on any crystallographic subject may be presented during the meeting.
Contributors are kindly asked to send their **abstracts** as a word file to hans-beat.buergi@krist.unibe.ch with a copy to radovan.cerny@cryst.unige.ch and jurg.schefer@psi.ch **no later than Sept. 15, 2006**

Detailed meeting information:
http://www.sgk-sscr.ch/SSC_meeting/ssc_meeting_bern06/

Program Annual Meeting of the SGK/SSCr in Berne, October 20, 2006

09h45 – 09h50	**Welcome by the President Walter Steurer**
09h50 – 10h35	**Michael Wulff**, ESRF, Genoble (F), "Molecular dynamics studied by single-pulse X-ray diffraction"
10h35 – 10h45	Discussion
10h45 – 11h00	Coffee break / Poster session
11h00 – 11h45	**Samuel Leutwyler**, University of Bern, "Hydrogen Bonding and π-Stacking, a Gas Phase Perspective"
11h45 – 11h55	Discussion
11h55 – 12h15	**'Appetizer Presentations'** to the Poster Session: (oral, 5 Min. each)
12h15 – 13h30	**Lunch at the Posters**, Sandwiches and Soft Drinks provided
13h30 – 14h15	**Roman Fasel**, EMPA, Dübendorf, "Expressions of chirality upon two-dimensional crystallization"
14h15 – 14h25	Discussion
14h25 – 14h55	**Vladimir Dmitriev**, Swiss Norwegian Beam Lines: "Scientific highlights from SNBL and other important developments", Information by the Swiss Steering Committee of the SNBL
14h55 – 15h25	**Bruce Patterson**, SLS, **Jürg Schefer**, SINQ "Scientific highlights from SLS and SINQ"
15h25 – 15h45	Coffee break / Poster session
15h45 – 16h30	**Nenad Ban**, ETH, Zürich, "Crystallographic studies of fatty acid synthases: supersize enzymes"
16h30 – 16h40	Discussion
16h45 – 17h45	**General Assembly** of the SGK/SSC
18h00	**Apero followed by Dinner** at a Restaurant close to the train station. Hans Grimmer, former president of the SGK/SSCr, will be our invited guest on the occasion of his retirement.

Call 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	March 15, Nov. 15	user.web.psi.ch
Protein beam lines (PX)	Feb. 15, June 15, Oct. 15	user.web.psi.ch
SINQ: Swiss Spallation Neutron Source		
All instruments except irradiation	May 15, Nov. 15	user.web.psi.ch
SμS: Swiss Muon Source		
All instruments	Dec. 5	user.web.psi.ch
ESRF: European Synchrotron		
All instruments, long term proposals	Jan. 15	www.esrf.fr
All instruments, short term proposals	March 1, Sept. 1	www.esrf.fr
SNBL: Swiss Norwegian Beam Line		
	March 1, Sept. 1	www.esrf.fr/ exp_facilities/BM1A
ILL: Institut Laue Langevin		
All instruments	Sept. 19, 2006	www.ill.fr
FRM-II		
All instruments	Aug. 11, 2006	user.frm2.tum.de

Outstanding Member Fees

If your membership account balance on the back side of the mailing letter **is not stating zero** (status June 2, 2006), we remind you to pay the full amount as soon as possible by bank transfer to the UBS account: IBAN CH39 0027 9279 C029 1110 0 (old system: BLZ 279, account No. C0291110.0)
Please add CHF 1.20 if paid at a PTT counter (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0). **Empty forms are available at any PTT counter** (We apologize for not attaching them anymore. Printing costs are considerably high).

