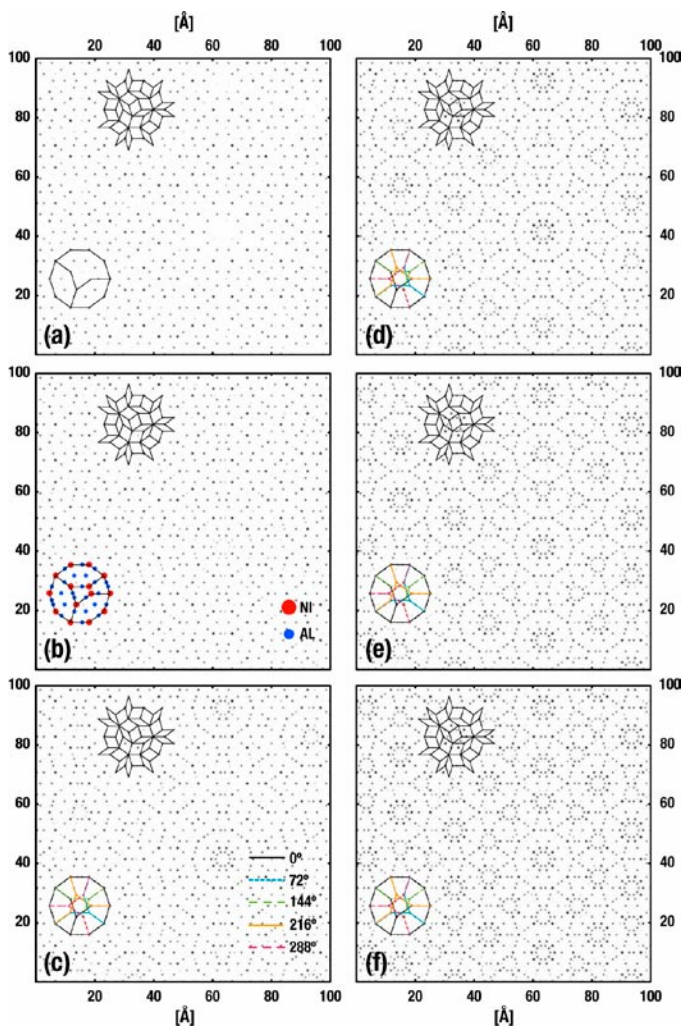




Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie

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



SGK/SSCr Newsletter No. 64

Contents :

Society News

<i>Letter of the president</i>	1
<i>Annual Report for 2004</i>	2
<i>SGK / SSCr Annual Meeting 2005</i>	5
<i>Minutes of the General Assembly 2004</i>	5
<i>SSCr and SCT Accounts 2004</i>	8
<i>2005 Membership Fees</i>	11
<i>Travel Grants</i>	11
<i>News of Members</i>	12
<i>Pictures of the Annual Meeting 2004</i>	13
Thesis Abstract: Modelling Disorder in Quasicrystals	15
SNBL Status Reports	17
New Protein Crystallography Beamline at SLS	19
Paul Scherrer Institute - Call for Proposals	21
Third International Workshop on Crystal Growth Technology	22
Calendar of Forthcoming Meetings	23

Cover page:

Depicted is the influence of phasonic fluctuations on the atomic configurations of a rhombic Penrose tiling (modelled by radii fluctuations of the atomic surfaces of the rhombic Penrose tiling in the higher-dimensional description). Average structures of the rhombic Penrose tiling with increasing amount of phasonic disorder are shown in (a-f), respectively. The highlighted cluster in (c) reveals an ordering, which can be described by a fivefold orientationally disordered version of the cluster from (a). Further increase of the amount of phasonic disorder leads to an increasing number of clusters, which are best described by fivefold orientational disorder. This means that phasons induce orientational disorder of clusters. See also the abstract of the thesis by Miroslav Kobas on page 15.

Lettre du président

Tout d'abord, j'aimerais vous souhaiter une très bonne année 2005, avec beaucoup de bonheur dans votre vie privée et de succès dans votre travail. J'aimerais aussi remercier, au nom de vous tous, mes collègues du comité qui ont assuré un très bon fonctionnement de la SSCr pendant l'année 2004.

C'est la dernière fois, que je m'adresse à vous comme président de la Société Suisse de Cristallographie. Lors de notre prochaine réunion annuelle, en octobre 2005, nous allons élire notre nouveau président ainsi que plusieurs nouveaux membres du comité. C'est peut être le moment de faire le point et de discuter la position de la cristallographie dans la recherche actuelle.

Dans ma dernière "Lettre du président" j'ai proposé une enquête sur l'enseignement de la cristallographie en Suisse. Il n'y a pas eu beaucoup de réactions ce que j'interprète comme une satisfaction générale avec la qualité et accessibilité de l'enseignement de la cristallographie aux étudiants suisses. Néanmoins, je m'adresse encore une fois à nos membres enseignants des Universités et Hautes Ecoles en Suisse: Le futur de la cristallographie dans le développement rapide de la science ne pourra être assuré que si les connaissances de la théorie et des méthodes cristallographiques sont correctement transférées à tous les chimistes, physiciens de la matière condensée, chercheurs en science des matériaux, minéralogistes et bien sûr tous les autres qui s'y intéressent, comme par exemple les biologistes. C'est sans aucune importance si les futurs chercheurs ne s'appellent plus "cristallographes" mais "chimistes" ou "scientistes de matériaux". Ce qui compte est leur connaissance en méthodes et théorie de cristallographie, car elles sont non seulement indispensables pour leur recherche, mais aussi porteuses de nouvelles idées.

Lors de notre dernière réunion annuelle, le 6 octobre 2004 à Neuchâtel, nous avons passé en revue les activités de la cristallographie en chimie, domaine traditionnellement le plus dépendant des résultats fournis par les cristallographes. Notre prochaine assemblée va être organisée par nos collègues de l'EPF Lausanne sur un thème consacré à la cristallographie en physique, domaine qui pose habituellement les questions les plus difficiles aux cristallographes. A savoir que l'année 2005 est déclarée par l'ONU "année internationale de physique" à l'occasion du 100^{ème} anniversaire des travaux importants d'Albert Einstein.

