Schweizerische Gesellschaft für Kristallographie Société Suisse de Cristallographie
Swiss Society for Crystallography

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

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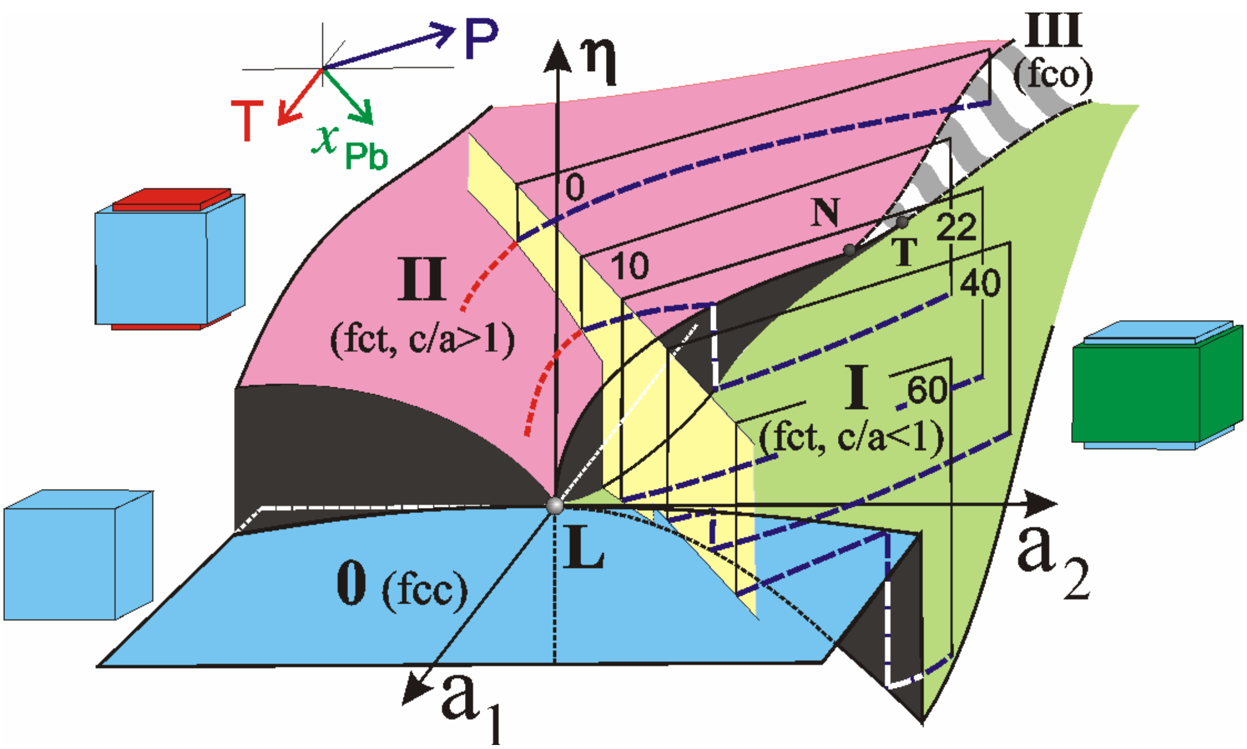


SGK/SSCr NEWSLETTER **No. 71**

April 2007

In this issue:

Anti-isostructural phase transitions
Laboratory of Solid State Chemistry and Catalysis at EMPA
Annual membership fee
Annual meeting 2007: call for abstracts

On the Cover:

Anti-isostructural phase transitions are induced by variations of external thermodynamic parameters such as temperature (T), pressure (P) and composition (*x*), and occur between phases that have a common parent structure but different signs of *symmetry breaking* distortions

from V. P. Dmitriev, D. Chernyshov, Y. E. Filinchuk, V. F. Degtyareva, Phys. Rev. **B 75**, 024111 (2007)

More details in our new section: Did you hear … ?

SGK/SSCr Newsletter No. 71

Letter from the President

Walter Steurer (steurer@mat.ethz.ch)

Are you familiar with photonic or phononic *quasi*-crystals? No? Not even with simple periodic photonic or phononic crystals (PTCs or PNCs)? Well, this is not mainstream crystallography admittedly, but even so I will draw your attention for a few minutes to this exciting field. PTCs and PNCs are periodic heterostructures which consist of at least two materials differing in their dielectric or elastic properties, respectively. To some extent, PTCs are to electromagnetic waves what PNCs are to elastic or acoustic waves and what crystals (semiconductors) are to electron waves: their way of ordering determines band structure and transport properties. Of course, the period of the structure has to be of the same order as the wave length.

Well trained from numerous evaluations, I made some amazing publication statistics. In the two decades since their discovery, the number of publications on PTCs has been growing exponentially surpassing already 8700 this year. The reason behind this is the big promise of gaining full control of light on the sub-micrometer scale, the prerequisite of optical computers and communication devices. Frequency filters, waveguides with sharp bends, absorption-free mirrors, optical microcavities or aberration-free negative-refraction-index lenses are just a few of the possible applications. There are also many potential engineering applications of PNCs such as thermal barriers, elastic/acoustic filters, acoustic lenses, waveguides and non-absorbing mirrors, sound-protection devices and even earthquake shields. However, the innovation potential and market volume for PNC-based devices seem to be much smaller than for PTCs if we neglect the somehow speculative earthquake shields. Consequently, only about 350 papers have been published in this field up to now. Of the more than 9000 publications in total, around 300, most of them published in the past two years, deal with quasiperiodically ordered heterostructures, trying to exploit their high degree of isotropy. Here we are!

