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].*

J. Appl. Cryst. (1988). **21**, 380

CRYSPLANES – description of the bounding faces of a polyhedral crystal.

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The crystallographic problem: To produce a precise description of a polyhedral crystal, specified in terms of Miller indices, for use in absorption correction [*e.g.* as input to *SHELX*76 (Sheldrick, 1976) or *ABSCOR* (Alcock, 1970*a*)].

Method of solution: For the program as written, data on the planes bounding the crystal (which may be cleavage planes or approximate faces as well as true crystal faces) are provided from measurements made under a microscope with the faces edge-on in 'eclipsed' position, following the method of Alcock (1970*b*). These measurements are made while the crystal is still mounted on the goniometer head, and the diffractometer orientation matrix is used to locate the crystallographic axes. The program could readily be adapted for data obtained through a diffractometer-mounted telescope providing φ, χ and distance from an arbitrary origin for each face.

Views are produced on the monitor and on line-printer output of the crystal as mounted on the goniometer head (for comparison with its observed appearance), and as oriented on crystal-based orthogonal axes. With these axes, equations of faces and coordinates of vertices are calculated, edges identified, and the validity of the measurements checked by application of Euler's rule. Finally, the Cartesian face equations are converted to specify the face planes as Miller indices plus the distance of the face from the arbitrary origin within the crystal. An approximation to whole-number Miller indices is calculated by normalizing relative to the smallest index obtained, provided the original value of this index exceeds 0·8 (a value that has proved relatively effective at identifying indices whose true value is zero).

Software environment: *CRYSPLANES* has been implemented under Unix. The program is written in Fortran 77, but is closely based on earlier programs in Fortran IV. It should be readily adaptable to the latter language. No overlay structure is used. Crystal drawings are produced as line-printer output and displayed as characters on a VDU, rather than by using graphics subroutines.

Hardware environment: The program is implemented on a Vax 780 computer, but should be immediately transportable to any Unix-based machine. Only minor changes should be needed for the program to run under a VMS operating system. As implemented, 32-bit words are used; 16-bit words might result in imprecision in small dimensions. Hard copy is most conveniently produced on a 132-character-wide printer, but could be adapted to 80-character width.

Program specification: 1500 lines of code; running time is small.

Documentation: This is provided in the form of test data and sample output. Input is *via* a keyboard, with prompts and full checking.

Availability: Copies may be obtained by sending a 600 ft magnetic tape to the authors (NWA), or by electronic mail (msrbb@uk.ac.warwick.cu); hard copy can also be provided.

Keywords: Crystal measurement, absorption correction.

References

Alcock, N. W. (1970*a*). *Crystallographic Computing*, edited by F. R. Ahmed, pp. 271–278. Copenhagen: Munksgaard.

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Sheldrick, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

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).

Goro Honjo 1918–1987

Goro Honjo, emeritus Professor of Physics, Tokyo Institute of Technology, passed away unexpectedly from a heart attack in his home on 29 November 1987 after a long period of ill health.

He was born on the 28 July 1918 in Hyogo prefecture and educated at the University of Tokyo where he graduated with BSc in Physics. From 1942 to 1945 he served as a Navy officer. After the war he began to study diffraction crystallography in Kobayashi Institute of Physical Research in Professor Miyake's group. Soon after, he took part in the establishment of Professor Miyake's new laboratory in the Department of Physics at Tokyo Institute of Technology (TIT). His distinctive work in this early stage was the discovery of the double refraction effect in electron diffraction patterns from some powder samples, which led to his degree of Doctor of Science awarded by the University of Nagoya in 1954. In 1958 he became a full Professor of Physics at TIT.

Goro Honjo contributed to a wide range of topics in solid-state physics by establishing various new techniques in electron diffraction and electron microscopy. In particular, his development of a cooling stage in electron diffraction allowed his students to study structure of cubic ice for which he put forward the idea of a double minimum in the potential for the proton in this structure. He extended the method to analyse the structure of solid hydrogen sulfide and its phase transitions. He was also one of the first people to develop a tilting stage for an electron microscope and this led him to observations of anomalous diffuse streaks in electron diffraction patterns from various materials, such as Ge, Si, metals and some other crystals. The diffuse streaks are now well known as being similar to those found in X-ray diffraction photographs by the late Professor K. Lonsdale and are understood as being due to low-frequency transverse phonons in the crystals. The study was also extended to confirm the existence of a ferroelectric mode in $BaTiO_3$.

On the basis of his recognition of the importance of carrying out *in situ* obser-

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vations of structural changes under various conditions, he directed his students to observe the motion of domains in ferroelectric crystals under an applied electric field. When he turned his scientific interests to the study of thin films and surfaces, he also put emphasis on the importance of *in situ* observations which led him with great success to see the growth process of thin films on various crystalline substrates. In fact he pioneered the field on UHV electron microscopy and surface studies and the work he has performed in this field is undoubtedly valued as absolutely outstanding. As conveyed in a letter to Mrs Honjo from Dr C. J. Humphreys, 'his death is a great loss to our field but his life has really been one in which he pioneered and led the world in various important aspects of electron diffraction and electron microscopy'.