Cette année l'Europe accueillera le Congrès Mondial de Cristallographie à Florence. Je vous invite tous, et surtout nos jeunes collaborateurs, à y participer en grand nombre. La SSCr dispose de fonds pour soutenir la participation des jeunes chercheurs aux conférences. La SSCr est aussi active en organisation de conférences internationales en Suisse. La Section de Croissance et Technologie des Cristaux de la SSCr, notamment notre vice-président Hans J. Scheel, organise

le 10-18 septembre 2005 le 3^{ème} Workshop International sur la Technologie de Croissance Cristalline, IWCGT-3, à Beatenberg. L'organisation de la Conférence Européenne sur la Diffraction sur Poudres, EPDIC-10, qui aura lieu 1-4 septembre 2006 à Genève, est en cours. C'est un évènement organisé conjointement avec l'Université de Genève et je vais y consacrer toutes mes forces après ma retraite du poste de président de la SSCr. Toutes les personnes intéressées d'y participer sont bienvenues, n'hésitez pas à me contacter!

Nos installations-sources de radiations synchrotrone (SNBL et SLS) ainsi que neutronique (SINQ) ont commencé l'année 2005 en bonne santé, la SNBL avec le nouveau directeur, Vladimir Dmitriev, à qui je souhaite beaucoup de succès dans son travail.

Le nombre de nos membres est de 165 et la société semble être en bonne santé, avec des membres qui participent à sa vie active. Néanmoins, si vous avez dans votre entourage des personnes susceptibles de devenir membre de notre société, encouragez-les à s'inscrire directement sur notre site web <http://www.sgk-sscr.ch>.

L'année 2005 va être, comme les autres années, pleine de travail. Nous avons toutes les conditions réunies pour poursuivre nos recherches, faire progresser les théories de la cristallographie et la faire valoir dans nos enseignements. J'en suis certain que 2005 va être de nouveau une bonne année.

Radovan Cerny, Président de la SSCr

Annual report of the President of the SGK/SSCr for 2004

Work of the committee:

The committee met twice in 2004; in between the committee members stayed in contact by e-mail. The committee dealt mainly with managing the society, with its relationship with the ECA and with the preparation of the annual meeting 2004.

The treasurer of the SSCr, John Priestle, resigned from the committee of the SSCr at the end of this year, because he assumed new, non-crystallographic tasks within Novartis Pharma. He is replaced by Michael Henning from Hoffmann-La Roche, elected at the annual meeting 2004 of the SSCr.

Eight members joined (Fabrice Camus, Eric Germaneau and Marc Schiltz from the EPFL, Kurt Clausen from the PSI, Eva Freisinger from the University of Zürich, Gael Labat from the University of Neuchatel, Frank Stowasser from Novartis and Olaf Grassmann from Hoffmann-La Roche), and seven (Bernard Bertheville, Melchior Fehlmann, Frank Kubel, John Priestle, Guillaume Renaudin, Andreas Rüegg and Hans Peter Weber [Hochwald]) left the society during the year, so that the number of members increased to 162.

The committee has nominated Gervais Chapuis as a candidate for the Executive Committee of the IUCr, and Hans J. Scheel as a candidate for the Commission on Crystal Growth and Characterization of Materials of the IUCr.

In 2004 three SGK/SSCr Newsletters, and five IUCr Newsletters have been distributed to the members. The web page (<http://www.sgk-sscr.ch/>) and membership database of our society were regularly updated.

The committee awarded a travel grant of 700 CHF to I. Orlov (PhD student at EPFL), who gave a lecture "Ferrites through the looking glass of aperiodic crystallography" at ECM-22 in Budapest.

The committee has regularly discussed the situation at the two Swiss synchrotron sources, SNBL and SLS.

Annual meeting of the SGK/SSCr:

The annual meeting 2004 of the SGK/SSCr was held at the University of Neuchâtel, October 6, under the theme "Chemical Crystallography". Five lectures were invited:

- Jack Dunitz (ETH-Zürich), Are crystal structures predictable?
- John Helliwell (University of Manchester, UK), The molecular basis of the colouration mechanism in lobster shell.
- Irene Margiolaki (ESRF, Grenoble, France), Recent advances in protein powder diffraction at the ESRF.
- Katharina Fromm (University of Basel), Polymorphism in coordination polymers.
- Ute Kolb (University of Mainz, Germany), Nanodiffraction - a key to beam sensitive material? Unfortunately, Ute Kolb had to cancel her presentation due to health problems. She was replaced by
- Philip Pattison (SNBL, Grenoble), who gave a talk on The nature of halogen ... halogen interactions in molecular crystals.

Other 4 oral and 26 poster presentations gave an overview of crystallographic research in Switzerland.

Information on the activity of the Swiss Steering Committee of the SNBL (Swiss-Norwegian Beamline) at the ESRF, Grenoble, was given during the SGK/SSCr annual meeting.

Relation with the ECA:

The ECM-22 took place in Budapest, Hungary, August 26-31, and was attended by 650 paying participants. A satellite meeting «Crystallography at the start of the 21st century: Mathematical and Symmetry Aspects» has been organized by the Commission on Inorganic and Mineral Structures of the IUCr just before the ECM. During the ECA council meeting Hans Grimmer represented individual members, and Radovan Černý acted as representative of the SGK/SSCr.

Swiss crystallography was well represented on the ECM, it was placed on the fourth place with 42 paying participants, behind UK with 108, Germany with 103 and France with 47 paying participants.

The poster «*Atomic Displacement Parameters of the α -Polymorph of p-Dichlorobenzene Measured between 15 and 300 K*» by Aree, Thammarat; Hostettler, Marc; Chernyshov, Dmitry and Bürgi, Hans-Beat from University of Bern was awarded a Cambridge Crystallographic Data Centre (CCDC) Poster Prize in chemical crystallography.

The ECA (Max Perutz) Prize 2004 was awarded to Prof. George Sheldrick from the University of Göttingen, Germany, for his major theoretical and practical contribution to the development of direct methods and for his help to transfer the methodology into a straightforward procedure for solving small molecule structures.

