Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) 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. (1988). **21**, 76

Publish your Crystallographic Computer Programs

A large number of new crystallographic computer programs (or modifications to existing programs) presented at international and national conferences, summer schools, private demonstrations, or referred to only passingly in other publications remain unpublished. Consequently, potential users are deprived of valuable information and access to state-of-the-art computer code. The IUCr Commission on Crystallographic Computing is well aware of this problem and is particularly anxious to encourage authors of computer programs to publish their software. The journal of choice for crystallographic computer programs is:

Journal of Applied Crystallography – a publication of the IUCr – which provides two categories of publication concerned with crystallographic computer programs: *Computer Programs* is intended for complete articles giving in-depth information on the program and algorithm whereas *Computer Program Abstracts* provides a condensed format that contains only essential details.

In *Computer Programs*, a brief description of the purpose, strategy, computer language, machine requirement, input requirements and the type of results obtained should be included. Ordinarily, it is required also that the adequacy of the documentation shall have been proven by the successful use of the program by someone outside the authors' institution. Examples of *Computer Programs* are: *TREOR*, a semi-exhaustive trial-and-error powder indexing program for all symmetries [Werner, P.-E., Eriksson, L. & Westdahl, M. (1985). *J. Appl. Cryst.* **18**, 367–370]; *STRUPLO*84, a Fortran plot program for crystal structure illustrations in polyhedral representation [Fischer, R. X. (1985). *J. Appl. Cryst.* **18**, 258–262]. Notes for Authors may be found in *Acta Cryst.* (1983), A**39**, 174–186 and a checklist in *J. Appl. Cryst.* (1985), **18**, 1–2.

Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing programs. Following normal submission, a *Computer Program Abstract* will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given in *J. Appl. Cryst.* (1985), **18**, 189–190. Examples of publications in this category are: *PATMET* – program for determination of orientation and position of a known fragment in the unit cell [Wilson, C. C. & Tollin, P. (1986). *J. Appl. Cryst.* **19**, 411–412], *DREAM* – data reduction and error analysis routines for accurate single-crystal diffraction intensity measurements [Blessing, R. H. (1986). *J. Appl. Cryst.* **19**, 412].

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, BP*166, *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. (1988). **21**, 76

INRAD Forms New Optics Company

INRAD has formed a wholly owned subsidiary, **INRAD Optical Systems, Inc.**, that will specialize in the manufacture of precision optics and optical systems. Using INRAD's optical coating facility, the new company will provide finished optics for aerospace and defence applications. INRAD Optical Systems will complement and expand the parent company's present capabilities in these areas.

INRAD develops and manufactures crystals, crystal devices, and laser systems for the research, industry, and defence markets.

J. Appl. Cryst. (1988). **21**, 76

INRAD'S Autotracker II now Available with BBB Crystals

INRAD now offers its **Autotracker II system with beta barium borate** (BBB). BBB produces the second and third harmonics of dye laser outputs more efficiently than most previously available materials. It also has a broad phase-matchable range, good ultraviolet transparency, and a high damage threshold.

INRAD's Autotracker II system extends the wavelength coverage of pulsed dye lasers using nonlinear frequency mixing to allow high-resolution spectroscopy in regions not easily reached by dye lasers alone.

INRAD, 181 *Legrand Ave*, *Northvale*, *NJ* 07647, *USA*.

J. Appl. Cryst. (1988). **21**, 76

Philips 300 kV Transmission Electron Microscope

With the **transmission electron microscope CM30/STEM** Philips is completing their new generation of TEM/STEM instruments. Principal characteristics of this TEM/STEM are the 300 kV accelerating voltage, its further refined electron optics and the new operating concept – the **Microcontroller**.

The high acceleration voltage allows the investigation of specimens of greater thickness giving a deeper insight into the three-dimensional structure of the live-science or materials-science object. In high-resolution structure analysis the point resolution of 0·23 nm can be combined with local chemical analysis by X-rays or diffraction down to an area of 2 nm ∅.

The CM30/STEM is equipped with all necessary facilities to support the advanced technologies applied in fundamental and applied research. The list includes high-resolution imaging in TEM and STEM, small electron probes for local analyses in energy-dispersive X-ray spectroscopy, convergent-beam electron diffraction or electron energy loss spectroscopy.

