

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 13 · Issue 3

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Yuji Ohashi

It is an honor for me to have been elected as the President of the IUCr from 2005 to 2008 at the General Assembly in Florence. Although I have been serving the IUCr for more than 15 years as a member of the Commission on Structural Chemistry, as a Co-editor of *Acta Crystallographica* Sections A, B and C, and as a member of the Executive Committee, I appreciate my increased responsibility to the IUCr as President.

At the same Assembly, it was officially confirmed that the 21st IUCr Congress will be held in Osaka, Japan, August 29-31, 2008. The 9th Congress was held in Kyoto in 1972 and so it will be 36 years since the last Congress was held in Japan, which was also my first opportunity to attend an IUCr Congress.

In the three decades since the Kyoto Congress, X-ray crystallography has grown extensively, especially in structural chemistry and biology, compared with the former six decades from 1912, when the first X-ray diffraction experiment was performed by Laue. This growth is due in part to the development of methodologies such as direct methods and isomorphous replacement. Additionally, automated diffractometers, such as the four-circle diffractometer and more recently CCD or IP diffractometers, have enabled very rapid and accurate data collection. Computers have made the difficult task of structure analysis fast and convenient. Recently, the advent of synchrotron radiation has made structure analysis even faster and easier than before. The above methodological and technical developments have made crystallography one of the most pervasive basic sciences. Nowadays, many scientists, not formally trained as crystallographers can analyze crystal structures by themselves.

Furthermore, in the past fifteen years genomics and nanotechnology have been pursued extensively in many countries. In these projects, crystallography has played an important role. Many scientists want to analyze the three-dimensional structures of target molecules and crystals. In other words, using an Asian expression, in the last ten years a very good “wind” has been blowing in the field of crystallography, especially in structural biology and nano science. We have been studying crystallography without anxiety in the stream of the good wind.

The relation between structure and function in more complex biological systems such as membranes or nerves has become the object of public attention. Inorganic and organic substances with more specific functions than before have become increasingly important in material sciences. Not only the structure but also the dynamic nature of the interacting molecules should be analyzed. We must take steps to ensure that crystallography continues to flourish. To accomplish this I believe we need to promote the following two initiatives.

The first is the development of new crystallographic techniques. More complex structures of crystalline or non-crystalline substances and their dynamically changing structures should be analyzed more precisely. Time-resolved experiments or surface diffraction, for example, may give rise to new areas for crystallographic studies. The IUCr will strongly encourage crystallographers to hold seminars on new techniques and to publish articles and books on new developments.

The second is the wider expansion of crystallography to scientists in other scientific fields. This will bring more difficult but challenging problems to crystallographers and crystallography will develop even further. Moreover, crystallography should be expanded to include scientists in the developing countries.

Because of expensive equipment and the difficulty of accessing large facilities with synchrotron radiation or neutron sources, the numbers of crystallographers and teaching systems are insufficient in the developing countries. The IUCr will provide strong encouragement to crystallographers in developing countries not only by providing support for young scientists to enable them to attend international conferences, but also by supporting schools and seminars held in those countries by sending experts as lecturers. The IUCr will also ask large facilities to support scientists from the developing countries.

I have made efforts to promote these initiatives as a Commission member and when I was AsCA President. I plan to continue to promote these as the IUCr President in collaboration with the Executive Committee, all Commission members and the staff in the Chester Office. However, we cannot accomplish this ourselves. I hope that all crystallographers will give us strong support to enable further development in crystallography to take place. I am confident that we will be able to show progress in these areas at the Osaka Congress in 2008. Furthermore, we will be able to celebrate the 60th anniversary of the IUCr in 2008.

Yuji Ohashi, yohashi@cms.titech.ac.jp

LETTER TO THE EDITOR

Letter to the Editor

Dear Prof. Daux,

In your President's Letter in Vol. 12, No. 1 (2004), you quoted from a speech of UN Secretary, Kofi Annan, who touches upon very important problems. We share Mr. Annan's view that all independent countries should develop self-governed scientific centers in order to address questions of vital importance and immediate interest to their country and to all humanity, (such as terrorism, preservation of the environment, struggle against contagious diseases, and above all, struggle against extension and production of weapons of mass destruction).

We share your anxiety concerning these problems and your concern with the destiny of our beautiful planet.

Taking into account the importance of X-ray crystallography to advancing an understanding of science and the structure of substances and in particular the structure of crystals and also the peaceful character of crystallography and its complexity, we opened a new laboratory on our own initiative, the "X-Ray Bunch Laboratory", for development of this science in Armenia. We hope to become a useful and important center in our region.

An article written by M. Navasardyan, entitled "Controllable variation of the intensity of diffracted X-ray beams and double modulation of such beams for transmission and reception of audio information", published in the *J. Appl. Crystallography* was cited in the *IUCr Newsletter*, Vol. 10, No.1, p.6 (2002).

We hope to determine the cause of this phenomenon of "Controllable Complete Reflection", the absolute diverting of an X-ray beam in the direction of diffraction in the presence of external influences. We shall also look for different applications for a powerful oscillating stream of X-ray and synchrotron radiation with the help of our modulator of X-rays. We ask for the support of the IUCr.

K.T.Hayrapetyan, Director of the "X-Ray Bunch Laboratory",

M.A. Navasardyan, and S.N. Noreyan

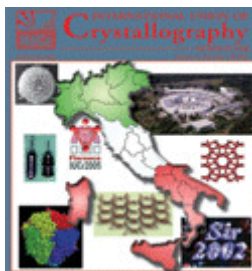
I urge members of the IUCr community from throughout the world to find ways in which they can assist crystallographers such as Drs. Hayrapetyan, Navasardyan, and Noreyan in Armenia and other developing countries to develop crystallographic capabilities with gifts of books, used instruments and research collaborations.

William L. Duax

IUCr Past President

LETTER TO THE EDITOR

Letter to the Editor



Dear Judith,

I really liked the newsletter booth in Florence, with all the colorfull posters of the cover pages. You are really doing a great service to the Union!

I noticed that our idea of having in the cover page a map of the country surrounded by smaller pictures of crystallographic interest (Vol. 12, No. 1), had been carried over to all subsequent issues with a national Cover Story. Unfortunately in the printed edition of our Cover Story on "Crystallography in Italy", the due acknowledgment to Dr. Gianluca Croce, the young crystallographer who had the idea and made the graphical composition, was cut out.

Davide Viterbo

Davide,

Thank you for the lovely compliment and for correcting our inadvertent omission of giving credit to Gianluca for the beautiful cover for issue 12#1.

Judith

EDITORIAL

Editorial



I came away from the IUCr Congress in Florence with two lasting impressions: One – that Carlo Mealli, Paola Paoli and their respective committees did an incredible job in putting together a most memorable Congress and two – a deep disappointment with the way the Executive Committee (EC) organized the election process.

Let me give you a little background on the process. In the spring of 2004 the IUCr Executive Secretary, Mike Dacombe, sent notices to the National Committees of all countries adhering to the Union requesting nominations for the Executive Committee (EC) and for the various commissions. By the deadline two nominations had been received for both IUCr President and General Secretary/Treasurer; 16 names had been submitted as candidates for Ordinary Member positions and no nominations had been received for IUCr Vice-President. However, the slate of candidates presented to the delegates in Florence was surprisingly sparse in that it listed one candidate each for President, Vice-President and General Secretary and 6 candidates for the 3 Ordinary Member positions.

Since I have been old enough I have voted in every US election possible, and while I have often been less than pleased with the results I at least knew that the ballot would contain the names of all candidates that had qualified to be there. This is a fundamental part of the democratic process and, therefore, as a defender of choice in all areas I was extremely distressed with the slate as it was presented to us in Florence. I could not help but feel that the top three offices had been pre-selected and that the field for ordinary members had been pre-filtered by the EC.

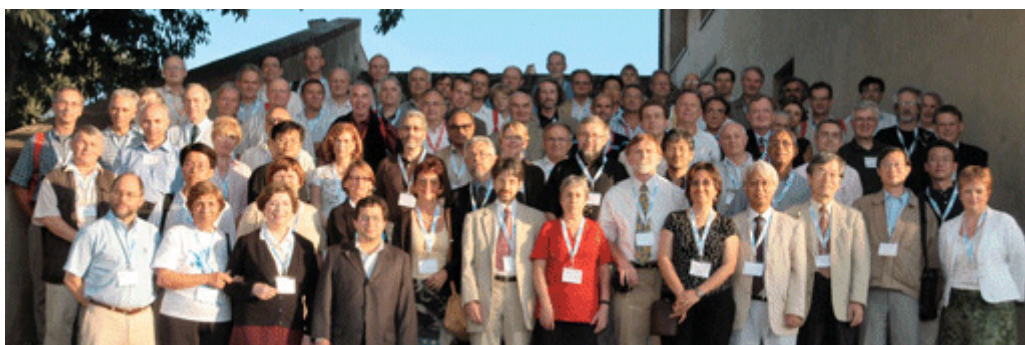
My four companions on the US delegation shared this frustration as did a significant number of delegates from various other countries. As a result Maria Carrondo was re-nominated by petition. The petition carried the signatures of delegates from seven separate countries. We had expected that her name would simply be added to the ballot without bias, but instead there were expressions of strong disapproval by some members of the sitting EC both before and during the General Assembly meetings. It would be counter-productive to elaborate on this here and I would instead offer the following simple suggestions:

1. That, subject to current by-laws, all candidates who are nominated should be included on the ballot.
2. That the entire process should be carried out in the open – using the IUCr Newsletter to keep the community informed of progress.
3. That prior to the Congress an issue of the IUCr Newsletter should carry the following on each candidate: Background information (educational, relevant professional or organizational experience and research interests) and a personal statement describing why they think they should be elected and what they would hope to accomplish if elected.

I have high hopes that the newly elected members of the EC already share many of these views and that change will come from them. However, to ensure that change takes places I would further suggest that the National Committees give serious consideration to proposing changes to the IUCr by-laws governing election procedures.

Please understand that I hold the elected President, Yuji Ohashi, in the highest esteem and that my comments have been directed solely at the process and not at him personally. I also have only the greatest admiration for Maria Carrondo who was willing to be the flag bearer for those of us who

attempted to change the status quo – to be willing to say that ‘because that’s the way it has always been done’ is simply not acceptable.



National Committee Delegates to the Congress

Unfortunately, many of us left Florence with the impression that there was also an undercurrent of gender bias in the elections. This is wrong-headed thinking that has no place within any scientific community, especially one that has benefited greatly from the contributions of women. Maria responded to the undercurrent most eloquently in the closing remarks of her statement presented at the general assembly – “I would like to think that all women crystallographers around the world (young and not so young) would regard a woman as President of IUCr as a stimulus and incentive for their careers, in the sense that they would feel encouraged in pursuing and achieving important goals, no matter how difficult, inaccessible or controversial they might seem.”