One new ECA member (Algeria) and three potential members (Belorussia, Moldova and Tunisia) were presented during the council meeting.

The new web-master of the ECA web site is Massimo Nespolo from the University of Nancy.

A discussion was held about the role of the SIGs in the program of the future ECMs. The actual situation, where the SIGs are directly responsible for organizing microsymbosia, was conserved.

The ECM-23 will be organized in Leuven, Belgium, August 6-11, 2006, and ECM-24 in Marrakech, Morocco, August, 26-31, 2007.

The next ECA council meeting will take place during the XX congress of the IUCr in Florence, between August 23 and 31, 2005.

Relation with the SANW/ASSN:

Hans Grimmer represents the SSCr in the Senate and Radovan Černý in Section I of the SANW/ASSN, which contributed this year 1000.- CHF to the travel grants for young scientists, 2500.- CHF for the organization of the annual meeting, and 500.- CHF for our delegation on the council meeting of the ECA.

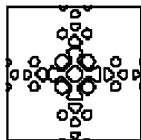
The Annual Meeting of the SANW/ASSN was held in Ob- and Nidwald, October 7-8, (<http://limits04.scnatweb.ch/>) under the title *Limits 04*.

International meetings in Switzerland:

The Third International Workshop on Crystal Growth Technology will be organized by H. J. Scheel, S. Uda and D. Witter in Beatenberg, September 10-18, 2005.

The EPDIC-10 conference will be held in Geneva, 1-4 September 2006, Uni Mail, organized by the SSCr and the University of Geneva.

Radovan Černý
President of the SSCr



SGK/SSCr
SKT/SCT

Swiss Society for Crystallography
Section for Crystal Growth and Crystal Technology

Annual Meeting 2005

October 13

Lausanne (Dorigny/Ecublens Campus)

General Theme

Crystallography in Physics

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

SECRETARY: HANS GRIMMER, PAUL SCHERRER INSTITUT, CH-5232 VILIGEN PSI
PHONE: 056 310 24 21, FAX: 056 310 31 31, E-MAIL: HANS.GRIMMER@PSI.CH

Minutes of the General Assembly

at the University of Neuchâtel, Institute of Chemistry, Av. de Bellevaux 51
October 6, 2004, 16h45 - 17h40

R. Černý, President of the Society, presided over the meeting.

Present: 21 Members and 1 Guest (Céline Besnard)

- 1) The proposed **Agenda** of the meeting is accepted.
- 2) The **Minutes of the last General Assembly** in Zürich on October 17, 2003 are accepted.
- 3) **Report of the President** (R. Černý)

Work of the committee

The committee met twice in 2004; in between the committee members stayed in contact by e-mail. The committee dealt mainly with managing the society, with its relationship with the ECA and with the preparation of this annual meeting. Eight

members joined and three left the society during the year, so that the number of members increased to 166. The committee nominated Gervais Chapis as a candidate for the Executive Committee of the IUCr and Hans Scheel as a candidate for the Commission on Crystal Growth and Characterization of Materials of the IUCr. In 2004 three SGK/SSCr Newsletters and, so far, three IUCr Newsletters have been distributed to the members. The web page and membership database of our society were regularly updated.

Relationship with the SANW/ASSN:

Hans Grimmer represents the SGK/SSCr in the Senate and Radovan Černý in Section I of the SANW/ASSN, which contributes this year 1000,- CHF towards travel grants for young scientists, 2500,- CHF for the organization of the annual meeting, and 500,- CHF for our delegation on the council meeting of the ECA.

The 2004 Annual Meeting of the SANW/ASSN will be held in Ob- and Nidwald on October 7-8.

International meetings in Switzerland:

The Third International Workshop on Crystal Growth Technology (IWCGT-3) will be organized by H. Scheel, S. Uda and D. Witter in Beatenberg, September 10-18, 2005. H. Scheel will act as one of three Co-chairmen and as member of the International Program Committee; K. Fromm will act as Treasurer.

The EPDIC-10 conference will be held in Geneva, September 1-4, 2006, Uni Mail, organized by the SGK/SSCr and the University of Geneva.

4) Report of the Section Head

K. Fromm, proxy for H.J. Scheel presents the budget of IWCGT-3, which foresees incomes and expenditures of 89000 CHF each, and asks the SGK/SSCr for a deficit guarantee of 2000 CHF, which is accorded by the assembly.

5) Report of the Section Treasurer (K. Fromm)

The Accounts for 2003 were published in SGK/SSCr Newsletter 61, the report of the auditor, M. Neuburger, in Newsletter 63. The accounts for 2003 are accepted by the assembly. The financial situation on October 5, 2004 is presented. The assets of the section have been transferred to an online-account, which charges no fees.

6) Report of the Treasurer (J. Priestle)

The Accounts for 2003 were published in SGK/SSCr Newsletter 61, the report of the auditors in Newsletter 63. The accounts for 2003 are accepted by the assembly. Credits and Debits for 2004 are presented up to October 1. Also the budget for 2005 is presented. The annual membership fees remain unchanged.

7) Report of the delegate to the ECA Council Meeting (R. Černý , proxy for H. Stoeckli-Evans):

The ECA council meeting was held in Budapest during ECM-22. Hans Grimmer represented individual members and Radovan Černý acted as representative of the SGK/SSCr.

One new ECA member (Algeria) and three potential members (Belorussia, Moldava and Tunisia) were presented during the council meeting.

The new web-master of the ECA web site is Massimo Nespolo from the University

of Nancy.

A discussion was held about the role of the SIGs in the program of the future ECMs. The current situation, where the SIGs are directly responsible for organizing respective microsymposia, is maintained.

ECM-23 will be organized in Leuven, Belgium, 6.- 11. August 2006, ECM-24 in Marrakech, Morocco, 26.- 31. August 2007. The next ECA council meeting will be held during the XX congress of the IUCr in Florence, which takes place 23.- 31. August 2005.