Interested in basic research on real, intermetallic quasicrystals I am often asked about industrial applications. However, there are only a few niche applications, from coatings for frying pans to surgical steels. This is different for photonic and phononic quasicrystals, there seem to be the really interesting technological applications of quasiperiodicity. The arbitrarily high rotational symmetry and the pure point spectra of 2D and 3D quasiperiodic structures can be practically exploited to manufacture isotropic band-gap materials, which are perfectly well suitable to host waveguides or cavities, for instance. With the massive promotion they currently enjoy, there could be a bright future for devices based on photonic or phonic quasicrystals.

Walter Steurer
President of the SGK/SSCr

Hydrogenography: a High-Throughput Look at Hydrides

Contribution of R. Griessen (griessen@nat.vu.nl)
Faculty of Sciences, Department of Physics and Astronomy,
Condensed Matter Physics, Vrije Universiteit,
De Boelelaan 1081, 1081HV Amsterdam, The Netherlands

To reach high mass and volumetric densities for hydrogen storage in solids one is limited to alloys or compounds of the upper part of the Periodic System including Rows 1 to 4 and Groups IA up to VB. With these ± 22 elements a huge number of binary, ternary and quaternary materials can be conceived. Their potential use for hydrogen storage can only be investigated by means of high-throughput techniques. To this end we have developed HYDROGENOGRAPHY. This is a novel technique based on the optical changes induced by hydrogen ab- and desorption in metal films. Hydrogenography on thin films with a compositional gradient has the great advantage that it allows to measure simultaneously a large number of samples (up to thousands) of different elemental compositions on only one wafer (each pixel of the recording camera corresponds essentially to one alloy composition). This enormously facilitates the search for new metal-hydrides with specific physical properties [1]. The compositional gradient thin films necessary for hydrogenography are synthesized by co-sputtering on a 3” wafer from three (up to six) off-centered magnetron sources. The hydride formation during hydrogen absorption at well-defined temperatures and hydrogen gas pressures is monitored through the transparency of the films. From these optical measurements it is possible to determine simultaneously the enthalpy and entropy of formation of thousands of compositions and, consequently, to identify the most attractive compositions for specific applications. As an illustration of our technique I describe how hydrogenography is used to optimize Magnesium-Transition metal hydrides. Some of these hydrides have gravimetric hydrogen capacities approximately 4 times higher than that of conventional NiMH batteries. In addition, the hydrogen sorption kinetics is directly amenable to the experiment as hydrogenographic data are continuously recorded during hydrogen ab/desorption. Hydrogenography is also of great help in the search and optimization of catalytic layers [3], optical fiber hydrogen safety sensors [4] and smart solar collectors [5].

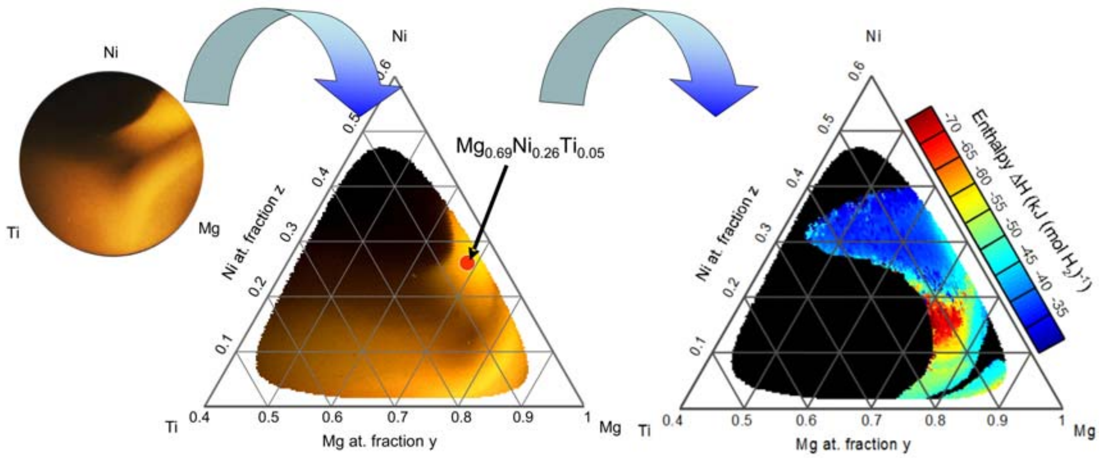


Figure 1: Optical transmission for the example of the ternary phases of hydrated Ti-Mg-Ni. On the left the optical transmission of the wafer measured, on the right the same values calibrated by the scaled correct composition. Scaling is done by the determination of the composition on a few spots using Rutherford scattering and interpolating the values for the remaining area of the wafer. Please visit our internet site for the colour version of this figure (http://www.sgk-sscr.ch/Newsletters.html).

[1] B. Dam et al.:
Combinatorial thin film methods for the search of new lightweight metal-hydrides,
Scripta Materialia **56** (2007) 853-858

[2] R. Gremaud et al.:
Structural and optical properties of $Mg_xAl_{1-x}H_y$ gradient thin films: a combinatorial approach,
Applied Physics A: Mat. Science & Processing **84** (2006) 77

[3] A. Borgschulte et al.:
Catalytic activity of noble metals promoting hydrogen uptake,
J. of Catalysis **229** (2006) 263

[4] M. Pasturel et al.:
Stabilized switchable 'black state' in Mg_2Ni/Ti/Pd thin films for optical hydrogen sensing,
Appl. Phys. Lett. **89** (2006) 021913

[5] D. M. Borsa et al.:
Mg–Ti–H thin films for smart solar collectors,
Appl. Phys. Lett. **88** (2006) 241910

Laboratory of Solid State Chemistry and Catalysis at EMPA

Contribution of Christoph N. Zwicky (Christoph.Zwicky@empa.ch)

Swiss Federal Laboratories for Materials Testing and Research (EMPA),
Überlandstrasse 129, CH-8600 Dübendorf

The new Laboratory of Solid State Chemistry and Catalysis at EMPA (Abteilung 131: www.empa.ch/abt131) was founded in May 2006 and consists of the three groups **Solid State Chemistry, Heterogeneous Catalysis** and **Inorganic Solid State Analysis**.

