

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



The National Committees and adhering bodies of the IUCr of 24 countries nominated candidates to fill offices of the Executive Committee and the 15 Commissions of the IUCr for the triennium 2005-2008. The list of nominees has been posted on the IUCr website. Two candidates for President, two candidates for Secretary/Treasurer, and sixteen candidates for general membership on the Executive Committee were nominated. I want to express my appreciation to all the members of the national committees of all countries who have made nominations. Traditionally, national committees have tended to recommend crystallographers from their country for membership on the Executive Committee. It is gratifying to see national committees go beyond their own borders to support nomination of candidates regardless of gender or country of origin. The list of candidates demonstrates how many highly qualified and capable people are willing to serve the Union. In accordance with the by-laws, the Executive Committee, meeting in Budapest, Hungary, August 25-26, began a review of the nominations in order to compose a slate of candidates for presentation to the delegates to the the XX General Assembly in Florence, Italy. The results of the Executive Committees deliberations will be sent to the Secretaries of all National Committees as soon as possible, after which time the results will be posted on the IUCr website. In accordance with the by-laws, additional nominations for election to any executive office can be proposed at the Congress. It may be time to consider an expanded Executive Committee coming from an increased number of Union countries that could advance the goals of the Union more effectively. A review of the list of candidates for membership on the Executive Committee indicated how well each of these excellent candidates could serve the needs of the IUCr throughout the world. The composition of the IUCr Executive Committee has changed very little in the 50 years since its inception. Any expansion of the size of the Executive Committee would require revision of the bylaws, another matter for the consideration of the delegates to future IUCr General Assemblies.

Since my election as President, I tried to attend the meetings of all the regional affiliates to the IUCr in order to learn more about the needs and activities of crystallographers everywhere. I have attended meetings with crystallographers in Canada, Moldova, Novosibirsk, Algeria, Australia, South Africa, Germany, Morocco, Italy, Spain, Hong Kong, Budapest, and Chicago. Later this year, I will attend meetings of crystallographers in Venezuela, Argentina, the UK and Moscow. While in these countries, I try to meet with members of the national crystallographic associations and national committees and especially crystallographers from nonmember countries to discuss how the Union can serve them better. I have prepared summary reports of highlights of my visits for the members of the Executive Committee. Excerpts from these reports will be distributed to national committees and appear in future issues of the Newsletter.

At some of the meetings, I have also been able to meet with other members of the Executive Committee to discuss a range of issues facing our community. We are very fortunate to have an active Executive Committee that has accepted new responsibilities, including the preparation of special issues of the IUCr Newsletter that review crystallography in their country. In this issue, Leonid Aslanov, assisted by crystallographers throughout Russia, begins a comprehensive survey of crystallography in Russia covering the Moscow region. The next issue will include reports from other major centers in Russia.

Bill Duax

duax@hwi.buffalo.edu

EDITORIAL

Crystallography in Russia



This short message introduces a collection of papers describing “Crystallography in Russia”. A number of laboratories and institutes have contributed to give readers a chance to learn about the activities of Russian crystallographers. Last year the Institute of Crystallography of the Russian Academy of Sciences (IC RAS) celebrated its 60th anniversary jubilee. The corresponding paper reflects the achievements of IC RAS both in retrospective and with a look toward future prospects of the Institute.

Due to space constraints, some very active and well known crystallographic laboratories will be featured in future issues of the *IUCr Newsletter* (e.g. Institute of Chemistry in Vladivostok, Institute of Elemento-Organic Chemistry in Moscow, Institute of Problems of Chemical Physics in Chernogolovka, and the Institute of Chemistry of Silicates in St. Petersburg). The activity of Russian crystallographers is clearly illustrated by the crystallographic conferences held in Russia in 2003: on chemical crystallography in May in Chernogolovka, mineralogical crystallography in September at St. Petersburg, physical crystallography in November in Moscow, on metal alloys in October in Moscow, Fedorov’s Session in December, at St. Petersburg, and Belov’s memorial conference in December in Nizhnii Novgorod.

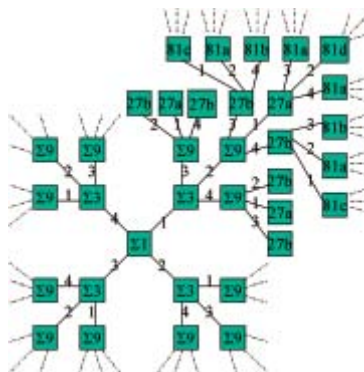
All these conferences were organized under the supervision of the National Committee of Crystallographers of Russia, which is a body of RAS. Members of the committee were active in the conferences, both as organizers and as participants. In 1990, the National Committee, as well as many members of the Russian crystallographic community, experienced some problems which are hopefully in the past. The National Committee hopes that this review, “Crystallography in Russia”, will strengthen the ties of Russian crystallographers to the world wide crystallographic community.

Yurii A. Osipyan

Chairman, National Committee of Crystallographers of Russia

The structure of the cubic coincident site lattice rotation group

***Acta Cryst.* (2004). A60, 263–277 [doi:10.1107/S010876730400772X]**



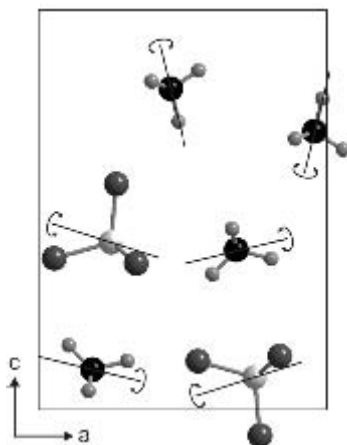
A map of a portion of the twin-related group $\Sigma 3^{\omega}$, which governs the grain boundary networks in ideal twin-dominated materials.

The field of grain boundary engineering aims to improve the properties (e.g. fracture toughness) of polycrystalline materials by optimizing their networks of grain boundaries. The idea is to enhance the frequency and connectivity of so-called “special boundaries,” which arise from particular relative orientations of adjacent crystal grains and which tend to have relatively high strength, diffusion resistance, etc. The group theory of crystallographic misorientations imposes strong constraints on the network only now beginning to be understood. This article develops the mathematical underpinnings of these kinds of constraints, synthesizing and generalizing previous work in a simple, unified, and extensible framework.

B. W. Reed, R. W. Minich, R. E. Rudd and M. Kumar

Structure of incommensurate ammonium tetrafluoroberyllate studied by structure refinements and the maximum entropy method

Acta Cryst. (2004). B60, 127-137 [doi:10.1107/S0108768104000874]



Projection of the basic structure of $(\text{NH}_4)_2\text{BeF}_4$. Rotation axes describing the modulations of the complex ions are indicated. Be atoms light gray; N atoms black.

Ammonium tetrafluoroberyllate has an incommensurately modulated phase that is stable in a narrow temperature interval (175–182 K) between the paraelectric and low-temperature ferroelectric phases. The structure of this phase is difficult to determine because of a narrow interval of stability and partial overlap of reflections. Structure refinements and the Maximum Entropy Method in superspace show that the modulation comprises single harmonic rotations and translations of rigid BeF_4^{2-} and NH_4^+ complex ions. The development of the modulation is driven by changes in the network of hydrogen bonds. The ferroelectric transition is driven by the development of the ferroelectric polarization, as evidenced by the presence of second harmonic modulation amplitudes in the low-temperature crystal structure.

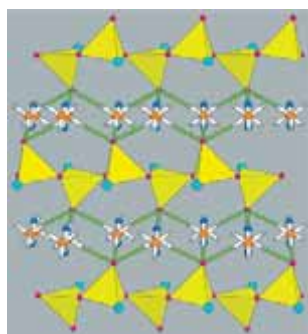
L. Palatinus, M. Amami and S. van Smaalen

IUCR JOURNALS NEWS

The catena-arsenite chain anion, $[\text{AsO}_2]_n^{n-}$: $(\text{H}_3\text{NCH}_2\text{CH}_2\text{NH}_3)_{0.5}[\text{AsO}_2]$ and NaAsO_2 (revisited)

The *catena*-arsenite chain anion, $[\text{AsO}_2]_n^{n-}$: $(\text{H}_3\text{NCH}_2\text{CH}_2\text{NH}_3)_{0.5}[\text{AsO}_2]$ and NaAsO_2 (revisited)

Acta Cryst. (2004). C60, m215-m218 [doi:10.1107/S0108270104007450]



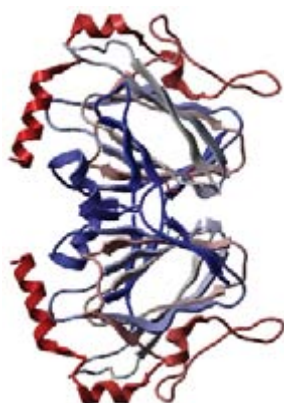
The catena-arsenite chain anion, $[\text{AsO}_2]_n^{n-}$, has been known in minerals for many years. The As^{III} atom in this species shows a distinctive pyramidal geometry, due to its stereochemically active lone pair of electrons. The *catena*-arsenite anion results from these AsO_3 pyramids fusing together *via* O atoms to result in an infinite chain. We have prepared the first example of the $[\text{AsO}_2]_n^{n-}$ grouping accompanied by an organic cation, ethylenediammonium. The discrete $[\text{H}_3\text{NCH}_2\text{CH}_2\text{NH}_3]_{2+}^{2+}$ cations and $[\text{AsO}_2]_n^{n-}$ chain anions interact strongly by way of N–H...O hydrogen bonds.

C. Lee and W. T. A. Harrison

IUCR JOURNALS NEWS

Mycobacterium tuberculosis RmIC epimerase (Rv3465): a promising drug-target structure in the rhamnose pathway

Acta Cryst. (2004). D60, 895-902 [doi:10.1107/S0907444904005323]



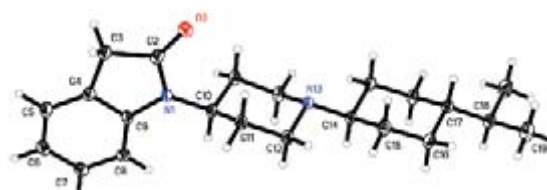
The 1.7 Å native structure of *Mycobacterium tuberculosis* rmIC (PDB entry 1UPI) has been recently reported by the TB Structural Genomics Consortium, and implications for virtual ligand screening are discussed. Rhamnose synthetic enzymes have been of particular interest in the development of novel antimycobacterial therapeutics, because L-rhamnose, a sugar not present in the human host, plays a key role as a structural link between the mycobacterial cell-wall components arabinogalactan and peptidoglycan. dTDP-4-keto-6-deoxyglucose epimerase (rmIC), the third enzyme in the dTDP-L-rhamnose pathway, is considered to be the most promising target in the pathway for structure-guided drug design, because rmIC is structurally unique, highly substrate specific, and does not require a cofactor.

K. A. Kantardjieff, C.-Y. Kim, C. Naranjo, G. S. Waldo, T. Lakin, B. W. Segelke, A. Zemla, M. S. Park, T. C. Terwilliger and B. Rupp

1-[1-(trans-4-Isopropylcyclohexyl)piperidin-4-yl]indolin-2-one, one of a novel series of nociceptin receptor ligands

1-[1-(*trans*-4-Isopropylcyclohexyl)piperidin-4-yl]indolin-2-one, one of a novel series of nociceptin receptor ligands

Acta Cryst. (2004). E60, o791-o792 [doi:10.1107/S1600536804008682]



A series of *N*-(4-piperidinyl)-2-indolinones have been discovered as a new class of nociceptin (NOP) receptor ligands. The physiological role of the NOP receptor and its ligand has been the focus of intense research. This paper reports on a member of this new series based on the 1,3-dihydroindolin-2-one heterocyclic scaffold. This series is particularly interesting because subtle changes in the piperidine N-1 substituent result in the production of both antagonists and agonists, the title compound being a weak agonist. In this example changing only the configuration of the cyclohexyl-isopropyl group from *trans* to *cis* converts this weak agonist to a strong agonist.