8) **Award of travel grants** (R. Černý)

I. Orlov (PhD student at EPFL), who gave a lecture "Ferrites through the looking glass of aperiodic crystallography" at ECM-22 in Budapest, receives a travel grant of 700 CHF.

Yaroslav Filinchuk proposes to make young scientists travel grants also available also to Postdocs. The SGK/SSCr committee will look into this at its next meeting.

9) **Election of a successor for J. Priestle as member of the SGK/SSCr committee** (R. Černý)

John Priestle, will resign from the committee of the SGK/SSCr at the end of this year because he assumed new, non-crystallographic tasks within Novartis Pharma. R. Černý thanks J. Priestle for his work on behalf of the SGK/SSCr and presents Michael Hennig (Hoffmann-LaRoche) as candidate for his succession, who is willing to act as the new treasurer of the SGK/SSCr. M. Hennig is elected unanimously.

10) **Next Annual Meetings of the SGK/SSCr** (R. Černý)

) **2005:** The European Physical Society will hold its 13th general meeting at the University of Bern on July 11-15 to commemorate Einstein's famous three contributions on the special theory of relativity, the quantum theory of the photoelectric effect and the explanation of Brownian motion by statistical mechanics, published in 1905, when he was employed at the Swiss patent office in Bern. This is also the main reason why 2005 has been declared the World Year of Physics. The Swiss Academy of Sciences (SANW/ASSN) and the Swiss Physical Society will take this opportunity to hold their annual meetings in Bern, on July 14-15, 2005.

J. Dunitz recalls that Einstein contributed also to the theory of the specific heat of solids, a topic of interest to crystallographers.

H.B. Bürgi offers to organize the annual meeting in Bern either in 2005 or 2006.

R. Černý is in contact with the French Crystallographic Association concerning a joint annual meeting in Les Houches (near Chamonix).

2006: This annual meeting was planned to take place in Konstanz together with the annual meeting of the DGK. Our society accepted the change of venue from Konstanz to Freiburg im Breisgau. However, the change of date from March to April, which was announced later, causes problems because the new date will fall into the summer semester at Swiss Universities. The committee has informed the organizer, Prof. A. Cröll, that the proposed date will prevent our participation.

It has been suggested to devote the meeting in Freiburg to the 100th birthday of Fritz Laves, who became the successor of Paul Niggli at ETHZ from 1954 until his

retirement in 1976. In this case, H. Scheel is interested in helping to organize the Freiburg meeting. If we cannot hold our annual meeting 2006 in Freiburg, we may consider combining it with EPDIC-10 in Geneva.

11 **EPDIC-10 in Geneva, 2006**

) R. Černý presents the organizing committee and the organizing agency of ERDIC-10 and encourages members interested in helping with the organisation of the meeting to let him know. He presents the budget of this conference and asks the SGK/SSCr to pay 25% towards a possible deficit but not more than 4000 CHF. This deficit guarantee is accepted.

12 **Varia**

) D. Schwarzenbach reminds the assembly of the Symposium in honour of the 60th anniversary of Prof. G. Chapuis, which will be held on October 22, 2004 at Auditoire D, Collège Propédeutique 1, Université de Lausanne.

Villigen, November 5, 2004

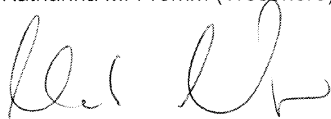
Hans Grimmer, Secretary of the SGK/SSCr

FINANZSITUATION DER SKT AM 31.12.2004

Saldoübertrag vom 31.12.2003	+ 4'282.30
Eingang SGK-Beitrag 2004	+ 600.00
Bankspesen (+Zinsen + Verrechnungssteuer)	- 24.00
<hr/>	
GUTHABEN AM 31.12.2004	+ 4'906.30



Katharina M. Fromm (Trésorière)



Markus Neuburger (Kassenprüfer)

SGK/SSCr Financial Report 2004

UBS Account
 Status 1.1.2004 9'491.26

Credits:

Membership dues (118 members)	4'814.55
ECA dues (8 members)	180.00
SANW reimbursement for Annual Meeting 2003	2'292.00
SANW reimbursement for Annual Meeting 2004	1'185.00
SANW reimbursement for ECA delegation	500.00
SANW funds for young scientists travel grants	1'000.00
Interest	67.90

Total Income **10'039.45**

Debits:

Membership dues to SANW (162 members)	1'134.00
ECA dues (SGK + individuals)	276.75
Sekt. Kristallwachstum (2004)	600.00
ECA delegation	750.00
Young Scientist travel grant	700.00
Post Giros / "Global" forms	95.50
To Cash on Hand	800.00
Gifts	70.00
Annual Meeting	1'544.40
Travel expenses, speaker (annual meeting)	485.00
Banking charges	174.40
Withholding Tax	23.75

Total Expenses **6'653.80**

Income - Expenses **3'385.65**

Starting Balance + Income - Expenses **12'876.91**

UBS Balance 31.12.2004 **12'876.91**

Cash on Hand - 2004

Status 1.1.2004	31.00
	(+ EUR 75.00)
<u>Credits:</u>	
Bank Transfer	800.00
EUR 75.- to Swiss Francs	114.25
Membership dues (1 person)	30.00
	<hr/>
Total Income	944.25
<u>Debits:</u>	
Software for Webpage editing	110.85
SWITCH (Web address "sgk-sscr.ch")	35.00
Travel Expenses, Auditors	96.00
Travel Expenses, Executive Committee	208.60
	<hr/>
Total Expenses	450.45
Income - Expenses	493.80
Starting Balance + Income - Expenses	524.80
 Cash on Hand 31.12.2004	 524.80

Status of other Accounts

CS (savings account)

Status 1.1.04	16'418.90
Interest (1.0%)	164.20
Withholding Tax (35%)	-57.45
	<hr/>
Balance 31.12.04	16'525.65

Post Account

Status 1.1.04	367.27
Interest (1.0%)	3.65
Withholding Tax	-1.30
	<hr/>
Balance 31.12.04	369.62

2005 MEMBERSHIP FEE

I would like to take the opportunity to thank all the members for promptly paying their membership fees. These will remain unchanged for 2005 and stand at:

full member	30 CHF / year
student member	10 CHF / year
institutional members	130 CHF / year

- Please use the enclosed red PTT form to pay the fee for 2005 by the end of March (Bank transfers and post giro are preferable to payments at the PTT counter as this saves us CHF 1.20 / transfer).
- Several of the fees for 2004 and even a few for 2003 or earlier are still missing. A letter indicating the total amount due has been included with this newsletter to the members concerned.
- Institutional members will be mailed a special invoice.
- Members of the ECA can also use this opportunity to pay their annual ECA dues (EUR 10.- = CHF 15.-). This way we can make a single foreign bank transfer to the ECA and avoid having each member make an individual one (typically CHF 15.- each). Please note on your payment whether you are also including your ECA membership fees.

