

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President

Science for all nations

In the world of the 21st century, critical issues related to science and technology (S&T) confront every nation. How can we prevent global and regional environmental damage? What is the best way to introduce beneficial new technologies, thwart acts of terrorism, or respond quickly to the rapid spread of new diseases? Today, no nation that wants to shape informed policies and take effective action on such issues can afford to be without its own independent capacity in S&T.

Kofi Annan, Secretary-General of the United Nations, Science, Vol. 303, 13 February 2004



As members of the International Union of Crystallography, we have the means to assist the UN in its efforts to empower all nations to develop powerful independent programs in science and technology. X-ray crystallography is arguably the most powerful of all technologies vital to the infrastructure of science everywhere.

This issue of the Newsletter features a cover story on crystallography in Italy that was organized by Davide Viterbo and Paola Spadon. When we conceived of articles such as this one and asked members of the Executive Committee of the IUCr to prepare the first of them for publication, we did not have a clear picture of what might emerge. I was very pleased and impressed with the overview of Latin American Crystallography organized by Iris Torriani (Vol. 11, No. 3). I am equally impressed with the picture that Davide, Paola, and their colleagues have provided of the history and current activities in the field of crystallography in Italy. The material reminds us of how powerful the technique of diffraction (X-ray, neutron, and electron) is to understanding the structure of matter of all kinds. The information so carefully gathered, organized and presented is potentially very useful. Dozens of web sites are listed as part of summaries of specific areas of crystallographic analysis, including crystal growth, material science, chemical, mineralogy, and biocrystallography. Anyone interested in expert advice or potential collaboration in any of these areas can take advantage of the information presented here.

It is especially fitting that we should have the wonderful overview of crystallography in Italy as we look forward to the XXth Congress, which will take place in Florence, Italy in August 2005. The activities of Italian crystallographers in almost all areas of crystallography bodes well for the program being so carefully crafted by Carlo Mealli with representation from all committees of the Union who are gathering input from throughout the crystallographic community.

It would be very nice to have an IUCr Newsletter cover story on each of the 40 countries in our Union. Leonid Aslanov has gathered material from numerous laboratories in Russia for the next issue. Gernot Heger has told me of his plans for an issue on Crystallography in Germany and I will be writing to the members of the National Committees of Denmark, Finland, Norway, and Sweden asking them to work together to produce a special issue on Crystallography in Scandinavia. The nature of the articles written for each issue will be different because of the difference in the size, history, and interest of the member countries. It is precisely those differences that give our community its strength and vitality.

It is important that we share information, respect differences, and work together for a more tolerant, harmonious, and equitable future. We must take Kofi Annan's advice seriously to help each nation develop its independent capacity in science and technology.

Bill Duax
duax@hwi.buffalo.edu

EDITORIAL

European Crystallographic Association



Hartmut Fuess

The science of Crystallography has a long tradition in “Old Europe”. Basic principles of symmetry, description of crystals and their classification were well established before the discovery of x-rays and their application to crystals. Immediately after the discovery by von Laue (1912) the first crystal structure was solved by the Braggs (1913). In the following years Britain and Germany were the leading nations in radiocrystallography. Whereas in Britain crystallography has been widely connected with physics, mineralogy has been the “bigger” brother for crystallography in Germany. Thus, our British colleagues created an independent organization with the British Crystallographic Association (BCA) while Germany had a working group (Arbeitsgemeinschaft Kristallographie) somehow connected to the societies of mineralogy, chemistry and physics. An independent society was only founded after the unification of the two German states in 1991. Similar developments were observed in the other European countries. Crystallography was mostly connected with another scientific society, only a few independent organizations exist.

As a result of this heterogeneous situation a first European Crystallographic Meeting (ECM) was organized in 1973 at Bordeaux under the guidance of André Authier. Without any formal organization a small group of people organized the following ECM-conferences in years with no IUCr-congress. The name European Crystallographic Committee (ECC) was created and all European countries were invited to take part. Besides about 20 of them Israel and Egypt were always present. One of the - unwritten - guidelines of ECC was the alternation of ECM-meetings between Eastern and Western European countries. This approach was definitely very important and contributed considerably to overcome the isolation of colleagues in many countries and to a cohesion of crystallography in Europe. The ECM conferences attracted more and more scientists culminating in more than 1000 delegates in Vienna, Austria in 1988.

This tremendous success led to the consideration of a more formal organization. After lengthy discussions among ECC delegates, a formal organization was finally created under the chairmanship of Hartmut Fuess at ECM 17 in Lisboa. The legal act of registration was prepared by Paul Beurskens from Nijmegen, The Netherlands. Dutch is therefore the official language of the statutes.

Carmelo Giacovazzo was the first elected president. In 1978 the IUCr statutes were amended at the Warsaw Congress and the European Crystallographic Assn (ECA) became the first Regional Associate of the IUCr (at that time it was still the ECC). The ECA admits three categories of members (i) The crystallographic organizations of countries (ii) individual members and (iii) cooperative members. Most European nations are now represented, the number of individuals is about 500. In 1995 South Africa was admitted first as an observer and then as a regular member. The ECM 21 conference was held in 2003 in Durban. The presence of Egypt and South Africa in ECA most naturally led to the idea to include Africa in the organization. Under the presidency of Claude Lecomte several African countries were admitted as members. On the other hand some countries in Middle and Eastern Europe have experienced increasing

difficulties keeping in contact. To reintegrate those crystallographers is one of the important tasks of the present Executive Committee which was elected in Durban. The members, Teresa Duarte (Portugal), Giuseppe Filippini (Italy), Hartmut Fuess (Germany), Mariusz Jaskolski (Poland), Claude Lecomte (France), Anders Liljas (Sweden), André Roodt (South Africa), Chick Wilson (U.K.) represent well a European-African partnership.

The forthcoming meetings of ECM 22 in Budapest (Hungary) in August 2004, ECM 23 in Leuven (Belgium) in 2006 and ECM 24 in Marrakech (Marocco) in 2007 are already scheduled.

Hartmut Fuess, ECA President

LETTER TO THE EDITOR

50 Years of DNA continued a little further

Rex Palmer's criticism of Mark Spackman's commentary on the origins of the DNA structure can be extended to correct a regrettable omission in Watson's *The Double Helix* and Watson and Crick's 1953 *Nature* paper. As Palmer says "the whole thing is based largely on crystallographic results..... **from other groups!**". One of the experimentally derived factors mentioned by Palmer used in the DNA model building was "The possible base pairing H-bonding patterns and their geometry. This could be derived from a **wealth of crystallographic data**, and was revealed to Watson and Crick by Jerry Donohue, a world renowned expert on H-bonding in 1953."

Robert Olby's 1974 *The Path to the Double Helix* shows that Watson was working on base pairing before Donohue was brought into the discussions. He was studying June Broomhead's papers and thesis of 1948-1951 on the crystal structures of adenine HCl and guanine HCl. Happily for him the thesis was available close at hand in the Cavendish Laboratory. These papers were part of a series of five in *Acta Crystallographica* which Clews, Cochran and Broomhead published in those years on the structures of pyrimidines and purines. This work had been undertaken in close collaboration with the chemical work on nucleotides by Professor A.R. Todd and his colleagues.

Watson p184 writes "..... I was drawing the fused rings of adenine on paper. Suddenly I realized the profound implications of a DNA structure in which the adenine residue formed hydrogen bonds similar to those found in crystals of pure adenine. If DNA was like this, each adenine residue would form two hydrogen bonds to an adenine residue related to it by a 180-degree rotation." Watson had very cleverly abstracted the pair bonding from Broomhead's diagrams of the layers in her structures of adenine and guanine. But Broomhead is not named. Nor does Watson mention his good fortune in having available the Cavendish work on pyrimidines and purines.

At this stage Donohue, with his H-bonding knowledge, entered the action to point out that Watson should be using keto rather than enol forms. Shortly Watson saw that like-with-like pairings "led nowhere". Then brilliantly he spotted that adenine-thymine pairs would be identical in shape to guanine-cytosine pairs. Hence this type of double helix would immediately explain the Chargaff ratio rules. Crick then joined in to check and thrash out more features of their double helix model – and the rest is history. But it is sad that the famous duo omitted to acknowledge their debt to Broomhead and her colleagues.

Durward Cruickshank, Manchester

LETTER TO THE EDITOR

A correction



Dear Judy,

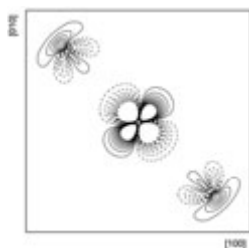
May I point out an error in Newsletter Volume 11, Number 3, which I have just received? In the photo on p.14, taken in 1983, which shows five lecturers at the International School, the man in the centre is not Weinstein (as written), but the late Sig Weissmann of Rutgers U.

Lisa Heller-Kallai

γ -ray and neutron diffraction studies of CoF₂: magnetostriction, electron density and magnetic moments

γ -ray and neutron diffraction studies of CoF₂: magnetostriction, electron density and magnetic moments

***Acta Cryst.* (2004). A60, 51-57 [doi:10.1107/S0108767303022803]**



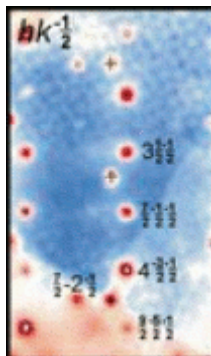
Contour map of the model deformation electron density with Co being located in the center. Preferred occupation of 3d orbitals gives rise to excess densities as large as $4 \text{ e}\text{\AA}^{-3}$.