Change is healthy and should be a stimulus for the continued growth and evolution of the crystallographic community in which we are all equal partners.

Respectfully,

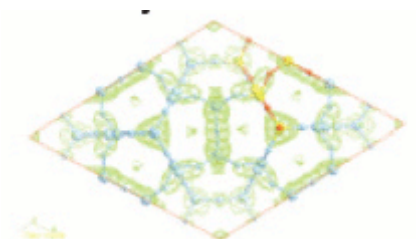
Judith L. Flippen-Anderson

flippen@rcsb.rutgers.edu

IUCR JOURNALS NEWS

Electron crystallography of zeolites - the MWW family as a test of direct 3D structure determination

***Acta Cryst.* (2005). A61, 516-527**



Direct methods [001] MWW potential map compared to actual structural framework.

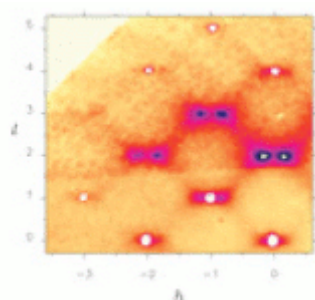
The 3D crystal structure of zeolites in the MWW framework family is determined from electron diffraction intensities by direct phasing using maximum entropy and likelihood. Although the 'missing cone' left from incomplete goniometric data sampling leads to a somewhat distorted model, the true zeolite framework geometry may be recovered by imposing conservative bonding restraints.

D. L. Dorset, W. J. Roth and C. J. Gilmore

Diffuse scattering and ordering in the short-range modulated paraelectric phase of sodium nitrite, NaNO_2

Diffuse scattering and ordering in the short-range modulated paraelectric phase of sodium nitrite, NaNO_2

Acta Cryst. (2005). B61, 473–480



A portion of the hkl layer of NaNO_2 containing diffuse satellite reflections recorded at 442 K and reconstructed by the program *CrysAlis*.

Contrary to the well known modulated structures with sharp satellite reflections, the diffraction pattern of a short-range modulated structure contains diffuse satellite reflections. The crystal structure of NaNO_2 above $T_N = 437.7$ K in the paraelectric phase is short-range modulated. The nanodomains elongated in the $[001]$ direction are remnants of distorted fragments of the sinusoidally modulated crystal structure of antiferroelectric NaNO_2 . The size of the nanodomains and the range of order decrease with temperature. Above 480 K diffuse satellite reflections are replaced by broad diffuse streaks and the nanodomains become hardly visible.

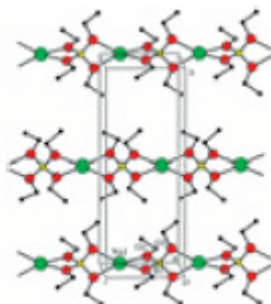
K. Lukaszewicz, A. Pietraszko and M. Kucharska

IUCR JOURNALS NEWS

catena-Poly[sodium(I)- μ -tetraethoxyborato]

catena-Poly[sodium(I)- μ -tetraethoxyborato]

***Acta Cryst.* (2005). C61, m417-m418**



View of the unit-cell contents of the title compound along the *a* axis, showing the one-dimensional polymers along the twofold *c* axis.

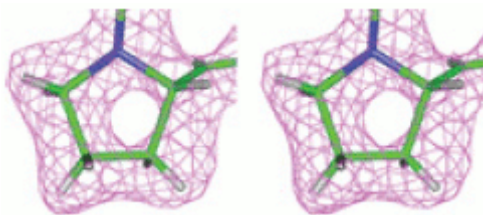
Recent interest in using borohydrides as hydrogen storage media for a future 'hydrogen energy economy' initiated our interest in alcoholysis derivatives of sodium borohydride. The title compound, $\text{NaB}(\text{OEt})_4$, is accessible from both sodium borate and sodium borohydride. The crystal structure shows the compound existing as a one-dimensional polymer, incorporating 4-coordinated sodium atoms. The simplicity of the structure is in contrast with the methoxide derivative, which contains methanol molecules bridging 5-coordinated sodium atoms in a two-dimensional structure, and the ethylene glycol derivative, which incorporates 6-coordinated sodium atoms.

G. J. Gainsford and T. Kemmitt

IUCR JOURNALS NEWS

High-resolution neutron protein crystallography with radically small crystal volumes: application of perdeuteration to human aldose reductase

Acta Cryst. (2005). D61, 1413-1417



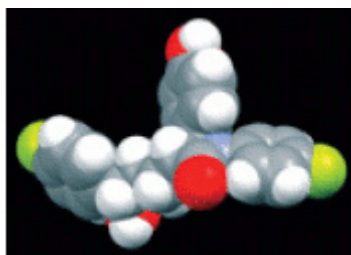
Full deuteration of human aldose reductase (MW = 36 kDa) significantly improved the neutron diffraction signal/noise ratio compared with that obtained with hydrogen/deuterium partially exchanged samples. Consequently, a good quality data set (2.2 Å resolution at room temperature) was collected on the LADI diffractometer at the ILL neutron source (France), with a crystal volume (0.15 mm³) radically smaller than usual for neutron diffraction studies. Deuterium atoms are clearly visible in neutron scattering density maps at 2.2 Å resolution (see proline 13, $2F_o - F_c$ map, 1.5 r.m.s. contour).

I. Hazemann, M. T. Dauvergne, M. P. Blakeley, F. Meilleur, M. Haertlein, A. Van Dorsselaer, A. Mitschler, D. A. A. Myles and A. Podjarny

IUCR JOURNALS NEWS

Ezetimibe monohydrate

***Acta Cryst.* (2005). E61, o2907–o2909**



Crystal structure of ezetimibe displayed through a CPK model.

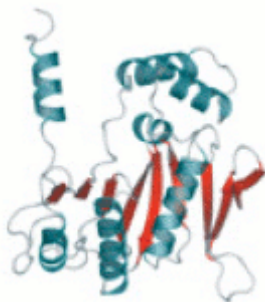
This paper describes the structure of a medically important compound, belonging to a class of agents that inhibit cholesterol absorption in the intestine. It has a favorable pharmacokinetic profile, which allows it to be administered daily and to be given in conjunction with a statin. Considering the X-ray crystal structure from the point of view of a structure–activity model, it may be speculated that the binding site accommodates a “T” shape, with the two arm ends occupied by the two fluorophenyl rings and the tail end by the hydroxyphenyl ring, while the azetidinone ring is located at the junction.

Krishnan Ravikumar and Balasubramanian Sridhar

IUCR JOURNALS NEWS

The structure at 2.5 Å resolution of human basophilic leukemia-expressed protein BLES03

Acta Cryst. (2005). F61, 812-817

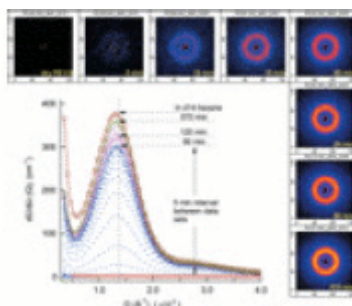


The crystal structure of the 27.5 kDa human basophilic leukemia-expressed protein (BLES03, p5326, Hs.433573) was determined at 2.5 Å resolution. Despite having an undetectable sequence relationship, the structure adopts a fold similar to that of eukaryotic initiation factor 4E with minor variations. The observed similarity extends beyond the shared fold and encompasses the conservation of both the electrostatic surface potential and the location of a binding cavity. It is hypothesized that BLES03 itself may be involved in a biochemical process that requires recognition of nucleic acids.

Eduard Bitto, Craig A. Bingman, Howard Robinson, Simon T. M. Allard, Gary E. Wesenberg and George N. Phillips Jr

Application of in situ vapor sorption small-angle neutron scattering (SANS) to semicrystalline polymers: vapor pathway and structure evolution in semicrystalline linear polyethylene

J. Appl. Cryst. (2005). 38, 734–739



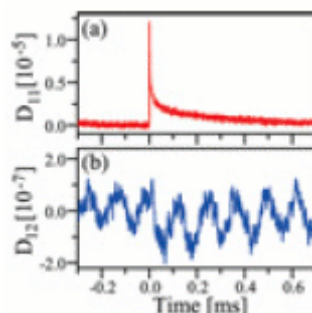
SANS 2D detector patterns, and circularly averaged profiles, as a function of d_{14} -hexane sorption time. The peak comes from the lamellar structure of the crystalline and amorphous regions in the polyethylene sample. SANS from the dry sample is at the bottom (circle) of the 1D profiles.

Unlike SAXS, SANS has not been successfully applied to study the structure of semicrystalline polyolefins due to the fundamental limitation of negligible neutron contrast between the crystalline and amorphous phases. We demonstrate an *in situ* vapor sorption SANS technique that circumvents this limitation by diffusing a contrast-generating vapor selectively into the amorphous phase. The enhanced contrast enables the sorption to be followed in real time and structural changes to be correlated with adsorption isotherms. The quality of the data is comparable with synchrotron SAXS data on dry samples.

M.-H. Kim and C. J. Glinka

Determination of the dynamic deformation tensor by time-resolved triple-crystal diffractometry

J. Synchrotron Rad. (2005). **12**, 685–689



Time dependence of (a) dilational component, D_{11} , and (b) shear component, D_{12} , of a deformation tensor with ultrafast laser irradiation at 1 kHz. Laser shots are at time = 0.

The brightest X-rays from the SPring-8 27 m undulator have enabled fast time-resolved measurements with a triple-crystal diffractometer. This was applied to detecting minute and fast dynamic deformation in nearly perfect GaAs crystals in a manner that dilational and shear components of the deformation tensor were separately determined. A digital storage oscilloscope recorded the time-varying signal from a photodiode detector with less than 100 ns time resolution. With ultrashort laser pulse irradiation, pulsed photothermal deformation and a following flexural standing wave were clearly detected.

Y. Hayashi, N. Tsukuda, E. Kuramoto, Y. Tanaka and T. Ishikawa

IUCR ACTIVITIES

International Tables Online announced at the XX IUCr congress in Florence



Congress delegates were invited to a wine and cheese party to celebrate the upcoming launch of International Tables Online (it.iucr.org) and the arrival of the IUCr's latest journal, *Acta Crystallographica* Section F: Structural Biology and Crystallization Communications (journals.iucr.org/f). Details of the online version of *International Tables* were also presented during an Open Commission meeting.

