

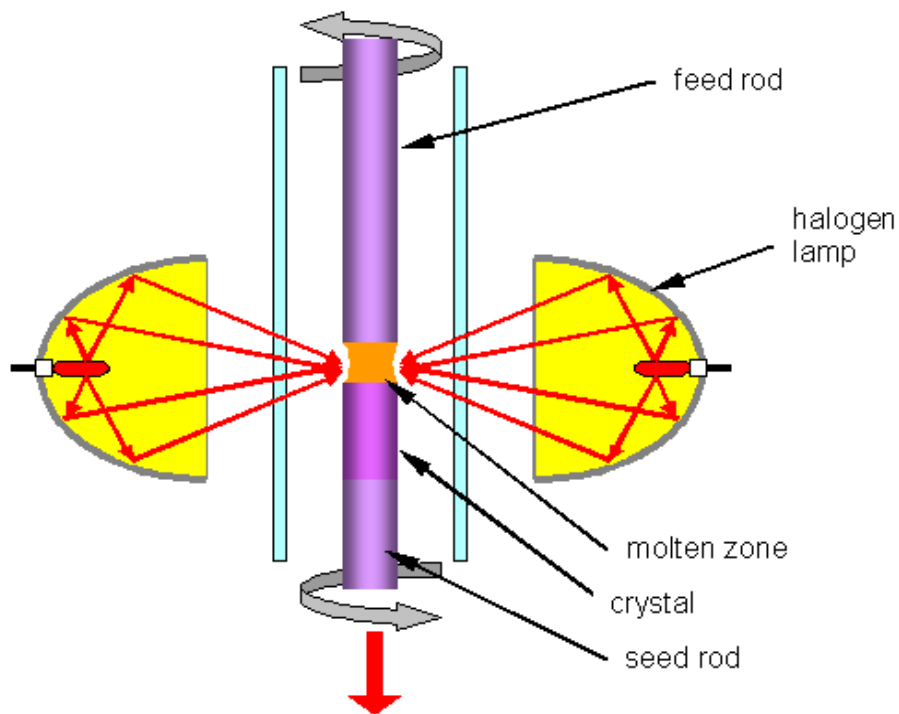


Schweizerische Gesellschaft für Kristallographie  
Société Suisse de Cristallographie

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

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the Swiss Academy of Sciences



SGK/SSCr NEWSLETTER

**No. 65**  
July 2005

# SGK/SSCr Newsletter No. 65

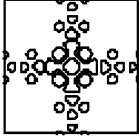
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Operation principle of a mirror furnace for crystal growth by the Travelling Solvent Floating Zone method. See also the article on p. 7 f.



*SGK/SSCr*  
SKT/SCT

*Swiss Society for Crystallography*  
Section for Crystal Growth and Crystal Technology

# **Annual Meeting 2005**

Thursday, October 13

Auditoire 410, Collège propédeutique 2,  
Université de Lausanne, Dorigny

**Lausanne**

*General Theme*

**Crystallography and Physics**

## Programme

### Thursday, the 13th October 2005

Lecture room :     Auditoire 410, Collège propédeutique 2,  
                           Université de Lausanne, Dorigny, 1015 Lausanne

09h25 – 09h30	<b>Welcome by the President Radovan Cerny, and the local organisers Gervais Chapuis and Marc Schiltz</b>
09h30 – 10h20	Edgar Weckert, DESY, Hamburg « The new radiation sources, PETRA III and the European XFEL at DESY »
10h20 – 11h10	Andras Sütö, Hungarian Academy of Science, Budapest « Ab initio structure determination by charge flipping »
11h10 – 11h50	<b>Coffee break / Poster session</b>
11h50 – 12h10	Contribution from the University of Geneva
12h10 – 12h30	Contribution from the EPFL
12h30 – 14h00	<b>Lunch / Coffee / Poster session</b>
14h00 – 14h50	Jean-Louis Hodeau, CNRS Grenoble « Resonant diffraction »
14h50 – 15h40	Franz Pfeifer (PSI, Würenlingen) « Coherent x-ray diffraction »
15h40 – 16h00	Selected poster presentation
16h00 – 16h40	<b>Coffee break / Poster session</b>
16h40 – 17h00	Contribution from the ETHZ
17h00 – 18h00	<b>General Assembly of the Swiss Society for Crystallography</b>
18h00 – 18h20	<b>Information of the Swiss Steering Committee of the SNBL</b>
From 18h30	<b>Apero followed by Dinner at the Restaurant de Dorigny</b>

