Vladimír Syneček 1929–1990

Vladimír Syneček died suddenly on 4 March in Prague. Born in Bílina (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 strutures 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.

JIŘÍ 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

Announcements of new commercial products are published by the Journal of Applied Crystallography *free of charge. The descriptions, up to* 300 *words or the equivalent if a figure is included, should give the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Dr A. M. Glazer, Editor* Journal of Applied Crystallography, *Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX*1 3*PU, England.*

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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-suppllied 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, meridional 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 CB*4 4*WS, 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 epitaxic 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.

*Bede Scientific Instruments, Lindsey Park, Bowburn, Durham DH*6 5*PF, England*