Accurate structure factors up to $\sin\theta/\lambda = 1.6 \text{ \AA}^{-1}$ have been measured from CoF₂ at room temperature and in the antiferromagnetic state at 10 K using 316.5 keV gamma radiation. Extended time-of-flight neutron diffraction data allowed an accurate determination of the fluorine positional parameter. A complete charge-density analysis has been carried out for the ordered phase. On magnetic ordering, a small shift of the fluorine ions is found which confirms a prediction from theory of optical birefringence. The effect of magnetostriction on the distortion of the ligand coordination octahedra is compared for the late members of the 3d transition-metal difluorides, and is shown to follow a remarkably simple scheme. From neutron powder diffraction, an ordered magnetic moment of $2.60(4) \mu_B$ per cobalt ion is found. Despite the strong deviation from the spin value of $3 \mu_B$ for the free atom there is still an appreciable orbital contribution to the local magnetic moment.

W. Jauch, M. Reehuis and A. J. Schultz

Local and long-range order in ferroelastic lead phosphate at high pressure

***Acta Cryst.* (2004). B60, 1-9 [doi:10.1107/S0108768103026582]**



$hk\text{-}\frac{1}{2}$ reciprocal lattice section collected from a single crystal of $\text{Pb}_3(\text{As}_{0.52}\text{P}_{0.48}\text{O}_4)_2$ shows diffuse maxima that are indexed with half-integer indices of the $R\text{-}3m$ unit cell.

Lead orthophosphate, $\text{Pb}_3(\text{PO}_4)_2$, undergoes a phase transition from $C2/c$ to $R\text{-}3m$ symmetry at a pressure of 1.8 GPa at room temperature. Structures determined from neutron powder diffraction data indicate that the $R\text{-}3m$ phase includes disordered positions for several atoms. Observation of X-ray diffuse scattering from the $R\text{-}3m$ phase at high pressure suggests that this disorder is static and arises from the presence of several orientations of ordered microdomains of monoclinic local structure, and thus there is no significant change in the local structure at the phase transition. This is in contrast to the high-temperature $R\text{-}3m$ phase in which the disorder is dynamic in nature.

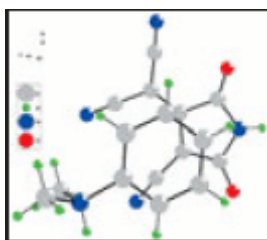
R. J. Angel, U. Bismayer and W. G. Marshall

IUCR JOURNALS NEWS

N,N-Dimethylanilinium 3-cyano-4-(dicyanomethylene)-5-oxo-4,5-dihydro-1H-pyrrol-2-olate

N,N-Dimethylanilinium 3-cyano-4-(dicyanomethylene)-5-oxo-4,5-dihydro-1H-pyrrol-2-olate

Acta Cryst. (2004). C60, o62-o64 [doi:10.1107/S0108270103025940]



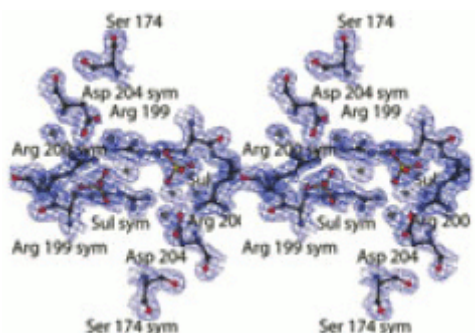
On the basis of the structural data and the calculated charge distribution on the atom of the title anion, the following types of the anion-cation interaction can be postulated: a) “isotropic” interaction with each outer heteroatom of the anion taking part in the formation of a polyhedron enclosing the cation (alkali, alkali-earth metals); b) π - π stacking interaction, involving planar cations (e.g. pyridinium); c) transition metal - π -system of the anion interaction (e.g. ferrocene); and d) interaction of the heteroatoms of the anion and transition metals to form a coordination compound, chelate complex or polymeric structure. In the title salt, anions and cations overlap to form π - π stacks along the *a* axis.

Viktor A. Tafeenko, Rene Peschar, Olga V. Kaukova, Henk Schenk and Leonid A. Aslanov

IUCR JOURNALS NEWS

The impact of Lys → Arg surface mutations on the crystallization of the globular domain of RhoGDI

***Acta Cryst.* (2004). D60, 275–280 [doi:10.1107/S0907444903026271]**



A stereo figure illustrating a crystal contact in crystals of a double mutant of RhoGDI in which two adjacent lysines (199 and 200) were replaced with arginines. Both the electron density and the model are shown. The arginines from adjacent molecules sequester two sulfate ions from the precipitant. A crystal structure can only be determined if X-ray quality crystals are available. In the case of proteins, the preparation of such crystals is often difficult or even impossible. One possible way of circumventing the difficulties is to modify the protein's surface by site directed mutagenesis. Previous work (*Acta Cryst.* D57, 679–688 and *Acta Cryst.* D58, 1983–1991) showed that introducing patches with low conformational entropy by mutating lysines and/or glutamates to alanines, promotes formation of crystal contacts mediated by these epitopes. However, such mutations reduce solubility. The present study showed how sometimes mutations of lysines to arginines can also be useful. In the particular case reported in the paper, two arginines introduced in place of lysines create a crystal contact by sequestering a sulfate ion.

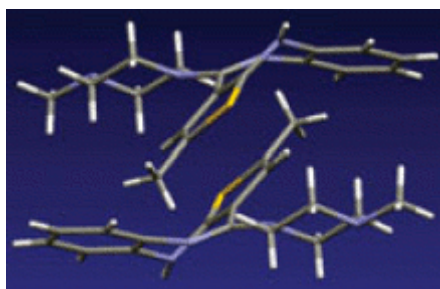
J. Czepas, Y. Devedjiev, D. Krowarsch, U. Derewenda, J. Otlewski and Z. S. Derewenda

IUCR JOURNALS NEWS

Polymorphic form II of 2-methyl-4-(4-methyl-1-piperazinyl)-10H-thieno[2,3-b][1,5]benzodiazepine

Polymorphic form II of 2-methyl-4-(4-methyl-1-piperazinyl)-10H-thieno[2,3-b][1,5]benzodiazepine

Acta Cryst. (2004). E60, o66-o68 [doi:10.1107/S160053680302806X]

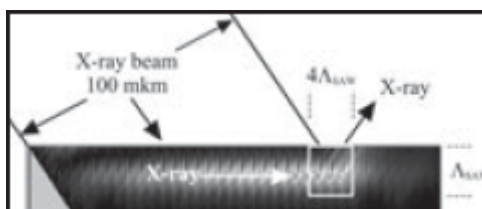


The title compound, generic name olanzapine, is one of the newer generation atypical antipsychotic agents. Approved pharmaceutical formulations contain stable polymorphic form II of olanzapine, which is one of five known and patented forms. Crystalline unsolvated form II was obtained from solutions in anhydrous toluene and esters of acetic acid. The main building block of this crystal net is a molecular dimer. The centrosymmetric olanzapine dimer is stabilized by multiple C-H... π contacts which occur between the aliphatic (methyl or methylene groups) and aromatic (thiophene or phenyl rings) parts of the molecules. Similar dimers have been found also in the crystal structure of olanzapine solvates.

I. Wawrzycka-Gorczyca, A. E. Koziol, M. Glice and J. Cybulski

Dynamical theory for calculations of X-ray spectra from crystals modulated by surface acoustic waves

***J. Appl. Cryst.* (2004). 37, 52–61 [doi:10.1107/S0021889803023847]**



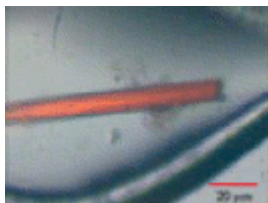
Surface acoustic wave (SAW) excitation in the YZ-cut LiNbO_3 causes crystal lattice deformation and leads to “quasi”-waveguide propagation of X-rays in the region under incident beam illumination (see figure). In this region the crystal virtually ceases to reflect despite the fact that the incidence angle is equal to the Bragg angle of the ideal case (perfect crystal). As a consequence, splitting of diffraction peaks on the rocking curve during the experiment are registered. The effect has been explained using direct calculations of the SAW deformation field and simulation of wavefield distribution inside the crystal by numerical integration of the Takagi-Taupin equations. So, the direct problem of X-ray diffraction on a crystal modulated by SAW is believed to be solved.

I. A. Schelokov, D. V. Roshchupkin, D. V. Irzhak and R. Tucoulou

IUCR JOURNALS NEWS

Recent developments in microdiffraction on protein crystals

***J. Synchrotron Rad.* (2004). 11, 4-6 [doi:10.1107/S090904950302541X]**



Cryocooled crystal of bovine rhodopsin visualized on the microgoniometer. (Courtesy of G. Schertler, Cambridge)

A dedicated microgoniometer for synchrotron radiation protein crystallography has been developed at EMBL-Grenoble in collaboration with ESRF. Beam sizes down to about 5 µm and a compact pinhole collimating system allow reducing background scattering from the sample environment, which is important for small and weakly scattering crystals such as membrane proteins. A microscope, coaxial to the X-ray beam, facilitates sample alignment. Needle-like protein crystals of about 10 µm diameter of trigonal bovine rhodopsin belong to the currently smallest protein crystals studied.

C. Riekel

SPECIAL REPORT

Crystallography in Italy



Italy can boast an old tradition in the field of Crystallography. It suffices to remember that in the 16th century, the Medici Family gathered in Florence one of the oldest and most precious collections of natural crystals and morphological studies were initiated by Vannoccio Biringuccio. Here, however, we wish to concentrate on the birth and growth of modern structural crystallography in Italy.

The first structural work with X-ray diffraction was carried out around 1923-24 in Milano by the group headed by G. Bruni and formed by G.R. Levi, A. Ferrari, G. Peyronel and G. Natta. Not only did G. Natta pioneer X-ray crystallography in Italy, but, when he moved his interest to polymer science, with his co-workers P. Corradini and G. Allegra, he applied X-ray diffraction to the structural characterization of synthetic polymers. For his outstanding results in this field he became Nobel Laureate for Chemistry in 1963. A. Ferrari was the founder of the crystallographic school in Parma, where his co-workers, L. Cavalca and M. Nardelli, were very successful in creating and maintaining a large and productive group.

