Laboratory Notes


A miniature Peltier-effect goniometer-head attachment

Fraase Storm & Tuinstra (1986) have described an attachment for a single-crystal head in which the crystal is maintained anywhere in the range between 248 and 353K by means of a temperature-controlled air stream. The air passes through a labyrinth, cooled (or heated) by a ring-shaped Peltier device mounted immediately below the crystal. The advantages of the arrangement are that only thin-walled flexible tubes for air and water and electrical leads for the Peltier device carrying 9A need to be attached to the device. The labyrinth is thermally insulated by a hard form cover.

We have appreciably reduced the size of the device by making the air labyrinth in the form of a hollow rod of square cross section. Four Peltier elements are mounted between this rod and four water-cooled brass pieces. In this way the room-temperature parts are on the outside and the cooled (or heated) parts are on the inside, so that no external heat insulation is required. Consequently, the device can be made very compact (see Fig. 1), so that it can be mounted either on an XYZ head or a standard eucentric goniometer head, although in the latter case the crystal is above the centre of the arcs. The semi-angle of the blind cone subtended at the crystal is only 25° and the attachment imposes no additional restrictions to the accessible angles in the k geometry. Furthermore, by connecting the four Peltier elements (Melcor, type FC073250L) electrically in series the maximum supply current is only 1.5A.

As in the original design the crystal is mounted in a capillary tube which in turn is glued to a thin steel tube. The latter is pushed into the central hole in the nylon part at the bottom of the device. A 'perspex' tube is then inserted in the recess turned in the top of the water-cooled brass assembly to act as a guide for lowering the concentric Mylar tubes attached to nylon bushes at both ends. The tubes, made by welding from 0.04 mm foil, are sufficiently strong to allow the screw thread to be started. The tube assembly is screwed down after removing the guiding tube.

The performance of our device is very similar to that described by Fraase Storm & Tuinstra (1986).

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Reference

Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. 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 on page 189 of the June 1985 issue of the Journal (J. Appl. Cryst. 1985, 18, 189–190).


EASY-REFINE, X-ray powder diffraction refinement program.
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The crystallographic problem: EASY-REFINE refines crystal structural parameters against data obtained from integrated Bragg intensities measured by means of X-ray diffraction on powder samples. Ease of use has been one of its design features.

Method of solution: X-ray powder intensities are generated with an adaption of the LAZY-PULVERIX program (Yvon, Jeitschko & Parthé, 1977) from an initial set of atomic and crystal parameters. An adaption of the ANDEGE (Zapata, 1985) program is then used to perform multiple linear regression of the calculated against the observed integrated intensities. The parameter shifts are controlled by using the Fischer test and normalized residual plots (Draper & Smith, 1981).

Software environment: Operating system VM/CMS. Programming language Fortran IV. No overlays. Subroutine libraries: Global TXTLIB VFORTLIB.

Hardware environment: IBM 4331 model L02 Computer of the Computing Centre, University of Santiago of Chile. The program requires 750 kbytes of memory, eight bits per word. The peripherals used are virtual IBM disks and IBM 3262 printer.

Program specification: The restrictions on the complexity of the calculation are the same as for the LAZY-PULVERIX program. The program has 4000 source code lines and is written in modular form using top-down concepts. A typical run
time for 18 \((hkl)\) planes in a spinel mixed-oxide system is 20 s. The form of the input data is designed to be easy to enter.

**Documentation:** A user's manual is available giving details (1) of the program input and (2) for program modification.

**Availability:** The program, in the form of a small magnetic tape, is available on request to the authors.

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**Keywords:** X-ray powder diffraction; refinement.

**References**


**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).

Dr Michael Elder was killed in a climbing accident on 7 March 1987. Originally a New Zealander, though latterly of British nationality, he studied chemistry at Canterbury University, New Zealand and obtained the degree of PhD under the supervision of B. R. Penfold in 1967. After six years of postdoctoral peripatetics he was appointed to the UK SRC Atlas Computer Laboratory at Chilton in 1973, finally moving to the Daresbury Laboratory in 1977 where he became Head of the Applications Group in the Computing Systems and Electronics Division and eventually, in 1984, the Head of the Division. He was a member of the British Crystallographic Association and served on various Crystallography and Chemical Information committees.