Starting in 2006, the full series of all eight volumes of *International Tables for Crystallography* (including the latest volume, Volume G, *Definition and Exchange of Crystallographic Data*) will be available through SpringerLink by payment of an annual licence fee.

The advantages that the online volumes will have over the the printed volumes are clear: users will be able to follow cross-references from one chapter to another in the series using hyperlinks, rather than having to have eight large, heavy books at hand at any one time, and will also be able to search the full text of all volumes. The volumes will also be quicker to update, as revised articles and new data can be made available online straight away, rather than only when the volume is reprinted. It will also be possible to 'break away' from the restrictions imposed by print media by including interactive features and multimedia presentations.



Andrea Sharpe (IUCr Promotions Officer), Hartmut Fuess (Chair, Commission on International Tables), and Peter Strickland (IUCr Managing Editor)

It is envisaged that the initial implementation of International Tables Online will have the following features: (1) The full text of all eight volumes (6000 pages) will be available as PDF and HTML. (2) Users will be able to navigate rapidly through the volumes. (3) Contents lists will be available down to and including the chapter level. (4) Users can choose to view a chapter, a section or a subsection, or even just a single table or a figure. (5) Hyperlinks will be provided from each chapter to related chapters in the series. (6) Advanced search facilities will be available. (7) Indexes will be available at the volume and individual chapter levels, and later at the series level. (8) Links will provided from reference lists to the original literature through CrossRef, ChemPort and PubMed. (9) The online volumes will be intergrated

with Crystallography Journals Online and the World Directory of Crystallographers. (10) The space-group tables will contain links between each space group and its sub- and supergroups. (11) Updated content will be immediately available to subscribers.



IUCr cheese and wine party in Florence

The online Tables have been designed to be simple for nonspecialists to use: users do not need to know the printed volumes in great detail to be able to find what they need online. A particular aim of the design is that it should not take more than two clicks of the mouse to deliver content to the user. Every dialogue box will have a menu of options to choose from and all the appropriate pages will contain bibliographic information, so that it will be clear how to cite the page. Above all, the system has been designed to be quick to use and to rapidly deliver content. In addition to all the information in the printed volumes, it is expected that the online Tables will also include 'resources': supplementary information, databases and programs that enhance the material within the printed volumes. For example, a chapter that discusses a CIF dictionary will be linked to a browsable HTML version of the dictionary, so that the user can use the dictionary while reading the chapter. From 2007 on, the IUCr will further develop International Tables Online. Space-group information in more nonstandard settings than covered at present by Volume A will be included. The user will be able to download data in well defined electronic formats (such as CIF or XML). 'Playing' with symmetry will be possible with interactive space-group diagrams and large tables of data will be converted into databases, allowing the user to select and plot graphs of the data within the tables if they wish. To register your interest in International Tables Online and find out more about online access and pricing, please visit it.iucr.org or contact support@iucr.org.

Hartmut Fuess

Chair, Commission on International Tables for Crystallography

SPECIAL REPORT

CRYSTALLOGRAPHY IN JAPAN

This issue completes the series of articles describing crystallography in Japan that started in Vol 13 No 2. Our thanks to Yuji Ohashi for assembling the information.

Recent developments

Chemical crystallography

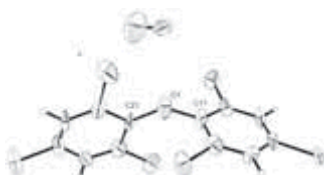


Fig. 1 Photo-produced triplet diphenylcarbene and nitrogen molecule

In Japan, many chemical crystallographers are doing forefront research in solid-state reaction-mechanisms, supra-molecular chemistry, phase transition, and materials science. Multi-dimensional structural chemistry which depends on time, temperature, and humidity etc. is actively investigated together with the development of equipment with two-dimensional detectors.



Fig. 2 The MSGC detector set up at SPring-8. The detector and the data acquisition system are installed in a cubic box of ca. 25 cm. Rotating the crystal around a vertical axis by 360 degrees on the goniometer, the intensity data can be observed within 0.2 msec.

At the Tokyo Inst. of Technology, Y. Ohashi, H. Uekusa and their coworkers developed crystalline-state reaction, which means the reaction occurs in a single crystal without degradation of crystallinity. Any stage of the reaction process, therefore, can be observed by X-ray crystal structure analysis and the reaction mechanism can be analyzed using the intermediate structures as eyewitness accounts. They defined the reaction cavity, which explains quantitative reactivity in solid-state reactions. Recently, in collaboration with Rigaku, they have developed a new diffractometer with an imaging-plate detector, R-Axis RAPID, which enables three-dimensional intensity data collection within 2 or 3 hours. Using this new diffractometer, they analyzed a variety of metastable intermediate structures, such as radical pairs of hexaarylbiimidazolyl derivatives, triplet carbenes (Fig. 1) and triplet nitrenes. Moreover, they analyzed the excited-state structures of a series of Pt complexes and a vanadium complex at the equilibrium state between ground and excited states. In order to analyze more rapid structural changes, they are now developing a new detector, Micro-Strip-Gas-Chamber (MSGC). Using this detector and a rotating anode, preliminary intensity data were collected within 2 seconds and the structure was successfully analyzed. Combining the detector and Synchrotron radiation at SPring-8 (Fig. 2), they found that the cell change of the Pt complex due to the formation of the excited state continued for more than 20 seconds and then the equilibrium state appeared.



Fig. 3 A cutaway view of the $[V_{12}O_{32}]^{4-}$ anion that traps an otherwise unstable NO^- anion.

T. Ozeki (Tokyo Inst. of Technology) is working on the structural chemistry of polyoxometalates. His research interests include the crystal structure determinations of novel polyoxometalates, hydrogen bonds involving the polyoxometalates, extended structures using polyoxometalates as building blocks, and inclusion compounds using the polyoxometalate as the host (Fig. 3). He is also in charge of two diffractometers in the synchrotron radiation facilities: an imaging plate Weissenberg camera at the BL04B2 beamline of SPring-8 and a CCD diffractometer at the NW2 beamline of the Advanced Ring (AR), Photon Factory (PF) of the High Energy Accelerator Research Organization (KEK). Using these facilities, he is exploiting the advantage of the high energy (typically $\lambda=0.33\text{\AA}$) and high flux X-rays to do atomic-resolution single crystal structure analyses of polyoxometalates and other chemically synthesized molecules (sometimes the size of which is stepping out of the realm of smallness and thus the common name “small molecules” is not used here).

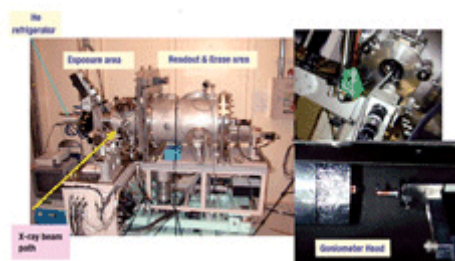


Fig. 4. Low-temperature vacuum X-ray camera at SPring-8 BL02B1 beamline.

K. Toriumi and Y. Ozawa (Univ. of Hyogo) and their coworkers have developed a new low-temperature vacuum X-ray camera (LTV X-ray camera) and installed it at the SPring-8 BL02B1 beamline (Fig. 4) for photo-excited crystallography, phase transition studies at low temperature, and micro-crystal structure analyses. By eliminating X-ray scattering from air and windows, high quality diffraction data with high S/N ratio can be automatically obtained down to 20 K. Direct observation of geometrical changes accompanied by photo-excitation of molecules provides essential information for transient species such as metastable states of chemical reactions. They have developed the multiple-exposure IP method for accurate measurement of intensity changes due to photo-illumination. A photo-excited molecular structure has been observed for the luminescent diplatinum(II) complex $[Pt_2(pop)_4]_4$. The observed electron density map shows positive and negative peaks with heights of 1–2 $e/\text{\AA}^3$ near the Pt atoms (Fig. 5). This indicates that small portions of the metal atoms move toward the positive peaks in the light-on crystal.

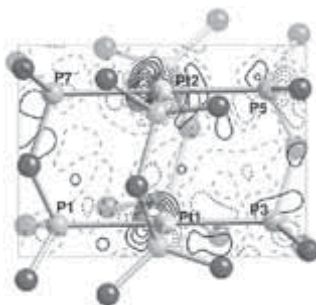


Fig. 5 Difference Fourier map (superimposed with a molecular diagram) of $|F_{on}| - |F_{off}|$ in a plane containing Pt(1)–Pt(2) vector and coordinated four P atoms of the ligands. Continuous lines and dashed lines indicate positive and negative density, drawn at every $0.2e/\text{\AA}^3$, respectively.

The main subjects of H. Kobayashi (Inst. of Molecular Science) and A. Kobayashi (The Univ. of Tokyo) are: (1) development and physical properties of molecular metals and superconductors and (2) molecular design, development and physical properties of single-component molecular metals. Until the early 1990s they engaged in the development of various molecular superconductors including a k-type BEDT-TTF superconductor ($k\text{-(BEDT-TTF)}_2\text{I}_3$) and a p-acceptor (M(dmit)_2 , $\text{M}=\text{Ni, Pd}$) superconductor without TTF-like donors. Recently they have reported an organic conductors exhibiting colossal magnetoresistance and field-induced superconductivity, $\text{I-(BETS)}_2\text{FeCl}_4$ and the first antiferromagnetic organic superconductor, $k\text{-(BETS)}_2\text{FeBr}_4$ ($\text{BETS} = \text{Bis(ethylenedithio)tetraselenafulvalene}$). They have also developed a single-component molecular metal with extended-TTF (tetrathiafulvalene) ligands, $[\text{Ni(tmdt)}_2]$ ($\text{tmdt} = \text{trimethylenetetraethia fulvalenedithiolate}$). The planar molecules are closely packed and three-dimensional S...S interactions were observed in the crystal (Fig. 6). The room temperature conductivity was 400 S cm^{-1} and metallic behaviour was observed down to 0.6 K. Experimental evidence for the existence of Fermi surfaces was obtained by detecting the quantum oscillations in magnetization (the de Haas-van Alphen (dHvA) effect). Metallic $[\text{Au(tmdt)}_2]$ is isostructural with $[\text{Ni(tmdt)}_2]$ and has an unusually high temperature SDW antiferromagnetic transition at around 85 K.

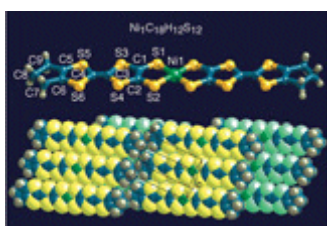


Fig.6 The molecular and crystal structure of $[\text{Ni(tmdt)}_2]$.