In the mid thirties G. Giacomello in Rome and S. Bezzi in Padova were the first to apply X-ray crystallography to organic compounds and in 1954 they founded the first Centres for Structural Chemistry of the National Research Council (CNR) and established international collaborations. G. Giacomello had among his co-workers V. Caglioti, P. Corradini, A.M. Liquori and A. Ripamonti. Today, the important "G. Giacomello" Institute for Structural Chemistry, located in Monterotondo (near Rome), bears the name of its founder. When A.M. Liquori moved to Naples in the early sixties, he encouraged the young L. Mazzarella to visit M.F. Perutz in Cambridge. There he contributed to a pioneering paper on the crystal structure of haemoglobin, thus becoming the first Italian protein crystallographer.

In Padova, S. Bezzi initially dedicated his interest to set up and improve the experimental and computational methodologies of crystal structure analysis and in 1940 he published the structure of p-dibromobenzene. In the CNR Centre he founded in Padova, Bezzi's co-workers were U. Croatto, V. Scatturin, and C. Panattoni, who carried out relevant research in the field of structural inorganic chemistry, and M. Mammi with his group, who developed the initial route of organic crystal chemistry into protein crystallography. In 1975 Mammi became the director of the CNR Centre for the Study of Biopolymers.

The structural study of organic compounds in the late fifties was also promoted by M. Simonetta in Milano. He was mainly a theoretical chemist, but his farsightedness led him to pursue the direct interaction between crystallographers and theoreticians.

In the sixties, in Florence, L. Sacconi, an internationally renowned transition metal chemist, was among the first in Italy to understand the enormous potential of crystallography in coordination and organometallic chemistry, especially if aimed at establishing basic correlations between structure and properties. Today, the members of the former Sacconi's team propose themselves as the enthusiastic organisers of the XXth IUCr meeting in 2005.

In the field of mineralogical crystallography, the first structural work was carried out in the late thirties in Rome by the group of E. Onorato. After the war, the structural analysis of minerals continued to be developed by various groups. In Rome, F. Sgarlata developed a very efficient set of crystallographic programs for the Olivetti ELEA computer (at that time a valid competitor of IBM 1620). In 1958 the group directed by M. Fenoglio in Turin, already active before the war, acquired the first 3-circle single-crystal diffractometer in Italy and initiated the era of modern structure analysis. In Florence, the Mineralogy Institute of the University, directed by G. Carobbi, was home to the early work of F. Mazzi, G. Cocco and C. Garavelli, who later developed important crystallographic schools in Pavia, Perugia and Bari. In Pisa, S. Bonatti started major research in crystallography, which was then successfully developed by G. Gottardi, S. Merlino and co-workers. The groups in Florence, Genoa, Pavia, Pisa, Rome and Turin soon joined their efforts and founded the CNR National Center of Crystallography, later concentrated only in Pavia.

In the mid sixties the role of Crystallography started to enlarge towards other fields.

The Italian Crystal Growth Association (AICC) was created soon after the birth of the IOCG (International Organization for Crystal Growth) and collected practically all the Italian growers from industry, CNR and the academic world. Italian growers proved very active not only from the scientific point of view, but also in the organisation of many national and international schools and meetings.

In the field of protein crystallography, after the groups in Naples and Padova a third important group was established in Pavia and today Italy can count more than 15 groups.

The role of Italian crystallography within the IUCr (of which Italy has been an official member since its creation in 1947) received a first important recognition when Rome was chosen as the site of the VIth IUCr Congress in 1963.



Rome 1967 foundation meeting of the Italian Crystallographic Association.

In 1967 the need to coordinate crystallographic activities led to the foundation of the Italian Crystallographic Association (AIC). From the 108 founding members, mainly chemists and mineralogists, the association rapidly enlarged its membership (reaching now over 300) as well as its interests. Physicists, Biologists, and Materials Scientists joined AIC and in 1993 the unification with AICC was the last important step to enlarge the scope of the association.



Participants to the AIC School on Interaction Forces in Crystals, Perugia September 1989.

The first AIC president was F. Mazzi and the first congress was held in January 1968 in Perugia. The annual meetings have become the most important occasions of scientific interchange. Joint congresses with Yugoslav and Swiss colleagues have also been organized. A separate section of this presentation is devoted to the last XXXIII AIC Congress held in Trieste. Teaching all basic aspects of crystallography, especially to young people, is one of the AIC main goals and, since 1971, the "Summer School" has become the other important event in our scientific life (usually organized in Perugia by A. Nunzi). M.M. Woolfson, with the help of M. Nardelli and his group, organized the "Nato Advanced Study Institute on Direct and Patterson Methods" in Parma in 1970. This event led to the first School of Crystallography held in Erice in 1974. Thanks to the invaluable organizational skills of Lodovico (his surname is redundant among crystallographers), recently enriched by the charm and efficiency of Paola Spadon, the Erice School (www.crystalalice.org) is now a regular international event touching all innovative aspects of Crystallography, with 36 Courses organized, gathering more than 4000 participants.

In 1972 L. Cavalca and M. Nardelli founded the journal *Crystal Structure Communication* in Parma. The quality of the structural papers, together with the powerful automatic procedures developed by the editors to control the quality of the numeric data, convinced the IUCr to transform *CSC* into *Acta Cryst. C* in 1983.

Many Italian crystallographers have been chairpersons and members of numerous IUCr commissions and Co-editors of *Acta Cryst.* M. Nardelli was elected President of the IUCr in 1987, and in 2002 D. Viterbo was elected to the Executive Committee. The 154 Italian entries in the 3rd edition (1965) of the World Directory of Crystallographers have increased to 337 in the last 1997 edition, making Italy the sixth largest country in the world.

Italy has always been active within the European Crystallographic Committee since its founding in 1972, and in the period 1984-90, G. Filippini was secretary of the committee. In 1985 the IXth European Crystallographic Congress (ECM-9) organized by G. Ferraris in Torino was attended by more than 650 people and showed the first large attendance from East European countries. Also ECM-13 in 1991, initially planned in Ljubljana, was finally held in Trieste. When in 1997 in Lisbon the European Crystallographic Association (ECA) was founded, C. Giacovazzo was elected to be the first Chairman. More recently, G. Filippini and D. Viterbo were elected to the ECA Executive Committee in 2003 in Durban (ECM-21). C. Giacovazzo was awarded the third ECA Prize for his outstanding achievements in the field of Direct Methods.



Italy will host the XXth IUCr Congress in 2005 in Florence, a city of unequalled history, beauty and receptivity. The high level of the scientific activity carried out in Florence, the enthusiasm and competence of C. Mealli, P. Paoli and our other Florentine colleagues and the guaranteed help and support of the whole Italian crystallographic community, will make Florence 2005 an unforgettable event from both a scientific and social point of view. Italian Crystallographers welcome all of you in Florence!

Davide Viterbo

NOTE - The Cover Story on Crystallography in Italy is the result of the cooperation of several people, but the main responsibility for its structure goes to Davide Viterbo and Paola Spadon, who have coordinated the work. We are aware that we have certainly missed or forgotten something, and we apologize in advance to all those who may feel they have been underrepresented. This presentation has suggested creating a special page in the AIC web-site (<http://aic.istm.cnr.it>) in which more details on the crystallographic activities in Italy are given and constantly updated. A special thanks to all those who have contributed to this work and helped us in this task.

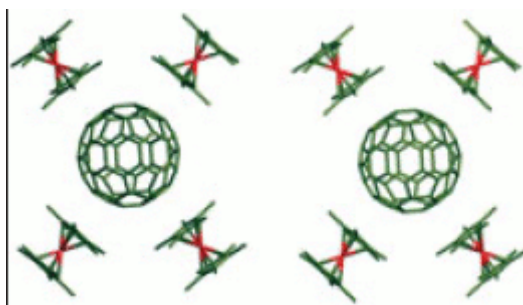
Davide Viterbo (member of the IUCr Executive Committee)

Paola Spadon (president of the Italian Crystallographic Association)

Chemical crystallography

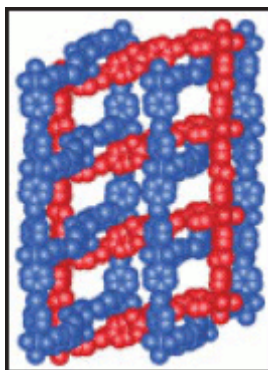
The pioneering and seminal work of the group of bright Italian crystallographers who worked in a number of strategic Italian Universities in the '60's gave birth to an Italian crystallographic Golden Age, and the urgency of "seeing the structure, understanding the chemistry" rapidly spread all over Italy. Today, along with the initial landmarks settled in Milan, Parma, Rome, Naples, Padua, Florence, Pavia, a large number of lively and creative laboratories has flourished in many other sites, playing crucial roles in the European landscape of Structural Chemistry.

In 2005, Florence will be the world's scientific capital of crystallography; the Florentine crystallographic community is centred around two laboratories, where the main research topics embrace structure-properties relationships of inorganic and organometallic compounds studied by experimental crystal structure analysis, systematic usage of structural databases, theoretical quantum-mechanical calculations^[1], structure-activity relationships for small pharmacological organic molecules and macrocyclic metal complexes, coordination compounds of biological interest, and the interaction of small molecules (P_4 , P_4S_3) with metal-ligand systems^[2].



Solid State Adducts between C_{60} and Decamethylferrocene (A. Arrais, E. Diana, R. Gobetto, M. Milanesio, D. Viterbo, P.L. Stanghellini, *Eur. J. Inorg. Chem.*, 2003, 1186-1192).

In Milan three laboratories operate in the field of structural chemistry, investigating: electrostatic properties by topological analysis of experimental electron density between 15K and 300K^[3]; supramolecular architectures assembled by halogen bonding and organometallic complexes, weak H-bonds and metal-metal interactions by multipolar analysis of electron densities^[4]; conventional X-ray single crystal diffractometry on organometallics and minerals, accurate LT structural determinations and topological analysis of experimental and theoretical charge densities, *ab initio* powder diffraction, structural characterisation of materials, neutron diffraction, synthesis and characterisation of coordination polymers and supramolecular architectures, molecular modelling, crystal structure prediction, and tomographic methods^[5].