J. R. Deschamps, D. Parrish, N. T. Zaveri and F. Jiang

Elucidation of zeolite microstructure by synchrotron X-ray diffuse scattering

J. Appl. Cryst. (2004). **37**, 187–192 [doi:10.1107/S0021889803028048]



Weissenberg image of diffuse structure within the sheet-like scattering distribution concentrated in the $l = 5$ plane of a natural mordenite single crystal.

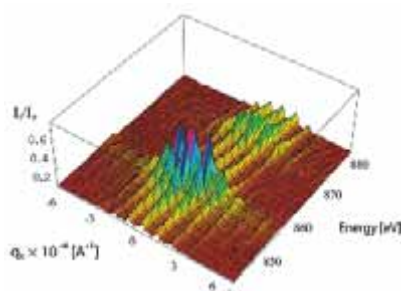
Zeolite mordenite, an important industrial catalyst, has long been suspected of framework variability. A broad single-crystal X-ray diffuse-scattering survey now reveals columnar framework fault defects and a block-mosaic network of planar stacking faults, which, even at very low concentrations, may significantly alter mordenite's fundamentally shape-selective properties. An experimental 3D diffuse-scattering distribution, mapped out using 20 keV synchrotron X-rays and a CCD camera, was compared with computer-simulated distributions that employed large-scale atomistic defect models. Isolated c -axis columns of 4MR rings are fault-shifted by $c/2$, while columnar faults also cooperate along the $\langle 110 \rangle$ directions to form planar antiphase boundaries.

B. J. Campbell, T. R. Welberry, R. W. Broach, H. Hong and A. K. Cheetham

IUCR JOURNALS NEWS

Soft X-ray resonant magnetic scattering from a Ni layer with modulated magnetic anisotropy

J. Synchrotron Rad. (2004). **11**, 254-260 [doi:10.1107/S0909049504004868]



2D plot of the photon energy- and scattering vector q_x -dependence of the scattered intensity measured by rocking scans with $2\theta = 10^\circ$ across the Ni $L_{2,3}$ resonance of the magnetically modulated Cu/Ni/Cu. Structural and magnetic characterization of a magnetically modulated, but nominally chemically homogenous, 5 nm Ni layer in a Cu/Ni/Cu thin film system was performed using specular reflection and rocking scans in X-ray resonant magnetic scattering, probing the scattering vector components in the perpendicular and in-plane direction to the Ni wires, respectively. Using polarized soft X-rays at the Ni $L_{2,3}$ resonance energy the measured magnetic scattering intensity reveals the magnetic modulation of the Ni layer. The results demonstrate the large potential of this element-specific scattering technique to study such complex magnetic structures in artificially patterned samples.

A. Haznar, G. van der Laan, S. P. Collins, C. A. F. Vaz, J. A. C. Bland and S. S. Dhesi

SPECIAL REPORT

Crystallography in Russia

Shubnikov Institute of Crystallography, Russian Academy of Sciences: 1940-2000

Foundation of the Institute



A. V. Shubnikov



B. K. Vainshtein



M. V. Kovalchuk

Aleksei Vasil'evich Shubnikov is justly considered one of the founders of the science on growth, structure, and properties of crystals. He initiated the physical direction in crystallography, broadened its horizons from the study of crystals within the framework of traditional mineralogy to the interdisciplinary science including physics, chemistry and mathematics. In 1934 Shubnikov organized the Crystallographic Section at the Lomonosov Institute of Geochemistry, Mineralogy, and Petrography in Moscow. In 1937, the crystallographic section was reorganized into the independent Laboratory of Crystallography of the USSR Academy of Sciences within the Dept. of Geological-Geographical Sciences. In November 1943 the Laboratory became the Institute of Crystallography in the Dept. of Physical-Mathematical Sciences of the USSR Academy of Sciences. A.V. Shubnikov was the first Director, Boris K. Vainshtein was the head of the Institute from 1962 to 1996, and Mikhail V. Kovalchuk has been the Director since 1998.

Development of scientific directions

The Institute of Crystallography was actively engaged in the fields of crystal symmetry and morphology, X-ray diffraction analysis, crystal growth and the synthesis of quartz. In 1939, N.N. Sheftal suggested a method for growing large crystals of Rochelle salt and high-quality piezoelectrics necessary for

constructing sensitive piezoelectric devices for use in the war. In the 1940s, Shubnikov put forward a concept of antisymmetry for studying magnetic properties of crystals and N.V. Belov composed a theory of close packings and performed detailed X-ray diffraction analysis of the atomic structures of silicate minerals. In 1945, G.G. Lemmlein found a spiral relief in crystal faces associated with the helicoidal structure of the crystal lattice. Methods for studying crystal structure were being rapidly developed at the Institute. Vainshtein used Fourier synthesis to calculate the distribution of electrostatic potentials in crystal lattices based on experimental electron diffraction data (1949). Vainshtein and Z.G. Pinsker determined the structure of paraffin, and the localized hydrogen atoms within it. In the 1950s, S.A. Semiletov and coworkers obtained fundamental results on the mechanism of homoepitaxial growth of thin germanium films. At the same time S.K. Popov designed an automated industrial apparatus for growing ruby rods. In 1940s-1950s, N.V. Belov and his coworkers initiated studies on the crystal chemistry of silicates related to geochemical and geophysical processes and the production of cements, glasses, and ceramics. Their studies were used to develop low-temperature cement and new types of concrete. In 1951, Shubnikov published *Symmetry and Antisymmetry of Finite Figures*, in which he discussed the notion of four-dimensional crystallography.



N. V. Belov



TRS triple-crystal spectrometer



A spiral growth step on the silicon carbide surface.

Sheftal and coworkers synthesized dislocation-free germanium single crystals and put forward the concept of artificial epitaxy for obtaining oriented films on amorphous substrates. In 1969, the scientists of the Institute grew oriented systems of whiskers on single-crystal substrates, a method useful for the

production of semiconductors. V.L. Indenbom found (1958) that the structural transformation observed in Rochelle salt is a second-order phase transition. Scientists at the Institute, headed by I.S. Zheludev and L.A. Shuvalov, worked on the general laws of formation of structures possessing spontaneous polarization and found new ferroelectric materials.

B.N. Grechushnikov, in cooperation with G.I. Distler, worked on the theory of Fourier-spectroscopy and designed and constructed a Fourier spectrometer. This instrument obtained well-resolved illumination light spectra from the Saturn disk and rings.

In 1962, the group, headed by Kh.S. Bagdasarov, built a stably operating laser. In 1972, laser radiation from chromium ions in garnets was achieved. At the beginning of the 1960s, the scientists of the Institute determined the structures of synthetic analogues of a protein (a complex polypeptide), crystallized enzymes into tubes with monomolecular walls, and determined the structure of leghemoglobin. In the 1980s, the scientists of the Institute developed an experimental approach to high-pressure studies of crystals using diamond anvils, increasing the range of attainable pressures (up to 100 GPa) and broadening the spectrum of problems solvable by this method.

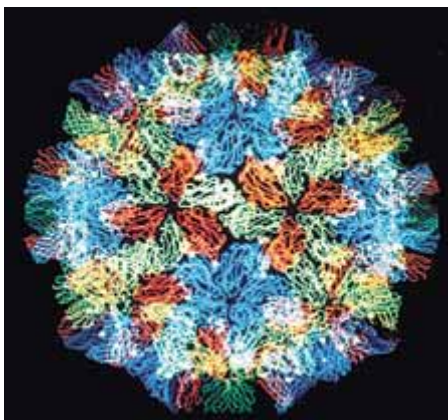
Fundamental studies in the theory of dislocations, the physics of plasticity, the theory of phase transitions in crystals, and the theory of symmetry were pursued. In particular, the existence of improper phase transitions was predicted. The studies of the statistical kinetics of spiral-layer crystallization helped to clarify many processes. In 1990s the scientists of the Institute developed the theory of electrooptical and ferroelectric properties of liquid crystals and designed many applicable devices.

Development of technology of crystal synthesis

L.M. Belyaev and his coworkers studied the synthesis of organic and inorganic crystal-scintillators with high scintillation efficiency. In the 1960s, A.A. Shternberg worked out the industrial synthesis of a rock crystal, piezoelectric quartz.

A method for horizontal crystallization for growing refractory single crystals was developed along with the technologies for growing large almost perfect single crystals of yttrium-aluminum garnet, sapphire, and yttrium aluminate. Industrial facilities for growing single crystals were constructed.

Methods of the thermal-compression junction and creation of solid-phase junctions of laser crystals that guarantee high optical quality of the interfaces were developed. New crystallization apparatus for growing crystals in space were also constructed, and crystallization experiments were performed on water-soluble crystals under the conditions of microgravity at the Salyut-5 orbital station (1976).



Atomic structure of a Carnation Mottle virus.



Synthetic crystals.

Instrument design

A series of specialized diffractometers have been designed at the Institute including the TRS triple-crystal X-ray diffractometer, the KARD-4 automated coordinate X-ray diffractometer, the RED-EL four-circle X-ray diffractometer, the DAR family of automated X-ray diffractometers, and the AMUR series of X-ray small-angle diffractometers. An automated 512-channel diffractometer for proteins was also constructed. In cooperation with the Laboratory of High Energies of the Joint Institute for Nuclear Research (JINR) in Dubna, a two-dimensional proportional chamber for the automated KARD diffractometer for studying protein single crystals was designed. Methods for studying polycrystalline materials, polymers and liquid crystals in X-ray diffractometers with two-dimensional detectors were also developed.

The Institute of Crystallography in the 21st century

New scientific priorities

At present, the Shubnikov Institute is focusing on the following problems:

- Creation of new crystals, films, and structures with specific properties;
- The study of the structures and properties of condensed matter using X-ray and synchrotron radiation, neutrons, and electrons;
- Further development of existing instruments and methods and creation of new ones;
- Study of properties of biological materials and organic systems;
- Study of condensed matter under microgravity;
- Study of surfaces, subsurface layers, interfaces, thin films, and track membranes;
- Development of X-ray optics; and
- Design and construction of apparatus for crystal growth.

The Institute also participates in the following projects of the Federal Scientific and Technological Program:

- Physics of Radiation,
- Condensed Matter,
- High-Precision Measurements,
- Quantum and Nonlinear Processes,
- Physics of Solid Nanostructures,
- Information Technologies and Electronics,
- New Materials and Chemical Products,
- Scientific Instrument Engineering.

Within the framework of the Russian Academy of Sciences, the Institute performs work on laser systems, strongly correlated electrons, nanomaterials and nanotechnologies. The Institute of Crystallography participates in the Federal Space Program of Russia.

Shubnikov participated in the organization of the IUCr and suggested the title *Acta Crystallographica* for its printed edition. Belov served as the IUCr President from 1966 to 1969, Vainshtein and V.I. Simonov were Vice-Presidents in 1975-1978 and 1984-1987, respectively. The Institute of Crystallography cooperates with more than twenty foreign scientific organizations participating in numerous interacademic and interinstitute agreements. The Institute holds annual Shubnikov, Vainshtein, and Belov lectures.

Structural studies



Computer simulation of growth of an icosahedral quasicrystal.

