

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.

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## 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 collection 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

were in their infancy. They were subsequently joined by Mike Elder and together, with their high standards of accuracy, reliability and dedication to the service of the scientific community, provided the UK Interactive Chemical Databank service which now seems to be indispensable. Pella's service to the protein crystallography community was greatly appreciated and especially with respect to the Collaborative Computing Project in protein crystallography (CCP4) and its organisation.

The contribution of Pella Machin and Mike Elder was vital to the development of new X-ray diffraction methods utilising the Synchrotron Radiation Source at Daresbury. Their experience and expertise in processing Weissenberg and protein oscillation film data was readily applied to the development of processing programs for synchrotron radiation Laue diffraction films from protein and small-molecule crystals.

As well as these academic achievements, Pella was an extremely good organiser and this was most evident at the series of Daresbury Laboratory Study Weekends for CCP4, which she co-organised. Pella was a delightful person to collaborate with. She is and will be missed.

Professor **Donald T. J. Hurle**, of the Royal Signals and Radar Establishment, Malvern, England, will receive the International Crystal Growth Award, sponsored by the American Association of Crystal Growth, at the Seventh American Conference on Crystal Growth in Monterey, CA, on 15 July 1987. The award is presented triennially for 'outstanding contributions to the field of crystal growth'. It consists of a framed citation, a commemorative medal (generously contributed by the Union Carbide Corp.), and an honorarium of \$3000. Previous recipients of this award are Professor Sir Charles Frank (University of Bristol, UK), Dr Robert A. Laudise (AT&T Bell Laboratories, USA) and Professor Bruce Chalmers (Harvard University, USA).

This International Award gives recognition to Professor Hurle's many contributions to the theory and practice of crystal growth of electronic materials. In particular, as emphasized in the citation, 'he possesses the rare talent to combine major theoretical insights with the ability to test his discoveries experimentally and to see their impact on crystal growth technology'. For example, his basic calculations of fluid convection in crystal growing systems have been experimentally verified on earth and on space

missions, and they have also led to automatic control during Czochralski growth.

Professor Hurle has been with RSRE, then called the Royal Radar Establishment, since 1959. While there, he obtained a DSc in 1972 from the University of Southampton, and in 1985 he became a Deputy Chief Scientific Officer at RSRE. He has recently been appointed visiting Professor of Physics and Mathematics to the University of Bristol. His dedication to the organization of international conferences is boundless, and, as Editor of the *Journal of Crystal Growth*, he has helped propagate our ideas, methods, and results.

At the same time, in Monterey, the AACG Young Author Award will be presented to Drs **Thomas F. Kuech** and **Bernard S. Meyerson**, both of the IBM T. J. Watson Research Center in Yorktown Heights, NY. This award is presented 'for significant contributions to the field of crystal growth'. It consists of a framed citation and an honorarium of \$1000. Specifically, Drs Kuech and Meyerson will be recognized for advances in epitaxial techniques used for the production of III-V compound semiconductor and of silicon thin films. Dr Kuech obtained his PhD from the California Institute of Technology in 1981. He joined IBM that year, and he is currently the manager of the III-V Epitaxy Group. Dr Meyerson obtained his PhD from the City University of New York in 1981. He also joined IBM that year, and he is currently the manager of the Electronic Materials Group.

Professor **Otto Kratky**, Graz, Austria, has been awarded the 1987 Gregori Aminoff gold medal and prize for his development of small-angle methods for X-ray studies of the structure of macromolecules. This, the 8th such award, was presented to Professor Kratky at the Royal Swedish Academy of Sciences meeting on May 26. Previous recipients of the award are Professor P. P. Ewald (1979), Sir Charles Frank (1981), Professors C. Hägg (1982), J. M. Robertson (1983), D. Harker (1984), A. Guinier (1985) and E. F. Bertaut (1986).

Professor **Ingvar Lindqvist**, Professor of Inorganic and Physical Chemistry at the Swedish University of Agricultural Sciences, Uppsala, has been elected President of the Royal Swedish Academy of Sciences.

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