New polycatenation type in $[Ni_6(bpe)_{10}(H_2O)_{16}](SO_4)_6 \times xH_2O$ [bpe = bis(4-pyridyl)ethane] (L. Carlucci, G. Ciani, D.M. Proserpio, S. Rizzato, *Cryst.Eng. Comm.*, 2003, **5**(34), 190-199).

In Parma more than 20 researchers and technicians operate in the Laboratorio di Strutturistica^[6], which has inherited the legacy of the Centro di Studio per la Strutturistica Diffraattometrica del C.N.R., founded in 1968. The scientific activity spans from structural and theoretical aspects of supramolecular chemistry and crystal engineering of organic/inorganic hybrid networks, to bioinorganic and bioorganic medicinal chemistry, from structure-reactivity relationships of organometallic compounds, to the characterization of superconducting and magnetic materials and to computational crystallography.

In Bologna, four groups operate in the laboratories of the Dipartimento di Chimica^[7], where research topics cover: hazard monitoring of asbestos, bone crystal growth, self-assembly of collagen fibers, drug delivery, hydroxyapatite based materials, chrysotile nanotubes, silica xero-gels, quantum wires, chemical-physical characterization of morphology and surface activity; design and development of new inorganic and composite materials with tailored functional properties (nano- and micro-crystalline inorganic phases, oriented growth of inorganic phases on nanostructured matrices, and new biomaterials); group 8 metal carbonyl clusters and stereochemistry of low valent metal complexes; design of crystalline materials for applications in solid/solid and solid/gas solvent-free reactions, and polymorphism.

In Rome structure-activity studies on compounds of biopharmaceutical and industrial interest are a traditional interest of the IC-CNR Institute^[8]. The research activities address: antiviral compounds; inhibitor-resistant β -lactamase to design new powerful inhibitors; design and synthesis of new peptide inhibitors of Zn-proteinases involved in inflammatory processes; polyamine catabolism in plants; inorganic compounds with possible antineoplastic activity; coordination and organometallic compounds of industrial interest. Researchers at the Dipartimento di Chimica^[9] have been active for many years studying the theoretical/experimental study and design of molecular adducts of nucleobases as a model for the DNA/RNA bases recognition.

Research activity at the U. of Genova^[10] started in the early fifties. Since then, more than one thousand intermetallic compounds have been synthesized and structurally characterised; seventy new structure types have been discovered, and currently the crystal chemistry of intermetallic compounds, and

structure-activity relationships for pharmaceutical organic compounds by XRD and QM methods are studied.

In Ferrara the structural physical chemistry group^[11] has contributed remarkably to the study of hydrogen bonded systems, and is currently involved in quantum-mechanical calculations of H-bonded systems, proton-transfer pathways, Bader's AIM topological analysis, molecular pharmacology, biothermodynamics, and molecular modelling.

In Turin crystal and molecular structures of coordination compounds and organometallic complexes have been studied by X-ray and neutron diffraction since the 1970s at the Laboratorio di Chimica Strutturale^[12]. Study of experimental electron density and multipolar analysis from low temperature diffraction data of model molecules have been addressed since the late 1990s.

In Padua at the Dipartimento di Scienze Farmaceutiche solid-state structural analyses of bioinorganic drugs, psychotropic agents belonging to the classes of cognition activators and nootropics, and theoretical analysis of coordination complexes and psychotropic agents are performed^[13], while at the CNR Istit. di Chimica Biomolecolare crystallographic work is devoted to the conformational characterization of peptide antibiotics (peptaibols) and analogs thereof, synthetic peptides carrying non standard amino acid residues, and peptide foldamers^[14].

In Messina the Interdepartmental Centre^[15] shares human resources from many departments in the University. It is organized into three groups whose research topics cover physical and chemical crystallography, X-ray applications in cultural heritage materials, X-ray applications in materials science and engineering.

In Alessandria, the structural physical chemistry group^[16] is involved in the study of biopharmacological compounds and of zeolites of catalytic interest. Weak interactions in molecular crystals and organic-inorganic interactions in relation to the biomineralization process are also being investigated.

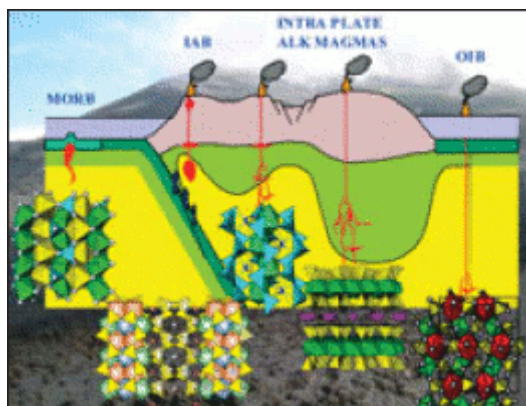
At the U. of Calabria^[17] the current scientific fields of interest are the study of structure and magnetic behaviour of paramagnetic coordination compounds, and the interaction between metal ions and DNA components.

In Perugia^[18] layered metal phosphates and phosphonates and synthetic hydrotalcites are designed for potential application in catalysis, proton conduction, ionic and molecular recognition and their structures are studied by powder diffraction.

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Crystal-chemical studies of rock-forming minerals allow a better understanding of petrogenetic processes, either related to subduction or to magmatic activity. (courtesy of R. Oberti)

Mineralogical crystallography

Internationally, Italian research in the field of Mineralogy is very highly regarded, thanks to its strong crystallographic character, as recently witnessed by the role played by Italian mineralogists in founding and ruling the Mineralogical Crystallography SIG of ECA^[1] and the Commission on Inorganic and Mineral Structures of IUCr^[2]. The Italians also play a fundamental role in the organizing and contributing to crystallography-oriented symposia and schools organized by the International Mineralogical Association^[3] and the European Union of Mineralogy^[4]. Italy is a leader in the characterization of new and rare mineral species^[5,6,7,8,9,10,11,12,13], a topic where the structural characterization by X-ray and electron diffraction plays a crucial role. Low crystallinity and complexity of the structures that are met in this type of research, often do not allow the use of automatic methods for structure solution; thus, the development and use of other modern experimental (TEM^[9,10,11]; spectroscopy like EXAFS^[7,11,14], IR, Mössbauer, NMR, XANES^[7,11,14], XPS) and theoretical approaches have been stimulated. Important theoretical contributions have been published in the field of modular crystallography (OD theory, polysomatism, polytypism, twinning, incommensurate structures)^[5,9,10,11], an approach applicable to large families of technological materials as well. The spectroscopic methods mentioned have also been applied to the study of local geometry, oxidation state and short-range ordering. The experimental results are often supported by theoretical calculations, e.g. molecular dynamics and modelling of crystal structures and of absorption spectra^[7,8,10,12,14,15,16].



HRTEM image of carlosturanite (after Carlo Sturani, Professor in Torino), cylindrical chrysotile and polygonal serpentine intergrown fibres as seen along the fibre axes. (Deriu, A., Ferraris, G., Belluso, E. *Phys. Chem. Minerals*, **21**, 1994, 222-227).

The crystal-chemical investigation of some main groups of rock-forming minerals (amphiboles^[8,10], carbonates^[8], feldspars^[10,14], garnets^[8], micas^[7,10,13,15,17], pyroxenes^[8,10,18], pyroxenoids^[9],

serpentines^[10,11], spinels^[6,10,18], staurolites^[8], zeolites^[7,9,15,16], including meteorites^[11]) is another outstanding feature of Italian mineralogical crystallography. In particular, this type of research led to the development of crystallographic investigations at non-ambient conditions (in order to study the stability, transformations and kinetics of phases and to establish state equations) and of detailed crystal-chemical analysis and structure modelling (with the aim to relate cation order and site geometry to the *P*, *T*, *X* conditions of formation)^[7,8,9,10,11,15,17,19]. The latter results combine structure refinement, SIMS and IR analysis when light elements are involved^[8]. For most of the mentioned groups of minerals, unique databases of crystal-chemical data have been established^[8].

Some of the results obtained by Italian mineralogical crystallographers are of primary interest for materials and environmental sciences, technology and industrial processes, like those concerning the properties of cationic exchange, diffusion, heterogeneous catalysis and gas dehydration of microporous minerals (zeolites^[7,15,16], titanosilicates^[9,10], layered silicates^[7,15]) and the calcium silicates hydrates so important in the chemistry of cement (e.g. the tobermorite group)^[9].

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Crystal growth



Participants to the 10th Summer School on Crystal Growth (ISSCG-10), Rimini, Hotel Continental.

Relevant aspects of crystal growth (CG) are currently investigated in universities, private and governmental laboratories and industries. Advanced characterization techniques are usually available for crystal quality assessment. Not all the Italian crystal growers are AIC members, but most of them attend the annual AIC meetings, which always include a specific symposium. The proceedings of these symposia are occasionally published. A look at the last of them^[1] might give an idea of the CG activity in Italy. Its favorable acknowledgement abroad helped promote international meetings and schools in Italy in recent years, see, e.g., [2-5].

Most of the CG research has been devoted to the deposition and characterization of epitaxial and polycrystalline layers, prepared by vapour phase (CVD, MOCVD, MBE, sputtering, pulsed-laser ablation, etc.) and sol-gel techniques. The motivations are usually the improvement of solid-state devices for special applications. The main activity is on semiconductors, such as silicon and Si-Ge alloys^[6-9], III-V and II-VI compounds^[1-6,10-17]; but also on magnetic materials^[18-19], superconductors^[10-11,20], diamond coatings and others.

Bulk CG technology is developed: (a) in industries: MEMC Electronics Materials grows silicon in Meran^[9] while Venezia Technologies grows III-V compounds (GaAs, InP^[21]) in Venice; (b) in governmental laboratories: crystals of II-VI^[10,22] and III-V semiconductor compounds and organics (urea and derivatives, urotropine, etc.^[10,23]) are grown by IMEM-CNR in Parma; (c) in universities: crystalline samples, usually grown from solution, are proteins^[25], carbonates, phosphates and sulphates^[26,27], zeolites^[28], and sugars^[30].