Thank you for your cooperation.

Your treasurer,
Michael Hennig

Travel Grants for Young SGK/SSCr Members

The Swiss Academy of Sciences (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.

News of Members

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

Donat Jozsef Adams (Laboratorium für Kristallographie, ETH Zürich)

Vladimir Dmitriev (Swiss-Norwegian Beam Lines, Grenoble, France)

Gael Charles Labat (Institut de Chimie, Université de Neuchâtel)

Oksana Zaharko (Labor für Neutronenstreuung, Paul Scherrer Institut, Villigen)

Important birthdays in 2005:

80th birthday Prof. Hans Wondratschek - Uni Karlsruhe

65th birthday Prof. Marc Ilegems - EPD Lausanne
Dr. Pedro Moeckli - Zürich

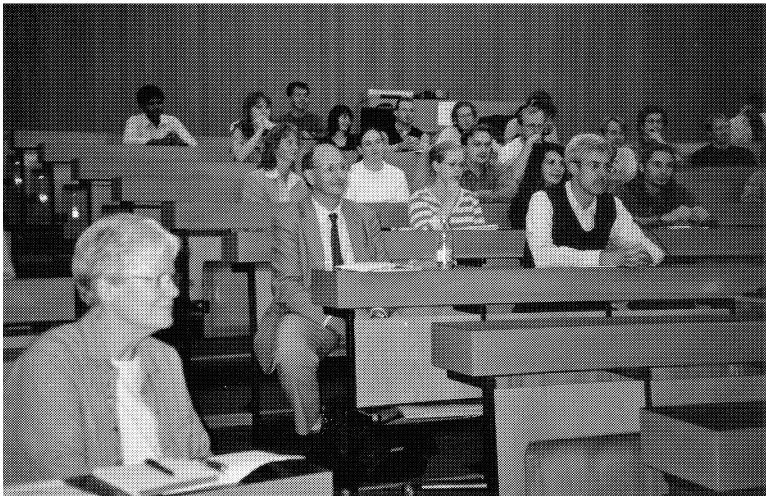
60th birthday Dr. Gérald Bernardinelli - Uni Genève
Dr. David F. Sargent - ETH Zürich
Paul Seiler - ETH Zürich
Dr. Jan-Derk Smit - Bonstetten
Dr. Phillip Smith - New York University

50th birthday Dr. Franco Rossi - Wetzikon
Dr. Jürg Schefer - PSI

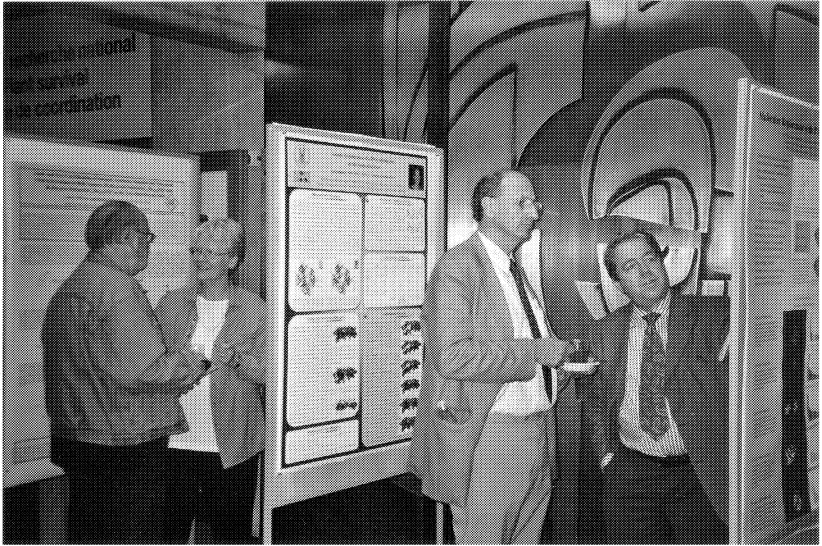
Impressions from the Annual Meeting 2004 in Neuchâtel



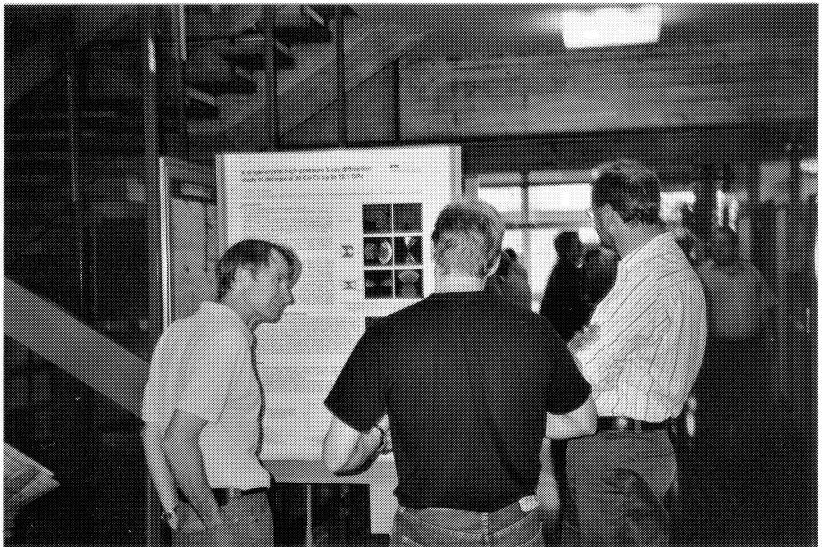
Lecturers and organizers gather on the evening before the annual meeting
(Picture taken by Katharina Fromm, the others were taken by Hans Grimmer)