K. Tanaka (Nagoya Inst. of Technology) has reported 4f-electron transfer to B6 with a decrease in temperature in the study of the electron density distribution (EDD) analysis of the Kondo crystal CeB_6 by X-ray atomic orbital methods. This analysis opened the door to many interesting heavy-atoms materials and they have tried to explain precise electron densities for high T_c superconductors, skutterudites and rare-earth garnets. Diffraction measurements under vacuum by the VCIP method is also being developed to get super accurate structure factors for retrieving molecular orbitals from X-ray diffraction.

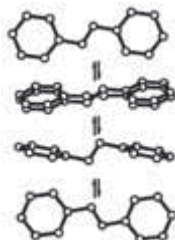


Fig. 7 Torsional motion and a conformational change through Pedal motion of (E)-stilbene.

The research activity of J. Mizuguchi and co-workers (Yokohama National Univ.) is focused on molecular structure, crystal structure and intermolecular interactions with potential electronic applications. Organic pigments are basically organic semiconductors which can be used in electronic materials such as photoconductors, electrophotographic photoreceptors, solar cells, optical recording materials, organic transistors etc.

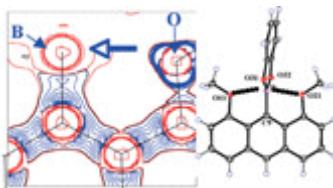


Fig. 8 Laplacian map of the five coordinated B compound.

Y. Sugawara (Kitasato Univ.), investigated humidity and temperature dependent phase transitions of nucleosides and nucleotide hydrates. Change in the numbers of water molecules or in their ordering at low temperature accompanies reconstruction of hydrogen-bonding networks. Structural transformations

and dynamics of phase transitions are being examined using X-ray and neutron diffraction methods, Raman spectroscopy, and computer simulation calculations. These phenomena are interesting from the view points of crystal engineering, pseudopolymorphism of pharmaceuticals, and water structure in biological systems.

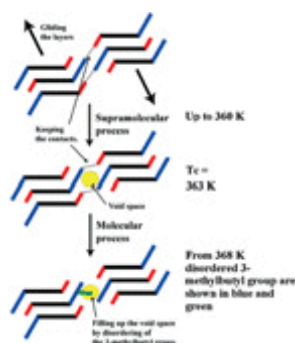


Fig. 9 Mechanism of phase transition of 1-ethyl-3-(4-methylpentanoyl)urea.

K. Ogawa and J. Harada (The Univ. of Tokyo) have discovered a pedal motion in crystals (Fig. 7), an essential molecular motion of stilbene-type molecules. They have also been successful in providing new insight into the chromism of organic crystals.

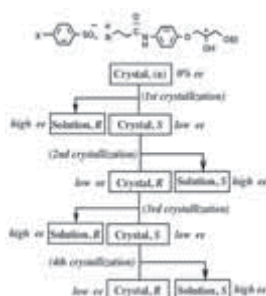


Fig. 10 Enantiomeric resolution of a racemic mixed crystal using preferential enrichment.

The main research interests of M. Yasui, F. Iwasaki (Univ. of Electro-Communications) and D. Hashizume (Riken) are: (1) weak intra and intermolecular interactions by a topological analysis of experimental charge density distributions, and (2) the mechanism of phase transitions of organic crystals using detailed temperature-resolved diffraction methods. Topological analyses for tetraazathiapentalenes, pentacoordinated hypervalent boron and carbon compounds show small positive Laplacian values at bond critical points which indicate the electrostatic character of these hypervalent bonds (Fig. 8). Analyses of intermolecular Br...Br contacts shorter than the normal van der Waals contacts revealed an electro-static interaction corresponding to the dispersion force. The magnitude of Br...Br interactions can be estimated to be about half of those of NH...O hydrogen bonds. They also studied intermolecular CH...O interactions in TEMPO radical derivatives. Topological properties prove that at least one H atom has a significant interaction with the p^* orbital of the radical O atom which can explain intermolecular magnetic interaction. They have developed a 'detailed temperature resolved diffraction method' during the phase transition of organic crystals. This method can make the mechanism of the transition clear by looking at a set of stop-motion photographs. The mechanisms of phase transition of acylurea derivatives and thiocatecholate crystals were clarified, and energy barriers of these transitions were estimated (Fig. 9). R. Tamura (Kyoto Univ.) reported the first instance where enantiomeric resolution by simple recrystallization of a racemic crystal was observed. This unusual enantiomeric resolution phenomenon was referred to as preferential enrichment. Mechanistically, it has been proven that preferential enrichment is a secondary, dynamic enantiomeric resolution phenomenon caused by a solvent-assisted solid-to-solid transformation of a metastable polymorphic form into a thermodynamically stable polymorphic form. It occurs during crystallization of certain kinds of racemic mixed crystals composed of two enantiomers in a supersaturated solution. This phenomenon has been detected in (i) the crystal structures of the stable and metastable polymorphic forms (ii) by a direct-space approach employing the Monte Carlo method followed by Rietveld refinement, (iii) in the *in situ* ATR-FTIR (ReactIR) spectral data

during crystallization, and (iv) in the DSC analytical and solid-state ReactIR spectral data of the deposited crystals (Fig. 10).

R. Kuroda's research group (Univ. of Tokyo) explores and exploits solid-state chiral chemistry. In crystals, interactions between molecules are expected to be orders of magnitude stronger than in solution. Thus, it is safe to assume that chiral discrimination, recognition, generation and transfer occur most strongly in the solid state. They have studied chirality recognition in solvent-free, solid-solid reactions. Upon co-grinding and heating (without melting) of the crystals of a template compound and a substrate compound, the chirality of the substrate compound was inverted to fit with the chirality of the template compound. They have developed two novel instruments, UCS-1 (Universal Chiroptical Spectrophotometer) and UCS-2, for measuring the chirality of solid materials.

Today, many scientists in Japan, whose main research involves organic or coordination chemistry, have their own diffractometers. Apart from the above examples, splendid work is going on related to chemical crystallography, such as, multicolor phototropism of single crystals by M. Irie (Kyushu Univ.), solid-solid synthesis using host-guest interactions by F. Toda (Okayama Univ. of Science) and K. Tanaka (Kansai Univ.), inclusion phenomena of choric acids by M. Miyata (Osaka Univ.), and synthesis of organic semiconductors with metallic luster by K. Ogura (Chiba Univ.).

F. Iwasaki, Univ. Electro-communication

Materials science

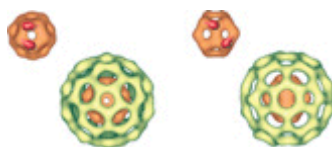


Fig. 11. A double shell of platonic solids formed by pentagonal-podecahedral La_2 charge density in [80-lh] fullerene: $\text{La}_2@C_{80}$

Structural science of materials in Japan is studied not only by crystallographers but also by materials scientists, physicists, chemists and many other researchers in science and technology. This report cannot be expected to cover all the aspects of structural science of materials in Japan but a few aspects of the field give some flavor of our country.

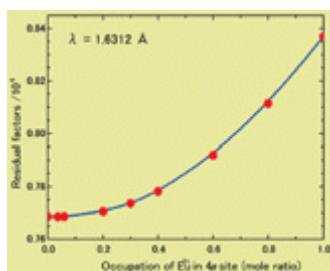


Fig. 12 Residual factors of Eu_3S_4 against the mole ratio of Eu^{2+} ions occupied in the 4a sites in the $I-42d$ structure.

In 1991, S. Iijima and coworkers (NEC Co. LTD.) reported a structure of a nanotube. There are many varieties, such as multi-wall, double-wall, and single-wall carbon nanotubes. These structures are mainly determined by TEM. Structural studies of nanotubes by X-ray are also active in Japan. One of the interesting properties of nanotubes is an inner hollow cavity of nanometer size. Kataura and coworkers reported that a one-dimensional crystal of fullerene molecules were found inside the nanotubes. Takenouchi and coworkers suggested that the nanotube absorbed not only fullerene molecules but also exotic molecules like TCNQ and TMTSF.

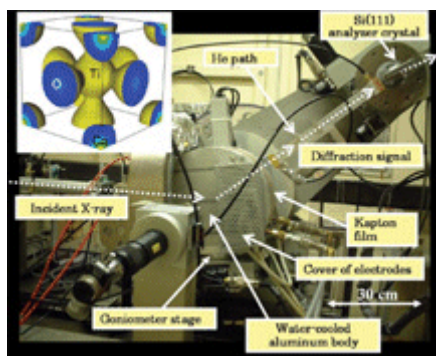


Fig. 13 A new furnace for high-resolution synchrotron powder diffraction study up to 1900K (BL-3A@PF). Iso-surface of electron density distribution of the cubic calcium titanate perovskite (1674K). *J. Appl. Cryst.* **37**, 786 (2004).

Another nano-structured carbon material, for which structures are mainly determined in Japan, is metallo-fullerene. M. Sakata, M. Takata and coworkers confirmed the endohedral nature of metallo-fullerene by X-ray powder diffraction at SPring-8. Since then, the structures of endohedral metallofullerenes have shown very unique structures including the disordered states of two La atoms in a C_{80} carbon cage (Fig. 11).

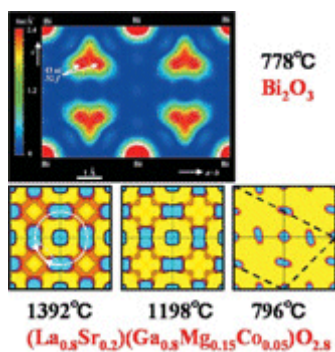


Fig. 14 Nuclear density distribution, disorder and the diffusion path of oxide ions in superionic conductors. *Chem. Phys. Lett.*, 378, 395, 380, 391 (2003).

J. Akimitsu and coworkers (Aoyama Gakuin Univ.) discovered that MgB_2 has one of the highest transition temperature ($T_c = 39$ K) of the known metallic superconductors. The superconductivity relating the BCS (Bardeen-Cooper-Schrieffer) mechanism has a superconducting energy gap associated with formation of the superconducting pairs. T. Takahashi (Tokyo Univ.) and S. Sasaki (Tokyo Inst. Tech.) suggested the existence of two kinds of superconducting gaps in MgB_2 on the basis of an ARPES (angle-resolved photoemission spectroscopy) study, where the σ and surface bands have large gaps of 6-7 meV and the σ band is dominant in the superconductivity with a stronger coupling to phonons. The electron-phonon coupling in MgB_2 causes the high T_c in a particular phonon mode with the E_{2g} symmetry at Γ . The electron-phonon coupling is only possible for phonons with momenta appropriate to move electrons within the neighborhood of a Fermi surface. The softening and broadening of the E_{2g} mode were observed inside the σ surfaces, by using a highly efficient X-ray spectrometer with a 4 meV resolution at SPring-8. K. Ohshima and coworkers reported a Kohn anomaly in TaS_2 from the phonon dispersion curves.