Calendar of Forthcoming Meetings

Date	Location	Meeting / Link	Abstract Deadline
2006			
July 22-27	Honolulu USA	ACA, American Crystallographic Association http://www.xray.chem.ufl.edu/aca2006	expired
Aug. 6-11	Leuven Belgium	ECM 23 European Crystallographic Meeting http://www.ecm23.be	expired
Aug. 19-26	Zuoz CH	5th PSI Summer School on Condensed Matter Neutrons, X-rays and Muons for Nanostructures http://num.web.psi.ch/zuoz2006	open
Aug. 27 - Sept. 2	Siena Italy	IUCr School on Basic Crystallography http://www.iucr.org/iucrtop/comm/cteach/siena2006/	expired
Aug. 28 - Sept. 2	Nancy France	Summer School: Analyse structurale par diffraction des rayon X, cristallographie sous perturbation	
Aug. 30 - Sept. 1	Geneva CH	EPDIC-10 Workshops: – Powder Diffraction Software Workshop 'Under the Bonnet' – Pharmaceutical Applications of Powder Diffraction – Nano-materials and Powder Diffraction – ICDD Workshop	
Sept 1-4	Geneva CH	EPDIC 10 : European Powder Diffraction Conference http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html	expired
Sept. 11-13	Bristol GB	EMPG XI: mineralogy, petrology and geochemistry http://www.empg2006.org	expired
Sept. 8 – Oct. 1	Dubna Russia	Crystallography at High Pressures http://nfdfn.jinr.ru/~denk/crhp06/main.htm	June 30, 2006
Sept. 28-29	Villigen CH	7th SLS User Meeting http://sls.web.psi.ch/view.php/users/affairs/umeetings/Umee2006/index.html	to be announced
Oct. 4-6	Hamburg Germany	Synchrotronstrahlung, Neutronen und Ionenstrahlen an Grossgeräten 2006, http://www.sni2006.de	expired
Oct. 20	Bern CH	SKG/SCCR annual meeting, Freiestr. 3 http://www.sgk-sscr.ch	**Sept. 15, 2006**
Nov. 27- Dec. 1	Boston USA	MRS Fall Meeting, http://www.mrs.org/s_mrs/sec_mtgdetail.asp?CID=6073&DID=167209	June 20, 2006
2007			
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	Nov. 30, 2006
July 21-26	Salt Lake City, USA	Annual Meeting of the American Crystallographic Society www.hwi.buffalo.edu/ACA	to be announced
August 13-17	Manchester UK	9th Int'l Conference on Biology and Synchrotron Radiation www.srs.ac.uk/bsr2007	March 31, 2007
Aug. 22-27	Marrakech Marocco	ECM-24: European Crystallographic Meeting http://www.ecm24.org.	to be announced
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	to be announced
June 25-29	Lund Sweden	4th European Conference on Neutron Scattering http://www.ecns2007.org	to be announced

2008

May	Gargnano Italy	Summer School on Mathematical and Theoretical Crystallography, http://www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm	to be announced
May 18-25	Beatenberg CH	IWCGT-4 Fourth International Workshop on Crystal Growth Technology http://www.beatenberg.ch/IWCGT-4	to be announced
May 31 – June 5	Knoxville USA	Annual Meeting of the American Crystallographic Society www.hwi.buffalo.edu/ACA	to be announced

For deadlines such as conference registration,
please contact the corresponding web-pages

Become a Member of SGK/SSCr

If your are working in the field of crystallography, you will be interested to become a member of our society. Please have a look on our website (http://www.sgk-sscr.ch) for more information as well as online registration. Presently, the yearly membership fee is sfr. 30 (sfr. 10 for students). For new members, the membership until the end of 2006 is free. Please note: SGK/SSCr members can also apply to be a member of the subsection crystal growth at no additional charge.
SGK/SSCr is a member of the Swiss Academy of Science.

Name	
Given name	
Title	
Institution	
Street	
Box/building	
ZIP Code	
Town	
Country	
Phone office	**+ ( )**
Fax office	**+ ( )**
Phone private	**+ ( )**
Mobile phone	**+ ( )**
E-Mail	**@**
Interest	
Membership subsection crystal growth	**Yes ( ) No ( )**
Birth date	**Day: Month: Year:**
Language(s)	
Major research interests	
Highest degree received	
from university	
Present position	

Date: …….. Place: ……..

Signature: ……

FAX **the completed form to: Dr. Radovan Cerny,** +41 (0) 22 37 961 08
or use our online application form **at** http://www.sgk-sscr.ch

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

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SGK/SSCr Newsletter

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Commercial advertisements of material of interest to members of the SGK/SSCr are welcome. Please contact the treasurer for details of the advertisement rates.