Modern energy- and pollution-control technologies are necessary to ensure our present quality of life and depend upon novel tailor-made functional materials as well as on a profound description and analysis of materials in the environment.
The inorganic elemental analysis of solid materials is a prerequisite to describe a material. It is further a research-tool for industry support, energy- and environmental technologies and support of EMPA's research programs.
The Inorganic Solid State Analysis group is working with wavelength-dispersive X-ray fluorescence spectrometry (WD-XRF), energy-dispersive X-ray fluorescence spectrometry (ED-XRF), synchrotron-based X-ray fluorescence spectrometry (SR-XRF), X-ray diffraction (XRD) and scanning electron microscopy (SEM). A great variety of materials such as environmental samples, building materials, rock samples, metals, ceramics, oil, etc. can be characterized. Present projects include aerosol analytics on PM10 emissions from road and railway traffic using WD-XRF and SR-XRF, WD-XRF analysis of heavy metals in forest soils, in-situ analysis of ashes derived from wood supplied firing systems with a portable ED-XRF spectrometer and E-learning projects. Furthermore a considerable number of commercial projects for industry, private and government customers are performed every year.

Facilities and applied methods

Inorganic Solid State Analysis group
contact: peter.lienemann@empa.ch

X-ray analytics have a long tradition at EMPA. For about 50 years EMPA operates X-ray fluorescence spectrometers (XRF) and X-ray diffractometers (XRD) to investigate the chemical and mineralogical composition of materials.

Wavelength-dispersive X-ray fluorescence spectrometry (WD-XRF)
We operate two WD-XRF spectrometers, a PW1404 and a PW2400 from Philips. The PW1404 is equipped with a chromium X-ray tube whereas the PW2400 contains a rhodium X-ray tube. The spectrometers are used for qualitative and quantitative analyse of metals, building materials, environmental and geological samples, ceramics, waste and dust samples, etc. Besides self-designed quantitative analytical programs a commercially available "standardless" quantitative analytical program is

used. For sample preparation an automatic bead machine Perl'X 3 from Philips (SOLED) is to disposition.

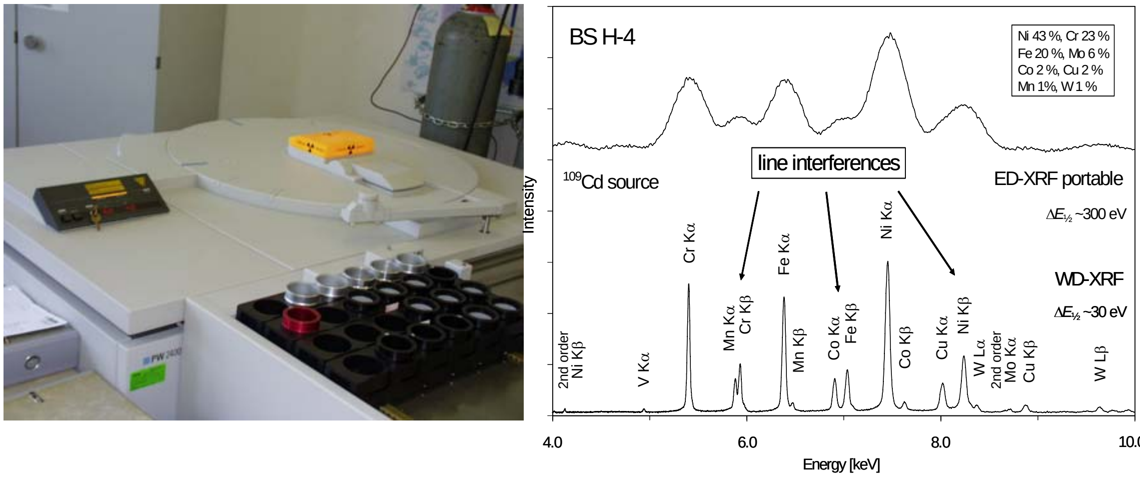


Figure 1: WD-XRF spectrometer PW2400. Spectral resolution of the laboratory-based and the portable XRF spectrometer. Line interferences with several element lines occur. The spectral resolution of the portable ED-XRF instrument does not resolve these element lines whereas the spectrum of the WD-XRF spectrometer shows clearly separated element lines [Zwicky C.N., Lienemann P. (2004), Quantitative or semi-quantitative? - laboratory-based WD-XRF versus portable ED-XRF spectrometer: results obtained from measurements on nickel-base alloys, *X-Ray Spectrom.*, **33**, 294-300].

Portable energy-dispersive X-ray fluorescence spectrometer (ED-XRF)

The new portable ED-XRF spectrometer XLt 898 from NITON contains a miniature Ag X-ray tube instead of radioactive sources. It provides fast and non-destructive identification of metal alloys by chemical composition and name. The instrument is also used for qualitative analyses of non-metallic materials.

X-ray diffractometry

The X-ray diffractometer X'Pert PRO from PANalytical is equipped with a copper X-ray tube and usually operates with the Bragg-Brentano geometry. Our versatile equipment allows performing analysis with parallel beam optics to investigate samples with uneven surfaces such as e.g. coins, statues, artificial hip-joints, etc. With the capillary technique texture-free measurements are possible and thin layers are analyzed with the grazing incidence technique. Besides a sealed proportional detector with secondary monochromator to extract the copper Kβ-radiation the diffractometer is equipped with an X'Celerator detector. The X'Celerator is an X-ray detection system based on RTMS (Real Time Multiple Strip) technology. This technology operates as if there were an array of over a hundred detectors at work simultaneously in an X-ray diffraction system and thus allows very short measuring times combined with good counting statistics. The X-ray diffractometer is used to analyze crystalline materials such as ceramics, building materials, metallic corrosion products, pharmaceutical products, medical implant materials, etc.