## ***Call for Posters***

Posters on any crystallographic subject may be presented during the meeting. Contributors are kindly asked to send their abstracts by e-mail to

Radovan.Cerny@cryst.unige.ch,

Hans.Grimmer@psi.ch,

Gervais.Chapuis@epfl.ch

and  
until

**August 31, 2005.**

The abstracts will be made available under the address

<http://www.sgk-sscr.ch/>

and will be included in the next issue of the SGK/SSCr Newsletter, which will appear in September.

## **Travel Grants for Young SGK/SSCr Members**

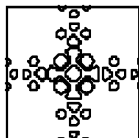
The Swiss Academy of Sciences ([www.scnat.ch](http://www.scnat.ch)) puts this year SFr. 1300.- (of which 300.- have been transferred from last year and 1000.- are new) at the disposal of our society to support the attendance of younger members at international meetings.

After the discussion we had on our last annual meeting, the committee of the SGK/SSCr decided that also post-docs may receive travel grants. The recipients should, however, not be supported by the Swiss National Science Foundation, because its contracts allow for travel expenses.

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

- Preference is given to students and 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.
- The candidate has to prove that he will present an accepted contribution.

If you wish to apply for a travel grant, please, send the above mentioned documents to the President of the SGK/SSCr (Radovan.Cerny@cryst.unige.ch) before October 1, 2005. The successful candidates will be informed on the annual meeting of the SGK/SSCr.



**SGK/SSCr Swiss Society for Crystallography**

**SKT/SCT**

Section for Crystal Growth and Crystal Technology

## **General Assembly 2005**

Thursday, October 13 at 17h00

### **Proposed Agenda**

1. Minutes of the Annual General Assembly in Neuchâtel on October 6, 2004  
(published in SGK/SSCr Newsletter 64)
2. Report from SGK/SSCr
  - Report of the President (R. Cerny)
  - Report of the Treasurer for 2004 (M. Hennig)  
(cf. SGK/SSCr Newsletter 64)
  - Report of the Auditors for 2004 (Ch. Bärlocher / K. Schenk)
  - Preliminary report of the Treasurer for 2005 (M. Hennig)
  - Presentation of the Budget 2006, Membership fee 2006 (M. Hennig)
3. Report from SKT/SCT
  - Report of the Section head (H. Scheel)
  - Report of the Treasurer for 2004 (K. Fromm)  
(cf. SGK/SSCr Newsletter 64)
  - Report of the Auditor for 2004
  - Preliminary report of the Treasurer for 2005 (K. Fromm)
  - Presentation of the Budget 2006 (K. Fromm)
4. Report of the delegates to the IUCr General Assembly (H. Grimmer / R. Cerny)
5. Report of the delegate to the ECA Council Meeting (H. Stoeckli-Evans)
6. Award of travel grants (R. Cerny)
7. International conferences in Switzerland related to crystallography (R. Cerny)
8. Election of the committee and the president of the SSCr for 2006-2008
9. Election of the delegate to the Senate of the Swiss Academy of Sciences and of his proxy
10. Election of the auditors
11. Next annual meeting of the SGK/SSCr (new President)
12. Varia

Suggestions for changes of the agenda are requested to the president of SGK/SSCr ([president@sgk-sscr.ch](mailto:president@sgk-sscr.ch)) until August 31, 2005.