Listening to Phil Pattison's lecture



Lively discussions during the poster sessions



Diss. ETH Nr. 15819

Modelling Disorder in Quasicrystals

Decagonal Al-Co-Ni

Dissertation
submitted to the

Swiss Federal Institute of Technology Zurich

for the degree of
Doctor of Natural Sciences

presented by

Miroslav Kobas

Dipl. Werkstoff-Ing. ETH
born 23 September 1975, citizen of Kirchberg SG

Accepted on the recommendation of

Prof. Dr. Walter Steurer	Examiner
Dr. Thomas Weber	Co-examiner
Prof. Dr. Friedrich Frey	Co-examiner

Summary

The theme of this doctoral thesis is the modelling of structural disorder phenomena from decagonal Al-Co-Ni quasicrystals by an analysis of full diffuse X-ray scattering data as a function of temperature. The motivation for this study is to reveal the complex ordering principles of decagonal Al-Co-Ni quasicrystals and, consequently, to understand the driving force for the formation and stability of these materials.

For the first time, the 3D difference Patterson (autocorrelation) function of a disordered quasicrystal (*Edagawa-phase*) has been analysed. A new technique, the *punch-and-fill* method has been developed to separate diffuse scattering and Bragg reflections. Its potential and limits are discussed in detail. The calculated difference Patterson maps are interpreted in terms of inter-cluster correlations as a function of temperature. Both, at high and low temperatures, clusters decorate the vertices of the same quasiperiodic covering. At high temperatures, medium-range

inter-cluster correlations are present, whereas at low temperatures, the ordering between the clusters becomes more complicated. Qualitatively, the Patterson maps may be interpreted by inter-cluster correlations, which take place mainly inside pentagonal superclusters below 1120 K, and inside larger decagonal superclusters at 1120 K. The pentagonal supercluster consists of five *Gummelt* clusters at the corners of a star-centred pentagon with ≈ 20 Å edge length; the decagonal supercluster is composed of one central *Gummelt* cluster edge-joiningly surrounded by a ring of ten further overlapping *Gummelt* clusters.

The hydrodynamic theory of phasonic and phononic disorder has been applied successfully to describe the short-range, disordered structure of the *Edagawa-phase*. Moreover, model calculations demonstrate that the main features of diffuse scattering can equally well be described by phasonic disorder and fivefold orientational disorder of clusters. The calculations allow distinguishing the different cluster types published so far and the best agreement with experimental data could be achieved with the mirror-symmetric Abe-cluster. Modelling of phasonic diffuse scattering associated with the S1 and S2 superstructure reflections indicates disorder of superclusters. The former basically show inter-cluster correlations inside quasiperiodic layers, while the latter exhibit intra- and inter-cluster correlations, both between adjacent and inside quasiperiodic layers. The feasibility, potential and limits of the Patterson method in combination with the *punch-and-fill* method employed is shown on the example of a phasonic disordered rhombic Penrose tiling. A variation of the elastic constants within the framework of the hydrodynamic theory does not change qualitatively the way phasonic disorder is realized in the *local* quasicrystalline structure. For the same model system it is also shown that phasonic fluctuations of the atomic surfaces give average clusters in the cut-space, which correspond to fivefold orientationally disordered clusters, *i.e.* phasons induce fivefold orientational disorder of clusters.

A Patterson analysis of the diffuse interlayers from the *Edagawa-phase* showed that the main unit for correlated displacements along the periodic direction is a disordered structure motif (cluster) with a diameter of ≈ 15 Å, the fine structure of which does hardly change as a function of temperature. At 1120 K, the displacements of the clusters are uncorrelated along quasiperiodic directions, while at lower temperatures ≈ 42 Å-sized superclusters of a well-defined shape are formed. The spatial distribution but not the internal structure of the superclusters differs significantly at 1070 K and 300 K.

SNBL status, January 2005

Gervais Chapuis, chairman of the Swiss Steering Committee

Since 1st January 2004, the SNBLs have a new administrative structure in the form of a Foundation under Swiss Law and established in Lausanne. The creation of this new administrative structure, the SNX foundation, was necessary following the transfer of the Institute of Crystallography from the University to the EPFL. The foundation was the best compromise in order to accommodate the spirit of independence required by our Norwegian partners and by the BBW (Bundesamt für Bildung und Wissenschaft), the funds providing institution for the Swiss partners.

Each country delegates three members to the SNX foundation. The present Swiss delegates are Rafael Abela, from SLS, chairman of the SNX foundation, Radovan Cerny from the University of Geneva and Gervais Chapuis from the EPFL in Lausanne. These delegates are designated by the Swiss Steering committee of the SNBL, an institution comprising members from the ETHs, SLS, interested Universities and a permanent guest from BBW.

Also at the beginning of 2004, an agreement has been signed between the two national institutions (BBW and the Norwegian synchrotron Association) to secure the funding of the SNBLs for the next four year period, *i.e.* 2004-2007. This period obviously corresponds to the Swiss parliamentary calendar for the funding of scientific and educational projects. We are glad to report that the SNBL funding that is expected to be attributed over the four year period represents a non negligible increase of the yearly budget of the SNBLs.

Concerning the technical aspects of the SNBLs, we refer to the report of Phil Pattison on the current situation and the future projects.

During the first meeting of the SNX foundation (the first meeting following the new organisation) which took place in May 2004, the SNX council has decided not to extend the mandate of the former beamline director beyond the end of 2004. The new position of the beamline director has been widely announced in various journals and the deadline has been set to the end of October 2004.

In the second SNX meeting, which took place in December 2004, the council has selected its new director, Prof. Vladimir Dmitriev along with Dr. Phil Pattison as deputy director. Both have started their new functions on 1 January 2005. Vladimir has been involved in the SNBLs for a few years as a member of the high pressure team and is therefore already familiar with the Grenoble synchrotron environment.