Other topics worth mentioning are the growth of nanocrystals (carbon^[29,11,22] and various oxides^[1,22]) and space growth^[1,4,23-25].

As to CG theory, research is developed from a phenomenological point of view, aiming at optimising, through modelling, CG processes in bulk and epitaxial technology (see, e.g., [1-7,23-25]), as well as at evaluating the relevance of space growth experiments^[1,4,24-25]. Surface energy concepts are also made use of to study nucleation and aspects of crystal morphology^[26].

Finally, research is also carried out on the development of methods for estimating unknown parameters through 'first-principles' calculations and the development of 'multiscale' approaches, in view of linking atomistic, crystallographic and phenomenological aspects in CG^[1,4,7].

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- [1] Proc. Italian Crystal Growth Symp., Naples, Sept.1999; *Materials Chem.Phys.* (single issue), R. Fornari, C. Paorici, A. Zagari eds., **66** (2000).
- [2] Proc. ISSCG-10, Rimini, June 1998 (promoted by IOCG and IUCr); published as *Theoretical and Technological Aspects of Crystal Growth*, R.Fornari, C.Paorici eds., Transtech, Zurich (1998).
- [3] Proc. Intern. School on *Crystal Growth of Materials for Energy Production and Energy-saving Applications* (promoted by IUCr), R. Fornari. L. Sorba eds., ETS, Trieste (2001).
- [4] Proc. Joint Italo-French Meeting on *Crystal Growth: from Basic to Applied*, S.Carrà, C.Paorici eds., Academy of Lincei, Rome (2003).
- [5] *Proc. European Workshop on Metalorganic Vapour Phase Epitaxy*, Lecce, June 2003, N. Lovergine, A.M. Mancini, P. Prete eds., U. of Lecce (2003).
- [6] *Silicon Epitaxy*, D. Crippa, D.L. Rode, M. Masi eds., *Semiconductors and Semimetals Series*, Vol.72, Academic Press, San Diego (USA) (2001).
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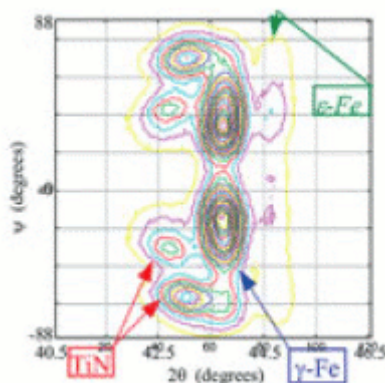
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Materials science

Materials science in Italy has a long tradition as an interdisciplinary area involving chemistry, physics and engineering research. The last 20 years has seen the creation of dedicated research centres, departments and consortiums, and the institution of university degrees in Materials Engineering and in Materials Science. This present report only mentions some Italian research groups most directly engaged in the development of crystallographic methodologies applied to materials science and technology, without trying to represent the vast category of users of crystallographic methods and related analytical techniques.

In Brescia^[1] crystallographers are engaged in investigations of thin films and multilayers for optical, catalytic, and sensor applications; optimization of structural and innovative techniques to investigate metallurgical problems; and synthesis and structural, chemical, and nanomechanical characterisation of magnetic multilayers and patterned magnetic nanostructures.

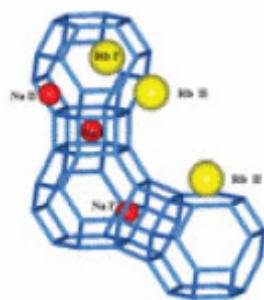
Crystal structure and properties of natural zeolites and clay minerals; Quantitative phase analysis by the Rietveld method of oxide mixtures, clays and glass-ceramics and amorphous/crystalline fractions; high temperature/high pressure dynamic studies of zeolites by *in-situ* X-ray synchrotron light (diffraction and spectroscopy) and *ab-initio* computational methods are being pursued in Modena^[2].



Residual stress - texture θ - $2\theta/\psi$ map. TiN on steel substrate. (P. Scardi & Y.H.Dong, *J. Mater. Res.* **16** (2001) 233-242.)

In Trento^[3] the following topics are being investigated: residual stress and texture analysis in thin films and coatings: new analytical methodologies based on laboratory and synchrotron radiation diffraction

techniques; and microstructure and lattice defects in nanocrystalline and severely deformed materials by diffraction line profile analysis: new methods for *ab-initio* modelling of the whole powder diffraction pattern.



Structure of faujasite, where the location of cation sites Na and Rb are shown. (G.L. Marra, A.N. Fitch, A. Zecchina, G. Ricchiardi, M. Salvalaggio, S. Bordiga, C. Lamberti, *J. of Phys. Chem. B*, **101**(50), 1997, 10653-10660.)

In Bologna^[4] research is focused on: isotactic polymers by WAXS/SAXS (polybutene-1, ethylene, polypropylene, polyvinylchloride); evolution of microstructure and morphology as a function of catalysis conditions; and high molecular weight polyethylene polymerized in different conditions; correlation between structural and morphological parameters and high-modulus properties of the materials.

In Venice^[5] the microstructure of materials is analysed by powder diffraction and small angle scattering: amorphous, partially crystalline and polycrystalline systems containing nanostructured phases are studied. The quantitative and qualitative analysis of small fractions of supported metal clusters with a size of a few nanometres are also investigated.

In Pavia^[6] structure-properties relationships in polycrystalline doped materials are investigated.

The Research Centre in Novara^[7] investigates: characterization by diffraction methods, using laboratory and synchrotron sources, of powders of heterogeneous catalysts used in oxidation reactions of H₂O₂ and application of full profile fitting procedures to study crystallographic aspects related to catalytic performance.

In Rome^[8], time resolved *in-situ* structural and morphological investigations are performed on magnetic nanostructured and high T_c superconducting thin films, organic gas sensors, electrochemical and fuel cells and amorphous alloys undergoing phase transitions. Energy dispersive X-ray diffraction and reflectometry are also used.

In Udine^[9] research involves: diffraction study of polymer (poly-organolphosphazenes and polydimethylsiloxane) structures from polycrystalline samples and synthesis and crystallographic and microstructural characterization of oxide based ceramic materials.

At the Politecnico in Milano^[10] the structure, morphology, crystallization and mesophases of synthetic organic polymers, oligomers and model compounds and the self assembly of new organic materials using specific intermolecular interactions are studied together with organic matrix nanocomposites with inorganic silicates.

At the U. in Milano^[11] the following are investigated: physical properties and crystal structures of materials and industrial minerals at high temperature and pressure, with particular emphasis on thermal expansion and vibrational properties and chemical reactivity at crystal surfaces and kinetics of nucleation and crystal growth, studied by atomic force microscopy and *in situ* synchrotron radiation techniques.

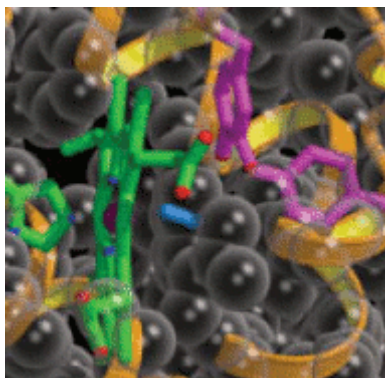
At Milano Bicocca^[12] materials science and theoretical methodologies are investigated. Neutron diffraction studies of ion mobility in inorganic ionic conductors as well as first-principle studies of phase transitions and physical properties of crystals are carried out.

In Cagliari^[13] ionic coordination in water solutions and in glasses by X-ray diffraction and EXAFS and structural investigation of nanomaterials by XRD, TEM, HREM and EXAFS are researched.

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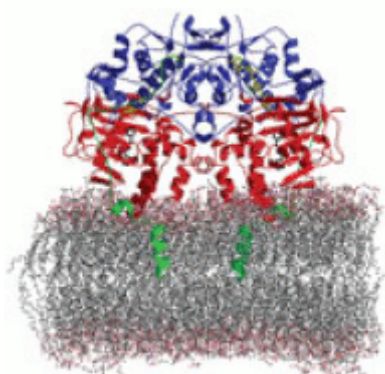
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Biocrystallography



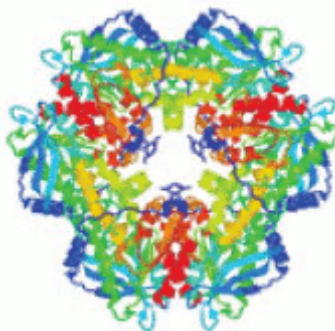
Tyrosine post-translational modification in a haemoglobin-like protein from *Mycobacterium tuberculosis* (M. Milani, P.Y. Savard, H. Ouellet, P. Ascenzi, M. Guertin, M.O. Bolognesi, *Proc. Natl. Acad. Sci. USA*, **100**, 2003, 5766-5771).

A survey based on the Italian scientists devoted to Biocrystallography provides a picture of a very productive community that dates back to the 1960s. After the pioneering start of L. Mazzarella in Napoli, a laboratory was established in the 1970s by M. Mammi in Padova, followed in the 1980s by A. Coda, the founder of the crystallographic school in Pavia.



Structure of Human Monoamine Oxidase B linked to a membrane lipid double layer (C. Binda, P. Newton-Vinson, F. Hubalek, D. E. Edmondson, A. Mattevi, *Nature Structural Biology*, **9**, 2002, 22-26.)

Nowadays there are 17 academic and 2 industrial, dynamic research groups located in: Roma^[1], Milano^[2], Napoli^[3], Trieste^[4], Siena-Firenze^[5], Bari^[6], Bologna^[7], Genova^[8], Pavia^[9], Padova^[10], and Verona^[11]. The groups based in Pavia and in Padova deserve a special tribute for their pivotal role in training many Italian researchers who are now working as leading scientists in the field of structural biology in Italy and in various foreign institutions. The current focus of the laboratories is on proteins of medical and biotechnological interest.