## News of Members

### We welcome the following new member of the SGK/SSCr:

**Kazimierz Conder** (Labor für Entwicklung und Methoden, Festkörperforschung mit Neutronen und Myonen, Paul Scherrer Institut, Villigen)

**Philippe Kocian** (Laboratoire de Cristallographie, EPFL, Lausanne)

**Deborah Gonzalez Mantero** (Institut de Chimie, Université de Neuchâtel)

**Lucile Pernot** (Département de Microbiologie et Médecine Moléculaire, Faculté de Médecine, Université de Genève)

### Unknown Address:

If you know the present address of Dr. Olivier Crottaz, formerly with Moltech SA at Carouge, please inform the Secretary of the SSCr, Hans.Grimmer@psi.ch.

The executive committee of IUCr intends to appoint **Gernot Kosterz** as Editor-in-Chief of all IUCr journals.

**Artem R. Oganov** (ETHZ) and S. Ono (JAMSTEC, Japan) have discovered a new high-pressure phase of  $\text{Al}_2\text{O}_3$  with a very unusual structure. This phase has been predicted theoretically and verified experimentally; its existence has implications for the interpretation of previous experiments and has important implications for the Earth's deep interior. The paper will soon appear in Proc. Natl. Acad. Sci.

The special issue "Computational Crystallography" of Z. Kristallographie (2005, **220**, issue 5/6), edited by **Artem R. Oganov**, has come out. It is available on-line at: <http://www.extenza-eps.com/extenza/contentviewing/viewJournalIssueTOC.do?issueId=5313>

## Nachrichten aus der Akademie der Naturwissenschaften Schweiz

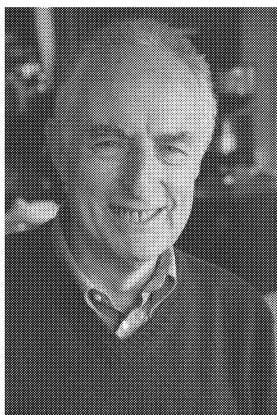
Anlässlich der 100. Senatssitzung vom 13. Mai 2005 in Bern wurde Prof. Denis Monard zum Präsidenten des Zentralvorstandes (ab 2007) gewählt. Gleichzeitig bestimmte der Senat Basel zum Vorort für die Periode 2007 – 2012. Denis Monard ist Professor für Zellbiologie an der Universität Basel sowie Gruppenleiter am Friedrich Mischer Institut Basel, welches er 2002 – 2004 leitete.

### Jahreskongress 2005 "Einstein heute"

Der Jahreskongress der Akademie der Naturwissenschaften findet im Rahmen des «World Year of Physics 2005» und der damit verbundenen Veranstaltungen zum Einstein-Jahr in Bern statt. Der zweitägige Kongress zum Thema «Einstein heute» wird von der Schweizerischen Physikalischen Gesellschaft mit Jean-Philippe Ansermet (Departement Physik EPFL, 1015 Lausanne) als Jahrespräsidenten organisiert. Er findet ausnahmsweise nicht im Herbst, sondern vom 14. – 15. Juli in der Universität Bern statt.

Das Programm des Jahreskongresses liegt diesem Newsletter bei und kann auch unter [www.einsteinheute.ch](http://www.einsteinheute.ch) eingesehen werden.

## News from the IUCr



The IUCr is pleased to announce that Professor Philip Coppens (Department of Chemistry, State University of New York at Buffalo, USA) has been awarded the seventh Ewald Prize for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states, and for his contributions to the education and inspiration of young crystallographers as an enthusiastic teacher by participating in and organizing many courses and workshops.

The presentation of the Ewald Prize will be made during the Florence Congress Opening Ceremony on 23 August 2005.

