Crystallographers

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).

J. Appl. Cryst. (1989). **22**, 398

Katarina Kranjc 1915–1989

Katarina Kranjc, retired professor of physics at the Faculty of Science of the Zagreb University, died on 23 March 1989 in Zagreb after a long and serious illness. Born in Zagreb in 1915, she was educated there at the Grammar School and the University, graduating with a degree in physics in 1936. She started her scientific career only after the war in X-ray diffraction crystallography and remained faithful to this field until the end of her life. Her first papers in *Acta Cryst.* (1954) and *J. Coll. Sci.* (1955) were based on her PhD thesis (1953) on the small-angle X-ray scattering of some colloid systems, suggested by Professor M. Paić. During her short stay in Paris (1954) in Professor A. Guinier's laboratory, she learnt new methods in the field and participated at the 3rd IUCr Congress. On this occasion she came into contact with her first international crystallographic acquaintances through Rosalind Franklin, with whom she had made friends in Zagreb, one year before, when Rosalind gave a lecture on her X-ray studies of graphitic oxide. In the years to follow Rosalind, as Katarina's guest, spent part of her holidays on the Adriatic coast and in Montenegro. Katarina's written reminiscences about their friendship were included by Mrs Anne Sayre in the book she published (1975) on Rosalind's life and work. Katarina also enjoyed a friendship with Alan L. Mackay and his wife Sheila, initiated also at the Paris Congress, which brought her many intellectual contacts through correspondence as well as talks at her home in Zagreb.

Being an excellent experimentalist with a remarkable knowledge of applied mathematics, she was able to satisfy her curiosity in diffraction phenomena by studying them in a variety of cases. Mentioned here are only some of her thirty papers.

After a study of the surface defects in sodium chloride crystals (*Glas. Mat. Fiz. Astron.* 1964), she used Berg–Barrett X-ray diffraction microscopy to investigate the domain structure (*J. Appl. Cryst.* 1968, 1969). Then she shared the success of her colleagues at the University Institute of Physics using X-ray microradiography (*Metallography*, 1969), small-angle X-ray scattering (*Fizika*, 1970; *J. Appl. Cryst.* 1974) and X-ray diffraction (*Metall. Trans.* 1973) in the investigation of alloys quenched from the liquid state, and found a distortion of scattering curves obtained with a Levelut–Guinier camera (*J. Appl. Cryst.* 1974). She particularly studied spherical particles of non-uniform electron density in precipitated alloys (*Fizika*, 1976) as well as moiré fringes in SnTe–Sn–SnTe layer crystals (*Phys. Status Solidi*, 1981, 1982). In short but exemplary articles on the Abbe theory (*Am. J. Phys.* 1962) and on lead dendritic crystals (*J. Appl. Cryst.* 1972), one recognizes her aim to reveal the essential as the main feature of Katarina's character.

As one of the initiators of the Yugoslav Centre of Crystallography (1966), as an active and devoted member of its executive Committee, as a regular participant of the Annual meetings of Yugoslav crystallographers and as the Sub-Editor of the Yugoslav section of the *World Directory of Crystallographers*, she greatly contributed to the Yugoslav crystallographic community. Respected as a scientist and a teacher, beloved for her open-mindedness and sense of humour, Katarina Kranjc will always be affectionately remembered among her colleagues and friends.

D. GRDENIĆ

Dr **Lynne B. McCusker**, Institut für Kristallographie, ETH Zürich, Switzerland, was presented with an award of £250 by the Physical Crystallography Group of the British Crystallographic Association at the April 1989 BCA meeting. This is the first time such an award has been made; it will be presented from time to time by the Group for recently published work on aspects of physical crystallography to individuals considered to show particular promise.

The award recognizes McCusker's work on *ab initio* structure determination of a new clathrasil compound – a material similar to a zeolite and consisting of carbon, silicon and oxygen – using synchrotron powder diffraction data [*J. Appl. Cryst.* (1988). **21**, 305–310]. She solved a complex crystal structure using direct methods with almost no prior information whilst at the Clarendon Laboratory, Oxford, where she held until recently an ICI Joint Research Scheme Fellowship.