Structure of *Bacillus Pumilus* AcetylXylan Esterase: a carbohydrate degrading enzyme (I. Krastanova, G. Degrassi, A. Cassetta, V. Venturi, D. Lamba, unpublished result).

Recent results include structural and functional studies on heme-proteins^[1a,1b,3a,8], DNA/PNA^[3b], DNA-drugs and DNA-protein complexes^[1c,4a], collagen models^[3a], metalloenzymes involved in denitrification and radical protection^[4b,5,8], flavodoxins^[2b], plant, viral and bacterial pathogenic proteins^[1a,1d,2c,5,10], carbohydrate processing enzymes^[4b], hydrophobic ligand-binding proteins^[10,11], metallo proteins^[4a,5], animal and vegetal lectins^[11], protein kinases^[10], proteins involved in NAD biosynthesis and iron homeostasis^[9], proteins involved in the coagulation and fibrinolysis pathways^[3b,4b,8], protein complexes involved in the regulation of mitosis^[2a], in neuronal differentiation^[2a], in immuno response^[2c], in amyloidosis^[8], and in muscle contraction^[4b]; cell activating receptors involved in natural cytotoxicity^[8]; target-based drug design proteins involved in various human diseases^[1a,1c,1d,2d,3a,5], in Alzheimer's and Parkinson's diseases^[4b,9]; proteins involved in the biomineralization processes^[7]. Research activities also include the growth of biological macromolecules crystals on engineered surfaces^[7]; macromolecular crystallization under microgravity on the international space station^[3a]; the use of soft X-rays as a phasing tool^[4b]; direct methods in macromolecular crystallography^[6].

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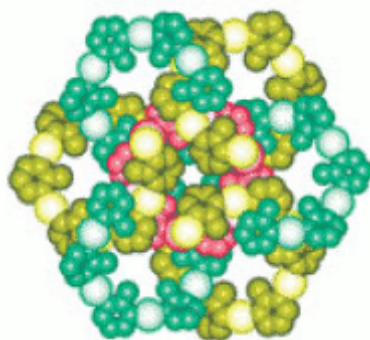
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Crystallographic methodologies

A number of Italian research groups are actively involved in the development of crystallographic methodologies, producing relevant results both in the field of structure determination and materials characterization and the investigation of new experimental techniques.

In Bari and Rome^{[1],[2]} research in the last thirty years has focused on the theory and application of the phase problem in crystallography (in collaboration with researchers at the University of Perugia), producing significant scientific contributions at an international level. Their research goals are the development of innovative procedures for *ab-initio* crystal structure solution. The methods, developed so far, have been implemented in computer programs used by the crystallographic community all over the world: Sir97 (small molecules), the heir of Sir92 and CAOS (least squares refinement); EXPO (powder data); and Sir2002 (proteins). A very recent methodological activity concerns the crystallographic characterization of materials (quasicrystals, nanocrystals) and the quantitative analysis of multicomponent polycrystalline mixtures (program QUANTO).

In Como^[3] and Milan^[4] research interests are the structural determination by *ab-initio* powder diffraction methods of covalent inorganic and organometallic polymers and the study of structure-property relations in functional materials (transition-metal-based molecular magnets; electroluminescent materials, organometallic catalysts). Most recent activity has been focused on the determination of the local structure of disordered materials by total scattering analysis with application to amorphous or paracrystalline metalcoordination polymers.



The unique formation of a crystal phase containing cyclic oligomers and helical polymers of the same monomeric fragment as discovered by *ab-initio* XRPD studies on conventional lab data (N. Masciocchi, G.A. Ardizzoia, G. La Monica, A. Maspero, A. Sironi, *Angew. Chem., Int. Ed. Engl.*, (1998), **37**, 3366). In Parma^[5] and Bologna^[6] Transmission Electron Microscopy (TEM) techniques, in particular High Resolution Electron Microscopy (HREM) and Electron Diffraction (ED), have been (and are still) used to support, in a strategic way, conventional diffraction techniques for the solution of complex structural problems. More recently, with the enlargement of the research group^[7] a significant effort has been concentrated on *ab-initio* crystal structure solution using ED data. Three main research lines are being developed: 1) the experimental reduction of dynamical effects on ED intensities (implementation of a beam-precession technique on a Philips CM30T microscope), 2) the development of computer programs for quantitative treatment of ED data (QED program package), and 3) the characterization of strategies

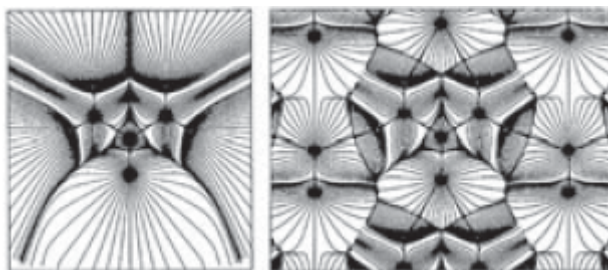
for direct methods application to ED data and synergetic use of HREM, ED, X-ray and neutron powder diffraction data for the structure determination of materials.

The group in Pisa^[8] is interested in X-ray diffractometry methods. In particular: technological aspects, production of prototypes, standardization and metrological aspects, and new approaches to round robin designs.

In Pavia^{[9],[10]}, Milan^[11] and Turin^[12] scientific activity is directed at improving crystallographic procedures for the characterization of materials. Research on least-squares refinement, electron density reconstruction, leverage analysis and maximum entropy methods are in progress.

In Salerno^[13] research is devoted to the study of stereoregular crystalline polymers from powder and/or fiber samples with particular attention to the solution and refinement of polymer structures (the program TRY has been developed) and to the indexing and extraction of integrated intensities from image plate detectors.

In Siena^[14], the main research lines are: improvement of the Gandolfi technique to minimize the number of missing reflections and to obtain reliable 'powder' diffraction patterns from a single grain as small as 20µm diameter; the quantitative determination of the diffraction aspect in pseudosymmetric crystal structures.



Gradient field of the electron density in the molecular plane of urea, in gas phase (left) and in the crystal (right), obtained using the TOPOND Code (C. Gatti, V.R. Saunders, C. Roetti, *J. Chem. Phys.* **101**, 1994, 10686-10696).

In Milan^[15], research is concerned with the development of software for 1) electron density distributions analysis, including topological and electrostatic properties (TOPOND, TOPXD and PAMoc), 2) lattice dynamics (VIBR) and 3) crystal structure and polymorphism's prediction (PROMET).

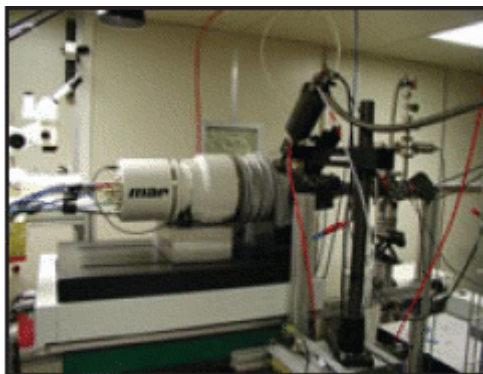
The group in Turin^[16] is studying the electronic structure and properties of perfect and defective crystalline materials. They have developed *ab initio* methods that have been implemented in program CRYSTAL that is distributed to the scientific community for applications involving the study of physical, chemical, electric and magnetic properties of ionic, covalent and molecular crystals.

Coordinated by Angela Altomare (angela.altomare@ic.cnr.it)

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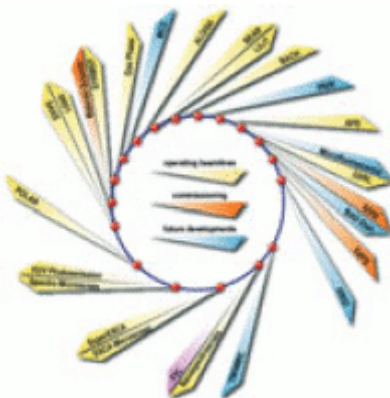
Elettra Synchrotron Radiation Source in Trieste



CCD on the diffraction beamline, with He purging path for long wavelength data collection (photograph by K. Djinovic).

Elettra (www.elettra.trieste.it) is the Italian third generation synchrotron radiation laboratory. It is built around a medium energy electron storage ring operated at 2 and 2.4 GeV. The Elettra beamlines cover a wide energy range, from the far infrared to hard x-rays, with wavelengths between 0.6 mm and 0.3 Å. The facility is operated by the Sincrotrone Trieste public no profit company, which built the accelerator system and some of the beamlines. Other beamlines are built in collaboration with external partners from various scientific institutions, both Italian and from other countries. Altogether, there are 15 operating beamlines and 4 under commissioning.

Elettra also hosts several support and complementary laboratories, which make it a multidisciplinary research and service centre, competitive at the international level. Researchers at Elettra are active in fields as diverse as genomics, pharmacology, biomedicine, catalysis and chemical processes, microelectronics and micromechanics.



Beamlines at ELETTRA.

The X-Ray Diffraction 1 beamline has been designed primarily for macromolecular crystallography. The light source is a multipole wiggler with a useful range from 4 to 25 keV. The optics consists of a double-crystal monochromator in non-dispersive configuration, followed by a toroidal focussing mirror with a horizontal acceptance of 2.8 mrad. The tunability of the wavelength provides the opportunity to use the MAD technique for solving the phase problem over a broad range of wavelengths, covering the absorption edges of all heavy atoms commonly used in protein crystallography. The multipole wiggler spectrum includes high photon flux at low energies, allowing optimisation of the anomalous signal at the Sulphur, Xenon and Calcium edges.

The high-flux Small Angle X-ray Scattering beamline is mainly intended for time-resolved studies on fast structural transitions in the sub-millisecond time region in solutions and partly ordered systems with a SAXS resolution of 1 to 140 nm in real-space. The SAXS-Beamline accepts 3 discrete energies, namely 5.4, 8 and 16 keV (0.077, 0.154, 0.23 nm). The beamline optics consists of a flat, asymmetric-cut double crystal monochromator and a double focusing toroidal mirror.