Kovalchuk and his laboratory developed different surface-sensitive and phase-sensitive X-Ray diffraction methods, among them - new modification of X-ray Standing Waves (XRSW) with photoelectrons. This method combines high resolution X-ray diffraction and spectroscopy. The XRSW method has been modified for the structural characterization of multicomponent crystals, semiconductor heterostructures, multilayer X-ray mirrors, X-ray waveguide structures, organic multilayer systems based on Langmuir-Blodgett films, and protein-lipid systems on solid and liquid substrates. Coherent interaction of X-ray and synchrotron radiations with condensed matter in the range of hard wavelengths have been studied. XRSWs with periods varying from 0.001 to 100 nm based on the phenomena of double- and multibeam diffraction, total external reflection, etc. have been developed.

M.V. Kovalchuk and S.I. Zheludeva used fluorescence in the range of total external reflection of X-rays for localization of ions inside organic multilayers. The study of protein-lipid systems on liquid surfaces and solid substrates revealed the effect of drugs on heavy atom positions. Today scientists at the Institute actively use synchrotron radiation in many fields of modern crystallography and they play a leading role in researches at Kurchatov Center of Synchrotron Radiation (KCSR).

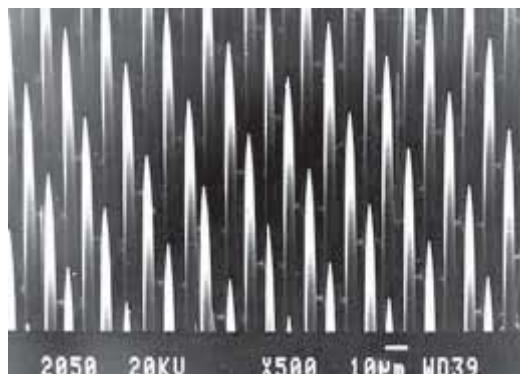
Studies of the semiconductor $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ demonstrated the value of X-ray diffraction in characterization of multilayer systems including determination of the thickness and compositions of individual layers, interface structures, and defects in the layers. Computer simulation of the growth of icosahedral quasicrystals has been performed. New types of diffraction reflections in crystals of germanium and a germanium-silicon alloy have been predicted. Defects arise because of distortion of the electronic state of germanium atoms by thermal vibrations and point defects. Such reflections have been observed in technologically important crystals and alloys. The group, headed by N.A. Kiselev, used high-resolution electron microscopy to study nanotubes with multilayer cylindrical walls and walls consisting of conic graphene layers and surface-modulated walls. L.A. Feigin's laboratory had a large contribution in the development of small angle scattering methods (theory, experiments and instrumentations) in application of X-R reflectometry in the study of different bioorganic materials.

Shortly before the 60th Jubilee of the Institute, a newly discovered mineral was officially named IKRANITE by the International Mineralogical Assn. Five other minerals have been named after scientists of the Institute: shubnikovite, belovite, lemmleinite, stishovite, and rastsvetsevite. The Institute regularly holds national conferences on crystal growth and annual schools on electron microscopy.

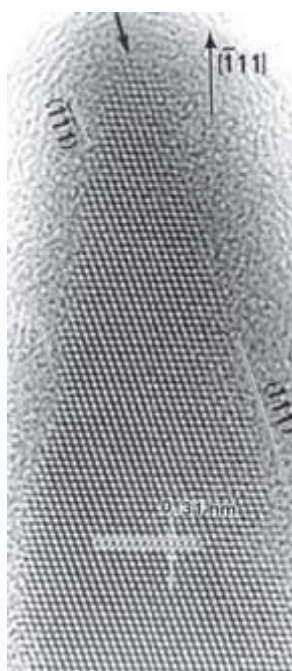
New crystalline media



Nanocrystalline zinc oxide powder.



(a)



(b)

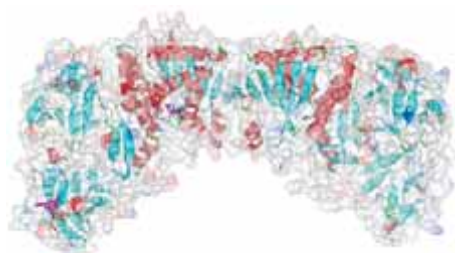
(a) Silicon whiskers, (b) HREM image of a nanodimensional tip.

Using hydro-thermal methods, nanocrystalline ZnO powders were obtained with luminescence characteristics significantly exceeding those of powders obtained by traditional methods (L. Demianetz group). The sol-gel synthesis in nonaqueous media produced cathode materials for lithium batteries. A method of diamond deposition onto silicon tips has been developed to enhance the autoemission of silicon cathodes. Systems of whiskers are used as the tips for autoemission cathodes. Single-crystal silicon wires with a diameter of 5 nm have been obtained, which are promising for potential nanoemitters.

A Gd-containing fast scintillator has been suggested in the fluoride family (together with the Russian

Research Center Kurchatov Institute). Such a scintillator is very promising for recording low-energy neutrinos. Languisites, a new family of highly efficient piezoelectrics, has been discovered by Pisarevsky's group in cooperation with Moscow State University.

Bioorganic materials science



Three-dimensional structure of *Ricinus communis* Agglutinin at a resolution of 2.5 Å.

The three-dimensional structure of a *Ricinus communis* Agglutinin was determined at a resolution of 2.5 Å using synchrotron radiation. The proteins of this group are used as stimulators of the immune system. The Institute developed a method and apparatus for protein crystallization that can also be used for growth of biocrystal films under the conditions of microgravitation. The Institute has developed a method for interactive modeling of structures of bio-polymer molecules in solution based on data from small-angle X-ray and neutron scattering. This allows one to determine not only the shape but also the inner structure of the particles, to analyze the domain structure and the dynamics of macromolecules in solution, and to reconstruct the structure of protein molecules in solution. Software designed at the Institute is used in many laboratories around the world.

Scientific engineering



PRO station of precision X-ray optics.

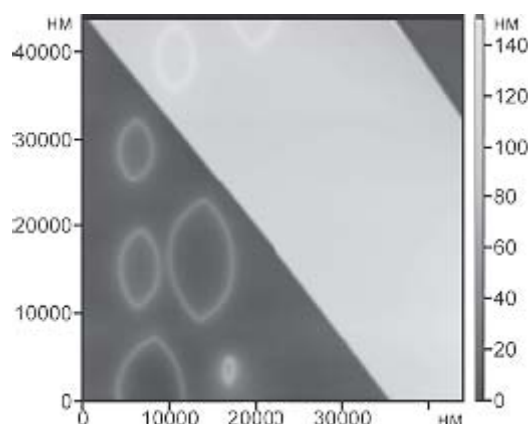


KROT setup for crystal growth.

Numerous instruments have been developed by Kovalchuk and co-workers for use on the synchrotron facilities at the Kurchatov Synchrotron Radiation Center including the experimental station for medical diagnostics (Mediana), protein crystallography (Belok), precision X-ray optics (PRO), material science

(RKFM) and EXAFS station. Instruments for robotic growth of large (75 mm diameter) high quality single crystals have been perfected. Of particular note are crystals of sapphire-titanium ($\text{Al}_2\text{O}_3:\text{Ti}^{3+}$) used in a new generation of terawatt lasers in the femtosecond range

Studies of physical properties



AFM topograph image of a portion of the polar (010) surface of a ferroelectric triglycine sulfate crystal. The effect of high pressures on the structural, magnetic, transport, and optical properties of magnetic materials is studied in high-pressure chambers with diamond anvils. Magnetic-nonmagnetic and dielectric-metal phase transitions, ferroelectric properties of ultrathin Langmuir-Blodgett polar films, and polarization switching in films of a P(VDF-TrFE) copolymer have been explored.

Active lithium niobate (a nonlinear optical material) was found to have impurities (Mg, Zn, In, etc.). By varying the doping level, it is possible to vary these properties. Magnetically stimulated strengthening of crystals manifests itself as a decrease in the dislocation mobility under the joint action of an applied mechanical load and a magnetic field. Atomic force microscopy (AFM) was found to be an efficient way to study the domain structure of polar surfaces of ferroelectrics. Analysis of the data revealed the effect of crystal-lattice distortions on dislocation mobility and a new type of dynamics of plastic flow in crystalline materials.

Track membranes

Track membranes allow one to create tip electrode nanostructures that release molecular hydrogen 100 times more intensely than traditional electrode systems. The Institute has obtained new products based on track membranes including systems for monitoring drinking water, systems of track-pore room and respirators based on the principle of diffusion gas exchange, tip structures for Raman spectroscopy and for increasing heat removal from reactor surfaces, and membranes for purification of crystallization solutions.

Innovative projects

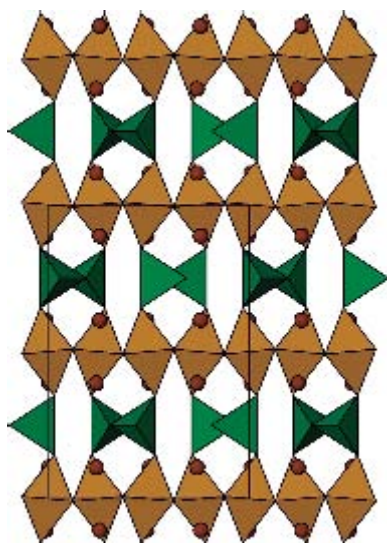
The experience of the Institute in solid-state physics and the development of technologies of crystal growth paved the way for participation in the State project on the development of an industry of synthetic dielectric crystals and their products. About twenty Russian institutes, industrial enterprises and companies participate in this project. The Institute coordinates the development of new instruments and technologies for the production of synthetic dielectric crystals. The new technology is based upon fundamental advances made by the Institute and benefit from past experience and industrial achievements in the field of growth and processing of crystals, and the manufacture of various crystal-based products.

Contact: Mikhail V. Kovalchuk (koval@ns.crys.ras.ru) Translated by L.I. Man

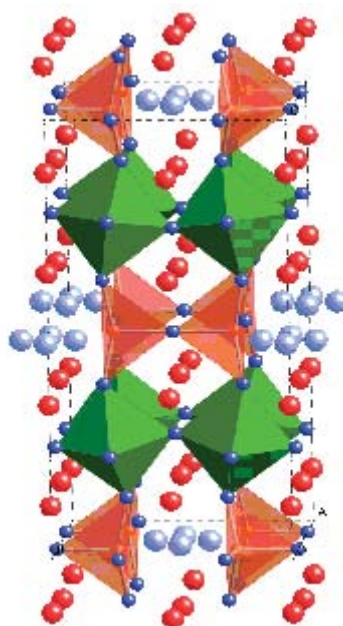
Inorganic Crystal Chemistry at Moscow State University



Chemists Holiday - Sr Day - celebrated at the Chemistry Department of Moscow State University. Probably the largest Mendeleev's Periodic Table of Elements.



The crystal structure of $\text{Sr}_2\text{MnGaO}_5$ with an ...LRLR... type of chain alternation (*Pcmb* space symmetry). Two different projections of the GaO_4 tetrahedra correspond of two different kinds of the tetrahedral chains.



Crystal structure of $\text{Sr}_{0.7}\text{Y}_{0.3}\text{CoO}_{2.62}$. Layers with Co_2O_6 octahedra alternate with oxygen-deficient layers.



The staff and students of the Inorganic Crystallochemistry Laboratory. From left to right front row: Yu. Velikodny, E. Antipov, A. Abakumov, S. Putilin; middle row: M. Rozova, R. Panin, O. Dyachenko; back row: R. Shpanchenko, S. Istomin, O. Lapshina, N. Khasanova, V. Govorov, V. Koutsenko, A. Alekseeva, A. Mironov.