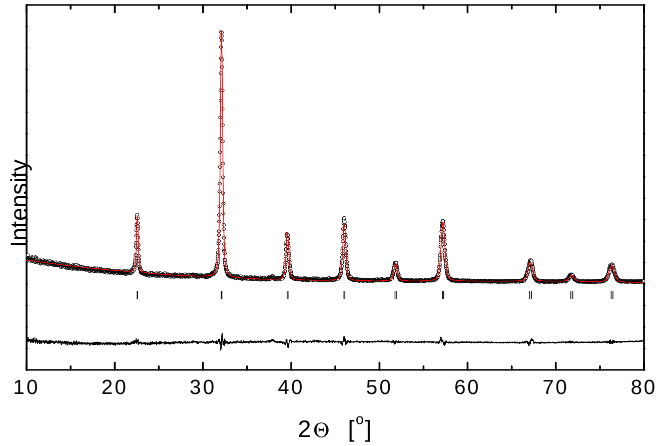


Figure 2: X-ray diffractometer. Calculated (red) and observed XRD pattern of $LaTiO_2N$ crystallized in perovskite-type pseudo-cubic unit cell [Logvinovich, D., Börger, A., Döbeli, M., Ebbinghaus, S.G., Reller, A. and Weidenkaff, A, Synthesis and physical chemical properties of Ca substituted $LaTiO_2N$, *Progr. in Solid State Chem.*, in press.]

Electron microscopes

Several electron microscopes at EMPA are used by the members of our laboratory, among them a scanning electron microscope (SEM) JSM-6300F from Jeol, which is equipped with a cold field emission cathode, an environmental scanning electron microscope (ESEM) XL30 from Philips and a transmission electron microscope (TEM) CM30 from Philips equipped with a thermoionic gun.

Solid State Chemistry and Heterogeneous Catalysis groups

contact: anke.weidenkaff@empa.ch

The goal of the Laboratory of Solid State Chemistry and Catalysis is to discover and develop novel functional materials by means of innovative solid state chemistry methods. Promising candidates are complex transition metal oxides with perovskite-type structure showing a broad multiplicity of interesting electrical, magnetic, catalytic and structural characteristics. Thus making them interesting in many applications as modern functional materials, such as dielectrics, ferroelectrics, thermoelectrics or CMR-materials.

The projects of the **Solid State Chemistry group** include the development of thermoelectric oxides, studies of structure and properties of oxynitride perovskites, studies of substitutional effects in ionic solids, as well as plasma enhanced anionic substitutions. Furthermore we work on the development of noble metal free car exhaust gas catalysts and on reversible alkaline fuel cells.

The improvement of current **catalytic systems** with respect to their efficiency and selectivity and the development of new catalytic material using some of the 20 most abundant elements for the substitution of noble metals in e.g. exhaust gas catalysis will be the goal of the new catalysis lab.

The projects of the **Heterogeneous Catalysis group** include in-situ spectroscopy of catalytic processes, studies on secondary processes of exhaust gas treatment including the assessment of risks and benefits, research on perovskites for catalytic exhaust gas treatment, the synthesis and evaluation of Ba-based perovskites as new NOx-trap materials and studies on the catalytic decomposition of diesel soot in particulate traps.

Thermal Analysis

For the analysis of the reactivity and chemical composition of solids we have a simultaneous thermoanalysis system, which combines thermogravimetry (TG) / differential thermal analysis (DTA) / differential scanning calorimetry (DSC) with mass spectrometry as well as a high resolution NETZSCH DSC.

The STA 409 CD from NETZSCH is based on the classic concept of a thermobalance in a vertically-arranged instrument with top-loaded samples. The STA 409 CD is designed for simultaneous TG-DSC or simultaneous TG-DTA measurements. There are two different furnaces to disposition. One furnace is suitable for measurements in any kind of atmosphere or vacuum from room temperature up to 1500°C. The second furnace allows working conditions under a defined partial pressure for water from 120°C up to 1200°C.

The QMS 403 C *Aëolos* ® is a quadrupole mass spectrometer with a heated capillary inlet system for routine analysis of gases and, in particular, volatile decomposition products of thermal analysis.

Figure 3: Pulse TA coupled to a mass spectrometer for studies on in-situ gas solid reactions.

B.E.T. Surface Area determination

With the sorption instrument ChemBET 3000 from QUANTACHROME processes of physisorption and chemisorption can be analyzed. Temperature programmed reactions are possible. With the Brunauer, Emmett and Teller method (BET) the specific surface of a material can be determined.

Measurement of the electrical conductivity and the Seebeck-coefficient

With the instrument RZ2001i from OZAWA SCIENCE measurements of the electrical conductivity and the Seebeck-coefficient from room temperature up to 1000°C in different gas atmospheres are possible.

Figure 4: High Temperature electrical conductivity and thermopower measurement system.

Large Area Bonder 5425

The manual bonder model 5425 from F&K Delvotec is an ultrasonic wedge-wedge bonder for aluminum and gold wires. The instrument is used to fix thin aluminum and gold wires to samples to measure their electrical conductivity.

Thermal Diffusivity and Conductivity

The laser flash system LFA 457 *MicroFlash*® from NETZSCH allows measurements of thermal diffusivity and conductivity from room temperature up to 1100°C. The infrared sensor technology employed in the system enables time resolved measurements of the temperature increase on the back surface of the sample after having shot on the front surface with a laser pulse of defined energy. Disc shaped samples of 10 mm, ½ inch and 1 inch diameter can be measured. The maximum thickness of the sample is 6 mm. The vacuum-tight design enables tests under defined atmospheres.