At present the X-ray Absorption Fine Structure (XAFS) beamline is under commissioning.

Giorgio Paolucci, Riccardo Spagna and Augusto Pifferi

Other non-conventional sources

Italy participates in the European Synchrotron Radiation Facility (ESRF: www.esrf.fr) in Grenoble. Most beamlines were constructed and are managed directly by ESRF, while additional Collaborating Research Group (CRG) beamlines were constructed by external groups. Italy constructed the GILDA beamline (www.lnf.infn.it/esperimenti/puls), which provides a high flux X-ray beam of mm² size in the energy range 4-80 KeV. The installed instruments allow performing X-ray absorption spectroscopy in transmission, fluorescence, total yield and REFLEXAFS mode, in the temperature range 4-1000 K, as well as time resolved powder diffraction with a translating imaging plate detector. An ultra high vacuum chamber is available for X-ray absorption studies on surfaces.

Other Italian activities at ESRF involve the development of a high resolution X-ray spectrometer for inelastic scattering in the meV regime installed on the ID26 beamline, the development of an inelastic soft X-ray scattering apparatus installed on the ID08 beamline, and the construction of a general support laboratory.

Italian activities on the use of available instrumentation and development of new ones for neutron diffraction and spectroscopy are based at the Institute Laue-Langevin (ILL, Grenoble, France; www.ill.fr) and at ISIS (Rutherford-Appleton Laboratory, Chilton, UK; www.isis.rl.ac.uk).

At the ILL, Italian teams from INFM (Istit. Nazionale per la Fisica della Materia) are involved in two CRGs: IN13 and BRISP, two instruments dedicated to study diffraction by non-crystalline media.

At ISIS, in the eighties, the CNR funded a project for building PRISMA, an inverse geometry crystal analyser spectrometer and high resolution diffractometer. In the nineties TOSCA, an instrument for molecular spectroscopy was built in collaboration with UK groups.

Several Italian groups have performed experiments on diffraction instruments at ISIS (SXD, POLARIS, HRPD, GEM) and ILL (D19, D1, D2) obtaining important structural results in the fields of chemical crystallography, materials science, mineralogy and polymer chemistry where the peculiar advantages of neutrons over X-rays as structural probe are outstanding.

Settimio Mobilio and Antonio Deriu

AIC-SILS Meeting

Trieste, July 21-25, 2003



The annual meetings of the Italian Crystallographic Association (AIC) and of the Italian Synchrotron Light Society (SILS) were held jointly in Trieste in July, 2003, in the beautiful area of Miramare by the International Centre of Theoretical Physics. More than 170 people from different Italian universities and research centres attended the conference. The goal of the joint meeting was to encourage interaction between two communities that have strong scientific common interests. The crystallographic community, which usually uses laboratory sources, had the opportunity to be informed of recent progresses in modern synchrotron radiation facilities and instruments. On the other hand synchrotron radiation scientists received an overview of many scientific problems of interest today in the structural characterization of different classes of materials, from amorphous materials to proteins.

The conference was structured in four common symposia, three parallel microsymposia, and a common poster section. In addition, a common section was dedicated to the presentation of the ESRF and ELETTRA Facilities. The common microsymposia were dedicated to "Diffraction in Materials Science", to "Progress of Structural Biology promoted by Synchrotron Sources", to "Spectroscopic Methods for Structural Investigations" and "Archeometry". The parallel microsymposia were organized separately by the two societies. AIC organized microsymposia on "Structural Crystallography" and "Experiments, Modeling and Theories on Crystal Growth Mechanisms at the Atomic- and Nano-scale level"; the SILS organized a microsymposium on "Studies with Synchrotron Radiation".

"Diffraction in Materials Science" aimed at presenting recent and innovative applications of synchrotron and laboratory based diffraction techniques in the structural and physical characterization of inorganic materials.

"Progress of Structural Biology promoted by Synchrotron Sources", was opened by J. Nyborg whose plenary lecture was focussed on the knowledge gained on the various elongation factors and how they are related to protein biosynthesis taking place on the ribosome. All the presentations stressed the increasing complexity of the biological systems studied in Italy and a common feature of all the experimental works was the utilization of European sources.

"Spectroscopic Methods for Structural Investigations" provided an overview of Synchrotron Radiation spectroscopic methods and their use in structural and morphological studies of different systems, from biological systems to semiconductor and nanostructures, focusing on the state of the art achieved in the different cases.

"Archeometry" was concerned with structural studies of archaeological materials by synchrotron radiation; it was shown how a microscopic comprehension of the structure favours the understanding of the origin of archaeological finds, of the treatments experienced during their production and of the transformations experienced during their ageing. For the first time in Italy, recent results obtained by X-ray methods in this field were illustrated in order to stimulate the use of these probes by archaeologists, cultural heritage operators and restorers.

The microsymposium "Structural Crystallography" was devoted to results and advances in structural crystallography. The plenary lecture by A. Fitch dealt with the use of synchrotron radiation in crystal structure solution and illustrated the instrumentation available for high-resolution powder diffraction measurements and different approaches to solve structures from synchrotron data. The following contributions were devoted to new trends in chemistry, frontier research on polymers and on incommensurate crystals. Two contributions were devoted to methodological research.



The 2003 AIC Prize winner with the organizers of the meeting in Trieste.

"Experiments, Modelling and Theories on Crystal Growth Mechanisms at the Atomic- and Nano-scale" focused on both experimental and theoretical results, and on fundamental mechanisms driving the growth of crystals at the microscopic (i.e., atomic and nano-scale) level. The Plenary lecture on "Probing Epitaxial Growth on a Microscopic Scale", was given by W. Richter. Other contributions were on the use of real-time small-angle synchrotron X-ray scattering, on the *in-situ* and *ex-situ* AFM investigations of crystal growth at both nano- and micron-scale, on advanced molecular dynamics simulation of growth by self-assembling of constituent atoms/molecules and on the application of density functional theory (DFT) to crystal growth chemistry.

In "Studies with Synchrotron Radiation" the contributions outlined recent achievements in the characterization of ordered and disordered materials by high energy and/or space resolved synchrotron radiation photoemission and X-ray microdiffraction experiments.

According to their tradition, both Societies awarded young researchers with special prizes. AIC gave the award to Marco Milanesio of the U. of Piemonte Orientale, who presented a review lecture on his scientific work on experimental and theoretical structural chemistry. SILS awarded four young scientists working in different fields. Namely R. Carboni from Bologna working in the characterization of semiconductor nanostructures, A. Sanson from Trento working on the dynamical properties of oxides, M. Merlini from Milano, working on heterogeneous catalytic systems for methane combustion and L. Di Costanzo from Trieste, working on protein crystallography.

The smooth and collaborative atmosphere present at the meeting favored deep and extensive discussions between the two communities and the birth of new scientific collaborations can be foreseen.

Settimio Mobilio and Gilberto Vlaic

The interdisciplinary crystallographic teaching activity in Erice, Italy



A. Zichichi, a nuclear physicist, founded the Ettore Majorana Centre for Scientific Culture (nowadays E. Majorana Foundation and Centre for Scientific Culture). He defined "International Schools" as any scientific field whose leaders would be willing to gather at the top of a mountain to review scientific progress in a restricted, stimulating atmosphere. He saw it as an appropriate setting for teaching and promoting generations of young scientists without ideological, political or racial barriers. The International School of Crystallography (ISCoC) was officially born in 1972 following a suggestion by Michael Woolfson during the 1972 Kyoto IUCr Congress. He personally inspected the site along with Herbert Hauptman, Gabriel Germain, Georges Tsoucaris and Lodovico Riva di Sanseverino. Michael was

also the scientific director of the very first Course on Direct Methods in 1974. Since then the ISCoC has been running courses every year (except 1979) on various crystallographic topics. Some of them became the foundation for repeated meetings with an approximate periodicity of six years to mark the most relevant contributions and exciting progress. The most popular titles have been: Direct Methods, Molecular Biology, Drug Design, Electron Diffraction, Material Science and Inorganic and Theoretical Chemistry.

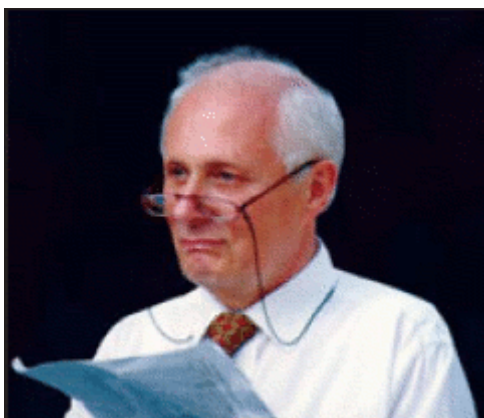
After a short period of stimulating directorship by Nobel laureate Dorothy Hodgkin, she passed the torch to Tom L. Blundell, FRS, Birkbeck College, now at Cambridge U., UK. Tom is responsible for the general planning of activities (mainly teaching courses) at the ISCoC and nominates the scientific director(s), who are dynamic leaders in the particular topic covered in each course. The director of the course is responsible for inviting lecturers and for setting up an attractive and stimulating scientific programme. The local organising staff consists of an executive secretary and a treasurer (who sign this text) and the IT expert, John J. Irwin, now at the UCSF, USA.

A typical Course in Erice consists of morning lectures, and afternoon tutorials run with the help of the most modern computing facilities. Poster sessions, round table discussions and sessions devoted to "short talks on hot topics" are always included in the programme. In recent years efforts have been made by the organizers to run a "virtual course" simultaneously with the traditional one. Thanks to the great work of the IT expert scientists from everywhere in the world can now follow the courses in real time and can even interact directly with the audience in Erice during the sessions.