For 50 years, the Inorganic Crystal Chemistry Laboratory in the Chemistry Department of Moscow State University has performed a full range of scientific studies from the syntheses of compounds to investigations of their structures and physical properties. The laboratory, previously directed by Yuri P. Simanov and Leonid M. Kovba, has been led by Evgeny V. Antipov since 1996.

The laboratory's goals involve the synthesis of new compounds, determination of their three-dimensional structures and correlation of structure and properties. Powder diffraction is used for phase analysis and cell parameter determination, followed by structure solution from either powder or single crystal X-ray data (XRD). For problem cases electron diffraction (ED) together with high resolution electron microscopy (HREM) and/or neutron diffraction are used. Sometimes other methods help to answer specific questions on structural details, and throughout the process measurements of physical properties are performed by collaborators.

The targets of study over the years have been mainly complex oxides. Intensive studies of superconducting complex cuprates in 1987 resulted in the discovery of a family of mercury based cuprates that exhibits the highest known transition temperature. In 1994, this work received the Lomonosov Award of the Moscow State University and the Superconductivity Award of Excellence given by the World Congress on Superconductivity. Our discoveries have included various superconducting

copper based oxides, oxycarbonates, oxyfluorides, and superconducting bismuthates. When $\text{Sr}_{1-x}\text{K}_x\text{BiO}_3$ was synthesized under high pressure it was found that both the symmetry of the unit cell and its superconducting properties depend on potassium content. The highest superconducting transition temperature was found for the composition $\text{Sr}_{0.44}\text{K}_{0.56}\text{BiO}_3$ when the phase crystallizes in a tetragonal unit cell.

The search for substances with colossal magnetoresistance effects resulted in the synthesis of $\text{A}_2\text{GaMnO}_{5+\delta}$ ($\text{A}=\text{Sr}, \text{Ca}, \delta \leq 0.5$) phases for the first time. These phases undergo interesting structural and magnetic phase transitions during the oxidation process. It has been shown that compounds with a Brownmillerite type structure crystallize in different space groups. Only the use of electron microscopy and a 3+d dimensional crystallographic approach helped to describe their structures correctly. The space group depends on the orientation of tetrahedral GaO_4 chains and their ordering in adjacent layers. Sometimes, such ordering occurs in a rather complicated manner forming commensurately modulated structures. For the Sr and Ca phases the insertion of extra oxygen resulted in the suppression of Jahn-Teller distortion for MnO_6 octahedra, a change of Ga coordination from tetrahedral to octahedral, and an increase of unit cell symmetry from orthorhombic to tetragonal.

The study of complex cobalt oxides as potential mixed conductors led to the discovery of $\text{Sr}_{0.7}\text{Y}_{0.3}\text{CoO}_{2.62}$ which has a perovskite-related crystal structure. Its tetragonal unit cell is formed of alternating cobalt oxygen layers. Half of the layers consist of CoO_6 octahedra, others are oxygen deficient tetrahedra with one additional oxygen at the long distance. The structure is considered as intermediate between brownmillerite and perovskite.

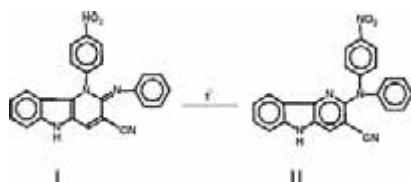
Many of these studies would not have been possible without our collaborators. We are grateful to Arne Magneli and Lars Kihlberg (Stockholm University) who were very helpful during the early 90's, a difficult time for Soviet and Russian science. Massimo Marezio and his colleagues (CNRS, France) have been collaborators in the syntheses and structural studies of superconducting complex copper oxides. Phillip Coppens (SUNY, USA) and Vaclav Petricek (Institute of Physics, Czech Rep.) helped us to understand what modulated structures are. Electron diffraction and high resolution electron microscopy studies are still carried out with Gustaaf Van Tendeloo and co-workers (EMAT, Belgium). Structure refinements from neutron data are based on experiments done in Dubna in the Joint Institute on Nuclear Research by the group of Anatoly Balagurov.

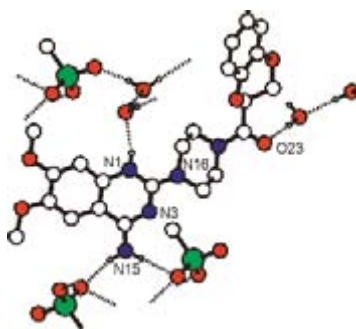
Information about the Inorganic Crystal Chemistry Laboratory can be found at www.icr.chem.msu.ru .
Contact: Evgeny Antipov (antipov@icr.chem.msu.ru)

Structural Chemistry, Moscow State University

Under the direction of Leonid A. Aslanov (aslanov@struct.chem.msu.ru), four main directions of research are being pursued in the Laboratory of Structural Chemistry at Moscow State University:

A. The laboratory is involved in the development of methods for structural characterization of polycrystalline materials from powder data in collaboration with H. Schenk (University of Amsterdam)^[1]. Two molecular structures solved recently from powder diffraction data demonstrate our achievements in this area.



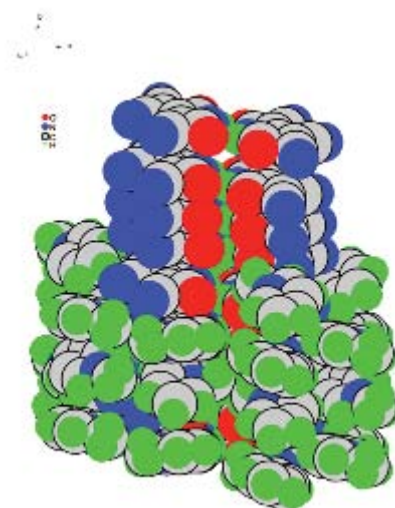


Hydrogen bonding in dG.

1. Evidence for thermal isomerization of compound (I), $C_{24}H_{15}N_5O_2$, into compound (II) (see Scheme) has been obtained^[2].

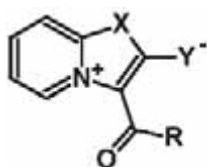
2. Elucidation of three-dimensional solid state structures of two modifications of doxazosin mesylate^[3], a commonly used antihypertensive agent, clearly showed the N1 protonation site in anhydrous (A) and hydrated (dG) solid forms, establish the conformations of the doxazosin molecule and define the hydrogen bonding in both forms.

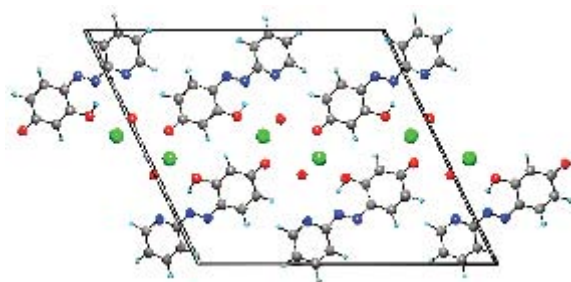
Contact: Vladimir V. Chernyshev (vladimir@struct.chem.msu.ru)



B. Organic compounds containing from two to four cyano-groups are widely used in preparation of photochromic materials and anticancer drugs. Such compounds contain several active chemical centers and participate in a diversity of chemical reactions. A new kind of organic anion, 3-cyano-4-(dicyanomethylene)-5-oxo-4,5-dihydro-1H-pyrrol-2-olate, was synthesized as a result of the reaction of tetracyanocyclopropane derivatives with an iodide anion. In the crystals of anion-containing organic salts there are various kinds of stacks due to π - π anion-cation or anion-anion interactions^[4].

Contact: Victor A. Tafeenko (tafeenko@biocryst.phys.msu.su)





Sodium pyridylazoresorcinolate monohydrate (PAR) – common metal indicator studied by X-ray powder diffraction.

C. The laboratory studies pathways for mapping reactions of mesoionic (MESOmeric+IONIC) compounds. Mesoionic systems may be transformed to highly reactive oxo(thio-, imino)[3,2-a]pyridinium cations which, in turn, undergo a variety of ring opening/transformation reactions leading to novel classes of heterocyclic compounds. For example, mesoionic azolopyridines are related to the family of condensed munchnones: a) $X=S$; $Y=S$, O, NR; b) $X=O$; $Y=S$, O, NR, c) $X=NR$; $Y=S$, O, NR. Crystal and molecular structures of novel anaesthetic drugs based on quiniline derivatives, novel pesticides based on urea heterocyclic derivatives, and novel radioprotectors based on pyrimidine derivatives were determined by both X-ray and neutron diffraction.

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D. A number of the traditional dyes and pigments, as well as modern materials for electrooptical and photonic applications and laser dyes, have been studied by means of single crystal and powder X-ray diffraction. Main research directions are the following: tautomeric interconversions in the solid state; intermolecular charge-transfer interactions and π -complexes; crystal packing effects on spatial and electronic molecular structure; crystallochromism, i.e. the difference in color of solid pigments due to molecular packing arrangements.

Contact: Alexandr V. Yatsenko (yatsenko@struct.chem.msu.su)

[1] Zhukov, S.G. *et al.* (2001). *Z. Kristallogr.* **216**, 5-9. [2] Chernyshev, V.V. *et al.* (2001). *Acta Cryst.* **C57**, 982-984. [3] Chernyshev, V.V. *et al.* (2003). *Acta Cryst.* **B59**, 787-793. [4] Tafeenko, V.A. *et al.* (2003). *Acta Cryst.* **C60**, o62-o64.

Crystallography in Physics, Moscow State University



Staff of the Physics Department at Moscow State University..

A chair of X-ray structure analysis was created in 1932 as one of seven chairs in the Physics Department of Moscow State University. In 1953, it became the Chair of Solid State Physics. Department Chairs have included S.T. Konobeevsky, the first Chair, V.I. Iveronova (a winner of the Fedorov prize of Soviet Academy of Science), and M.M. Umansky (a winner of the Lomonosov Prize of Moscow State University).

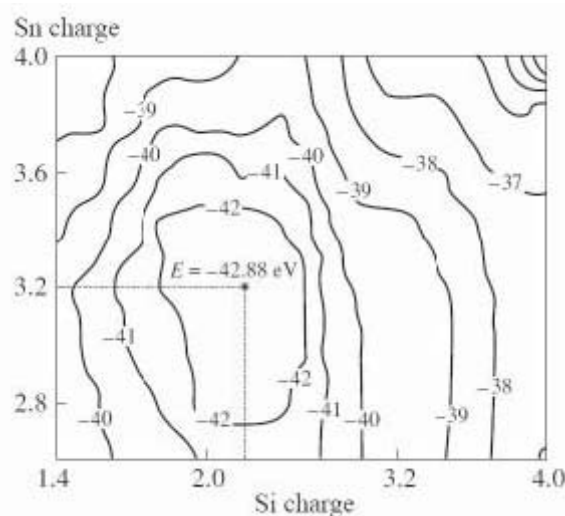
The current chair, A.S. Ilyushin, is a leader in the field of education programs on condensed matter among Russian Universities. The program combines the teaching of experimental methods (X-ray, Mossbauer etc.) with basic principles of solid state physics (atomic, electronic and defect structures of crystals, dynamics of the crystal lattice, and phase transformations).