Charge ordering and charge fluctuation of mixed-valence compounds are commonly investigated in Japanese universities and governmental institutes. The valence-difference contrast method with X-ray anomalous scattering and electron-microscopic techniques are used for materials such as RM_2O_5 (R: Y or a rare earth; M = Mn, Fe) by Y. Yamada, and K. Kohn (Waseda Univ.), $La_{1-x}Sr_xMnO_3$ by H. Sawa (Photon Factory), Fe_3O_4 by S. Sasaki (Tokyo Inst. of Technology), $CuIr_2S_4$ by H. Ishibashi (Osaka Prefecture Univ.), $Pr_{1-x}Ca_xMnO_3$ and $Nd_{1-x}Sr_xMnO_4$ by Y. Matsui (National Inst. for Materials Science(NIMS)), $CaFeO_3$ by S. Morimoto (Osaka Univ.), NaV_2O_5 by Y. Fujii (Univ. of Tokyo), and $La_{1-x}(Ba,Sr)_xCuO_4$ by Y. Noda (Tohoku Univ.). An example of the research by Noda is Eu_3S_4 , where Eu^{2+} and Eu^{3+} , in a tetragonal cell below

$T_C = 188.5$ K, occupy 4a and 8d sites, having the cation distribution of $[\text{Eu}^{3+}]^{4a}[\text{Eu}^{2+}\text{Eu}^{3+}]^{8d}\text{S}_4$, as shown in Fig. 12.

X-ray resonant magnetic scattering was found for Ni single crystals by K. Namikawa (Tokyo Gakugei Univ.) in 1985. Resonant magnetic scattering factors were then obtained from experimental data from Fe_3O_4 by H. Kawata (Photon Factory) and coworkers. Systematic work on nonresonant magnetic scattering has been devoted to metallic and simple oxides by M. Ito (Gunma Univ.). The resonant X-ray scattering technique has been proved to be a powerful probe of orbital states, and is now being applied to a wide range of systems with improved accuracy. One example is the case of $\text{La}_{0.45}\text{Sr}_{0.55}\text{MnO}_3/\text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3$ multilayers reported by M. Izumi (NIMS).

The horizontal-type high-speed four-circle diffractometer at beam line 14A at the Photon Factory has been used in a number of electron density studies. Recently a high-speed detector called a stacked avalanche photodiode detector (APD) was employed with the collaboration of S. Kishimoto (Photon factory) and N. Ishizawa (Nagoya Inst. Tech). Studies of $\text{La}(\text{Sr})_2\text{CuO}_4$ and MnS_2 revealed an enhanced accuracy of the experimentally determined electron densities.

Micro-beams obtained by using synchrotron radiation are powerful tools. Interplanetary dust particles and meteorites are usually examined by optical microscopy, chemical analysis, micro Raman spectroscopy, and so on. The lower limit of the area for these examinations is about a micrometer. Diffraction data from the same samples is indispensable especially in cases of polymorphs and polytypes. Interplanetary dust particles of iron sulfides and micrometer-sized areas of the same kind in a thin section of meteorite are identified, and the structure is refined based on intensities of the Laue spots obtained by using polychromatic synchrotron radiation at the Photon Factory by K. Ohsumi.

High-resolution synchrotron powder diffractometers are available at beam line 4B2 of the Photon Factory ($\delta d/d=0.04\%$) and at the BL15XU of SPring-8 ($\delta d/d=0.03\%$). Two angle-dispersive-type neutron powder diffractometers (HRPD) and HERMES are installed at the JRR-3M research reactor in JAERI. There are two time-of-flight (TOF) neutron powder diffractometers (Sirius and VEGA) at KENS of KEK in Tsukuba. The KENS facility will be shut down soon, but a new powerful neutron facility (JSNS at J-PARC) has been built. At the JSNS, a new high-resolution TOF neutron powder diffractometer will be installed. At the Ceramics Research Laboratory, Nagoya Inst. Tech., the profile functions of powder diffraction data are characterized by T. Ida. F. Izumi (NISM) developed computer programs for Rietveld analysis, maximum-entropy methods and visualization of crystal structure and electron/nuclear density distribution. The superspace group approach to structure analysis of composite crystals has been a successful collaboration between NIMS and Tohoku Univ. T. Ikeda (Tohoku Univ.) analyzed the crystal structures and properties of synthesized zeolites through *ab-initio* computational methods.

M. Yashima (Tokyo Inst. Tech.) and coworkers have been studying high-temperature neutron and synchrotron powder diffraction techniques for precise structure analysis up to 1900 K. By using the furnace diffusion path, the disorder in some ceramic superionic conductors were visualized (Fig. 13).

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High-pressure activity

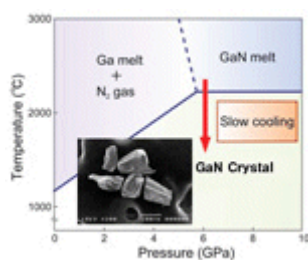


Fig. 15 High pressure-temperature phase diagram of GaN determined by in situ X-ray observation. Congruent melting of GaN occurs at high pressures above 6 GPa^[1]. Inserted figure is a SEM image of the GaN single crystals obtained by slow cooling from congruent melting at high pressure. For high pressure studies, a large volume press and diamond anvil cell (DAC) are used. There are two types of large volume presses; one is a DIA type cubic anvil system and the other is a Kawai type double stage anvil system.

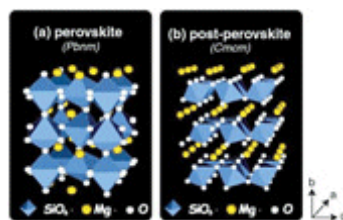


Fig. 16 Atomic arrangements of perovskite type (low pressure phase; left) and post-perovskite type (high pressure phase; right) structures^[2].

The DIA type apparatus, MAX80 at the Photon Factory and SMAP-180 at SPring-8, can generate a pressure and temperature around 10 GPa and 2000K, and it is mainly used for materials science. Recent work with SMAP-180 involved the observation of congruent melting of GaN under high pressure and temperature^[1]. Fig. 15 shows the phase boundaries of GaN obtained at high pressure and temperature. This observation enables one to obtain bulk single crystals of GaN by slow cooling from a high pressure congruent melt. GaN, a famous green fluorescent material, had so far been made only in thin films. Another exciting result is finding the pressure induced first order transition in liquid states. Phosphorus was found to show a clear first order transition at around 1 GPa and 1000K (Y. Katayama, SPring-8/JAERI). This was confirmed by measurements of XAFS, density, X-ray diffraction and X-ray transmission imaging at the transition. Density was measured by X-ray absorbance by filling the sample in a sapphire or diamond ring. A sharp liquid-liquid transition in liquid germanate accompanied by a fourfold to six fold coordination change was also found around 3 GPa at 1273 K(3) (O. Ohtaka, Osaka Univ.)

The first Kawai type press for SR study named SPEED1500 can generate pressure and temperature around 30 GPa and 2000K with tungsten carbide anvils, and will be used to study the interior of the earth across the lower mantle region. The first result using SPEED 1500 is the determination of the phase boundary of Mg_2SiO_4 (T. Irifune, Ehime Univ.). Assuming a geotherm of 1650K, dissociation pressure is estimated to be 21GPa, which is apparently lower than the previous result. This was a sensational result to understand the upper to lower mantle structures.

In order to extend the pressure range, a new system named SPEED Mk-II using sintered diamond anvils was developed at SPring-8. At room temperature, pressure generation higher than 60GPa can be routinely achieved. SPEED Mk-II has an oscillation mechanism to avoid the effect of preferred orientation and grain growth. With this oscillation mechanism, the diffraction profiles of NaCl were clearly observed with reasonable integrated intensities very close to the melting temperature, and the phase relations among the B1, B2 and liquid phases are precisely determined (N. Nishiyama, Ehime Univ.).

A unique technique with SR is viscosity measurements using a falling ball method. An image is recorded each 1/125 second and the linear part of the falling distance against time is fit to give an accurate viscosity. Sulfur content dependence in the Fe-FeS system is clearly seen, as well as temperature dependence.

We recently succeeded in measuring ultrasonic velocity at high pressure and temperature. A transducer is set outside the anvil to prevent damage by pressure and temperature. The length of the sample is measured directly by a transmission image of the sample using a CCD camera, and volume and pressure are measured by X-ray diffraction. With this technique, concentration dependence of bulk and shear moduli for ringwoodite are beautifully observed, which agrees very well with finite strain fitting simulations (Y. Higo, Ehime Univ.).

At dedicated DAC stations (BL10XU at SPring-8) one can perform high and low temperature diffraction experiments. Strongly correlated materials, nano-materials, etc. are extensively studied by using the quasi hydrostatic pressure medium of He. Structural behaviors of simple materials such as Sc, BeO, Hg, Cs, H₂, O₂, and LiH are investigated in the ultra high pressure region above 200GPa.

High temperature experiments with DAC are performed by use of a laser heated DAC. The characteristics of the system at SPring-8 are dual lasers (YAG and YLF) and dual detectors (IP for precise measurement and CCD for rapid measurement). The most exciting result with laser heated DAC is the structural phase transition of MgSiO₃ at 125GPa and 2400K^[2]. The structure of the lower pressure phase is a well known perovskite type structure with apical sharing. The structure of the high pressure phase, which is explained by a Cmc₂m structure type, is unique in that it is a layered type two dimensional one (Fig. 16). This pressure and temperature condition corresponds to the mantle to core boundary of the Earth, and this result is believed to help clarify the structure of earth's core.

Other experiments using DAC such as nuclear X-ray scattering, inelastic scattering, infrared spectroscopy, etc. are performed at each general beamline.

The high pressure neutron group, headed by H. Kagi (Tokyo Univ.) submitted a proposal for the construction of a high pressure system consisting of a DIA type high pressure cell to J-PARC. The proposal is on the waiting list.

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Electron diffraction

The electron microscope is unique in that it enables us to simultaneously conduct experiments in diffractometry, microscopy and spectroscopy on a nanometer scale.