## Solid State Chemistry Laboratory at Paul Scherrer Institute

Kazimierz Conder

*Laboratory for Developments and Methods, Paul Scherrer Institute*

Successful science in the field of condensed matter requires a strong collaboration between solid state physicists and chemists. Responding to the demand for specific, good characterised samples, primarily for the in-house performed science, a Solid State Chemistry Laboratory was established within the PSI Department NUM (Research with Neutrons and Muons). The laboratory is active in the synthesis and characterisation of the solid-state samples that are intended for detailed studies using research facilities installed at PSI. The synthesis capabilities for polycrystalline and powder samples include solid-state synthesis, sol-gel method and arc melting. Additionally the Laboratory is specialized in oxygen isotope exchange experiments. The samples can be characterised by chemical analysis methods, using Thermal Analysis, X-ray diffractometry and measurements of magnetic, transport and thermal properties. Scientific work performed during the last years based on polycrystalline/powder samples includes among others:

- study of the oxygen isotope effect (OIE) in  $HT_C$  superconductors (critical temperature, pseudogap temperature, penetration depth and other properties)
- OIE investigations in manganates, nickelates and cobaltates (magneto-resistance and metal-insulator transition)
- studies of the synthesis and oxygen content determination methods, oxygen thermodynamics and diffusion.

Since more than one year a commercial furnace (CSC Japan) for crystal growth by the Travelling Solvent Floating Zone (TSFZ) method is installed. The method enables the growth of large crystals ( $\varnothing$  7-8 mm, length up to 100 mm) of predominately oxide compounds. In the furnace a zone-melting process is realized using as heat source a focused light from four halogen lamps (up to 1500 W each). Once a small section of the rod is melted, the molten (floating) zone is translated along the sample length by moving the material with respect to the radiation focus with a controlled rate (0.1-20 mm/h). Crystal material is grown on the solidifying end of the float zone (see Fig.1). There is no crucible necessary, which reduces the impurity level in the crystals. A maximum operating temperature of 2200 °C can be reached, and the process can be performed in a controlled gas atmosphere from a high vacuum up to 10 bar. The laboratory is equipped with instruments for the

preparation of the feed rods (hydrostatic press, vertical sintering furnace) and also for cutting and polishing the crystals.

The TSFZ method was successfully applied for growing many different materials. High quality single crystals have been already obtained for  $\text{LaCoO}_3$  (see Fig.2),  $\text{SrCu}_2(\text{BO}_3)_2$ ,  $\text{YMnO}_3$ ,  $\text{YFeO}_3$ ,  $\text{ErFeO}_3$  and  $\text{Na}_x\text{CoO}_2$  ( $0.5 < x \leq 1$ ).

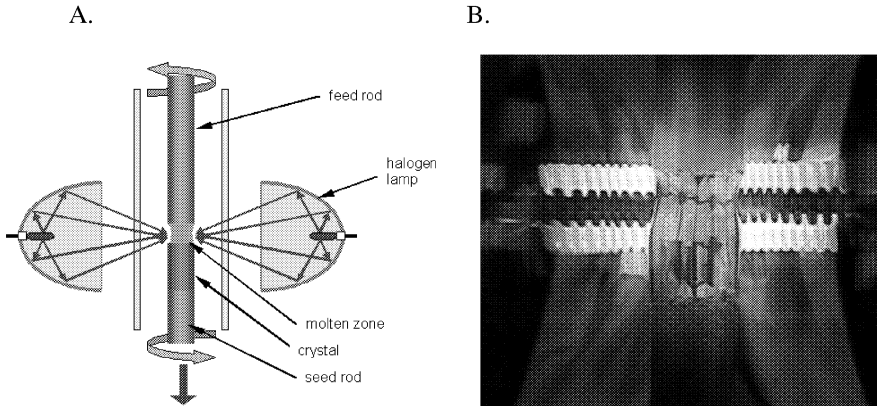


Fig. 1 A: Operation principle of a mirror furnace for crystal growth by the Travelling Solvent Floating Zone (TSFZ) method;

B: The crystallisation process can be observed using a video-camera.

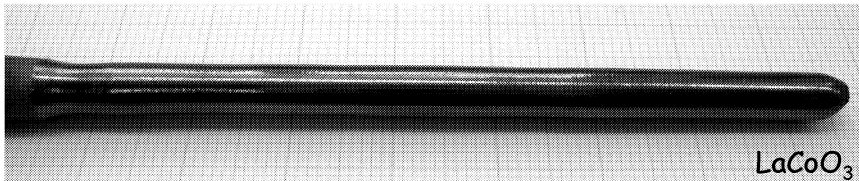


Fig. 2:  $\text{LaCoO}_3$  single crystal obtained by the TSFZ method (melting point  $\sim 1750^\circ\text{C}$ ). The rate of crystal growth was 5 mm/h.