Besides our research projects the instrument is used for industrial support, e.g. for investigations on the heat conductivity properties of ceramic coatings.

Raman Spectroscopy

The Raman Imaging Microscope Ramascope 2000 from Renishaw is equipped with two different lasers, a 633 nm HeNe-laser and a 780 nm diode laser. Besides our research projects the instrument is used for archaeometrical applications, e.g. for the identification of pigments in ancient paintings.

The Raman effect is exploited to identify and characterize the chemistry and structure of materials in a non-contacting, non-destructive manner. The Raman effect occurs when laser light is shone on a material; light is scattered, a tiny fraction of which is shifted in frequency as atoms in the material vibrate. Analysis of the frequency shifts (spectrum) of the light reveals the characteristic vibration frequencies of the atoms and hence the chemical composition and structure of the material.

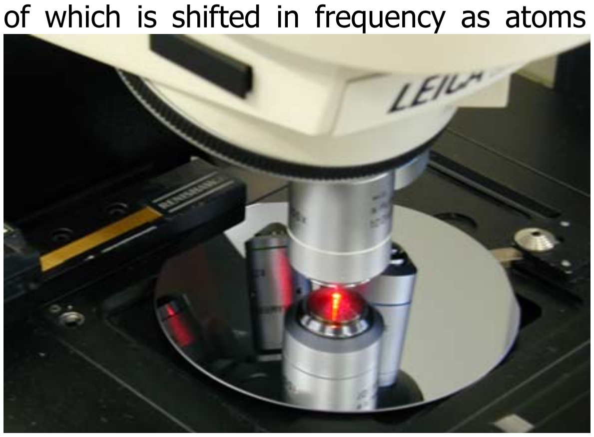


Figure 5: Raman Microscope for structural investigations and phase analysis.

DGK German Crystallographic Society
Annual Meeting 2007 in Bremen

Contribution of G. Schuck (Goetz.Schuck@PSI.CH)
Neutron Diffraction Group, ETH Zurich and Paul Scherrer Institut, 5232 Villigen PSI

More than 500 scientists from all over Europe came to Universität Bremen from March 5-9, 2007 to attend the joint annual meeting of the German Society for Crystallography (DGK) and the German Association for Crystal Growth (DGKK).

Plenary lectures:

J. Rodriguez-Carvajal (Grenoble):	Powder diffraction: instruments and methods
W. Schmahl (München):	Crystallography of Shape Memory and Superelasticity in NiTi Alloys - Investigations with Soft and Hard Synchrotron X-Radiation
W. Depmeier (Kiel):	Mikroporöse Strukturen: Neues zu einem alten Thema
M. Schmidt (Garching):	Time-Resolved Macromolecular X-ray Crystallography: Kinetics and Atomic Structures of Transient States
Ch. W. Müller (Grenoble):	Structural insight into RNA polymerase III transcription from X-ray crystallography and electron microscopy
A. Cröll (Freiburg):	Strömungskontrolle bei der Kristallzüchtung aus der Schmelze
S. Lutgen (Regensburg):	Entwicklung von InGaN-Laserdioden
A. Waag (Braunschweig):	ZnO Electronics : Opto - Magneto - Nano
A. Müller (Freiberg):	Herausforderungen bei der Kristallisation von multikristallinem Solarsilicium

Laureate lectures (Max-von-Laue-Price 2006):

Th. Höche (Leipzig):	Inkommensurable Modulationen in Fresnoiten
B. Dittrich (Crawley):	Invariom modelling: Introduction, current status and future outlook

Microsymposia (Chairpersons, Number of Abstracts)**:**

- Neutronenstreuung (M. Braden, H. Boysen, 9)
- Elektronenmikroskopie (M. Rodewald, 6)
- Kinetik von Oberflächen- und Grenzflächenreaktionen (G. Jordan, P. Rudolph, 8)
- Modulierte Strukturen, teilkristalline Verbindungen und Quasikristalle (A. Schönleber, S. van Smaalen, 13)
- Kristallographie in Lehre und Außendarstellung (R. Neder, 5)
- Hochdruckphasen (R. Pöttgen, U. Schwarz, 13)
- Kristallchemie anorganischer Strukturen (R. Pöttgen, S. van Smaalen, 78)
- Kristallchemie von Molekülverbindungen (Ch. W. Lehmann, R. Pöttgen, 25)
- New Macromolecular Structures (Th. Stehle, 22)
- Drug Design (U. Wendt, 7)
- Detectors for Macromolecular Crystallography (P. Tucker, 5)
- Enzyme Mechanisms (R. Ficner, 5)
- Pulverdiffraktometrie: Methodik und Kristallstrukturen (R. E. Dinnebier, M. U. Schmidt, 20)
- Elektronendichte (Ch. W. Lehmann, G. Raabe, 7)
- Textur (H.-G. Brokmeier, 15)
- Kristallographie und Spektroskopie (M. Fechtelkord, G. Amthauer, 15)
- Industrie-Symposium (M. Wendschuh, 10)
- Mineralogische und technische Kristallographie (H. Pöllmann, 19)
- Freie Themen (J. Birkenstock, R. X. Fischer, 19)
- Kristallphysik (J. Schreuer, 14)
- DGKK-Beiträge (M. Mühlberg, 32)

Max-von-Laue-Price 2007:

Dr. Dominik Schaniel from the University of Cologne, a former thesis student at Laboratory for Neutron Scattering (ETH Zurich & Paul Scherrer Institut, Villigen), was awarded the Max-von-Laue Price 2007.