The perspective of the SNBLs looks very bright, and we hope that the appointment of the new director and deputy director will correspond to a new era of successful exploitation and development of the SNBL and in a closer collaboration with the SLS.

SNBL Technical Status Report, November 2004

Phil Pattison, deputy director, SNBL

Both of the Swiss Norwegian Beam Lines at the ESRF are fully operational and there are no serious technical problems to report. There has been a heavy schedule of experiments on both stations, with a noticeable increase in the technical complexity of the proposals. In particular, there is a trend towards in-situ experiments aimed at investigating, for example, catalytic reactions, hydrogenation processes and structural phase transitions. In addition to the clear need to observe the sample in-situ, there has been an accompanying demand to use more than one experimental technique simultaneously (or at least sequentially), in order to provide additional characterization of the state of the sample. Considerable interest was generated by the test installation of an on-line Raman spectrometer which could collect data during a temperature-dependent powder diffraction measurement. Several proposals are now in preparation in which the aim is to exploit this combination (although the Raman spectrometer itself is only available on loan, for the moment). In another experiment, EXAFS data were collected in order to follow a catalytic reaction, and at the same time residual gas analysis provided a means to monitor continuously the progress of the chemical reaction. In a diffraction experiment on a myoglobin sample, micro-spectrophotometry (photoabsorption measurements on a single crystal) allowed the myoglobin-peroxide reaction to be followed both structurally and spectroscopically. In another series of single crystal experiments on various brominated organic crystals, the anomalous signal was followed both by observing the diffraction pattern and by measuring the directional dependence of the X-ray fluorescence from the K-edge absorption.

Two new detector systems have been installed and successfully commissioned on SNBL. On beamline BM1A, the CCD area detector on the KM6 multi-axis diffractometer is performing well. The data collection time for a complete structural study now takes about 1 hour, compared to 3-4 hours on the MAR345 image plate set-up. The combination of area detector and point detector simultaneously mounted on a 6-circle diffractometer is currently a unique crystallographic facility world-wide. On beamline BM1B, a new solid state fluorescence detector with 13 independent channels is now operational. This detector allows the concentration limit for fluorescence EXAFS measurements to be reduced dramatically. There is also an upgrade of the mechanical and x-ray optical layout of BM1B in progress, which when completed early in 2005 will provide substantially more space within the experimental hutch. This extra space will greatly facilitate the development of in-situ experiments and the combination of different techniques mentioned above.

A new Beamline for Protein Crystallography at the Swiss Light Source

*Michael Hennig (F. Hoffmann - La Roche AG)
and Clemens Schulze-Briese (SLS at PSI)*

After less than 2.5 years of planning and construction, the second beamline for protein crystallography X10SA was opened with a celebration on 19th of January 2005. In summer 2002, the pharmaceutical companies F. Hoffmann – La Roche and Novartis agreed to finance together with the Max Planck Society (Germany) the construction of a new undulator beamline using synchrotron radiation produced by the Swiss Light Source (SLS) at the Paul Scherrer Institute (PSI).

Synchrotron radiation has become indispensable for protein crystallography and the demand for beam-time has increased continually since the start of operation of the first beamline for protein crystallography X06SA at the SLS in September 2001. In the lectures of Hans Widmer from Novartis and René Imhof from Roche, the importance of crystal structure information for the drug discovery process was highlighted. Novartis showed the crystal structure of Abl kinase with Glivec and how this structural information will be used to overcome drug resistance and to further optimize this drug molecule. Roche presented examples of crystal structure determinations where the high quality of the existing beamline X06SA at the SLS was essential for the progress. The use of the structural information for drug design and rapid optimization of drug molecules was shown with DPP-IV as an example. Finally, the crystal structure of the monotopic membrane protein oxidosqualene cyclase was shown, which gave insight into the catalytic mechanism of the synthesis of lanosterol – a precursor of cholesterol. The importance of synchrotron radiation for structural biology and the MPG was highlighted by M. Baumeister from the MPG. He stressed that the investment in the SLS was financed despite major cutbacks of the budget of the society.

The users are looking forward to regular access to a state-of-the-art protein crystallography facility, high quality SLS-radiation and a continuation of the positive collaboration with the Macromolecular Crystallography group at the SLS.

Description of the main parameters of the new beamline

The concept of the new beamline X10SA can be summarised as *a high-throughput beamline for challenging projects*. The design and layout is based on its very successful predecessor X06SA. A U19 in-vacuum undulator operated between 4.5 and 7.5 mm gap produces high brightness X-rays in the energy regime of 5.5 to 20 keV. A liquid-nitrogen cooled Si(111) fixed-exit

monochromator selects an energy bandpass of $2 \cdot 10^{-4}$, compatible with the requirements of MAD-experiments. The second crystal of the monochromator focusses the beam in horizontal direction while the downstream mirror focusses in the vertical plane. The optical elements allow the focal spot size to be adjusted between $50 \times 10 \mu\text{m}^2$ and $500 \times 200 \mu\text{m}^2$. The flux on sample above 10^{12} photons/s can be adjusted by means of filters to suitable levels. The good access to the goniometer due to the A-frame geometry (Figure 1) was appreciated by the X06SA users and was hence implemented also at the new beamline. In addition to many mechanical improvements the new sample environment excels by its new sample microscope, which provides crystal images of outstanding optical quality, thereby significantly facilitating sample centring. The mar225 mosaic detector (3072×3072 pixel) with a read-out time of 1 second provides adequate performance even for very demanding experiments.