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 price and 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, Professor M. Schlenker, Editor* Journal of Applied Crystallography, *Laboratoire Louis Néel du CNRS, BP166, F-38042 Grenoble CEDEX, France.*

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

J. Appl. Cryst. (1989). **22**, 398

Image Storage Brings Quality Improvement to Philips SEMs

A novel **image-storage facility** has been introduced by Philips Analytical for use with the **Series 500 scanning electron microscopes**. The storage unit can be fully integrated into the microscope without in any way compromising its function.

Up to four images can be memorized and recalled at any time for image comparison and post-scan processing. This is a valuable feature, introducing new levels of image improvement. It makes possible such treatments as the identification and removal of noise interference, the introduction of enhancement techniques like linear and non-linear contrast expansion, the application of processing functions such as image inversion, signal mixing and image differencing, and the applying of high-pass filtering for detail sharpening.

The image store interfaces with the SEM *via* the 'Data Link' distributed intelligence architecture which is a feature of the Series 500 instruments, and functions are easily applied by simple keypad operation.

Philips image storage facility

Jeff Grimes, Philips Scientific, York Street, Cambridge CB1 2PX, England

J. Appl. Cryst. (1989). **22**, 398–399

3D Molecular Graphics on the Apple Mac II

Chemical Design is pleased to announce that the **Apple Macintosh II** is now supported as a **3D graphics terminal for molecular modelling.**

3D GKS graphics drivers have been developed for use with Chemical Design's Chem-X molecular modelling software. All graphics calculations are

offloaded to the Mac, while compute-intensive calculations are performed on the VAX server. The system is ideal for small-molecule modelling and offers advanced features including frame-based dynamic replay.

A Mac II with 3D GKS drivers represents a relatively inexpensive option for modellers who need the power of Chem-X but cannot justify a dedicated graphics terminal.

A 2-user industrial licence at £995 provides 3D graphics facilities at less than £500 per station. For larger numbers of users the cost per station is reduced still further. Academic institutions qualify for significant discounts.

Apple Macintosh II hardware is also available directly from Chemical Design.

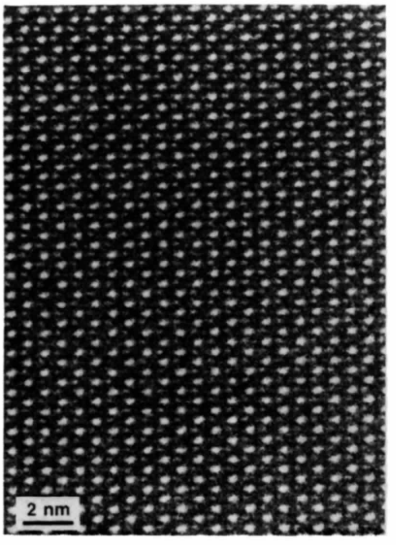
Helen Gasking, Chemical Design Ltd, Unit 12, 7 *West Way, Oxford OX*2 0*JB, England*

J. Appl. Cryst. (1989). **22**, 399

New High-Resolution Lens for Philips CM30 TEM/STEMs

Philips Analytical announces a new **SUPERTWIN lens** for use on its **CM30 transmission and scanning transmission electron microscopes.**

Complementing the instruments' 300 kV accelerating voltage and intelligent MICROCONTROLLER, the lens brings new capabilities in high-resolution structure imaging. It also provides microdiffraction, convergent-beam diffraction, electron energy loss (EELS) and energy-dispersive X-ray analysis (EDX) modes.



Ultra-high resolution imaging with the Philips CM30 TEM and SUPERTWIN lens. The specimen is hexagonal silicon nitride (Si_3N_4), showing the arrangement of atoms in hexagons.

Equipped with all these features, CM30 instruments are especially suitable for scientists needing to integrate high resolution, structural and chemical data.

The parameters of the new SUPERTWIN lens are a C_S of 1·2, point resolution better than 0·2 nm and a magnification range extending from $10^6\times$ right down to 50×. Minimum spot sizes are 1 nm in TEM microprobe and 1·5 nm in TEM nanoprobe and STEM modes. Full eucentric tilting is also possible using the lens.