From the 1940s through the 70s a group under M.M. Umansky developed an experimental set for X-ray studies of crystal structure which also won a Lomonosov Prize (M.M. Umansky, S.S. Kvitka, and V.V. Zubenko). Recent research has included the development of new methods of X-ray and Mossbauer structure analysis of ideal and real crystals and application of these methods to studies of phase transformations and defects in metals, alloys, semiconductors and multi-layer films; evolution and self-organization of crystals and their electronic structure; and non-equilibrium phenomena and surface layers. Significant results have included:

- a) A non-monotonic structural evolution, including a discrete (jump) evolution in the non-equilibrium metal-hydrogen systems was discovered, and a synergetic model was proposed (A.A. Katsnelson, G.P. Revkevich, and V.M. Avdyuhina).
- b) An effect of internal magnetostriction in the rare-earth intermetallic compounds was found and its atomic-ionic mechanism was estimated (A.S. Ilyushin).
- c) X-ray and Mossbauer diffraction near-edge spectroscopy of crystals and multi-layer films allowed depth-selective studies of atomic and magnetic structure (R.N. Kuzmin, V.A. Bushuev, M.A. Andreeva, and E.N. Ovchinnikova).
- d) A wave theory was proposed for 3D internal structure reconstruction in low-absorption non-crystals based on phase-contrast X-ray refraction tomography, featuring orders of magnitude higher image contrast and 1-2 orders lower dose of absorbed radiation (V.A. Bushuev, patented method).
- e) Molecular dynamics simulation and *ab initio* electronic structure calculations were used to study the formation of adsorbed nanostructures on metal surfaces and to predict the physical properties of surface layers (A.A. Katsnelson and V.S. Stepanyuk).

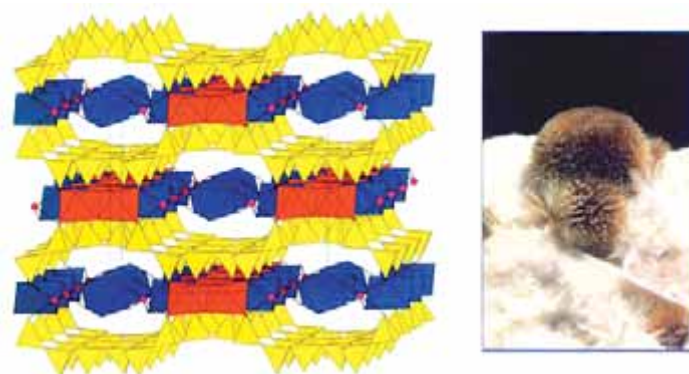
Contact: Albert A. Katsnelson (albert@sols3591.phys.msu.ru)

Crystallography and Crystal Chemistry of Geology, Lomonosov Moscow State University



The atomization energy distribution in malayaite CaSnOSiO_4 .

The Department of Crystallography and Crystal Chemistry of Geology was founded in Lomonosov Moscow State University by G.B. Bokii in 1949. In 1961 N.V. Belov became the head of the department. From 1983 on the department has been headed by V.S. Urusov. Currently the staff consists of 25 teachers, researchers, and engineers. Since its founding, X-ray crystal structure determination of minerals and their synthetic analogues has been the major focus of the department. More than 200 new crystal structures of minerals have been solved. Another important field of activity for this group (Corresponding Members of RAS D.Yu. Puscharovsky, E.L. Belokoneva, O.V. Yakubovich, Yu.K. Egorov-Tismenko, N.A. Yamnova, and N.V. Zubkova) is mineral systematics and classification based on their structural characteristics, especially crystal chemistry of the main rock-forming minerals: silicates, phosphates, borates, etc.



Silicate raite: X-rays from synchrotron source and its spherulite morphology.

In the past 2 decades precision X-ray diffraction studies and electron density distribution analysis in oxide and silicate minerals have also been conducted (V.S. Urusov, E.L. Belokoneva, O.V. Yakubovich, N.N. Eremin). Another group of scientists (Yu. K. Kabalov, N.V. Zubkova) is deeply involved in modern powder diffraction methods using Rietveld refinement of mineral crystal structures.

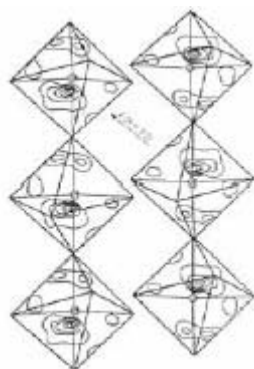
A central point in the domain of theoretical crystal chemistry is occupied by the development of energetic analysis of stability and properties of pure crystals and solid solutions. Recent activities of the group (V.S. Urusov, N.N. Eremin) have concentrated on the problem of computer modeling of structures and properties of mineral and inorganic solids using semi-empirical interatomic potentials as well as on the development of atomistic and phenomenological theory of isomorphous substitutions. Their original approach is minimization of crystal atomisation energy which accounts for the actual character of

chemical bonds in crystals.



The staff and students after the last exam.

In addition to crystal chemistry and X-ray diffraction groups, the department includes two laboratories doing single crystal growth: growth from high-T complex flux melts (N.I. Leonyuk, V.V. Maltsev) and growth from hydrothermal solutions (O.V. Dimitrova). Most crystals obtained in these laboratories possess technologically useful properties, e.g. lasers, fiber optics, ferroelectrics, high-T superconductors, superionic conductors, etc. Many have been the subjects of detailed crystal structure determination.



Electron density in titanite CaTiOSiO_4 .

The department is responsible for the crystallographic education of all students (about 200 per year) of the Geological Faculty of Moscow State University as well as for the special education of bachelors, masters and PhD students in the field of crystallography and crystal chemistry (5-6 students and 3-4 post-graduate students per year). Courses include general crystallography, theory of symmetry (Yu. K. Egorov-Tismenko), introduction to crystal chemistry and advanced theoretical crystal chemistry (V.S. Urusov, N.N. Eremin), X-ray diffraction and crystal structure analysis (D.Yu. Puscharovsky, N.N. Zubkova), crystal morphology (G.I. Dorokhova), and crystal growth (N.N. Leonyuk, E.V. Koporulina).



Our self made crystals.

In recent years the following text-books (in Russian) have been published by the teachers in the department: 'Crystallography' (1992) by Yu. Egorov-Tismenko et al., 'Theory of crystal symmetry' (2000)

by Yu. Egorov-Tismenko & G. Litvinskaya, 'Theoretical crystal chemistry' (1987) by V. Urusov, 'X-ray diffractometry' (2000) by D. Puscharovsky, 'Structural types of minerals' (1990) by D. Puscharovsky & V. Urusov, 'Design of probable crystal structures of minerals' by V. Urusov et al.

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Crystal Chemistry, Lomonosov Moscow State University (MSU)



Studies on crystal chemistry.

The laboratory was established in 1952 by G.B. Bokii, and first directed by M.A. Porai-Koshits. The current head of the laboratory is Peter M. Zorky and all students (200 to 250) of the department take the crystal chemistry course each year, which includes:

- The history of the X-ray structural methods and of crystal chemistry;
- Fundamentals of diffraction;
- General principles of characterization and interpretation of crystal structures, including the theory of symmetry;
- The thermodynamics of isostructurality, isomorphism, polymorphism, and morphotropy;
- Systematic description of crystals and properties of metals, non-metals, binary and ternary compounds, silicates, coordinate compounds, organic substances;
- The use of concepts from crystal chemistry and X-ray studies to characterize condensed phases with full and partial ordering: liquid crystals and liquids.

The study of crystal chemistry is not limited to crystallographic point and space groups, but has been expanded to include non-crystallographic axes and the symmetry of rods and slices.

A considerable portion of the course is dedicated to organic crystal chemistry and includes the following subjects: symmetry and structural classes of homo- and heteromolecular crystals; theory of close packing of molecules; calculation of the energy of intermolecular interaction in the atom-atom approximation; specific intermolecular contacts and their aggregation (hydrogen bonds, halogen-halogen contacts, and specific contacts involving benzene rings); and revelation of molecular aggregates in organic crystals; the influence of molecular aggregation on the properties of solid and liquid organic substances. The mastering of crystal chemistry requires visualization of structures (with the use of real ball-and-stick models, slides and animation).



P.M. Zorky, A.E. Obodovskaya and student Anna Soloshenko showing models of crystal structures. Since the 1970s theoretical studies in the field of organic crystal chemistry conducted under the direction of P. M. Zorky Crystal Chemistry, Lomonosov Moscow State University (MSU) have been a primary research focus. He has developed a topological classification system for organic crystal structures as ordinary, unordinary, and extraordinary, viewing molecular aggregation as optimal arrangements rather than molecular packing, and studied the coexistence of difficult conforms in the same crystal and the presence of common aggregate forms in difficult polymorphic hydrates or solvents. It is likely that the fragments of molecular aggregates that are present in crystals are retained in melts and in solutions, which is the cause of the microheterogeneity of liquid phases.

Correlations between the structures of liquids and crystals are another basis for generalization of crystal chemistry and the exploration of the interdependence of pharmacokinetical properties of drugs, crystal formation, and molecular aggregation in solution, computer simulation of the structures of solutions, and the interpretation of their melting temperatures, measurement of light scattering and of acoustic speeds in organic liquids and in their mixtures.

One of the most recent studies carried out in the laboratory of crystal chemistry is the refinement of the values of van der Waals radii of organogenic elements on the basis of the statistical treatment of structural data taken from 10000 crystal structures in the CSD.

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High-resolution protein structure at the Institute of Bioorganic Chemistry, RAS, Moscow



LMC in December 2003: (left to right) Tatiana Petrova, Natalia Lunina, Vladimir Y. Lunin, and Tatiana Skovoroda.



Research directions include X-ray studies of structure function relations of enzymes, molecular aspects of protein-carbohydrate and antibody-antigen interactions.

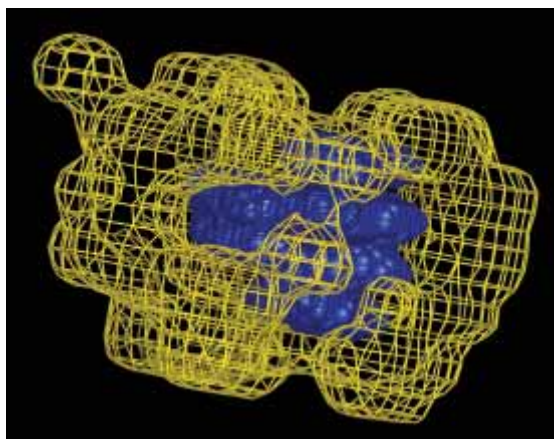
The crystal structure determinations (resolution 2.1 Å) of a series of Ca^{++} , Mn^{++} containing protein - pea lectin in complex with gluco- and mannopyranoside derivatives have revealed the stereochemical features of the binding site responsible for carbohydrate recognition and binding. Based on the determined structure, residue mutations were proposed to change carbohydrate specificity.

The three-dimensional structure (resolution 2.4 Å) of serine protease and bovine duodenase demonstrated the structural features of the active site compatible with effective accommodation of P1 residues typical of trypsin (Arg/Lys) and chymotrypsin (Tyr/Phe) substrates. These specificities in the past were considered to be mutually exclusive. The computer modeling of the complexes with the corresponding octapeptide substrates confirmed the experimental conclusions. The obtained results may permit design of enzymes with a specific ratio of trypsin and chymotrypsin activities.

The crystal structure of the Arg32His mutant of the human tumor necrosis factor (TNF- α), an important immune mediator, has been established at 2.5 Å. Models of the structure complexed with P55 and P75 receptors explained the decrease in its cytotoxic activity. The three dimensional structure of the antigen binding fragment of a monoclonal antibody to human interleukin-2 complexed with antigenic nonapeptide has been determined at 3 Å resolution. Antibody-antigen complexation involves a significant rearrangement of the epitope containing region of the interleukin-2 with retention of the α -helical character of the epitope fragment.

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Macromolecular crystallography in Pushchino



Low resolution crystallographic image of a lipoprotein particle obtained in collaboration with the Medical University of Freiburg (Germany) and Universities of Nancy and Strasbourg (France).