Tsuda *et al.*^[1] developed a method to refine crystal structural parameters and charge density using convergent-beam electron diffraction (CBED). The method is based on a least-squares fit between full dynamical calculations and energy-filtered intensities from two-dimensional higher-order Laue zone (HOLZ) and zeroth-order Laue zone (ZOLZ) CBED patterns. Application of this method to the rhombohedral phase of LaCrO₃ revealed clear anisotropy of thermal vibration of the oxygen atoms and charge transfer from the metal atoms to the oxygen atoms. With the aid of parallel computations, the structure (30 positional parameters and Debye-Waller factors) of the intermediate phase of hexagonal BaTiO₃ was refined. In the orbital ordering phase of LaMnO₃, the anisotropic charge distribution caused by orbital ordering of the 3d-electrons of the Mn atoms was found.

Fujiyoshi *et al.*^[2] developed a high-resolution electron cryo-microscope equipped with a top-entry specimen stage. Using the microscope, they determined the atomic structures of several membrane proteins with the use of two-dimensional (2D) and tubular crystals. Image shifts due to beam-induced specimen charging were found to be the most severe problem in imaging of biological macromolecular 2D crystals, especially at highly specimen tilt conditions. To reduce beam-induced movement, Gyobu *et al.* developed a new sample preparation method, the carbon sandwich method, in which the crystals are put between two carbon films. This method has improved the success ratio of obtaining high-resolution images from tilted specimens, namely from 30 to 90% at a tilt angle of 45 degrees. The method enabled them to collect a full data set (87.0% complete) of aquaporin-4 (AQP4), a water channel protein, and to conduct the structural analysis at 3.2 Å resolution with a Friedel factor and merging R-factor of 11.4 % and 22.3 %, respectively.

Nagayama *et al.*^[3] developed a series of transmission electron microscopes (TEM) capable of retrieving object-retarding phases in electron waves. The Zernike phase contrast (ZPC) method uses a classical $\pi/2$ phase plate in the form originally developed by Zernike. The Hilbert differential contrast (HDC) method uses a half-plane π phase plate to generate images similar to the differential-interference-contrast conveniently used in light microscopy. The Foucault differential contrast (FDC) method uses dynamical control for a Foucault knife-edge to perform an accurate differential operation for phases involved in the wave function of electrons. The remarkable high contrast achieved with these phase contrast TEMs without sample staining is now opening a novel field of in vivo electron microscopy in biology.

Matsui *et al.*^[4] carried out intensive structural studies of various new superconductors by means of high-resolution transmission electron microscopy (HRTEM). They found incommensurate superstructures in Bi-2212 and Bi-2223 superconducting phases, and proposed modulated structure models with strongly distorted lattice planes. They developed a new high-voltage (1300kV) HRTEM with an 0.1nm point-resolution and used it to identify new oxycarbonate superconductors which contain CO_3 groups forming various types of order/disorder structures. Since new phenomena of colossal magnetoresistivity (CMR) were reported, Matsui *et al.* also studied the magnetic nanostructures of various magnetic materials by cryo-Lorentz electron microscopy.^[5] They examined the formation of ferromagnetic domains in a “double-perovskite” $\text{Ba}_2\text{MoFeO}_6$, and proved that the crystallographic anti-phase boundaries tend to pin the ferromagnetic domains.

Saitoh *et al.*^[6] applied HAADF-STEM and ALCHEMI to quasicrystals and their approximants for the first time. Using the HAADF-STEM method, they first observed an asymmetric atom-cluster and a high degree of quasiperiodic arrangement of clusters in decagonal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, which led to the quasi-unit-cell model. Using the two-dimensional angular-scanning ALCHEMI, Saitoh *et al.* also found that, in decagonal Al-Ni-Co and Al-Ni-Fe, two kinds of transition metal elements occupy the same sublattice site (chemical disorder), which is compatible with the fact that the quasicrystals are stabilized by the Hume-Rothery mechanism.

Abe *et al.*^[7] demonstrated the real-space imaging of a local thermal vibration anomaly in a solid through atomic-resolution annular dark-field scanning transmission electron microscope (ADF-STEM) observations of an $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ quasicrystal. They found significant changes of the ADF intensity at some Al atomic sites, which depend on the observation temperature and the scattering angle range. This anomalous ADF intensity, which is due to an anomaly of the thermal diffuse scattering (TDS) intensity, is explained fairly well by an anomalously large value of the temperature (Debye-Waller) factor of Al at the sites or by a larger mean-square thermal vibration amplitude of the atoms. By introducing angle-resolved and/or *in-situ* heating/cooling techniques, they have extended the ADF-STEM method as a tool to determine local Debye-Waller factors that crucially affect the physical properties of materials.

Suenaga *et al.*^[8] demonstrated chemical analysis by means of electron energy-loss spectroscopy (EELS) with a sensitivity of a single atom limit and the high-resolution imaging of individual metallofullerene molecules encapsulated in a single-wall carbon nanotube. They directly observed nanotubes composed of single-graphene layers and their structural defects using phase contrast transmission electron microscopy.

Takayanagi *et al.*^[9] developed an ultra-high vacuum electron microscope combined with a scanning tunneling microscope to study structure and electronic conductance quantization of gold atomic chains and nanowires. They observed that a gold atomic chain, which was fabricated between the gold STM tip and the gold substrate, has the conductance quantum of $2e^2/h$, where e is electron charge and h is the Planck constant. They found gold nanowires having single-wall and multi-wall tubular structures (helical multi-shell magic number seven structure).

Using electron holography, Hirayama *et al.*^[10] observed two-dimensional electric potential distributions in a cross section of a Metal-Oxide-Semiconductor Field-Effect-Transistor (MOSFET) fabricated from a silicon wafer with a boron concentration of 10^{15}cm^{-3} . This implies that electron holography allows the

two-dimensional mapping of dopant distributions as low as 10^{15}cm^{-3} . This technique is useful for developing new devices for failure analysis in the semiconductor industry.

Kimoto *et al.*^[11] applied electron energy-loss spectroscopy (EELS) to the analysis of an ultra-thin film of amorphous- Al_2O_3 on Si. EEL spectra were successfully acquired with a small interval of 0.28 nm in depth using their spatially-resolved technique. From the spectra, they found different Al coordinations of an AlO_4 tetrahedron and an AlO_6 octahedron with the aid of first-principle calculations. They revealed the detailed depth dependence of Al coordination in the film with sub-nanometer resolution.

Terauchi *et al.*^[12] constructed a high energy-resolution EELS microscope equipped with a Wien-filter monochromator and a Wien-filter analyzer. The EELS microscope was used to measure the bandgap energies and the density of states (DOS) of the conduction bands of BN nano-cones and metal-doped boron micro-crystals with energy resolutions of 0.2-0.26 eV. Terauchi *et al.* have developed a high resolution soft-X-ray spectrometer for X-ray emission spectroscopy (XES) for a transmission electron microscope (TEM). This instrument enables us to obtain the DOS of the valence band with an energy resolution better than 1 eV from a small specimen area identified by observing an electron microscope image. They demonstrated using h-BN that the total DOS of the valence and conduction bands can be obtained in the electron microscope from XES and EELS spectra.

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XAFS activities

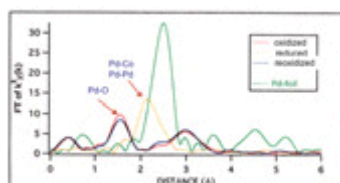


Fig. 17 Fourier transformed spectra of Pd K-edge EXAFS oscillations of the Pd-perovskite catalyst at oxidized, reduced and re-oxidized states together with that of a Pd foil.

XAFS activities in Japan started in 1982. The EXAFS beamline BL-10B, one of the first beamlines constructed at the Photon Factory (PF), is equipped with a Si(311) channel-cut type monochromator without any focusing optics. A number of papers for structural analysis of materials have been published using data from this beamline. New XAFS beamlines constructed include a sagittal focusing double crystal monochromator (BL-7B), and a Si(111) double crystal monochromator with curved cylindrical mirrors both up- and down-stream of the monochromator. Several upgrades of the PF ring lowered the emittance to 27 nm rad.

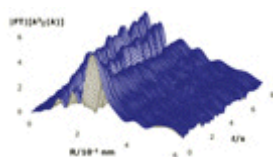


Fig. 18 The Fourier transformed spectra of Rh K-edge EXAFS oscillations of Rh/Al₂O₃ during the carbonylation process at 298 K measured every 100 ms.

SPRING-8, a third generation hard X-ray 8 GeV ring has two beamlines dedicated to XAFS experiments; BL-1B at the bending magnet port and BL-10XU in an undulator port. The former has been used for XAFS experiments in the higher energy region extending to 100 keV, and the latter for focused (0.1-1 mm²), high photon flux XAFS with more than 10¹³ photons/s. The latter beamline is especially useful for XAFS under high pressures. Micro XAFS experiments are conducted at BL37XU using Kirpatrick and Baez (K-B) mirror optics. The beam size was 2 (H) × 4 (V) μm², with a flux of more than 10¹⁰ photons/s at 10 keV.



Fig. 19 An illustrative mechanism for the disintegration of an Rh cluster on γ-Al₂O₃ by CO adsorption. Another 6 GeV storage ring in KEK, which had been used as a booster ring for the TRISTAN main ring (25 GeV), has been renewed as a high current ring with a single bunch mode dedicated for synchrotron radiation use. This is especially useful for time resolved XAFS. In the AR facility, the dispersive XAFS technique was installed, which enables one to measure EXAFS in less than 1 ms. Quick XAFS is also under construction and will be dedicated to structure analysis of catalysts. One unique feature of XAFS activities is that the laboratory XAFS instruments are prevailing in Japan. TECHNOS I.T Co. Ltd and RIGAKU Co. have independently developed compact XAFS instruments equipped with an X-ray tube. By using a Johansson-type curved crystal, EXAFS measurements can be taken in a reasonable time; typically, 20 min for Cu K-EXAFS of a Cu foil.

There are more than 150 users of XAFS experiments in Japan. The society of XAFS was organized in 2000. Its annual meetings attract more than 100 participants. More than 50% of its members specialize in catalysis and 15% are from industry.

Although XAFS studies are diverse in various fields, two recent highlights:

(1) Self-regeneration of a Pd-perovskite catalyst for automotive emission control. Catalytic conversion of exhaust gases is an essential part of automobiles. Recently, the Japanese motor company, Daihatsu Co. developed an intelligent conversion catalyst, LaFe_{0.75}Co_{0.38}Pd_{0.05}O₃, perovskite-based catalysts which has a much longer lifetime than the conventional catalyst, Pd/Al₂O₃. The structural change of the perovskite catalyst was studied in SPRING-8 by using Pd and Co K-edge XAFS as well as X-ray diffraction (Y. Nishihata *et al. Nature* **418**, 164 (2002)) Fig. 17 shows the Fourier transformed spectra of Pd K-edge EXAFS oscillations of the sample at oxidized, reduced and re-oxidized states together with that of a Pd foil. In the oxidized state, Pd is surrounded by oxygen, while in the reduced state, Pd is surrounded by Co and Pd. Combined with the XRD data, it revealed that Pd is in the B-site (octahedral site) of the perovskite lattice in the oxidized state and in the reduced state, Pd is segregated with Co to form a PdCo solid solution. This process is reversible and explains the retention of high catalytic activity during long-term use and aging.