**Swiss Spallation Neutron Source SINQ**  
**Swiss Synchrotron Light Source SLS**  
**Swiss Myon Source S $\mu$ S**

## Calls for proposals

The Paul Scherrer Institute, Villigen, CH (<http://www.psi.ch>) operates three major user laboratories for condensed matter research on one campus: a third generation X-ray synchrotron source (SLS), the only continuous spallation neutron source worldwide (SINQ) and the world's most powerful continuous-beam  $\mu$ SR facility (S $\mu$ S).

Please remember the following proposal submission deadlines:

**SLS:**

Protein crystallography beamlines	:	15/02, 15/06, 15/10
All other beamlines	:	15/03, 15/09

**SINQ:**

All instruments	:	15/05, 15/11
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**S $\mu$ S:**

All instruments	:	01/12
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The central PSI User Office offers a joint Web portal, from where all necessary information can be obtained: <http://user.web.psi.ch>

**Contact address:**

Paul Scherrer Institut	Phone:	+41-56-310 4666
<i>User Office</i>	Fax:	+41-56-310 3294
Bldg. WLGA/002	Web:	<a href="http://user.web.psi.ch">http://user.web.psi.ch</a>
CH-5232 Villigen PSI		

E-mail: [slsuo@psi.ch](mailto:slsuo@psi.ch), [sinq@psi.ch](mailto:sinq@psi.ch), [smus@psi.ch](mailto:smus@psi.ch)



## 3rd MEETING OF THE SNX COUNCIL

held in Sommarøy (Tromsø, Norway ) June 8 - 9 2005. Principal topics were:

### **ADMINISTRATIVE ASPECTS**

1. Report of the SNX Director on A-SNG/SNBL operations.
2. Financial Matters.

### **RESEARCH ASPECTS**

3. Status of the SNBL operations.
4. Midterm planning of the SNBL 2005 – 2007.
5. Applications for Beam Time / Review Process : New approach.
6. Discussion of Proposals.

### **Report of the SNX Director**

Good progress was reported on the refurbishment programme. The beam lines operations have been smooth and successful.

### **Financial Matters**

The total Baseline Budget plus Outside Baseline Budget for CHF 1'624'000 = 8'304'000 NOK was approved as a frame budget.

### **Midterm planning of the SNBL 2005 – 2007**

Some features typical for the current status and important for the Beam Lines future were noted: increasing fraction of papers published by SNBL users in high rated journals; stable increase of number of publications; increase of user groups requesting beamtime at SNBLs. The beam lines staff has already reacted to a number of needs expressed by the SNBL users. Given the fact that the SNX Council is the deciding organ about the future scientific directions the SNBL staff is ready to implement their decisions taken.

### **Applications for Beam Time**

It was decided **to keep the deadlines** for the Standard and Long Term Proposals. A new category of proposals was established, Urgent Research Proposals, and its concept was accepted. Urgent proposals should be indicated as urgent by the applicants, the special status should be clearly justified. Time requested should not exceed 6 shifts. The proposals will be handled with priority. The Beamline Director and a SNX council member review urgent proposals. If approved, beamtime will normally be allocated within 2 months of the proposal date.

The retiring members of the SNX Council Prof. Ed Hough (University of Tromsø) and Dr. Radovan Cerny (University of Geneve) were warmly thanked for their work. Dr. Helge Larsen (University of Stavanger) and Dr. Jan-Dierk Grundwaldt (ETH Zurich) will replace them as from September 2005.