The Institute of Mathematical Problems of Biology (IMBP) (www.impb.ru) was founded in the Pushchino Biological Centre of the Academy of Sciences in 1972 to create a link between mathematicians, computer scientists and biological laboratories interested in using mathematical and computer tools. A special program for development of protein crystallography was launched in 1976 that required huge computer support. The IMPB group spent its early years in close collaboration with the crystallographic laboratory (headed by Yu. Chirgadze) of the Institute of Protein Research (Pushchino), and benefitted from the advice of V. Borisov (Institute of Crystallography, Moscow). This era ended in the early 80's with the creation in Pushchino of a computational environment that supported all stages of macromolecular structure investigation, including model refinement (protein structure solution was not a routine procedure in those days).

Subsequently, the activities of the laboratory (see www.impb.ru/lmc for more details) have concentrated on development of new mathematical approaches and software for macromolecular crystallography, and collaboration with different laboratories on macromolecular structures. In particular, the laboratory has facilitated the use of the maximal likelihood principle in macromolecular crystallography (1982), the use of electron density histograms (1986) and the use of mixed (hybrid) electron density models (1984) for phase improvement etc. Most recently the main activity of the laboratory has concentrated on the development of *ab-initio* phasing methods suitable for low and middle resolution stages of crystallographic studies of macromolecular objects.

Contact: Vladimir Y. Lunin (lunin@impb.psn.ru)

Institute of Solid State Physics of the RAS

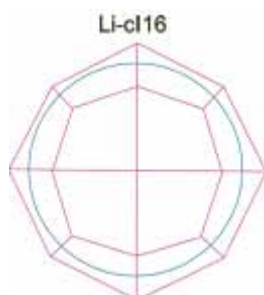


Panorama ISSP RAS.

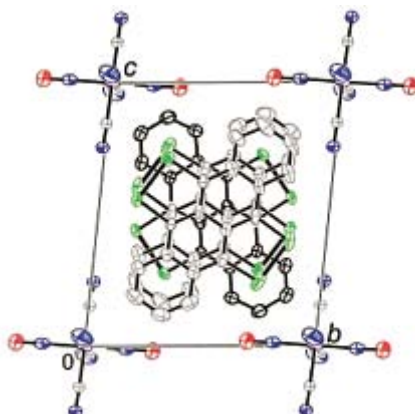
The ISSP RAS was founded in 1963 by George V. Kurdumov and Yurii A. Osipyan at the Research Center Chernogolovka in beautiful forests near Moscow. The focus of ISSP activities are: condensed-matter physics, materials science and new technologies. The Institute has laboratories for structural analysis by XRD and electron diffraction techniques. Microstructure investigations are carried out by the methods of X-ray spectroscopy, transmission electron microscopy (TEM), high-resolution transmission electron microscopy (HREM), scanning electron microscopy (SEM) and Mossbauer spectroscopy. Most of the facilities have low (liquid helium) and high (up to 2000°C) temperature capabilities. The staff includes five Doctors of Sciences, 12 PhD scientists, and 2-4 post-graduate students.

A variety of crystallographic problems are under investigation.

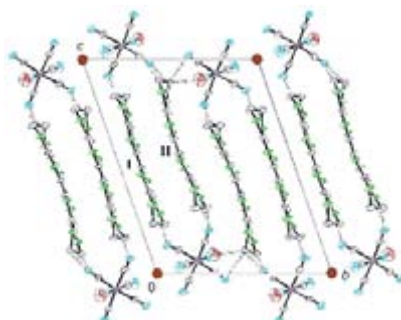
Crystallography of phase transformations and aperiodic crystals



Brillouin zone - Fermi sphere.



Crystal structure of 1D organic conductor (TSeT)₃FeNO(CN)₅I.



Crystal structure of 2D organic metal b''-(BEDT-TTF)₄Rb[FeNO(CN)₅]₂.

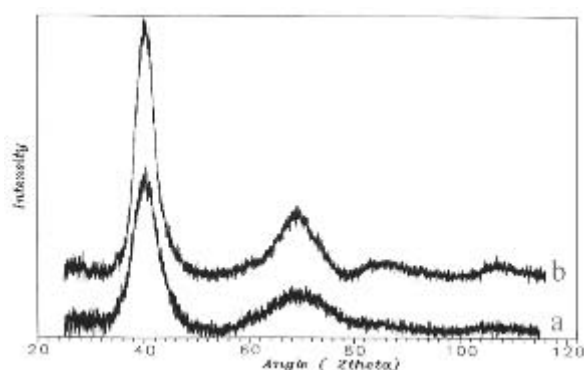
Since 1930s the name of Kurdumov has been associated with non-diffusion (martensite) transformations in steels and 'shape memory' effect in alloys. Today these ideas open up a large and diverse field of experimental research. Transformations connected with the cooperative motion of atoms occur in many crystal families. Data on structural changes at temperatures down to 4.2 K, under mechanical loading, in electric fields, and under optical pumping have been obtained from metals, dielectrics, ferroelectrics, and HTSC materials. Experts in the laboratory have studied domain systems in A-15 alloys and in high-T_c compounds; the para-ferro-electric transitions in KDP and perovskite crystals; and transformations of

polytypic systems of ZnS by oriented loading.

Another current focus is analysis of aperiodic crystals. The *invar effect* in incommensurate phases, i.e. the zero-coefficient of thermal broadening in the temperature region of the IC phase has been established. A new type of incommensurate composite structures has been discovered in $(\text{Rb}_x(\text{NH}_4)_{1-x})_2\text{SO}_4$ crystals. These composites exhibit incommensurability of host and guest substructures along all three crystallographic directions. To define the structure and properties of such composites, we examine changes in the structures as a function of temperature, pressure and electrical field. A sequence of phase transitions from an incommensurate composite phase into commensurate ones has been detailed and we have shown that the oriented stress causes the phase transition in the host or guest structure.

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Structure analysis of high pressure phases

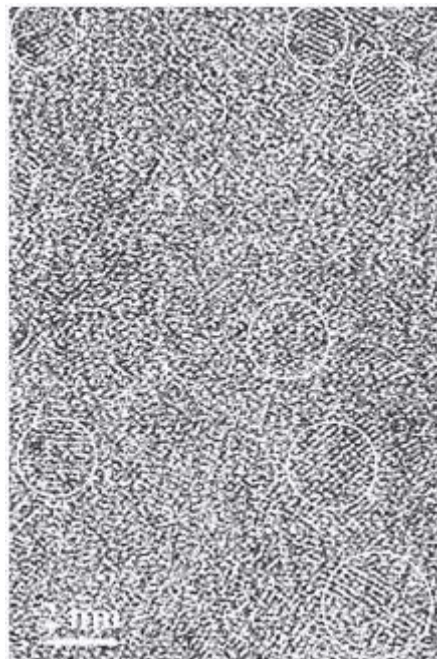


X-ray diffraction patterns from amorphous (curve a) and nanocrystalline (curve b) structure with very small grain size.

The high-pressure X-ray diffraction group is engaged in the study of phase transitions in metallic alloys. A series of intermetallic phases was synthesized under pressure and crystal structures analyzed. The concept of Brillouin zone - Fermi sphere interactions is applied to account for phase stability in sp metals and alloys. Enhanced Hume-Rothery arguments under high pressure are shown to be responsible for structural complexity in 'simple' metals. For instance, the Li-cl16 phase [Hanfland *et al.* (2000) *Nature* **408**, 174] is related to the classical Hume-Rothery phases with the Fermi surface close to the Brillouin zone boundaries.

Contact: Valentina F. Degtyareva (degtyar@issp.ac.ru)

Structure analysis of low-dimensional organic conductors



HREM image from amorphous.

The group, headed by R. Shibaeva, is studying the relationship between the crystal structures and physical properties of low-dimensional organic conductors. X-ray studies of organic radical cation salts with π -organic donors and various anions have been conducted. Compounds under investigation include semiconductors, organic metals with an M-I transition, stable organic metals and organic superconductors. The structural origin of first-order phase transitions are established, electronic band structures calculated, and theoretical and experimental electronic structures compared. Detected regularities in the structure of organic metals led to the development of some prescriptions for direct synthesis. Recently we have begun to study hybrid materials that combine π -electron donor networks, responsible for electronic conductivity, with counterion networks having distinct physical properties (magnetism, photochromism, etc.). Radical cation salts of organic π -donors with the photochromic metal mononitrosyl complexes and magnetic metal oxalates as counterions have also been studied.

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Amorphous and nanocrystalline systems

Metal-metal and metal-metalloid systems in amorphous and nanocrystalline states are being studied by X-ray diffraction and transmission and high resolution electron microscopy. Samples are produced by controlled crystallization of metallic glasses. Structure stability and evolution have been studied in Fe-, Co-, Ni-, Pd-, Al-, Mg-, Cu-, Zr-based alloys after the decomposition of amorphous alloys prepared by melt quenching. The Al-Ge, Zn-Sb systems were investigated under crystallization of an amorphous phase produced by high pressure with subsequent quenching to liquid nitrogen temperature. The grain size of the nanocrystals is 5-20 nm and the X-ray diffraction pattern contains broadened reflections for small nanocrystals (about 1-5 nm) the X-ray diffraction pattern (Figure below, curve b) is close to that of an amorphous phase (curve a). Both diffraction patterns contain only diffuse maxima, but the curves are different. Curve b corresponds to the structure consisting of both the amorphous phase and nanocrystals with the grain size of 1-5 nm. The high resolution electron microscopy image of this structure is shown in the figure. The structure contains a lot of very small nanocrystals. Analysis of the angular dependence of the diffraction line halfwidth allows us to estimate the main contribution to the broadening and draw conclusions about the fine structure of nanocrystals. All nanocrystals have been found to be defect-free, while Ni nanocrystals contain stacking faults, dislocations, microtwins etc.

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X-ray optics of real crystals

X-ray optical diffraction effects under investigation include diffraction focusing of X-ray Bloch waves in perfect single crystals, dynamic diffraction on bent single crystals, waveguide and channeling effects, and X-ray interferometry in a continuous radiation spectrum. Short-wave hard radiation scattering in a short-range field of deformation has been studied, schemes of focusing X-ray optical elements have been proposed, and specific features of diffraction in disordered quasi-crystals have been investigated. A software package has been written to interpret and simulate diffraction images obtained by Laue, Debye and rolling-crystal methods. The phase velocity of hard electromagnetic radiation in a medium is higher than the velocity of light in vacuum. Therefore the effects of both total external and total internal reflections exist for X-ray waves. Experiments on X-ray dynamic diffraction in limited perfect single crystals have been carried out under the conditions of total internal reflection of a scattered wave from a crystal-vacuum interface. The interference pattern, formed by a sum of the primary and mirror-like reflected scattered waves, is extremely sensitive to weak distortions of the crystal lattice. The results obtained open new prospects for diagnostics of defects in single crystals and development of new elements for X-ray optics.

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Leonid A. Aslanov



Leonid A. Aslanov was born in St. Petersburg, Russia in 1938 and studied chemistry at Lomonosov Moscow State University. After graduating from the University in 1960 he pursued his interest in crystallography and received his PhD in 1963 based on his studies of the synthesis and crystal structure determinations of ternary sulphides and selenides of alkali earth and some d-transition metals using powder diffraction. He is now employed by the Department of Chemistry of Moscow State University where he started as a junior researcher and is now a full professor.

Between 1965 and 1973 he investigated crystal structures of coordination compounds of rare earth elements and developed, in collaboration with M.A. Poraj-Koshits, a principle for determination of eight-vertexes polyhedra that has had broad application. (*J. Struct. Chem.* **13**, 244 (1972)).