News for and from Members

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

Mr. Daniel Jung
(Laboratory for Crystallography, ETH Zurich, 8093 Zürich, Thesis Student)

Dr. Felix Reifler (EMPA, Laboratory for Advanced Fibers, 9014 St. Gallen)

Dr. N. Penin (Laboratory for Crystallography, Université de Genève, 24 quai Ernest Ansermet, 1211 Genève)

Missing Addresses of SGK/SSCr Members

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

- Jean Philippe Rapin (Laboratoire de Crystallographie, Université de Genève)
- Dr. S. Rodriguez-Belluga

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

2007 SGK/SSCr Membership Fee

I would like to take the opportunity to thank all the members for promptly paying their membership fees. They will remain unchanged for 2007, only the ECA membership has been increased due to the updated exchange rate EUR/CHF.

SGK/SSCr full member	30	CHF / year
SGK/SSCr student member	10	CHF / year
SGK/SSCr institutional member	130	CHF / year
combined SGK/SSCr and ECA full membership	46	CHF / year
ECA individual membership	16	CHF / year

- Please pay the fee for 2007 by the end of May **by bank transfer** to the UBS account: IBAN CH39 0027 9279 C029 1110 0
  Please avoid to pay in cash at a post office (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0) if possible (or add an additional handling fee of CHF 1.20)
- Several of the fees for 2006 and even a few for 2005 are still missing. A cover letter indicating the **total amount due** has been included with this newsletter to the members concerned (a negative balance means that you paid in advance and no action is needed).
- **Institutional members will be mailed a special invoice.**
- Individual members of the ECA can also use this opportunity to pay their annual ECA dues (EUR 10.- = **CHF 16.-).** This way we can make a single foreign bank transfer to the ECA and avoid having each member make an individual one (typical bank charge is sfr. 10 per transfer). Please note on your payment whether you are also including your ECA membership fees for 2007.
  Application for ECA membership: http://www.ecanews.org/membership.htm

Thank you for your cooperation.

Your treasurer,
Michael Hennig

SGK/SSCr Annual Meeting 2007:

Call for Abstracts

The annual meeting of the SGK/SSCR and the general assemblies of SGK/SSCr and SKT 2007 will take place at PSI on September 12 (dinner) and 13 (meeting and general assemblies). It is organized by the diffraction group of the Laboratory for Neutron Scattering (LNS) of ETH Zurich & Paul Scherrer Institute. Please note, that the SLS User Meeting (Sept. 11/12) is preceding our meeting at the same place. A combined registration will be possible.

Invited Speakers: Prof. V. Petricek (Prague), Prof. F. Winkler (PSI)

Abstracts should be submitted to Jurg.Schefer@psi.ch (subject=SGK/SSCr Annual Meeting). They will be published in volume 72 of our newsletter.

Deadlines:
Abstract submission: **July 15, 2007**
Registration/Dinner: **Sept. 5, 2007**

Registration is processed through the DUO system of PSI. If you did not use SLS or SINQ up to date, **you have to open a new account** in this system**. Early reservation for accommodation** is recommended.

More detailed information (e.g. an abstract example) and links to relevant internet sites are given at:

http://diffraction.web.psi.ch/sgk-sscr-2007.htm

Call for Patterson Award Nominations (ACA)

Nominations are solicited for the 2008 A. Lindo Patterson Award, which will be presented at the annual ACA Meeting in Knoxville, TN. A special symposium will be organized in honor of the recipient and will provide the forum for the Patterson Award Lecture. The Patterson Award, established in 1980, is given every three years *to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information.*

Lindo Patterson's 1934 paper in *Phys. Rev.*: "A Fourier Series Method for the Determination of Components of Interatomic Distances in Crystals," signaled a major step forward in understanding diffraction theory; the Fourier series on F2, or Patterson function, greatly enabled subsequent structure determination. His section on Fundamental Mathematics in *International Tables, Vol. II* was another important contribution to the community. After working for the government during the war, and then teaching at Bryn Mawr, he moved in 1949 to the Institute for Cancer Research where he worked until his untimely death in 1966. Lindo Patterson was President of ASXRED in 1949 and played an important role in the formation of the ACA in 1950.

Selection committee members are: Frank Fronczek, Paul Langan, George Sheldrick, and Victor Young. Previous winners of the A.L. Patterson Award are: 2005: Alwyn Jones; 2002: Douglas Dorset; 1999: Gerard Bricogne; 1996: Christer E. Nordman; 1993: George Sheldrick; 1990: Michael M. Woolfson; 1987: David and Lieselotte Templeton; 1984: Jerome Karle and Herbert Hauptman; 1981: Wayne A. Hendrickson.

Please submit nominations to the ACA office, marcia@hwi.buffalo.edu, no later than May 1, 2007. The Nomination Guidelines and form are available http://www.amercrystalassn.org/Awards.htm

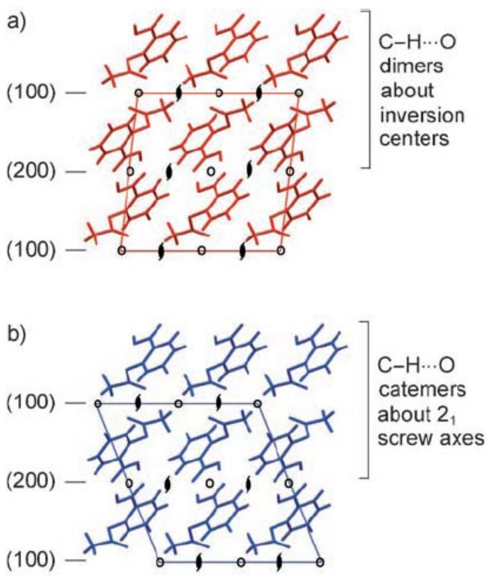
Did You Hear…?

We present in this new section recent results in the scientific area of crystallography. Your are invited to present recent papers, events, e.g. in the field of crystallography.