*Jeff Grimes, Philips Scientific, York Street, Cambridge CB*1 2*PX, England*

J. Appl. Cryst. (1989). **22**, 399

New High-Performance Molecular Modelling Workstations from Chemical Design

Chemical Design is pleased to announce the **P-GRAF 3 series of high-performance molecular modelling workstations**, based on the recently launched DEC VAXstation 3520 and VAXstation 3540. The powerful Chem-X modelling software is included as part of the package, and the whole system is maintained and supported by Chemical Design.

The multiprocessor architecture provides system performance and throughput up to twelve times that of a VAX 11/780. Custom VLSI processors make the P-GRAF 3 the fastest DEC-based 3D workstation, providing local manipulation, smooth shading, depth cueing and true colour display in hardware.

Chem-X is the most powerful and flexible molecular-modelling software on the market. It exploits the 3D raster graphics of the VAX hardware to the full, and is used in a wide range of applications, including drug design, protein engineering, petrochemical development and polymer research.

P-GRAF 3 systems may be configured either as standalone workstations or as part of a Local Area VAXcluster. Prices start at £28 000 for a networked system with the Chem-X licence on the server. Discounts are available to academic institutions.

The P-GRAF 3 systems are the newest members of Chemical Design's growing family of molecular modelling workstations. Others include P-GRAF 2 systems (based on the VAXstation 3100), MicroGRAF systems (based on the MicroVAX 3000) and the top-of-the-range MITIE superworkstation, a transputer-based parallel processing system running at up to 360 MIPS.

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J. Appl. Cryst. (1989). **22**, 399–400

Philips Upgrades AA Spectrometers to New Standards

Philips Analytical has upgraded two of its most popular atomic absorption spectrometers – the **PU9200 and PU9400 series** – to meet customer requirements.

The enhancements mean even better all-round AA capability, superior price–performance ratio, and improved automation, data handling and ease of use.

The new **fully automated PU9200X** now provides a quad data-coded lamp turret and full safety gas control as standard, together with high-energy beam-profiled correction. A high-performance spray chamber and finned burner system with tapered slot design ensure the very best in flame performance.

New for the PU9200X are full-colour VDU presentation and auto-turret options which together with the new extended software bring full multi-element capability at lower cost. Multi-element flame, furnace and vapour operation are now available for even the most demanding budget.

Further on-board options include a choice of single beam or unique Stockdale double-beam optics, a dual high-density disk system and flame autosampler. This ensures a factory quality-tested configuration to meet exactly any user requirement.

Other software enhancements underline the laboratory automation theme and include such features as full alphanumeric sample identification, on-line laboratory balance interfacing for full weight and dilution results correction and flexible user-definable hard-copy report formatting. Post-run results file manipulation has also been improved in the light of the increased importance of good laboratory practice.

Automation in furnace AA has also been extended. When employed with the new PU9390X furnace and PU9380X furnace sample-preparation system, the PU9200X is capable of automatically determining optimum temperature conditions for a particular analysis. This is achieved by a new ash-atomise facility featuring full graphics and storage capability. Together with the PU9385X autoprobe – the ultimate weapon in the control of furnace interference – the PU9200X offers the very best in furnace AA performance.

A new continuous-flow vapour system, the PU9360X, with full multi-element autosampling capability completes the perfect AA package.

The new **PU9400X** embraces all the improvements available in the PU9200X range and in a single compact unit provides the ultimate multi-element AA system. With fully automated 16-element capability and including as

standard an on-board flame autosampler, the 9400X takes automated AA analysis to new levels with its enhanced 'intelligent' mode of operation.

Not only will the system automatically optimize its own flame composition to achieve the best day-to-day performance, it can now choose for itself other optimum instrument parameters if required, such as wavelength and bandpass.

The 9200X and 9400X look set to continue where their predecessors leave off, playing a leading role in a wide range of application areas, including pharmaceuticals, metals, water, environmental studies, clinical, oils and foodstuffs.

Keith Andrews, Philips Scientific, York Street, Cambridge CB1 2PX, England

J. Appl. Cryst. (1989). **22**, 400

Cost-Effective and Flexible AA Analysis with Philips New Spectrometer

The new **PU9100X series atomic absorption spectrometer** from Philips Analytical offers an economic high-performance solution for flame, furnace or vapour analysis.