From 1973 to 1987 his research centered on the synthesis and crystal structure determinations of coordination compounds of tin, lead, and antimony and he found, in collaboration with V.S. Petrosyan and O.A. Reutov, a phenomenon of the trans-strengthening of bonds in octahedral complexes of tin and lead which is opposite to trans-effect in transition metal complexes (*Zh. Strukt. Khim.* **29**, 112 (1989)).

From 1979 to 1992 he developed crystal chemical models of atomic interactions (*Acta Cryst.* **B44**, 449 and 458 (1988), **A45**, 661 and 671 (1989), **A47**, 63 (1991), **A48**, 281 (1992)). During this period (1981 to 1991) he started an exploration of photocrystallography and together with his collaborators built a specialized four-circle diffractometer (*J. Appl. Cryst.* **22**, 42(1989)), developed software (*J. Appl. Cryst.* **24**, 293 and 910 (1991)) and performed investigations on ferroelectric materials (*J. Appl. Cryst.* **23**, FC1 (1990)). This research was stopped due to lack of financial support in 1992.

Since 1992 he has been doing research in materials science. During the period between 1992 and 1998 he proposed, and tested experimentally, an optoacoustic mechanism of latent image formation in silver halide materials (*Laser Physics* **6**, 1105 (1996)). Since 1999 he has been studying the crystallization of nanoclusters in ionic liquids.

L.A. Aslanov did postdoctoral research during the 1967-1968 academic year at the University of Sheffield, UK under the supervision of Ronald Mason. He had a Kapitsa Fellowship in 1993 with Judith A.K. Howard at the University of Durham, UK and from 1992 to 2003 he collaborated in the framework of NWO-grants with Henk Shenk at the University of Amsterdam.

L.A. Aslanov is now Vice-President of IUCr, Co-Editor of *Acta Crystallographica A, B, C, D, Zeitschrift für Kristallographie* and Associate Editor of *Crystallography Reviews* in addition to activities with other Russian journals and organizations. He has published over 300 papers, 6 books on crystallographic instrumentation, X-ray diffraction, crystal chemistry and another, on ionic liquids, is now in print. He has directed 28 PhD theses.

Hopefully, the articles on 'Crystallography in Russia' presented in this issue of the IUCr Newsletter have begun to provide an accurate picture of crystallography in modern Russia. With these articles, and those to come in the next issue, we will have demonstrated various branches of crystallography: X-ray, synchrotron, neutron instrumentation and methods; development of methods for crystal structure determination based on powder diffraction data; charge density; minerals, small molecules, proteins, aperiodic structures and amorphous materials; crystal growth; crystalline films; high pressure crystallography; Voronoi-Derichlet polyhedra; teaching crystallography and so on and so forth. All comments and remarks should be sent to

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IUCR ACTIVITIES

A few extra reasons to attend the XX Congress and General Assembly of the International Union of Crystallography August 23-31, 2005



Next year, the world crystallographic community will have the opportunity to attend an important international meeting immersed in the exciting and unique atmosphere of Florence. A visit to this city, with its magnificent attractions, is a striking experience for both first time and repeat visitors. Moreover, the Congress organizers are planning various activities that will give the delegates and accompanying persons the feeling of being not merely 'just another tourist'.



Florence was the cradle of the Renaissance, the cultural phenomenon which spread through Europe in the XVth century leaving for posterity famous masterpieces of architecture, sculpture and painting. The patronage that the Medici and other influential Florentine families gave to artists as well as to the development of science was unique for the times. One of the Medici ancestors, Cosimo il Vecchio (1389-1464), performed alchemic experiments personally, as is documented in the famous painting by Giovanni Stradano (the Italianized name of the Flemish painter Jan van der Straet), which can still be

admired in Palazzo Vecchio. And, we note that this painter is a significant example of the attraction that Florence held for artists and artisans of the period, thanks to the attention that the city and its governing families paid to human ingenuity, resulting in a unique collection of talented persons in a small geographical area. This favoured the growth of a fruitful mixture of handicraft and scientifically based activities which were performed by melting metals, molding waxes and glass, extracting dyes for textiles, pigments for painting, medicaments to treat diseases, just to name a few. Some of the outcomes remain as milestones in human history. The Medici family felt a special attraction for gems and beautiful crystals and their collection of minerals, one of the oldest in existence, is still visible in the University Museum of Mineralogy. Another 'must' for the scientifically inclined visitor is the History of Science Museum which contains a unique collection of research instruments, the most famous of which are Galileo Galilei's telescopes and his devices to demonstrate the laws of falling bodies. There are also many objects of historical interest for pharmacists, botanists, physicians and chemists. In particular, the alchemist's 'Tabula Affinitatum', represents an astonishing precursor of Mendeleev's Periodic Table and should not be missed.



Another historical curiosity of note is that Florence was for many years the home of the Danish scientist Niels Steensen, later Latinised as Nicolaus Steno, one of the fathers of modern crystallography. In Florence, where he had settled, Steno made a fundamental contribution to modern geology. In particular, he established one of the most basic principles of crystallography by using three simple words: 'non mutatis angulis'. Converted to Catholicism and nominated as a bishop, he is now buried in the Church of San Lorenzo. In the third centenary of his death (1986), he was beatified by Pope John Paul II, the first step toward sainthood. Thus, crystallographers may soon have their own patron saint, one who might occasionally intercede to solve problems regarding some difficult structure! Also, we organizers trust in Beato Steno for the success of the Congress, although we place absolute faith in the interest and dedication of crystallographers for their own discipline.

The Program Committee, formed by 23 international members, met June 17-19 in Erice (Sicily) to finalize the topics and the timetable. When this article will be published, most important decisions will have already been taken and approved by the Executive Committee. Obviously, I cannot provide any information in advance, but the community of crystallographers can rest assured that the quality of the presentations and the names of the speakers are of the highest scientific level and that the Conference will confirm that crystallography is really the most multidisciplinary of the sciences.

Carlo Mealli, Program Chair

MEETING REPORT

Aperiodic 2003



Belo Horizonte, Brazil, September 2003



Aperiodic 2003 was held at the Institute of Physics, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, September 8-13, 2003. The scope of the conference was designed to promote research on aperiodic systems, both from the experimental and theoretical points of view, and to encourage scientific exchange among groups working in the various fields of aperiodic materials. A total of 90 participants were present with an equal number of contributions from students and researchers from 22 countries of 5 continents. The papers presented were related to the following topics: incommensurate modulated structures, incommensurate composites, quasicrystals, mathematical modelling and symmetry, physical properties, structure determination, polytypes, and applications. Most of the prominent names in each area attended this conference. The sessions were organized into tutorials (4), oral presentations (20 invited) and posters. Most of the oral presentations were followed by very interesting discussions. Abstracts and proceedings of the congress are available at the website (<http://agora.grude.ufmg.br/aperiodic2003>). The proceedings will be published by Francis & Taylor as a special issue of *Ferroelectrics*.

A total of 19 scientists were granted partial support for travel and living expenses (2 from Brazil, 1 from Czech Republic, 1 from France, 1 from Germany, 2 from Mexico, 2 from Poland, 1 from Romania, 6 from Russia, 1 from Switzerland and 1 from Vietnam). In addition, 18 young scientists had their registration fee waived and ten students were partially or totally supported thanks to the funds granted by the IUCr.

Nivaldo Speziali, Iris L. Torriani

MEETING REPORT

ISCGChA 2003**La Pedrera, Uruguay, December 2003**

The International School on Crystal Growth, Characterization and Applications (ISCGChA) was held December 9-13, 2003, in La Pedrera, Uruguay, a small resort on the Atlantic Ocean. The ISCGChA was supported and promoted by the Commission on Crystal Growth and Characterization of the IUCr and sponsored by the IUCr, the United Nations Educational, Scientific and Cultural Organization (UNESCO), the IKZ (Inst. für Kristallzüchtung, Germany), and the Scientific Research Commission (CSIC) of the U. of the Republic, Uruguay. The ISCGChA was held under the auspices of the Faculty of Chemistry of the U. of the Republic, Uruguay. The organizers are very grateful to all sponsors because without their support this important school for young scientists in Latin America would not have been possible. Additionally, the efforts of the members of the scientific and organizational committees were also a big factor in the success of this event.

The ISCGChA promoted effective training of students and young scientists in the fundamentals and methods of crystal growth, their characterization and applications. For several of the young attendees this was their first opportunity to take part in such a meeting, and it was undoubtedly an important step in their careers. The school provided the chance for some of them to make new professional contacts, which may well develop into lasting friendship. The ISCGChA showed the stage of research in this field that is being done in Latin America as a whole. IUCr Executive Committee member, I. Torriani, gave an overview about the progress of crystallography in Latin America and emphasized the role of the IUCr in this development. This meeting was an excellent opportunity for researchers from all over the world, but especially from this region, to meet each other, share their experiences, start new cooperative projects and reaffirm current ones, all in an environment of friendly comradeship.

Forty-nine scientists participated in the ISCGChA. There were lecturers and attendees from eleven nations, six of them of Latin America. That is the highest number of Latin American countries represented at a gathering of crystals growers in this region. Seventeen students and young scientists were able to attend (out of the thirty who originally applied) thanks to grants from the IUCr, UNESCO and IKZ.

The ISCGChA included twenty lectures and two poster sessions, covering fundamental and recent advances in crystal growth. The lectures were given by prominent scientists in the field of crystal growth, characterization and applications. Introductory lectures in the theory of crystal growth were given by P. Rudolph (Germany) on thermodynamics, kinetics and historical development of the knowledge about defects in grown crystals, by R. Sekerka (USA) on fundamental concepts about crystal morphology, and by J. Derby (USA) on crystal growth modeling.

Four lecturers from Uruguay introduced the crystallographic and materials groundwork. Aspects of structural determination were explained by A. Mombrú and R. Mariezcurrena. The influence of crystal imperfections on material properties was covered by E. Quagliata and R. Marotti.



Participants of the ISCGChA 2003 on the Dunes in Cerro de la Buena Vista.

Lectures on crystal growth methods and their experimental results were given by A. Ibañez (France) on modern solution growth techniques and by A.C. Hernandez (Brazil) on laser heated pedestal fiber growth. Numerous lectures demonstrated the importance of crystal growth for modern applications. Basic aspects of MOVPE growth, especially nitride layers, were explained by M. Bosi (Italy). T. Ohachi (Japan) showed newer results of heteropitaxy of GaN on Si by MBE. A. Moreno (Mexico) reported the 2D and 3D characterization of biological macromolecules by AFM and XRD. Some lectures covered further crystal growth advances for specific technological applications carried out in Latin America. G. Nieva, H. Cánepa and M. Sade spoke about the progress made in Argentina in the area of high temperature superconductor single crystals, epitaxial growth of HgCdTe for infrared detectors, and single crystals of Cu alloys with shape memory properties, respectively. L. Fornaro (Uruguay) gave a lecture about the growth of thick films of heavy metal iodides for ionizing radiation imaging. Finally, an overview on future applications of crystals and nanostructures was given by E. Diéguez (Spain).

The poster sessions were held during two afternoons. However, all thirty-nine posters were displayed over the whole meeting to ensure maximum exposure and interaction between participants, who engaged in very lively discussions throughout the sessions. These contributions showed the activities of twenty-three research groups worldwide. Five awards, consisting of the last five years of the American Crystallographic Assn (ACA) Transactions, were given by I. Torriani to selected participants. Further, a prize from the IUCr, a one-year complimentary on-line subscription to all of the IUCr journals, went to the Faculty of Chemistry, U. of the Republic, Uruguay. Last, the best posters were awarded by I. Torriani with a two-year complimentary membership in the ACA to Erick Juarez (Mexico) and Ana Lía Noguera (Uruguay).