New headaches with aspirine

(contribution of Katharina M. Fromm, University of Fribourg)

Polymorphism is a big problem in structure prediction, especially when it comes to the protection of compounds in patents concerning pharmaceuticals. Theoretical calculations allow the prediction of possible structures. Thus, Sally L. Price et al. had predicted a polymorph "Form II" for the well-know Aspirine. "Form I" was well studied, and nobody had discovered any other form so far, until in 2005, when M. J. Zaworotko et al. published a communication on Aspirin form II.



Positions of the symmetry elements in the form I (a, on line version in red) and form II (b, on-line version in blue) crystal structures of aspirin. In both cases, centrosymmetric O–H···O dimers are formed about inversion centers in the (200) plane of the unit cell. In form I (a), centrosymmetric C–H···O dimers are formed about inversion centers in the (100) planes. In form II (b), the symmetry elements in the (100) planes are translated by ¼*c*, such that C–H···O catemers are formed about 2_1 screw axes running along *b*.

This new polymorph was repeatedly obtained during attempted 1:1 co-crystallization of aspirin and levetiracetam from hot acetonitrile, and was subsequently also observed in the presence of a molar equivalent of acetamide. This was of course a challenge for the Desiraju group to verify these findings, and they found out that the form I Aspirine data could be indexed with a different unit cell to yield the same structure as described by Zaworotko. Meanwhile, they have succeeded in the proof that a form II Aspirine does exist, but so far only in the form of intergrowths of two polymorphic domains. Now, the question arises if a new polymorph, which cannot be isolated in pure samples, is a real polymorph. Can it be protected by patents? Will it ever be isolated by itself?

Read more about it in:

- P. Vishweshwar, J. A. McMahon, M. Oliveria, M. L. Peterson, M. J. Zaworotko, *J. Am. Chem. Soc.* **2005**, *127*, 16802-16803
- A. D. Bond, R. Boese, G. R. Desiraju, *Angew. Chem. Int. Ed.* **2007**, *46*, 615-617, and idem 618-622

Anti-isostructural phase transitions

(*contribution of Klaus Yvon, Université de Genève)*

Isostructural phase transitions are relatively common in solid-state compounds, in particular those induced by external pressure such as in elements (Ce), oxides ($RFeO_3$ R=Pr,Eu,Lu), intermetallics (GdPdAl, $NdAl_xGa_{2-x}$), silicon clathrates etc. They generally lead to a volume collapse while leaving the space group symmetry unchanged.

Recently, *Vladimir Dmitriev* and collaborators of SNBL at ESRF have reported evidence for what they call ***anti-isostructural*** phase transitions. These transitions are induced by variations of external thermodynamic parameters such as temperature (T), pressure (P) and composition (x), and occur between phases that have a common parent structure but different signs of *symmetry breaking* distortions. Pure Indium, for example, crystallizes in a body-centered tetragonal structure (*I4/mmm*) that corresponds to a slightly distorted face-centered cubic (fcc) structure having an axial ratio of $(c/a)_{fct}$=1.076 if referred to the face-centered-tetragonal (fct) cell. High-pressure X-ray diffraction experiments show that c/a increases with pressure, reaching a maximum around 24 GPa, and then decreases with further compression. At 45 GPa the tetragonal phase transforms to a face-centered orthorhombic (fco) phase (*Fmmm*) as can be seen by the isoconcentration path ***0*** leading from phase **II** to phase **III** in Figure 1.

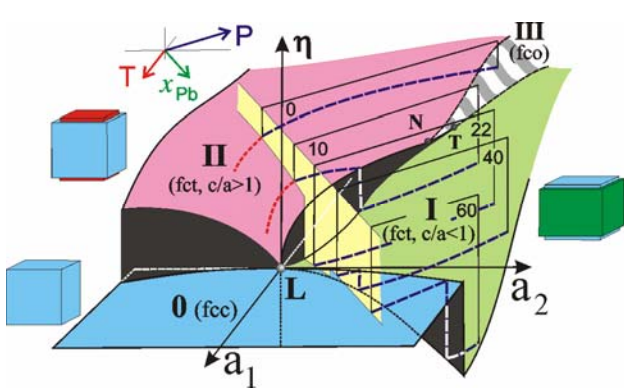


Figure 1: Equilibrium phase diagram of $In_{1-x}Pb_x$ alloys as obtained in the framework of a phenomenological model. The yellow plane (for colors see cover page) is an ambient isobaric plane. Vertical planes are isothermal-isoconcentration sections. Dashed and dotted lines show the order parameter η=(c/a-1) as a function of pressure and temperature, respectively (by courtesy from V. Dmitriev).

As Indium is partially replaced by Lead, a similar but distinctly different behavior is observed. An alloy of composition $In_{0.90}Pb_{0.10}$ (x=0.1) preserves the fct structure having c/a>1 (phase **II**) under ambient pressure conditions, but transforms discontinuously to a another fct structure having c/a<1 (phase **I**) under pressure (see path ***10***). A more Pb-rich alloy $In_{0.78}Pb_{0.22}$ (x=0.22) crystallizes in the latter fct structure (phase **I**) already under ambient pressure conditions and shows no phase transition up to, at least, 40 GPa (path ***22***). Finally, $In_{1-x}Pb_x$ alloys with 0.30<x<0.60 adopt a fcc structure (parent phase **0** in above Figure) that transforms under pressure into a fct structure having c/a<1 (phase **I**, paths ***40*** and ***60***). Thus **I** and **II** are anti-isostructural phases that derive from the parent phase **0**, and η=(c_t/a_t-1) can be considered as an order parameter of the phase transition.

Another example for an anti-isostructural phase transition was recently reported in the Ce_2Ni_7-hydrogen system. The system displays two hydride phases that derive from a parent phase having hexagonal symmetry and show different signs of orthorhombic lattice distortions. More such cases are likely to be found in the near future.