The basic instrument provides elemental analysis at a lower cost than any comparable system. Modular design enables the addition of quad lamp turret, full gas control system, and a high-energy background-correction facility.

The new spectrometer succeeds the popular PU9100, but is boosted by a number of enhancements, the most important of which is the PU9390X furnace system that combines unrivalled sensitivity and outstanding automation.

The system incorporates the most comprehensive interference control package available, including the unique furnace autoprobe. There is even a dedicated furnace instrument within the range.

The furnace can be rapidly interchanged with the burner system without disconnecting gas lines. The furnace head provides a totally replaceable all-graphite inert cuvette environment. High-pressure radial contacts ensure optimum electrical contact to all available cuvette types including the advanced totally pyrographite cuvettes.

The PU9380X furnace autosampler offers comprehensive sample and standard preparation together with automatic matrix modification.

Furthermore, addition of the Philips IBM-compatible AA data station to the PU9100X spectrometer now provides the option of full colour graphics and software.

Working within an IBM compatible environment, the menu-driven software is extremely easy to run, with extensive use of pop-ups and softkeys. No computer skills are required. Interfacing to commercial database software is also provided.

All spectrometers can employ the Philips AA data station to give full parameter, results and graphics presentation together with greatly improved storage of these items on the hard-disk system. Extensive help, cookbook and library facilities complete this exciting AA software package.

To improve system reliability and ease of use, the software package comes ready installed on the hard disk, ensuring 'out-of-the-box' start-up.

Keith Andrews, Philips Scientific, York Street, Cambridge CB1 2PX, England

J. Appl. Cryst. (1989). **22**, 400

PN4300 Profile Plotter

The **Bio-Rad PN4300** is the latest generation of the **Electrochemical Profile Plotter** which measures electrically active carrier concentration against depth in complex structures. Unlike conventional C-V analysis which employs a metal Schottky contact, the PN4300 uses an electrochemical contact which allows measurement to unlimited depth into the sample.

Electrochemical profiling offers a number of advantages including measurements over a wide range of carrier concentration (10^{13} to 10^{19} cm^{-3}) on a wide variety of materials (including GaAs, InP, AlGaAs, GaInAsP, GaP, GaAsP, CdTe and silicon) with no sample preparation.

In addition, the **PN4350 Photovoltage Spectroscopy** accessory is available which makes use of the optically transparent electrolyte/semiconductor interface in the PN4300 Profile Plotter to obtain a band-gap profile. In compound semiconductors the band gap gives a measure of chemical composition. The most important application of this is in the profiling of aluminium content in AlGaAs devices such as laser diodes or determining the active region of a long-wavelength laser device.

The PN4300 employs a 68008 based data station with a multiuser, multitasking operating system which allows measurements to be made while hardcopy is being printed. The data station has a high-resolution colour graphics display with data storage provided by a 20 Mbyte Winchester disk drive and a 1 Mbyte 3·5 inch disk drive. Hardcopy of both graphics and text are provided by the associated colour inkjet printer. The software includes a number of new features including series and parallel equivalent circuit treatment, LSS calculation of individual implants and summation for multiimplants, and extensive data editing facilities.

Additional software packages are available to enable PN4300 disks to be read by a PC compatible computer and disks from previous models of the Profile Plotter to be read directly by the PN4300.

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Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

J. Appl. Cryst. (1989). **22**, 400

Crystallographic computing 4: techniques and new technologies. (IUCr Crystallographic Symposia No. 3.) Edited by *N. W. Isaacs* and *M. R. Taylor.* Pp. xvi + 464. Oxford: International Union of Crystallography and Oxford University Press, 1988. Price £35.00. A review of this book, by Paul T. Beurskens, has been published in the June 1989 issue of *Acta Crystallographica*, Section A, page 444.

Dislocations in solids. Edited by *F. R. N. Nabarro.* Pp. xi + 434. Amsterdam: Elsevier Science Publishers, 1987. Price Dfl 235.00 or US $94.00. A review of this book, by A. S. Parasnis, has been published in the July 1989 issue of *Acta Crystallographica*, Section A, pages 499–500.