Key to the operational concept of the CM30/STEM is the reduction of the number of control elements like knobs and buttons to the minimum of those required in a given operational condition. Control functions which vary between the different modes of operation are assigned to 'multifunction controls' while components which are standard in all modes like the focusing operation are firmly assigned to one input control. The concept ensures maximum flexibility for the experienced microscopist with highest degree of simplicity and effectiveness for the scientist using the instrument purely as tool in his activities.

Specific attention has been given to the on-line quantification of microscope data and images or diffraction patterns. An example is the facility for direct read out of lattice spacing from a diffraction pattern.

Chief component of the optical system is the patented **TWIN objective lens**, unsurpassed in its capability of providing the illumination and imaging conditions for high-resolution information.

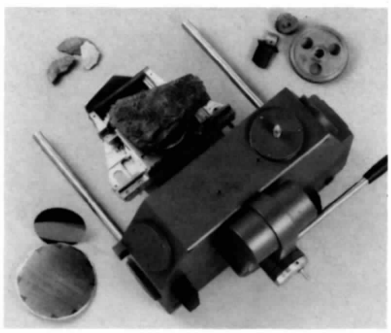
Philips Industrial and Electro-acoustic Systems Division, Building HKF, PO Box 218, 5600 *MD Eindhoven, The Netherlands.*

J. Appl. Cryst. (1988). **21**, 77

Philips Computer Control for SEM Specimen Stages

Philips has increased the extensive specimen handling capabilities of its most recent scanning electron microscopes, by offering the possibility of **controlling the motorized eucentric goniometer of the specimen stage from an external computer**. The microscopes, equipped with a specimen stage capable of handling objects larger than 200 mm (8 inches), have already found widespread acceptance in metallurgy, geology and the semiconductor industry.

The new facility uses an RS232C port for addressing and reading the coordinate memory of the specimen stage using the standard SECS protocol. Control can be performed for the standard analytical computers frequently associated with scanning electron microscopes, and control facilities can be easily incorporated into applications software for automating routines such as homogeneity analyses based on a matrix array of locations, or elemental distribution determinations across a boundary. Significant increases in efficiency and analytical throughput can be achieved for many applications.



The large sample capacity of the Philips motorized SEM stage is now enhanced by the possibility of external computer control.

Philips Industrial and Electro-acoustic Systems Division, Building HKF, PO Box 218, 5600 *MD Eindhoven, The Netherlands.*

J. Appl. Cryst. (1988). **21**, 77

Go-Faster Graphics Terminals from Chemical Design

Chemical Design is pleased to announce a new generation of high-performance raster graphics terminals for molecular modelling.

The new **S6236** and **S6266 terminals** are based on Sigmex's award-winning 6000 series displays, but incorporate customized hardware which improves their performance with Chemical Design's Chem-X molecular modelling software by an order of magnitude.

This latest development means that depth-cueing (an optical illusion giving 3D models their appearance of depth) is now controlled by hardware within the terminal rather than by the modelling software. Combined with existing 3D custom firmware for local transformations, this permits much more rapid rotation and translation of solid 3D structures on the screen.

By taking full advantage of the possibilities offered by customizing hardware and firmware for use with its Chem-X software, Chemical Design has produced devices with very impressive price/performance statistics. The S6236, for example, has a peak vector performance of 170 000 vectors s^{-1}, and costs only £17 000 ($26 000). The performance of the S6266 is equally impressive – it just has a higher screen resolution! (1448 × 1024 compared with 1024 × 724.)

The S6236 and S6266 are also included in some of Chemical Design's customized turnkey systems for molecular modelling.

Chem-X runs on VAX computers under VMS.

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

J. Appl. Cryst. (1988). **21**, 77

Low-Cost Workstations for Molecular Modelling

Very competitively priced molecular modelling workstations based on the MicroVAX 2000 and VAXstation 2000 are now available from Chemical Design. Both systems run Chemical Design's widely-used Chem-X molecular modelling software.

The new **P-GRAF 1** family of systems is based on a VAXstation 2000 CPU with 4 Mbyte memory and a 71 or 159 Mbyte disk. A complete system including a colour monitor, tailored VMS environment and the basic set of Chem-X modules is available to industrial users for less than £20 000.

P-GRAF 5 systems built around a MicroVAX 2000 are available in a variety of configurations and may be incorporated into local area clusters. The integrated high-performance raster graphics display is based on a 68020 processor, has a peak performance of 150 000 vectors s^{-1}, a pixel resolution of 1024 × 724, and can display 256 simultaneous colours from a palette of over 16 million. Depth-cueing and hidden-surface removal are hardware controlled, and the graphics system also contains firmware allowing transformation calculations to be performed locally. Industrial prices for a complete system with 4 Mbyte memory and a 71 Mbyte disk, including customized high-performance graphics display, tailored VMS environment and Chem-X, start around £36 000.