Read more about it in:

Anti-isostructural phases and anomalous thermoelasticity in In-based alloys: Synchrotron x-ray diffraction experiments and unified phenomenological model, by V. P. Dmitriev, D. Chernyshov, Y. E. Filinchuk, V. F. Degtyareva, *Phys. Rev.* B **75**, 024111 (2007)

Tetrahedral D Atom Coordination of Nickel and Evidence for Anti-isostructural Phase Transition in Orthorhombic $Ce_2Ni_7D_{\sim 4}$, by Yaroslav E. Filinchuk, Klaus Yvon, Herman Emerich, *Inorg. Chem.*; 2007; ASAP Web Release Date: 17-Feb-2007; (Article) DOI: 10.1021/ic062312u

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 imaging	May 15, Nov. 15	user.web.psi.ch
Imaging	anytime	
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. 18, 2007	www.ill.fr
FRM-II		
All instruments	26. Jan, 17. Aug.	user.frm2.tum.de

Calendar of Forthcoming Meetings

(please mail missing information on meetings of interest to Jurg.Schefer@psi.ch)

2007			**Abstract Deadline**
April 18-21	Engelberg CH	Landscape Development in Mountain Regions http://www.scnat.ch/d/Aktuell/Veranstaltungen/	
April 20	Bern CH	FEL: New Opportunities (Information day) SNF Plenarsaal, Wildhainweg 3, Bern, 09.30h	
April 26-29	Dongguang China	ICANS XVIII – Neutron Spallation Sources http://icans-XVIII.ac.cn	Expired
May 28-June 1	Strassburg France	E-MRS 2007 Spring Meeting http://www.emrs-strasbourg.com	Expired
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	Expired
June 25-29	Lund Sweden	4th European Conference on Neutron Scattering http://www.ecns2007.org	Expired
June 15-29	Istanbul Turkey	Nanoscaled Magnetism, ICNM-2007 http://web.gyte.edu.tr/ICNM/2007	Expired
July 15-20, 2007 **(new date)**	Havana Cuba	International School on Mathematical and Theoretical Crystallography www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm	
July 21-26	Salt Lake City, USA	Annual Meeting of the American Crystallographic Society aca.hwi.buffalo.edu	Expired
August 5-17	Zurich CH	The Zurich Crystallography School http://www.oci.uzh.ch/diversa/xtal_school	May 15, 2007
August 5-11	Turin Italy	41st IUPAC World Chemistry Congress http://www.IUPAC2007.org	Expired
August 5-11	Utah USA	International Summer School on Crystal Growth ISSCG 13 http://www.crystalgrowth.us/isscg13/index.php, Deadline Late News Posters	Expired May 15, 2007
August 12-17	Salt Lake City, USA	15th International Conference on Crystal Growth www.crystalgrowth.org/conferences/iccg15/index.php	May 15, 2007
August 13-17	Manchester UK	9th Int'l Conference on Biology and Synchrotron Radiation www.srs.ac.uk/bsr2007	March 31, 2007
August 20-22	Marrakech Marocco	ECM-23 Satellite Meeting "The enchanting beauty of Moroccan Ornaments (http://www.lcm3b.uhp-nancy.fr/mathcryst/marrakech2007.htm)	
Aug. 22-27	Marrakech Marocco	ECM-24: European Crystallographic Meeting http://www.ecm24.org	April 30, 2007 (2nd extension)
Sept. 10-13	Nürnberg Germany	Euromat 2007: Advanced Materials and Processes http://euromat2007.fems.org	Jan. 31, 2007
Sept. 11-12	Villigen PSI CH	User Meeting of the Swiss Light Source http://www.psi.ch/sls	to be announced
Sept. 12-13 **(new date)**	Villigen PSI CH	Annual Meeting 2007 of the SGK/SSCr http://diffraction.web.psi.ch/sgk-sscr-2007.htm	July 15, 2007
Sept. 21	Villigen PSI CH	Festkolloquium 10 Jahre SINQ	
Oct.7-9	Garmisch Germany	Size-Strain V http://www.mf.mpg.de/ss-v	Feb. 28, 2007

2008			Abstract Deadline
March 31-April 4	Villigen PSI CH	Workshop of the INTAS project Spintronics	to be announced
April 27– May 3	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
June 9-14	Zurich CH	10th International Conference on Quasicrystals, ICQ10, http://icq10.ethz.ch	Jan 15, 2008
August	Osaka Japan	IUCr-2008, 21st General Assembly and Congress of IUCr http://www.congre.co.jp/iucr2008	to be announced
Sept. 1-11	Warsaw Poland	EPDIC-11 European Powder Diffraction Conference	to be announced
Sept. 9-14	Sydney Australia	WATOC-08 World Association of Theoretical and Computation Chemists, http://www.ch.ic.ac.uk/watoc	to be announced
Nov. 17-20	Ghent Belgium	14th International Conference on Thin Films http://www.ICTF14.UGent.be	to be announced

2009			
August	Istanbul Turkey	ECM-25: European Crystallographic Meeting http://www.ecm25.org	to be announced

2010			
Sept. 29 – Oct. 5	Darmstadt Germany	ECM-26 and EPDIC-12	to be announced

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If your are working in the field of crystallography, you will be interested to become a member of our society. For more information as well as online registration, please have a look on our website (http://www.sgk-sscr.ch). Presently, the yearly membership fee is sfr. 30 (sfr. 10 for students). For new members, the membership is free until the end of 2007. Please note: SGK/SSCr members can also apply to be a member of the subsection crystal growth (no additional charge) or for individual membership of the European Crystallographic Association, ECA (additional charge: 10 Euro).

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from university	
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or use our online application form **at** http://www.sgk-sscr.ch

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