(2) Little has been known about the dynamical structural change of active metal sites in supported metal cluster/nanoparticles catalysts. The *in-situ* time resolved XAFS study of a CO-induced disintegration process of Rh clusters on an Al₂O₃ surface was performed at PF (Suzuki *et al. Ang. Chem. Int. Ed.* **42** (2003) 4795). Rh K-edge EXAFS of an Rh/Al₂O₃ catalyst was taken under 26.7 kPa of CO at 298 K every 100 ms with the energy dispersive mode. Fig. 18 shows a series of Fourier transforms calculated during the carbonylation process. The peak at 0.2 nm (Rh-Rh) suddenly reduces and the peak at 0.1 nm (Rh-C)

increases rapidly. Analysis of the coordination number and bond distances (Rh-Rh, Rh-C) as a function of CO exposure reveals that there are three elementary steps for the surface dynamic structural rearrangement of Rh clusters involving two intermediate states as depicted in Fig. 19. Before CO exposure, each Rh cluster consists of seven atoms in the first layer and three atoms in the second layer on Al_2O_3 . CO exposure causes Rh-CO bond formation for the second layer in 600 ms, and further CO exposure induces Rh-CO bond formation with cluster disintegration and finally each Rh atom adsorbs in the threefold hollow site, forming $\text{Rh}(\text{CO})_2$. These results demonstrate that dispersive XAFS is useful to elucidate the mechanism for dynamic surface processes.

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MEETING REPORT

National seminar on neutron and X-ray scattering

Serpong, Indonesia, August 2005



The 6th National Seminar on Neutron and X-ray Scattering was held at the National Nuclear Energy Agency of Indonesia (BATAN) in Serpong, Indonesia on August 3, 2005. The one-day seminar was attended by more than 120 participants coming from local universities and research institutes including 16 scientists from abroad. Eight speakers from India, UK, Australia, Japan, Singapore and Indonesia were invited to this seminar and presented oral talks. Meanwhile, 39 posters from the participants were also presented.

The seminar was officially opened by the Chairman of BATAN, Soedyartomo Soentono, and followed by a general talk on neutron scattering in soft condensed matter given by S. Goyal (UGC-DAE Consortium for Scientific Research, BARC, India). A. Ikram (Head of Neutron Scattering Lab from BATAN, Indonesia) gave a brief presentation on the neutron scattering facilities in Serpong. Another talk on some applications of small-angle X-ray scattering in complex liquid crystalline systems was delivered by G. Ungar (U. of Sheffield, UK). A review on small angle neutron scattering (SANS) in biological materials was presented by R. Knott (ANSTO, Australia). After a lunch break there was a presentation made by J.R.C. Van der Maarel (National U. of Singapore) with the title of ionic diblock copolymer micelles: small angle scattering estimates of charge ordering in the coronal layer. Z. Nurachman (ITB, Indonesia) presented a talk on protein X-ray crystallography. A talk on neutron stress measurement of W-fiber reinforced Cu composite was delivered by M. Nishida (Kobe City College of Technology, Japan). S. Mazumder (BARC, India) gave a talk on small angle scattering: the Indian scenario. Finally, the seminar was officially closed by the Deputy Chairman of BATAN, Pramudita Anggraita.

Prior to the seminar a two-day workshop was held in the neutron scattering laboratory in Serpong. The workshop was attended by more than 30 participants including 6 participants from abroad, i.e. Malaysia and Mexico. They were divided into two groups depending on their topic of interest, i.e. small angle neutron scattering and residual stress analyses. During the workshop, a lecture on basic theories of neutron and X-ray scattering was given by A. Purwanto (BATAN, Indonesia), meanwhile the lectures on theories of SANS, SAXS and residual stress analyses were given by the invited speakers mentioned above including a young scientist, V.K. Aswal (BARC, India), who gave an enlightening lecture on the principle of SANS and data reduction and N. Minakwa (Japan) gave an impressive talk on residual stress analyses. The participants were given an opportunity to experience hands-on training using the SANS machine and powder diffractometer for residual stress measurements and they carried out data analysis together with their tutors.

Besides facilitating an exchange of ideas, knowledge, and experience, the workshop and seminar were also aimed at attracting people especially the local researchers to make use of the neutron scattering facilities in Serpong for their research. Feedback from the participants revealed that they were impressed by the program and they looked forward to attending the continuation program planned next year in Bandung, West Java.

Edy Giri R. Putra & Sutiarso

MEETING REPORT

New frontiers in neutron macromolecular crystallography

Oak Ridge, TN, USA, July 2005



The conference “New Frontiers in Neutron Macromolecular Crystallography” was held at Oak Ridge National Lab., Oak Ridge, TN, July 12-13, 2005. The purpose of the conference was to highlight the impact of the proposed, state-of-the-art Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source (SNS), Oak Ridge, TN that can potentially make it routine to locate hydrogen atoms in biological structures. This ability stems from the fact that Neutron Macromolecular Crystallography (NMC) can provide accurate hydrogen atom positions, protonation states and hydration states, as well as information on hydrogen/deuterium exchange in macromolecular crystal structures, even at a moderate 2 Å resolution. In contrast, to observe hydrogen atoms via ultra-high resolution X-ray crystallography requires diffraction data beyond 1.0 Å. This limit accounts for less than 1% of all protein systems being studied by X-ray diffraction.

The advent of the SNS, with over an order of magnitude increase in neutron flux, combined with advances in neutron optics and detectors, promises to revolutionize NMC. In order to realize this potential, a dedicated, best-in-class high-resolution time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) has been proposed for the SNS. An optimized instrument design has been developed that will enable data collection rates over 50 times faster than at existing facilities. Furthermore, it will enable studies of crystals with lattice constants substantially larger than currently possible. The MaNDi Instrument Development Team secured beam line 11B at the SNS in October 2004. It is expected that the MaNDi will greatly advance the fields of structural biology, enzymology, and computational chemistry. The project is now at an advanced stage. It is necessary to secure funding for the engineering design and construction of the diffractometer and the associated infrastructure at SNS. This will be possible only with the strong support of the broader structural biology community.

An outstanding scientific program attracted about 100 macromolecular X-ray crystallographers and structural biologists from research institutions across the US, Europe and Japan. Invited talks by J. Glusker, H. Hauptman, W. Hendrickson, A. Joachimiak, A. Kossiakoff, B. Mathews, A. Podjarny, D. Ringe, G. Stubbs and B.C. Wang and posters on current research in high resolution neutron diffraction in structural biology as well as potential scientific problems for NMC were presented. In addition, the status of the SNS, MaNDi and of NMC programs worldwide was given by T. Mason, P. Thiyagarajan and D. Myles. A highlight of the conference was the tour of the SNS experimental hall containing the target and the instruments in various stages of construction.

The conference was highly successful in meeting its planned objectives: 1) To increase interest and awareness of the important new capabilities of neutron diffraction in structural biology 2) To engage and involve the community in defining challenge areas and problems that can be addressed at SNS, and 3) To showcase the novel and interesting macromolecular systems that will be amenable to neutron diffraction studies upon completion of MaNDi.

In the final panel-led discussion, highly enthusiastic remarks and unanimous support were expressed both by the audience and all the leading scientists. With such endorsement and with the active participation and support of the wider structural biology community, the US now has an opportunity to obtain a world-leading new facility for NMC. Further details of the conference can be found at www.sns.gov/MaNDi2005.

Organizers: Andrew Mesecar, Dean Myles, Arthur Schultz and P. Thiyagarajan

MEETING REPORT

Workshop on crystal growth technology

Beatenberg, Switzerland, September 2005



The Third Int'l Workshop on Crystal Growth Technology (IWCCT-3) was held in Beatenberg, Switzerland, September 10-18, 2005. 38 speakers lectured on research and numerical simulation of crystal growth processes, crystal growth industry, crystal machining and crystal characterization. Approximately 90 crystal growers and technologists from 12 different nations, some of them with their families, attended the workshop.



Assisted by a mountain guide, Hans Scheel led the participants over the Gries glacier.

The opening lecture on the growth of large halide scintillation crystals up to 450 kg weight was by A. Gektin (Inst. of Single Crystals, Kharkov, Ukraine). J. Telfer (Hilger Crystals Ltd, UK) gave an overview on crystal growth in the UK, focusing also on scintillation crystals. K. Jacobs (Inst. for Crystal Growth IKZ, Berlin, Germany) introduced the thermodynamics of crystal production processes from melt, solution and vapor. M. Mühlberg (U. of Cologne) followed up with phase diagrams as useful tools for crystal growth. The growth techniques of large (6 inch diameter) Nd-doped GGG-crystals ($\text{Gd}_3\text{Ga}_5\text{O}_{12}$) as well as of the classical garnets for high power lasers were presented by M. Randles (Northrop Grumman Synoptics, Charlotte, NC, USA). The series of talks on semiconductors was started by F. Börner (Freiberger Compound Materials FCM), who gave an overview on GaAs, focusing on its markets now and then, the production and future of wafers, and the economy of GaAs industry. Y. Makarov (Semiconductor Technology Research Inc. Richmond, VA, USA), presented a model for the Czochralski growth of large Si crystals in industrial systems, applying or not magnetic fields. F. J. Bruni (Santa Rosa, CA, USA) also talked on the Czochralski method, presenting ways to control the diameter and the interface shape stability of large industrial Si crystals, as well as lithium niobate and tantalate, GGG. The first day was closed with a panel discussion on world-wide crystal production.