A booklet with abstracts of the lectures and posters presented at ISCGChA were given to all participants. A special part included the sheet copies of the fundamental lectures of P. Rudolph on thermodynamics and kinetics of crystal growth. An internet connection, usable for all participants, was provided throughout the school. It is a special pleasure to gratefully acknowledge the work of people from the Instrument Dept. of the Faculty of Chemistry (L. Mussio, A. Gancharov, H. Bentos Pereira) who assembled the computer, media and internet facilities. The lectures, poster session, prizes ceremonies and the excursion to the Cerro de la Buena Vista, where the dunes reach up over a mass of granite rock, were partially recorded, and a special CD of highlights has been made. More details about the ISCGChA can be found at www.iscgcha2003.fq.edu.uy.

Laura Fornaro, Chairman of the ISCGhA

*Peter Rudolph, Member of the Int'l Scientific Committee of the ISCGhA
and IUCr Commission on Crystal Growth and Characterization*

MEETING REPORT

Advanced Workshop on Structural Biology at CBB in Poznan

Poznan, Poland, November 2003



The Center for Biocrystallographic Research (CBB) at the Inst. of Bioorganic Chemistry, Polish Academy of Sciences in Poznan, Poland, has again been the site of an intensive practical course in protein crystallography. It was organized as an external course for the Ph.D. students of the Int'l Max Planck Research School (IMPRS) at the Max Planck Inst. (MPI) for Plant Breeding Research in Cologne, Germany. The 15 students from Cologne were joined for the lectures and practicals by nine young structural biologists from Polish laboratories. The organization of the course was supported by the MPI under the coordination of Guntram Bauer. The Polish coordinator was J. Stepkowska. The teaching staff included local faculty members M. Jaskolski (head of the organizing team), G. Bujacz, M. Sikorski, and W. Rypniewski, as well as invited experts M. Bochtler (Warsaw), J. Otlewski (Wroclaw), and Z. Dauter (NSLS/NCI, USA), who also gave a special keynote lecture on phasing macromolecular structures. The program consisted of six hands-on exercises attended by small student groups, and of eight general lectures, covering subjects from protein expression and crystallographic fundamentals to crystallographic methodology and frontiers, to protein-protein interactions. The practical classes concerned protein purification and crystallization, macromolecular data collection and processing, the method of molecular replacement, and model building and analysis using molecular graphics. The topics instigated a lot of interest and discussions could be heard also during breaks and over an evening glass of beer. On one evening the group enjoyed a wonderful organ concert in the historical quarters of Poznan. It was the first external course offered by the IMPRS to their Ph.D. students. We hope that the seed of crystallographic fascination sown during the course will bear fruit in the future careers of the participants, who represented eight nations all over the world. Sponsorship was provided by UNESCO/PAN (Polish Network of Cell and Molecular Biology) and by Marresearch.

Mariusz Jaskolski (CBB, Poznan)

MISCELLANY

Does open data better serve the crystallographic community?

The many crystallographic databases, PDB, CSD, ICSD, CRYSTMET, ICDD, AMCSD, NDB, etc. are invaluable tools in crystallography. Essential uses for these tools are too numerous to list.

Unfortunately, many researchers do not have access to some of these data collections (open access being ensured for PDB, AMCSD and NDB only), which is detrimental to making good science (reviewers of crystallography papers may not be able to perform a correct evaluation, chemists will try to republish already known structures, etc). Further, the delays between publication and distribution of structures can be quite long, reducing the value of the tools for recent results. Following the ideal PDB, AMCSD and NDB models, the Crystallography Open Database (COD) wishes to establish a public domain Web repository and index for published and unpublished structural results (inorganic and organic, excluding proteins and nucleic acids covered by PDB and NDB). The COD advisory board members wish to open a discussion within the community of crystallographers on how this can best be accomplished.

We would like to see crystallographers deposit CIFs with the COD prior to publication, with the understanding that this disclosure should not be considered 'prior publication' when a paper is prepared for journal publication.

We would like to see the IUCr provide copies of CIFs for published papers to the COD, as the IUCr does with the other crystallographic databases. If this would endanger IUCr journal revenues, an alternative would be to only allow the COD to include information on recent structures in the COD indices for some period after publication. During this period, the COD would provide an URL pointer to the CIF on the IUCr site, where access could be restricted to journal subscribers. An outside organization of volunteers would bring new ideas for locating structural information, beyond what the IUCr can afford to develop internally for searching the IUCr's collection of CIFs. These innovations will be available to the established databases, strengthening their tools as well. For instance, an increasing COD subset is devoted to CIFs of predicted crystal structures (zeolites, etc).

If the IUCr takes a direct stance on open access to crystallographic data, we think this will establish the ethical standards for structure disclosure within the field, this can be used to encourage non-IUCr journals to also offer similar access.

Armel Le Bail on behalf of the COD Advisory Board

AWARDS AND PRIZES

Ivar Olovsson receives Marie Skłodowska-Curie Medal



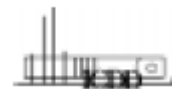
Ivar Olovsson.

The Polish Chemical Society awards its prestigious Maria Skłodowska-Curie Medal to outstanding chemists working permanently abroad. The Medal for the year 2003 went to Ivar Olovsson of the U. of Uppsala (Sweden) for his crystallographic studies of the structure of matter, especially for his fundamental studies of the hydrogen bond. The award ceremony had a particularly solemn character. It was part of a special session, organized jointly by the Polish Chemical Society and by the Polish Academy of Sciences (represented by Vice President, Janusz Lipkowski) to celebrate the 100th Anniversary of Maria Skłodowska-Curie's first Nobel Prize. The 1903 Nobel Prize in Physics Maria Skłodowska-Curie received jointly with her husband Pierre Curie and Henri Becquerel. (In 1911 she received her second Nobel Prize, this time in chemistry and all by herself.) In his prize award lecture, Ivar Olovsson spoke about Wilhelm Conrad Roentgen (the first Nobel Prize in Physics) and his discovery of X-rays in the context of the fertile times of fundamental discoveries in physics, which also included the discovery of radioactivity.

Mariusz Jaskolski (Poznan)

AWARDS AND PRIZES

ICDD announces Awards



The International Centre for Diffraction Data announces the following awards:

McMurdie Award

Winnie Wong-Ng, National Inst. of Standards and Technology, Gaithersburg, MD, USA, has been selected to receive the 2004 McMurdie Award. The award was presented at the 53rd Annual Denver X-ray Conference, Steamboat Springs, CO, USA, August 4, 2004. This award recognizes Dr. Wong-Ng's contributions to the computer-aided evaluation of X-ray powder patterns and editing of the Powder Diffraction FileTM, as well as her work in enhancing the accuracy of powder methods of X-ray crystallography. Named in honor of Howard McMurdie, long time editor of the ICDD Ceramics Subfile, the McMurdie Award is presented every two years for distinguished work, which improves the Powder Diffraction FileTM in its purpose of identifying and characterizing inorganic solids.

J.D. Hanawalt Award

Robert L. Snyder, of Georgia Inst. of Technology, Atlanta, GA, USA has been selected to receive the 2004 J.D. Hanawalt Award for excellence in the field of X-ray powder diffraction. Dr. Snyder will present the Hanawalt Award Lecture entitled, 'The Evolution of Total Pattern Analysis' at the 53rd Annual Denver X-ray Conference in Steamboat Springs, CO, USA, August 4, 2004. The J.D. Hanawalt Award is presented every three years for important, recent contributions to the field of X-ray powder diffraction and phase identification published within the last several years. The award consists of a commemorative plaque, an honorarium, and travel funds to attend the meeting at which the award and lecture will be presented.

OBITUARY

John Charles Taylor (1935-2002)



John Charles Taylor, MSc, PhD, DSc, died suddenly while playing tennis in Sydney on September 30, 2002. John spent the whole of his working life as a crystallographer using both X-ray and neutron diffraction methods. He authored or co-authored 99 fully refereed journal publications, 19 lightly or non-refereed publications, various conference papers, 4 seminar/workshop papers and 8 Internal (Lucas Heights) Divisional Publications. John also co-authored a book, 'Rietveld Made Easy'.

John's start in crystallographic research was in 'Old Chemistry' (now the Department of Pharmacy) at the U. of Sydney. He collected and visually estimated 929 diffracted intensities (another possible 331 were very weak and were not observed) on the crystal structure of potassium bis-biureto-cuprate (II) tetrahydrate using a Metropolitan- Vickers 'Raymax' X-ray generator with a demountable tube. He had manually corrected them for Lorentz, polarization and Tunell effects but not, at this stage, for absorption. He then disappeared home for quite a few weeks and graphically calculated absorption factors for all of his data. Subsequent cycles of Fourier and Least-Squares refinement (thanks to SILLIAC programs written by H C Freeman) led to the placement of all hydrogen atoms in the structure.

Sydney U. has a long history of X-ray analytical work, going back to the early 1930s. This short obituary is important for historical reasons as well as reflecting on the life of John Taylor and his early work (at Sydney U.) of which not many people have knowledge. John's work there commenced in the era before computers in Australia and was completed with the aid of the 'SILLIAC', Australia's second and then best electronic digital computer.

In August 1962, John met Mavis McKinnon who was to become his wife. John was awarded his Ph.D. in 1963 for his thesis 'Crystal Structure Analysis by X-ray and Neutron Diffraction Methods'. In 1981, the U. of NSW awarded John the Degree of Doctor of Science in recognition of his research excellence.

John became interested in the Rietveld method after reading Hugo Rietveld's initial papers on quantification of mineral phases from X-ray powder diffraction, adapting the single crystal program (ORFLS) for profile analysis for his research. This work was the early beginnings of the software program SIROQUANT that allowed multi-phase quantitative analysis of a wide range of materials. That John developed the algorithms from first principles allowed him to incorporate some innovative features, such as the use of observed HKL files for analysis of materials that have a poorly crystalline or amorphous nature. His research was leading edge although, to his colleagues, the apparent ease with which he succeeded in solving the most complex problems was daunting.

SIROQUANT has undergone considerable enhancements since those early days and is now one of the most popular programs for quantitative XRD sold throughout the world.

John was the classic individual researcher, best described as the quiet achiever, who shunned the tedium of budgets and management constraints but always delivered on his research. He was also an accomplished pianist and landscape painter of considerable merit. His painting commenced as a relaxation at the age of 40. He leaves a widow, Mavis, and two children, Phillip and Karen.

Chris Kelaart and John E.W. Lambert-Smith

OBITUARY

Rosemary Durley (1948-2003)



Rosemary Durley (nee Belford) was born in Edinburgh, Scotland in 1948, and grew up in Belfast, Northern Ireland. Rosemary received a B.Sc. degree from Bristol University in 1968, and then moved to Birkbeck College, London where she earned a master's degree. She went on to do research on crystal structures at University College, London with Jackie Truter and received her Ph.D. in 1973. She was appointed Assistant Professor at the University of Saskatoon, Canada in 1974, where she continued her research as well as teaching chemistry. After taking time off to raise two children, she returned to academia at Washington University, St. Louis, Missouri in 1988 to work with F. Scott Mathews. She used X-ray crystallography to study the crystal structures of enzyme complexes involved in oxidationreduction pathways and related redox co-factors. In particular, she studied the mechanism of flavocytochrome redox complexes and methylamine dehydrogenase redox chain complexes. She had many publications in this field and made many presentations. In 2000 she retired due to chronic illness. She passed away on December 29, 2003. She is survived by her husband, Richard, and two children, Alison and Stephen.

Scott Mathews, ACA Newsletter, Spring 2004