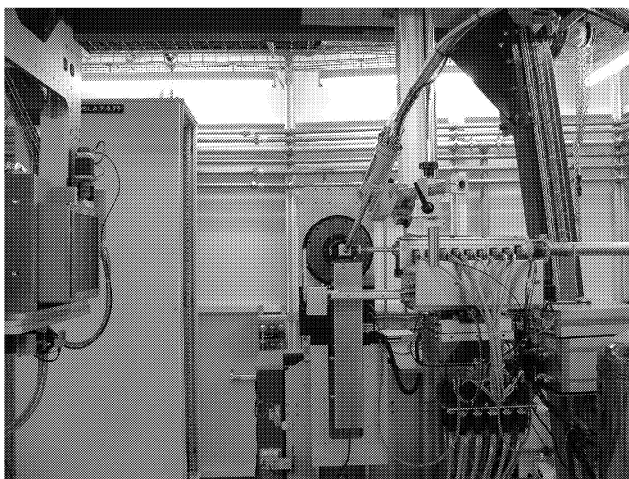


Figure 1: The setup in the experiments hutch of beamline X10SA. The X-ray beam comes from the right and impinges on the sample, which is mounted on a motorised goniometer head, which itself is mounted on an air-bearing rotary stage. The motorised beamstop prevents the direct beam from falling on the mar225 CCD detector, which is located at the left side of the picture. Note that the heavy detector is mounted on a separate support to prevent any coupling of its motion to the sample.

The graphical user interfaces at X10SA are similar to those at the old beamline to facilitate the user's adaptation. Future work will concentrate on further automation of the experiment, e.g. fully automatic MAD experiments and automatic crystal centring. Finally, the new beamline offers a larger laboratory for sample preparation, in particular to load robot magazines under liquid nitrogen, once a sample changing robot will have been installed by the end of this year.

PAUL SCHERRER INSTITUT



Swiss Spallation Neutron Source SINQ
Swiss Synchrotron Light Source SLS
Swiss Myon Source S μ 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 μ SR facility (S μ 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 μ S:

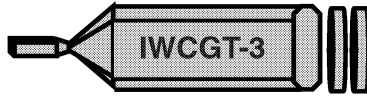
All instruments	:	01/12
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The central PSI User Office offers a joint Web portal, from where all necessary information can be obtained: <http://user.web.psi.ch>

Contact address:

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 E-mail : sinq@psi.ch,



Third International Workshop on Crystal Growth Technology*

Beatenberg above Interlaken, Switzerland

September 10 to 18, 2005

IWCGT-3 is organised under the auspices of the International Organisation of Crystal Growth IOCG
 With support from Asian Society for Crystal Growth and Crystal Technology; German Society for Crystal Growth (DGKK); Japanese Association for Crystal Growth; Korean Association of Crystal Growth; Swiss Society for Crystallography (SSCr), Section for Crystal Growth and Crystal Technology of the SSCr; and Northrop Grumman/USA

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► Approx. 40 one-hour lectures of top specialists in crystal fabrication and crystal machining

► Number of participants (involved in industrial crystal fabrication and crystal machining) limited (120)

Crystal technology was essential for the development of modern computer and communication technologies. Now it will become a key factor for development of GaN- and SiC- based technology for **saving energy** (high-temperature high-power electronics and LED-based illumination) and for progress in **renewable energy** (mass production of highest-efficiency photovoltaic solar cells, high-power and radiation-resistant Laser and nonlinear-optic crystals for Laser-fusion energy). Therefore, two evening panel discussions are planned, in addition to the related lectures, to discuss "Crystal Technology for Energy" and "Need for Education of Crystal Technologists (crystal growth engineers, epitaxy engineers)". The workshop is a chance for the half dozen Swiss companies - producing crystals and producing crystal slicing machines - to interact with international specialists.

For more information and for the Application / Registration Form see

www.beatenberg.ch/IWCGT-3 or contact hans.scheel@bluewin.ch

As a result of the first workshop in Beatenberg 1998, the book "**Crystal Growth Technology**" with 29 contributions of ISCGT-1, 694 pages, editors Hans J. Scheel and T. Fukuda, has been published by Wiley & Sons, Chichester UK in September 2003 (ISBN 0-471-49059-8) and as paperback April 2004 (ISBN 0-471-49524-7).

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>

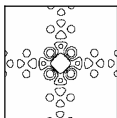
2005

16. – 18. March	Pisa (Italy)	Non Ambient Diffraction Workshop
18. March	Aachen (Germany)	Kolloquium über aktuelle Fragen der Kristallographie aus Anlass des 80. Geburtstages von Prof. Hans Wondratschek
7. – 8. April	Harwell (UK)	25th Anniversary of Condensed Matter Theory at ISIS and RAL
12. – 14. April	Loughborough (UK)	BCA Spring Meeting
17. – 21. April	Miami (USA)	Study of Matter at Extreme Conditions Conference (SMEC 2005)
12. – 22. May	Erice (Italy)	Evolving Methods in Macromolecular Crystallography
28. May – 2. June	Walt Disney World (USA)	ACA Annual Meeting
31. May – 3. June	Strasbourg (France)	E-MRS 2005 Spring Meeting: Symposium P
17. – 22. June	Helsinki (Finland)	Molecular Crystal Engineering Conference
19. – 28. June	Heidelberg (Germany)	7 th EMU School: Mineral Behaviour at Extreme Conditions
20. – 24. June	Nancy (France)	International School on Mathematical and Theoretical Crystallography
18. – 23. August	Siena (Italy)	IUCr Computing School (prior to the Florence congress).
23.	Florence (Italy)	XX Congress of the International Union of

– 31. August		Crystallography
30. August – 2. Sept.	Sheffield (UK)	The 10 th European Conference on Solid State Chemistry
2. – 8. Sept.	Brussels (Belgium)	Electron Crystallography School 2005 - ELCRYST 2005: New Frontiers in Electron Crystallography
5. – 7. Sept.	Dübendorf (Switzerland)	International Conference on Perovskites - Properties and Potential Applications
10. – 18. Sept.	Beatenberg (Switzerland)	3rd International Workshop on Crystal Growth Technology (IWCGT-3)
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
13. October	Lausanne (Switzerland)	Annual Meeting 2005 of the SGK/SSCr "Crystallography in Physics"
27. Nov. – 2. Dec.	Sydney (Australia)	International Conference on Neutron Scattering 2005

2006

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 rd European Crystallographic Meeting (ECM-23)
1. – 4. Sept.	Genève (Switzerland)	10th European Powder Diffraction Conference (EPDIC-X)



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Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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