Courses in Erice have a strong interdisciplinary character and are attended by specialists from various fields. The inimitable Erice environment and the efforts by the organizers have often led to closer scientific contacts and future collaborative research projects. Erice web page: www.crystallerice.org

Paola Spadon and Lodovico Riva di Sanseverino

Davide L. M. Viterbo



Davide L. M. Viterbo was born in Torino in 1939 and studied Chemistry at the University of Torino, where he joined the Physical Chemistry group and initiated his academic and scientific career.

He is now full professor of Physical Chemistry at the Faculty of Natural Sciences of the University of Piemonte Orientale "A. Avogadro" (Alessandria).

His research interests have been on the methodologies of structural analysis by diffraction methods, with particular emphasis on the so called "Direct Methods" for the solution of the phase problem. He spent three years in the Physics Dept. of the University of York (UK), working in this field with Prof. M. M. Woolfson and was also involved in research projects with Dr. H. Hauptman and Prof. C. Giacovazzo.

D. Viterbo has also carried out the structural investigation of several classes of organic compounds of bio-pharmacological interest (furoxans, azoxyderivatives, ranitidine analogues, sesquiterpenoids, taxane derivatives, squalenes, etc).

In the recent years he has also undertaken the analysis of the geometric and physico-chemical properties of molecular crystals, with particular attention to weak intermolecular interactions, by comparing the results of experimental charge density studies from accurate diffraction data, collected at low temperature, with those from *ab-initio* quantomechanical calculations.

In the last few years he has devoted his attention to the structural characterization of zeolite-like systems by diffraction techniques both on polycrystalline samples and on single crystals, taking advantage also of the powerful features of synchrotron radiation.

More recently he entered the fascinating world of siliceous spicules from marine sponges in order to elucidate their structural arrangement and to throw some light on the mechanisms of the biosilicification process.

D. Viterbo has been invited as lecturer at a number of International and National Schools. He is author of 130 publications and of a Chapter of the book "*Fundamentals of Crystallography*" (edited by C. Giacovazzo, Oxford U. Press, 2002) and he has been chairman of the "Commission for Crystallographic Computing" of the International Union of Crystallography in the period 1993-1996. He was elected chairman of the Italian Crystallographic Association in the triennium 1997-1999 and member of the executive committee of the European Crystallographic Association in the period 2000-2003. Presently he is member of the executive committee of the International Union of Crystallography.

MEETING REPORT

New Materials by Crystal Engineering Design

Singapore, December 2003

A symposium dedicated to *Crystal Engineering* was a key component of a larger International Conference on Materials for Advanced Technologies (ICMAT2003) held in Singapore in December, 2003. The symposium was attended by over 60 delegates from 17 countries with over 40 oral presentations covering a wide range of topics from rational design and synthesis of crystals (attracting quite some discussion), practical applications (electronic, magnetic, host/guest chemistry, etc.) and theoretical aspects of *Crystal Engineering*. A highlight of the Symposium was a day dedicated to honouring the pioneering contribution of Richard Robson. The symposium also featured Poster sessions with the ICMAT2003 prize being awarded to Makato Tadokoro (Osaka City U.) and the *CrystEngComm* prize being awarded to Bellam Sreenivasulu (National U. of Singapore). A collection of papers presented at the Symposium will be published in a dedicated volume of *Crystal Growth & Design* during 2004 and a photo gallery is available on the website (www.chemistry.nus.edu.sg/PSSO/Vittal/index.htm).

J.J. Vittal, E.R.T. Tiekink & S. Valiyaveetil



MEETING REPORT

Structure Determination Workshop

Leipzig, Germany, September, 2003

In September 2003 more than 60 German chemical crystallographers (ChemKrist) met in Leipzig to discuss various methods of X-ray structure determination structure analysis. G.M. Sheldrick, opening with a retrospective on the development of direct methods, was followed by lectures by P. Luger (derivation of atomic properties from experimental electron-density studies), H. Borrmann (K_1 diffractometry) and M. Ruck (dealing with very high absorption). Also M. Fechtelkord (combination of X-ray diffraction and NMR spectroscopy), G.M. Sheldrick (structure determination of large molecules), U. Kolb (electron microscopy), U. Schwarz (X-ray diffraction at high pressure), R. Dinnebier (structure determination from powder data), M. Hellenbrandt (ICSD database), N. Sträter (data collection strategies for macromolecules) and K. Fries (modulated structures) made excellent contributions. The organizer J. Sieler had invited two scientists from large-scale facilities: H.A. Graf (application of neutron diffraction) and E. Weckert (experiments with synchrotron radiation). In addition there were presentations by STOE and BRUKER AXS, which had generously supported this meeting. The last day began with an introduction by P.G. Jones into the secrets of a CIF file. Then I. Bruno and G. Battle demonstrated the enormous potential of the Cambridge Structural Database with the help of many instructive examples. Social activities included a visit of the famous Bibliotheca Albertina and a farewell dinner with a splendid view of Leipzig. One must admire Joachim Sieler for his excellent (and certainly time-consuming) preparation and organization of this really successful 'workshop conference', which gave a state-of-the-art overview on many important subjects.

Christian Näther and Ernst Egert



AWARDS AND PRIZES

2004 Clifford G. Shull Prize



J. Michael Rowe.

J. Michael Rowe (NIST Center for Neutron Research) is the first recipient of the 2004 Clifford G. Shull Prize of the Neutron Scattering Society of America (NSSA) 'For his seminal vision, leadership, and contributions to the field of neutron scattering'. The prize and \$5000 honorarium will be awarded at the 2004 ACNS, June 6-10, in College Park, MD (www.ncnr.nist.gov/acns).

The NSSA established the Clifford G. Shull Prize in Neutron Science to recognize outstanding research in neutron science and leadership promoting the North American neutron scattering community. The prize is named in honor of Clifford G. Shull, who received the Nobel Prize in 1994 with Bertram Brockhouse for seminal developments in the field of neutron science. The establishment of the prize was announced at the inaugural American Conference on Neutron Scattering (ACNS) in 2002.

Early in his career, Mike Rowe was at the forefront of research on the dynamics, structure and fundamental properties of materials, including influential work on hydrogen in metals, orientationally disordered solids and monatomic liquids. In addition, he has made significant contributions to the development of inelastic spectrometers and other instruments that utilize cold neutrons and is a leader in the design of the latest generation cold neutron sources, including the most efficient hydrogen cold source currently operating in the world at the NCNR. Dr. Rowe's talents and his profound impact on American neutron science go far beyond his individual contributions to research and instrumentation. Through his leadership and engineering creativity over the past 15 years, the NCNR has become the most important and widely used neutron facility thus far developed in the US.

AWARDS AND PRIZES

2004 ASBMB-AMGEN Award



Steven Almo.

Steven Almo, Albert Einstein College of Medicine, has been elected to receive the 2004 ASBMB-AMGEN Award. This award is made to a new investigator, with no more than 15 years experience since receipt of a doctorate, for significant achievements in the application of biochemistry and molecular biology to the understanding of disease.

Dr. Almo has achieved a position of world-leadership in structural biology by developing a unique program in the cytoskeleton and functional analysis of contractile and allergenic proteins. His recent work has been on the co-stimulatory molecules that modulate the T cell response of the adaptive immune response and the structural and biochemical analysis of the molecules that regulate the actin cytoskeleton and contractile and motile cellular processes. He is a founding member of the New York Structural Genomics Research Consortium, one of the nine NIH-funded National Centers charged with the development of a high throughput structure discovery pipeline to provide a useable model for all individual protein structures.

AWARDS AND PRIZES

2004 Ludo Frevel Crystallography Scholarship

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected six recipients for the 2004 Scholarship Program. These recipients were selected on a competitive basis from fifty-one commendable applications received by the ICDD Scholarship Committee. The recipients are:

- G. Kwai-Wai Kong (U. of Melbourne/St.Vincent's Inst. of Medical Research, Australia) with exploration into 'Crystallographic Studies of the Amyloid Precursor Protein (AAP)';
- C. Lim (U. of Illinois at Urbana-Champaign, USA) with research concerning 'Reaction Path and Crystallography of CoSi_2 Formation on Si(001) by Reactive Deposition Epitaxy';
- A. Locock (U. of Notre Dame, USA) with interest in 'Crystal Structure and Synchrotron Radiation Study of Uranyl Oxysalts of Phosphate and Arsenate – Implications for Remediation';
- R.T. Macaluso (Louisiana State U., USA) with research involving, 'X-ray and Neutron Diffraction Studies for Understanding Geometrically Frustrated Systems';
- P. Simoncic (U. of Bern, Switzerland) with studies on 'Defect Structure of the Natural and Synthetic Zeolites Mordenite – Structure Characterization of Dye Modified, Synthetic Mordenite';
- K. Tait (U. of Arizona, USA) whose research is entitled 'Investigations into the Stability, Morphology and the Crystal Structure of the Coexistence of Structure I and Structure II Methane-ethane Clathrate Hydrates – Occurrence and Geological Implications'.

Each student will receive \$2,250 to assist in the continuation of studies in their selected fields of crystallographic research. The application deadline for the 2005 Awards is October 31, 2004. The applicant should be enrolled in a graduate degree program during the 2005 calendar year with major interest in crystallography.

The scholarship term is one year. Further information is available at www.icdd.com.

These scholarships are made possible through corporate and private donations. If you would like information on how you can make a donation, contact ICDD at 610-325-9814.

NOTICE

New Amorphous Materials Group

A Special Interest Group of The Society of Glass Technology

A Structure of Amorphous Materials Special Interest Group has been formed by The Society of Glass Technology to provide a valuable forum for discussion and presentations of issues of current interest and significance in the areas relating to the structure of any non-periodic materials. Individuals actively engaged or

interested in this research field are encouraged to join the Special Interest Group.

The 1st Meeting of the Structure of Amorphous Materials Group will coincide with the Annual Spring Meeting of the Soc. of Glass Technology, held at the U. of Liverpool, UK, April 21–23, 2004.

Membership of the Special Interest Group is independent of that of The Soc. of Glass Technology. The membership fee is £15. Applications and further information is available at www.sgt.org.