

Crystallographers

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This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

C. W. Bunn 1905–1990

The following obituary is based on a longer one published in *Crystallography News* No. 34, the September 1990 Newsletter of the British Crystallography Association, which was prepared by Dr Bunn's son and was based mainly on autobiographical notes left by his father.

Charles William Bunn was born in 1905 in Camberwell, South London. His education commenced at the Denmark Hill School. In 1923 he gained an open scholarship to Exeter College, Oxford, to read honours chemistry. He gained his BSc in 1927, coming second in the first class honours list. From Oxford he joined the research staff at ICI Alkali Division at Northwich, Cheshire, soon after the formation of ICI. The research manager, H. E. Cocksedge, sent him back to Oxford for one summer term to learn crystal morphology and optics. He returned to Northwich and became skilled in the art of identifying crystals or fragments in mixtures of solids produced in chemical processes or phase equilibrium investigations. At the same time, Cocksedge started him in the study of the growth of crystals, with a view to controlling the size and shape of crystals in the company's products.

This work led him to an explanation of crystal habit modification by dissolved additives. It also led to a quest for 'the laws of crystal growth in solution' in terms of supersaturation of solution at the crystal face and in terms of diffusion gradients. He was soon disillusioned: the experiments showed no relation between the rate of growth of a crystal face and the supersaturation of the solution in contact with that face. His attention turned to the nature of the surfaces on which deposition of solute occurs. This led him to a concept of reciprocal interaction between surface contour and solute diffusion down concentration gradients. He credited diffusion momentum with creating surface nuclei as well as maintaining the high-index surfaces on which deposition can continue. This work in the early 1930's was published much later in the 1949 Faraday Society Discussion on crystal growth. However, little notice was

taken of it at that time as having a major role.

Also in the early 1930's, he worked on the identification of crystalline solids by X-ray powder diffraction patterns, notable achievements being the definite identification of the crystalline phases in bleaching powder, and an understanding of the changes that take place in the setting of plaster of Paris. He gradually built up a card index of the powder patterns of many species and this later formed one of the initial collections in the ASTM index. This work led on naturally to the interpretation of diffraction patterns and to the determination of the atomic arrangements in crystals. He examined the very first specimen of polyethylene (polythene) which was discovered in the Northwich laboratory in 1933 and determined its structure and those of several other polymers. He recognised the importance of the two-phase texture in its influence on the physical properties, the interplay between bond orientations and the attractions or repulsions of non-bonded atoms, and the importance of the flexibility of the molecules.

At a suggestion by C. N. Hinshelwood, he wrote his text book *Chemical Crystallography*, working mostly in the evenings during the war years. This was published in 1945, and has since been widely used in universities all over the world. A second edition was published in 1961, and there is a Japanese translation. In the 1940's, he developed an optical analogue method of solving crystal structures by trial. This had been suggested by Sir Lawrence Bragg, and is known as the fly's eye method. On the strength of this method, Dr Dorothy Hodgkin suggested collaboration in the attempt to settle the chemical structure of penicillin by crystal structure determination. He used the fly's eye method in the early stages of work on the sodium salt (monoclinic) and later developed a new Fourier method of correction and refinement. This led to a detailed solution (with A. Turner-Jones) of the structure of the central part of the molecule, which chemical methods had left doubtful. His solution was simultaneous with Dr Hodgkin's solution (with B. Low) of the structure of the K and Rb salts (orthorhombic). The two conclusions were identical.

In 1946, he was transferred from the Alkali Division at Northwich to the Plastics Division laboratory at Welwyn Garden City, Herts, where he was in charge of, at first, the Molecular Structure Division of the Research Department and, later, of the Physics Division which combined measurements of the useful properties of polymer materials with studies of their molecular structures.

He was elected a Fellow of the Chemical Society in 1941, a Fellow of the Institute of Physics in 1944, and awarded the degree of Doctor of Science of Oxford University in 1953.

At Plastics Division his further studies of crystalline polymers led to a knowledge of the molecular conformation and arrangement in crystalline regions in many polymers. He also made studies of optical properties, electron-microscopic studies of texture and further contributions to the understanding of the conformations of polymer molecules and the relation between molecular structure and texture and the physical properties. His interest in the melting points of polymer crystals led to a comprehensive survey of the melting points of molecular crystals in general, monomeric as well as polymeric, revealing that melting temperatures are determined by the general overall shape symmetry of molecules as well as intermolecular forces (cohesion energy) and molecular flexibility.

In 1963 he retired from ICI. He had become very interested in the stereochemistry of biological macromolecules and, as a natural extension of his interest in synthetic macromolecules, had indulged in much speculation on protein-chain conformations. Sir Lawrence Bragg invited him to join his group at the Royal Institution and, as Dewar Research Fellow, he attempted to find the structure of crystalline calf rennin (chymosin), a proteolytic enzyme. When Sir Lawrence Bragg retired and the main protein crystallography group under D. C. Philips migrated to Oxford, he continued his work at the RI with the assistance of a small group. Calf rennin, however, proved to be an intractable subject and was discontinued when financial support from the Medical Research Council came to an end in 1972, by which time he was 67 years of age.

He could now devote more time to his other interests; horticulture and classical music. He was an accomplished violinist and shared the leader's desk in the local orchestra for many years. He would play the piano, and also his gramophone, for at least two hours every day.

He published fifty scientific papers and contributed chapters in several other books besides his own text book and in 1964 published a second book, *Crystals, Their Role in Nature and in Science*, for general readership.