Academic users qualify for further discounts.

P-GRAF workstations provide a ready-made solution for small laboratories which require some serious modelling capability but cannot afford the larger VAX-based systems. They also provide a relatively inexpensive way of expanding existing VAX-based modelling facilities in a distributed network environment.

All Chemical Design workstations are supplied as fully integrated packages with their own built-in system management procedures and are supported by Chemical Design. They are easy to operate and are designed to be used by chemists, not computer experts.

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

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Molecules on the Menu

Computer models of chemical structures can now be generated and studied more easily, thanks to a new **menu-driven interface** to Chemical Design's powerful Chem-X molecular modelling software.

Chem-X can now be controlled entirely by picking items (not commands) from a carefully constructed series of menus using a data tablet or mouse.

The menu system is based on a tree structure, with branches and sub-branches covering different areas of Chem-X functionality. With more than 230 menus containing over 1500 items, it reaches all parts of Chem-X and allows access to more than 90% of Chem-X commands.

The menu display has been designed for maximum clarity and ease of use while keeping the screen area occupied to a minimum. Two menus are displayed simultaneously on the right-hand side of the screen, one above the other; the upper menu contains general options, such as HELP, while the lower menu changes with position in the tree. It is possible to pick an item from either menu at any time.

The new menu-driven interface is combined with ChemGuide, a knowledge-based Chem-X module intended to lead novice users towards specified modelling goals.

Experienced users may choose not to invoke the menu system – it is still possible to enter commands directly at the keyboard if desired.

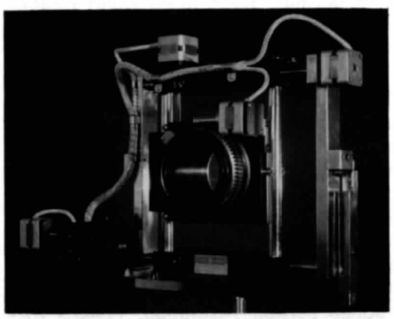
Chem-X runs on VAX computers under VMS.

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

J. Appl. Cryst. (1988). **21**, 78

Bede Scanning Stage for Double-Axis Diffractometry

Double-axis X-ray diffractometry has now become widely used for the characterization of epitaxial layers of electro-optic materials. For device manufacture, such layers have to be extremely uniform in composition and thickness across the whole wafer area. Point-by-point measurement of rocking curves provides an accurate and automatic means of determining any such variations. Bede Scientific Instruments has now introduced **scanning stages** for its **Model 150** and **300 double-axis X-ray diffractometers** whose novel design permits accurate scanning of wafers up to 50 and 75 mm diameter respectively. The stages provide stepping-motor-driven *X* and *Y* translation in the plane of the specimen, a stepping-motor-driven tilt adjustment and a manual adjustment normal to the specimen plane to accommodate specimens of varying thickness up to 5 mm. A full 360° stepping-motor-driven rotation of the specimen in its own plane permits measurement of substrate orientation at the arc second level, differentiation between lattice tilts and dilations, and rapid adjustment of tilt. The current IBM-compatible software already incorporates routines for driving the stages and performing various scanning sequences with automatic data collection and recording.



75 mm translation stage for the Bede Model 300 diffractometer

*Bede Scientific Instruments Ltd, Church Street, Coxhoe, Durham DH*6 4*HE, England.*

J. Appl. Cryst. (1988). **21**, 78

Spectrolab Bench Top Multichannel X-ray Diffractometer

A completely new compact **bench top XRD spectrometer** is available from Spectrolab Limited that should revolutionize X-ray diffraction spectroscopy. The spectrometer uses a curved multichannel detector instead of conventional scanning detectors and can, therefore, reduce analytical time from hours to just a few seconds.

Features of the design include: Ultrafast analytical time; Compact, only 1500 × 600 × 300 mm; IBM PC-compatible interface and software; Low prices; Vertical or horizontal geometry.

The new diffractometer will take all types of accessories including furnaces and is particularly well suited to kinetic or dynamic studies, powder diffraction, phase transitions, texture and stress analysis.

Spectrolab Limited, PO Box 25, *Newbury, Berkshire RG*16 8*BQ, England.*