D. Keith Bowen explains X-ray and synchrotron characterization of industrial crystals.

P. Capper (Selex Sensors and Airborne Systems Infrared Ltd, Milbrook, UK) spoke on the use of forced mixing by acceleration of crucible rotation (ACRT H.J. Scheel 1971) in the Bridgman technique for CMT (Cd-Hg-Telluride, $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$) used in infrared detectors. J.J. Derby (U. of Minnesota) introduced the possibilities of simulating flow effects during crystal growth as compared with the state of the art in modeling melt and solution crystal growth processes. K. Kakimoto (Kyushu U., Japan) analyzed the effects of magnetic field configuration on the melt-crystal interface shape and melt flow during the growth of a Si-crystal obtained via the Czochralski method, whereas T. Hibiya (Tokyo Metropolitan U.) gave an overview of the thermophysical properties of crystal growth melts. K. Schaffers (Lawrence National Lab., Livermore, CA, USA) talked on the growth of large laser crystals for fusion energy, highlighting the current problems of crystalline materials, and the largest YCOB-crystals ($= \text{YCa}_4\text{O}\{\text{BO}\}_3$) that could be produced so far. She was awarded best speaker of the conference for her talk. S. Uda (Tohoku U., Japan) presented the crystal growth of langasite-type crystals and their device properties. V.A. Klipov (Sawyer Technical Materials, Eastlake, OH, USA) dealt with the hydrothermal production of quartz crystals. A second talk by Y. Makarov on the modeling analysis of vapor pressure-controlled Czochralski Growth of GaAs bulk crystals and other low-gradient crystal pulling concluded the series of presentations of the second day.



U. Kerat, F. Dupret, Mrs. Dupret, A. De Potter and V. Regnier.

After a full-day excursion onto the Faulhorn, P. Rudolph (IKZ Berlin, Germany) started the day with a review on defects, their thermodynamics, origin and characterization. J. Friedrich (Fraunhofer Inst. Erlangen, Germany) combined thermal modeling with experimental studies of the vertical gradient freeze technique for the synthesis of large industrial semiconductor crystals, focusing on the example of InP. His talk was followed by a contribution by S. Eichler (FCM, Germany), who explained first the different crystal growth techniques of GaAs, followed by methods of doping for micro-electronics and opto-electronics. Then, A. Mühe (Crystal Growing Systems GmbH, Asslar, Germany), gave insights into the design of crystal growing systems, focusing on the interplay of material sciences and economy. Industrial crystal growth technologies of III-V compound semiconductors including GaN were presented by M. Tatsumi (Sumimoto Electric Industries, Japan). In-doped GaSb solid solution crystal growth using the vertical Bridgman technique with ACRT was discussed by P. S. Dutta (Rensselaer Polytechnic Inst., NY, USA). He was followed by G. Siefer (The Fraunhofer Inst. for Solar Energy Systems, Freiburg, Germany), who presented a new type of solar cell, Flatcon, based on III-V tandem cells and using a concentrator system, he explained its performance as compared with traditional solar cells. H. Scheel (Beatenberg, Switzerland) concluded the talks with a discussion on saving energy and renewable energy in which crystal growth technology can play a crucial role. The day ended with a panel discussion on that very subject.



The Swiss Award for outstanding contributions is passed to Shin Miyazawa of Waseda Univ. The picture shows Hans Scheel, chairman of the section, giving the laudatio.

The next day, dedicated to crystal machining, started with an animated presentation by H.J. Moeller on the physics of crystal sawing technology focusing on processes happening at the crystal surface upon different modes of multi-wire sawing and properties of the final products. P. Nasch (HCT Shaping Systems, Switzerland) gave a historical overview of multi-wire slurry slicing techniques for silicon crystals, and described the recent technology with examples and analysis. Y. Sano (Osaka U., Japan) introduced the technique of plasma chemical vaporization machining (PCVM) applied to SiC and Si crystals, and it was shown that this method allows slicing with a precision down to 7 nm. His colleague, K. Yamauchi, presented the revolutionary elastic emission machining (EEM) that is used for the generation of ultra-flat and crystallographically well-ordered surfaces of functional materials, such as total reflection X-ray mirrors. Over lunch time, a general assembly of the board of the Section of Crystal Growth and Technology of the Swiss Society of Crystallography was held in the presence of interested persons from the Swiss crystal industry in order to discuss the future of industrial crystal growth in Switzerland. In the afternoon, two lectures were given. The first one by F. Schmid (Crystal Systems Inc., Salem, MS, USA) dealt with the new technique of improved multi-wire slicing with fixed abrasive slicing technology (FAST) for cutting sapphire and SiC used in LED applications. J. Neugebauer (Max Planck Inst. Düsseldorf, Germany) uses DFT methods with concepts of thermodynamics, continuum theory and/or statistical mechanics. He presented applications to microscopic growth mechanisms, as well as limits of the method. The crystal growth prize, as well as the crystal technology prize of the Section of Crystal Growth and Technology of the Swiss Society of Crystallography were awarded by H. Scheel to Shintaro Miyazawa (Waseda U., Japan) for his contributions to crystal growth and epitaxy technologies and for establishing the role of dislocations for GaAs micro- and optoelectronics, and to Yuzo Mori (Osaka U., Japan) for his development of PCVM and EEM, respectively. This ceremony took place during the banquet at the Hotel Jungfrau-Victoria in Interlaken. Another full-day excursion onto a glacier, together with a glaciologist from ETH Zurich, was organized on Friday. The scientific program continued on Saturday with D.K. Bowen (Bede Scientific Inc., Englewood, UK), who presented on high precision digital X-ray diffraction imaging for quality analysis of industrial crystals before further processing, which is an important market due to the very high price of large crystals. D. Bliss (US Air Force Research Lab. and President of the American Crystal Growth Assn) highlighted recent advances in InP bulk crystal growth, focusing on the special care to be taken in order to avoid formation of white phosphorous during crystallization conditions, and the influence of dopants upon twinning. His talk was followed by G. Wehrhan (Schott Lithotec AG, Germany), who presented the recent development in CaF_2 -production used in optical lenses for UV lithography. Also dealing with CaF_2 , Y. Oyama (Canon Research Center, Japan) discussed the Bridgman technique and other production methods of large crystals, presenting various results of physical parameters of CaF_2 and its melt. H. Scheel and L. Lytvynov shared a talk on the flame-fusion (Verneuil) growth of oxides before W. Assmus (U. of Frankfurt am Main, Germany) gave an overview on the skull melting of zirconia, ZrO_2 , which is widely used as an imitation gem stone for diamond, highlighting the special conditions under which this material of 2700° C melting point can be obtained. Liquid phase epitaxy, LPE, is used for large rare-earth iron garnet layers, as presented by T. Iino (Sumitomo Metal Mining, Japan). The final talk was given by F. Dupret (U. Catholique de Louvain, Belgium) on numerical modeling of different aspects of industrial crystal production, using the software FEMAG. Finally, the conference ended in the evening with a panel discussion on the future of crystal growth and the awarding of the three best lecturers of the conference.

Overall, H. Scheel and his wife R. Hauser-Scheel have put together an appealing and successful conference with an intensive, high-level, and interdisciplinary scientific program, and a perfectly well organized social and ladies program. Many participants expressed their hopes for a future workshop to be held in this region, so we all look forward to IWCGT-4 to be held in 2008.

The Book of Lecture Notes of this workshop can be ordered at a cost of \$50 from Hans Scheel, hans.scheel@bluewin.ch, and the full papers of most lecturers will be published in the planned book *Crystal Growth Technology II* (editors P. Capper and H.J. Scheel, Wiley and Sons 2006).

Katharina M. Fromm

NOTICE

Call for nominations for Fankuchen and Trueblood Awards

Nominations are solicited for the 2007 Fankuchen Memorial Award and the 2007 Kenneth N. Trueblood Award. Both awards will be presented at the annual ACA meeting in Salt Lake City in July, 2007. The recipients will give their lectures at special Award Symposia organized to honor them. Both awards are given every three years and each consists of an honorarium plus travel expenses to accept the award. There are no geographic or age restrictions. The Fankuchen Award carries the additional responsibility that the Award Lecture should also be presented at an academic institution of the recipient's choice. Nominations should be submitted to the ACA no later than May 1, 2006. A nominating letter clearly indicating the accomplishments of the individual is required; an additional supporting letter and a c.v. for the nominee may be provided, but are not required.



Isidor Fankuchen

The Fankuchen Award was established in 1971 in memory of Isidor Fankuchen, Professor of Physics at the Polytechnic Inst. of Brooklyn, 1942-1964. It is given to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Previous winners were: 2004: Alexander McPherson; 2001: James Stewart; 1998: E. Dodson; 1995: Jenny Glusker and Kenneth Trueblood; 1992: L. D. Casper; 1989: David Sayre; 1986: Michael S. Rossmann; 1983: Lyle H. Jensen; 1980: David Harker; 1977: Dorothy Hodgkin; 1974: A. Guinier; 1971: Martin J. Buerger.



Kenneth N. Trueblood

The Kenneth N. Trueblood Award was given for the first time in 2004 to Richard E. Marsh. It was created to recognize exceptional achievement in computational or chemical crystallography. The award was established in 2001 in memory of Professor Kenneth N. Trueblood, UCLA 1949-1998, who was a major force in the early use of computers and the development of crystallographic computer programs. He applied these programs to the examination of chemical and molecular details of many structures at the frontiers of research. His contribution to the work on vitamin B12 is one example. Prof. Trueblood was a leader in the development of techniques for analysis of anisotropic motion and was also a superb teacher and a lucid author.

Further information about the awards can be found on the ACA website (hwi.buffalo.edu/ACA/)

NOTICE

UK resource centre for women

Return campaign

The United Kingdom Resource Center's Return Campaign to encourage women to return to careers in Science, Engineering and Technology was officially launched on in May, 2005 (visit news.bbc.co.uk/1/hi/sci/tech/4534177.stm for BBC coverage).

The Return Campaign encompasses:

- Information, referral and follow-up support from the UKRC;
- On-line course run by the Open University - T160;
- Mentoring and networking support;
- Links with employers (under development); and
- Services offered by regional hubs in the JIVE project and other partners.

For further information, contact J. Butcher, Women Returners Manager (j.butcher@bradfordcollege.ac.uk).

SET for women unit resources

As a result of the reorganization of the DTI the UK Resource Center (UKRC) has received a valuable collection of resources, including books, reports and papers, which have been built up over the 10 years since the Promoting SET for Women Unit was established. These will be catalogued and incorporated into the UKRC Library. All the resources held at the UKRC are available to anyone wishing to reference them for research purposes. The online Publications Catalogue is an ever growing bibliography signposting to many other available resources on Women in SET. Visit the Resource Bank (www.setwomenresource.org.uk/), your feedback and comments would be most welcomed. For further information contact E. Williams (e.williams@bradfordcollege.ac.uk).

AWARDS AND PRIZES

Franklin Award



Rosalind Franklin

Christine Davies (Glasgow U., UK), who is an active member of the Women In Physics Group of the IoP, has won the 2005 Royal Society Rosalind Franklin Award.

The Award, made annually to an individual for an outstanding contribution to any area of natural science, engineering or technology (SET) consists of a medal and about £30,000 and the recipient is called upon to deliver a lecture as part of the Society's public lecture series.