C. Heurtebise (Administrative Manager SNBL)

# Calendar of Forthcoming Meetings

**Meetings held in Switzerland are printed in bold letters.**

More details on most meetings can be found on the WWW under

<http://www.ch.iucr.org/iucr-top/index.html>

2005

<b>14. – 21. August</b>	<b>Zuoz (Switzerland)</b>	<b>4<sup>th</sup> PSI Summer School on Condensed Matter Research – Spectroscopy / Microscopy</b>
18. – 23. August	Siena (Italy)	IUCr Computing School (prior to the Florence congress).
23. – 31. August	Florence (Italy)	XX Congress of the International Union of Crystallography
29. August – 1. Sept.	Sheffield (UK)	ECSSC 10: The 10 <sup>th</sup> European Conference on Solid State Chemistry
1. – 2. Sept.	Edinburgh (UK)	Magnetism, Neutrons and High-Pressure
2. – 8. Sept.	Brussels (Belgium)	Electron Crystallography School 2005 - ELCRYST 2005: New Frontiers in Electron Crystallography
4. – 7. Sept.	Grenoble (France)	Neutrons in Biology – A satellite Meeting of the IUPAB/EBSA Biophysics Congress
<b>5. – 7. Sept.</b>	<b>Dübendorf (Switzerland)</b>	<b>International Conference on Perovskites - Properties and Potential Applications</b>
5. – 15. Sept.	Oxford (UK)	9 <sup>th</sup> Oxford School on Neutron Scattering
8. – 10. Sept.	Grenoble (France)	Neutron Spin Echo Workshop 2005
<b>10. – 18. Sept.</b>	<b>Beatenberg (Switzerland)</b>	<b>3<sup>rd</sup> International Workshop on Crystal Growth Technology (IWCGT-3)</b>
15. – 17. Sept.	Murnau (Germany)	Structural Biology of Molecular Recognition
<b>19. – 21. Sept.</b>	<b>Les Diablerets (Switzerland)</b>	<b>2005 Swiss Workshop on Materials with Novel Electronic Properties MaNEP</b>
<b>3. – 7. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>4<sup>th</sup> NCCR Practical Course – Synchrotron Data Acquisition Techniques in Macromolecular Crystallography</b>

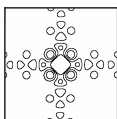
4. – 7. Oct.	Hofgeismar (Germany)	Fortbildungskurs: Anwendung der Gruppentheorie in der Kristallchemie
6. – 7. Oct.	Stuttgart (Germany)	Watching the Action: Powder Diffraction at Non-Ambient Conditions
<b>13. October</b>	<b>Lausanne (Switzerland)</b>	<b>Annual Meeting 2005 of the SGK/SSCr "Crystallography and Physics"</b>
<b>17. – 18. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>6<sup>th</sup> SLS Users' Meeting</b>
27. Nov. – 2. Dec.	Sydney (Australia)	International Conference on Neutron Scattering 2005

2006
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<b>25. – 27. January</b>	<b>Villigen (Switzerland)</b>	<b>SpS Users' Meeting</b>
<b>10. May</b>	<b>Villigen (Switzerland)</b>	<b>8<sup>th</sup> SINQ Users' Meeting</b>
9. – 18. June	Erice (Italy)	The Structure and Function of Large Molecular Assemblies
4. – 6. August	Leuven (Belgium)	Satellite Conference of ECM-23 on "Mathematical and Theoretical Crystallography"
6. – 11. August	Leuven (Belgium)	23 <sup>rd</sup> European Crystallographic Meeting (ECM-23)
<b>1. – 4. Sept.</b>	<b>Genève (Switzerland)</b>	<b>10<sup>th</sup> European Powder Diffraction Conference (EPDIC-X)</b>

2007
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7. – 17. June	Erice (Italy)	Engineering of Crystalline Materials Properties
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**Schweizerische Gesellschaft für Kristallographie**  
**Société Suisse de Cristallographie**  
**Società Svizzera di Cristallografia**  
**Societad Svizera per Cristallografia**

Membres du Comité pour la période 2003 – 2005

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The newsletter of the SGK/SSCr is published 3 times a year. Word files are welcome at any time, as well as illustrations for the cover. Articles in English, German or French may be submitted. Please send all interesting information to the Editor.

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