O. S. Mills writes that it is rare that the death of the head of a computing service is mourned by the crystallographic community but such is the case with Mike Elder. He entered into research at the time in the late sixties when computers had transformed crystallography not only in the way that they could be utilised both to solve structures and interpret the results but also with an increasing application to the study of intensity data. Mike was to play an important role with the latter from the moment that he was employed by the Science Research Council and was destined to make important contributions to the handling of results stored in data banks. His first task was to plan, initiate, offer and maintain a national facility for microdensitometer measurements on scanned X-ray crystallographic films. In the course of this work he became intensively aware of the needs for high standards and accuracy in service work devoted to supplement the skills of other scientists and his dedication to this aim can be traced throughout his subsequent career. He was closely involved with IUCr activities in microdensitometer and related measurements.

Whilst at the Atlas Computer Laboratory he joined Pella Machin who by then had already started to implement, with me, Richard Feldmann’s data-retrieval system. They brought complementary skills to this project. Mike contributed much original thought to the algorithms fundamental to ensure those standards of efficiency of method necessary for a national facility whilst at the same time understanding the need for simplicity to the inexperienced user and simultaneous battery of powerful aids for the expert. It is a recognition of their contributions that the system, extended well beyond the initial crystallography data bank, is so widely used.

After a couple of years this work was transferred to the Daresbury Laboratory as was also the now enhanced microdensitometry service. The synchrotron radiation source being located there provided yet further inspiration for programs which called for his geometric ability and coding skills. In particular, effort was directed towards, and success achieved in, the large-scale acquisition of intensities by techniques which use Laue geometry. Eventually his increasing appreciation for the service element and his administrative ability were satisfied by his appointment as division head.

Mike was a man of many facets. We will be reminded of some of his scientific achievements whenever we search those data banks. He was a keen competitive sportsman to whom any ball game, whether it be croquet or squash, came seemingly naturally. He enjoyed a knowledge, both theoretical and practical, for fine wine and food and was always a gracious host. He could, however, both become exasperated and be exasperating at times, but fortunately the storm clouds which then gathered, and were deplored by his friends, usually persisted but briefly. His inventiveness and enjoyment of challenge led to him being good at such diverse entertainments as crosswords and chess whilst that of the outdoors led to that appointment on a Scottish hillside.

**Penelope Anne (Pella) Machin** died on 7 March 1987 in a climbing accident in which Michael Elder was also killed. Pella was educated at the University of Bristol, obtaining a first class honours degree in Physics, and joined Professor D. C. Phillips at the Laboratory of Molecular Biophysics, Oxford University in 1967, undertaking graduate research in protein crystallography. She joined the Science Research Council (now Science and Engineering Research Council, SERC) in 1970 working at the Atlas Computer Laboratory and moved to SERC Daresbury Laboratory in 1977 where she became Group Leader of the Applications Group of the Computing Division in 1985. Pella served as Secretary of the Working Group of the Collaborative Computing Project in protein crystallography (CCP4) from 1979 until her death. She was also a member of the British Crystallographic Association and the British Biophysical Society.

J. R. Helliwell writes that Pella’s career has been tragically ended and she has left many friends and collaborators greatly saddened by her loss. Her field was primarily computational crystallography. This inclination was evident from her earliest work. In particular her collaboration with Dr John Woodhead-Galloway, while she was in Oxford and at Atlas, led to a series of papers on the calculation of X-ray scattering from disordered systems. This work was part of an effort to understand the diffraction patterns from collagen. The methods and programs developed were taken up by research workers elsewhere, particularly in the USA and Israel. While in Oxford she was also a co-author on papers about crystal structures of hen egg white lysozyme substrate complexes.

At the Atlas Computer Laboratory she helped with the first implementation there of the XRAY suite of programs on the IBM and ICL machines which then provided a backbone to crystallographic computing for the UK Universities. She also collaborated with Mike Elder on the X-ray film data scanning service made available nationally and used by many crystallographers and fibre diffractionists. She was later to join O. S. Mills and initiate work on the provision of an on-line data-retrieval service in the days when networking and on-line working...