In his group he trained many fine young scientists who are now leading figures in the field of diffraction crystallography in Japan. He will long be remembered by his students not only for his scientific guidance but also for his openness and personal warmth.

Goro Honjo played a leading role in many scientific societies: Japanese Association of Crystal Growth and The Japanese Society of Electron Microscopy. In particular, he performed an excellent job as a former Chairman of the Commission on Electron Diffraction of the International Union of Crystallography for a period of six years and President of the Crystallographic Society of Japan. He was also for some time a member of the Japan National Committee for Crystallography.

J. HARADA

Professor **T. L. Blundell**, Head of the Department of Crystallography, Birkbeck College, University of London, has been awarded the CIBA Medal and Prize for 1987. During the past 20 years Professor Blundell has been concerned with the development of protein crystallography. Over the past decade he has been concerned with using known structures to provide a basis for the determination of tertiary structure from amino acid and DNA sequences. He is now involved, with others at Birkbeck College, in the development of a relational database of protein tertiary structure for use in protein prediction and protein engineering.

Dr **Alan Kenneth Head**, Acting Head of the Division of Material Science and Technology, CSIRO, Australia, has been elected a Fellow of the Royal Society, in recognition of his contribution to the understanding of dislocations of crystals, especially near surfaces and under conditions of crystal anisotropy. He pioneered the computer simulation of dislocation images in the electron microscope, which has led to the identification of many types of such defects in engineering materials.

Sir **Peter Hirsch**, Isaac Wolfson Professor of Metallurgy at the University of Oxford, has been awarded the 1988 Holweck Medal and Prize of The Institute of Physics and the French Physical Society. His general research interests are the electron microscopy of defects in crystalline solids, and the relation between structural defects and physical properties of materials. Currently he has been working with Dr S. G. Roberts on a theory to explain quantitatively the ductile–brittle transition of intrinsically brittle materials. He is also concerned with developing an understanding of the plastic deformation processes which occur in an indentation in single crystals, and the mechanisms responsible for hardness anisotropy. Other interests include the effect of doping on mechanical properties of covalently bonded solids, and the observation of dislocations at surfaces by diffraction channelling contrast in a scanning electron microscope.

Dr **P. Horn**, Acting Director of the Physics Sciences Department, IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, NY, USA, and Professor **R. Birgeneau**, Cecil and Ida Green Professor of Physics at the Department of Physics, MIT, Cambridge, MA, USA, are the joint recipients of the 1988 Bertram Eugene Warren Diffraction Physics Award in recognition of their many contributions in the field of solid-state physics including studies of surface physics, inhomogeneous superconductivity, organic conductivity and charge-density-wave phenomena, magnetic critical phenomena, the structure of quasicrystals and high-temperature superconductivity.

Professor **G. A. Jeffrey**, Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260, USA, will receive the Martin J. Buerger Award in recognition of his outstanding crystallographic studies of clathrates and carbohydrates by the use of both X-ray and neutron diffraction techniques and the many contributions he has made to the crystallographic community.

Dr **Alan Lindsay Mackay**, Reader in Crystallography at Birkbeck College, London, England, has been elected a Fellow of the Royal Society, in recognition of his contributions to crystallography. He correctly predicted the occurrence of fivefold symmetry in nature, and is a leading authority on the geometry and symmetry of crystalline and quasicrystalline materials.

Professor **John Wickham Steeds**, Professor of Physics at the University of Bristol, England, has been elected a Fellow of the Royal Society, in recognition of his wide-ranging investigations of the microstructure of materials by means of electron microscopy and convergent-beam electron diffraction. His work on dislocation arrangements, solitons and precipitates has had significant applications to steels and other materials.

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)

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Synchrotron Radiation News

A new magazine with this title has just been published by Gordon and Breach. Volume 1, which will comprise six bimonthly issues, is being distributed free of charge to over 5000 synchrotron users worldwide. The editorial to the first issue states that the backbone of the coverage will be provided by correspondents at each facility who will report regularly on local developments. In addition, issues will include articles ranging from teaching and historical articles to conference reports, book reviews, a calendar of events, and a letters and comments section.

Sample copies of Volume 1 and subscription details for Volume 2 may be obtained from the Editorial Office, Gordon and Breach Science Publishers SA, PO Box 401, 2130 AK Hoofddorp, The Netherlands.

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Computer program for calculation of interface structures

A computer program is now available for calculation of interface structures, based upon methods contained in the book by W. Bollman: *Crystal Lattices, Interfaces, Matrices*. The book was reviewed in *J. Appl. Cryst.* (1984), **17**, 123–124 and is an introduction to the mathematical methods for dealing with practical problems in crystallography, especially the structure of interfaces in crystals. The author has now released a set of computer programs, written in Basic for the