After a full scientific life and a long retirement he died suddenly at Easter 1990.

R. BUNN

Vladimír Syneček 1929–1990

Vladimír Syneček died suddenly on 4 March in Prague. Born in Bilina (northern Bohemia) he later resettled in Prague. After finishing secondary school, he studied physics at the Faculty of Sciences of Charles University in Prague in 1948–1952. From the autumn of 1952, he worked in the Institute of Technical Physics of the Czechoslovak Academy of Sciences (later the Institute of Solid-State Physics and, since 1979, the Institute of Physics). As his thesis for the degree of RNDr (equivalent to MSc), he presented, in 1952, the solution of the structure of NH_4VO_4 . In 1956, Syneček presented his CSc (equivalent to PhD) thesis *Fundamental sets of inequalities among structure factors*. Later he studied the structures of minerals and inorganic substances. After the foundation of the Department of Metals, he shifted his attention to the study of transformation processes in aluminium alloys and structures of solid solutions. He was the head of the research team which obtained the State prize in 1971.

In 1966–1968 he was a visiting professor at the Department of Physics of the State University of New York at Albany.

Syneček also cooperated with the Department of Mineralogy, Faculty of Sciences, Charles University, in Prague. He participated in the description and structure determination of the new minerals kettnerite and krupkaite. He trained several students of mineralogy in X-ray crystallography.

In the last decade, Syneček dedicated himself to X-ray diffraction studies of the surfaces of Al alloys treated by a laser beam.

During his career he published more than 100 papers. He is survived by his wife and close co-worker Dr Marie Simerská.

JIRÍ HYBLER

Professor **Jack David Dunitz**, Laboratorium für Organische Chemie, ETH-Zentrum, Zürich, Switzerland, has been awarded the 1990 Gregori Aminoff Gold Medal and Prize of the Royal Swedish Academy, in recognition of his outstanding scientific accomplishments, primarily in the field of small-molecule crystallography. Among the previous recipients of the Aminoff Prize there are numerous distinguished crystallographers, including P. P. Ewald and J. M. Robertson who had a great influence on the scientific life and career of the present awardee.

New Commercial Products

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Four New Software Products from Cambridge Molecular Design

Cambridge Molecular Design offers four new software products for researchers who study crystals or use diffraction techniques. These four products, **CERIUS Crystals**, **CERIUS Diffraction I and II** and **CERIUS Diffraction Data**, are part of a family of products for molecular modelling in materials research.

CERIUS Crystals combines crystal model visualization, building, editing and property calculation in a single user-friendly program. **CERIUS Crystals** is designed for studies of molecular crystals, inorganic crystals (*e.g.* zeolites, ceramics) and polymer crystals. Symmetry can be specified using space-group symbols or general positions. Crystal models are constrained according to the user-specified symmetry. Applications include crystal visualization, theoretical studies (*e.g.* lattice energies, packing), structure analysis (in conjunction with **CERIUS Diffraction I**) and the teaching of crystallography and crystal symmetry.

CERIUS Diffraction I simulates X-ray, electron and neutron diffraction patterns from crystal models. Simulations are very fast, allowing *real-time* diffraction-pattern simulations simultaneous with the manipulation of crystal variables such as cell parameters, atom site occupancy, rotations and translations of atoms, and bond length and angle changes. Simulated diffraction can be presented as powder, fibre or zone patterns, and can be compared to user-supplied experimental patterns. Applications include analysis of crystal structure (*e.g.* polymer structure solution, ion or molecule location in zeolites, site occupancy in ceramics), estimation of crystalline morphology in materials (crystallite size, lattice/strain distortion) and teaching of diffraction methods.

There are two other closely related products: **CERIUS Diffraction II** simulates X-ray, electron and neutron diffraction patterns from non-crystalline models, calculating isotropic, meridio-

nal or 2D cylindrical forms. **CERIUS Diffraction Data** performs data reduction, radial and cylindrical distribution function analysis and orientation analysis on experimental diffraction data.

Computer requirements for **CERIUS** software are Silicon Graphics IRIS/Unix workstations or DEC VAX/VMS computers.

Cambridge Molecular Design, St John's Innovation Centre, Cowley Road, Cambridge CB4 4WS, England; 100 Sea Beach Drive, Stamford, CT 06902, USA

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A New Software Product from Bede Scientific Instruments

A new crystallographic software product has recently been released by Bede Scientific Instruments. **Rocking curve analysis by dynamical simulation (RADS)** uses the Takagi-Taupin equations to simulate double-axis X-ray rocking curves from epitaxial layer systems on a variety of substrates. Until recently, the algorithms used in such simulations have necessitated the use of mainframe computers to give results within a reasonable time, seriously limiting their widespread use. Fully supported codes have not previously been released by any manufacturer or institution. RADS, by the use of several novel computational methods, has cut the CPU time required to simulate rocking curves to an extent that it is now feasible to run the program on fast IBM-compatible PCs. Computation time on a PS/2 model 70 is typically only a few seconds for a simple single heteroepitaxial layer, and a (100) layer superlattice with a large scan range takes less than ten minutes.

An extensive crystal database is included in the software, which can be edited and supplemented by the user to customize it to their particular needs. Scattering factors and absorption parameters for all elements are included. Comprehensive graphics and file utility routines allow for high-resolution presentation and manipulation of the data. The software is fully documented and supported.

Combined with the user-friendly menu-driven user interface developed from Bede's experience in controlling double-crystal cameras, this new product means that simulation is generally available for the first time as a routine tool for the analysis of experimental double-crystal rocking curves.

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