Laboratory Note

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An inexpensive structure-model digitizing device

A simple system is described which transfers information contained in photographical reproductions of structure models into the digital form necessary for further computer evaluation.

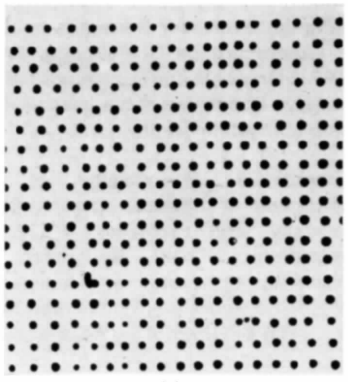
The model structure to be digitized is reproduced on photographic film to give a black-and-white transparent positive measuring approximately 60 × 60 mm. This film is fastened to the faceplate of an ordinary laboratory oscilloscope set to *x*–*y* deflection mode. The scope inputs are driven by two digital-to-analog converters which are part of a display controller in a PDP-15 digital computer system. By suitable programming, pairs of digital words move the light spot of the scope to distinct positions, thus enabling a raster scanning of the model structure. A lightproof housing fastened to the scope carries a photomultiplier, the photocathode of 14 mm diameter being approximately 150 mm from the screen.

The output voltage of the multiplier, determined by the amount of light passing through the film at this light spot position, is amplified, converted into a binary signal, fed back to the computer and stored in a core or disc memory array which may be output on punched cards or magnetic tape for further evaluation on a computer with sufficiently large computing capability. Alternatively the system can be built as a very simple and low-cost stand-alone system invoking a microprocessor for raster control and a cassette tape deck for data storage. The resolution of our system is determined by the following parameters: light spot size, distance between the fluorescent screen and the photographic emulsion (given mainly by the faceplate thickness), distance between screen and photocathode and multiplier window diameter. If compared with very expensive flying-spot scanning systems with optical imaging the resolution is low, but due to the limited capacity of the computer used for the Fourier calculations on the stored data there exists a heavy restriction on the useful size of the array.

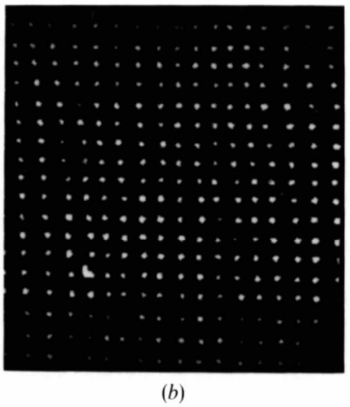
In our case the instrument is used especially as an input device for a program which calculates the scattering curves of medium resolution models mainly for comparison with small-angle scattering data (Labischinski & Bradaczek, 1977). The maximum array size was 64 by 64 raster points (leading to about a quarter of a million raster points in the three-dimensional case) which called for an overall resolution capability of the system of better than 1·0 mm. This was easily attained with a spot of approximately 0·5 mm diameter using a Tektronix Type 502 laboratory oscilloscope and the dimensions of the apparatus given above. The maximum resolution of the system would allow a raster of approximately 150 × 150 points.

For checking the quality of the digitizing process, a Tektronix graphics display was connected to the computer system to output the array contents immediately after scanning.

The system described above allows only the digitizing of two-dimensional pictures. In many cases this is sufficient, as *e.g.* for oriented structures. Fig. 1 gives an example of a paracrystalline structure model (Hosemann & Bagchi, 1962). The computer input of three-dimensional models can be done in two ways. One uses a set of two-dimensional cross-sections which are scanned one by one. In most cases this calls for a large amount of work in supplying all the drawings needed. A much better way for getting the necessary information is by the use of a small number of views of the model from different viewing angles. Normally three views (for convenience orthogonal ones) are sufficient for generating a model in the computer.



(*a*)



(*b*)

Fig. 1. Two-dimensional paracrystalline lattice consisting of about 400 lattice points. (*a*) Reproduction to be scanned, (*b*) array content after scanning as output on the display screen.

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Hosemann, R. & Bagchi, S. N. (1962). *Direct Analysis of Diffraction by Matter*. Amsterdam: North-Holland.

Labischinski, H. & Bradaczek, H. (1977). *J. Appl. Cryst.* **10**, 363–364.

International Union of Crystallography

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Commission on Journals Decisions taken at meetings in Warsaw, August 1978

The attention of authors planning to submit papers to *Acta Crystallographica* or *Journal of Applied Crystallography* is drawn to the following actions taken by the Commission on Journals at meetings held in Warsaw, 1–3 August 1978.

Estimated Standard Deviations

All measured or derived quantities which are of importance either to the conclusions or understanding of the paper, or to use by others, are required to be accompanied by their estimated standard deviations. The value of such quantities without estimated standard deviations is regarded as being sufficiently ill-defined as not to warrant publication.

International Symbols for Units

The system of units known as SI is to be used, except that the ångström (symbol Å, defined as 10^{-10} m) is preferred to the nanometer (nm) or picometer (pm).

When there is good reason for using other units (for example, when a dimension is determined by a standard machine tool or commercial practice) the SI equivalent should follow in parentheses [see *Notes for Authors. Acta Cryst.* (1978), **A34**, 143–157]. A useful publication on the SI system is *A Guide to International Recommendations on Names and Symbols for Quantities and on the Units of Measurement* (1975) by D. Armstrong Lowe (Geneva: World Heath Organization).

Structural Data

Routine checking of papers containing structural data, for consistency between the atomic coordinates and lattice constants and the quoted bond lengths, bond angles and torsion angles, is now being introduced by all Co-editors. Since the detection of inconsistency will result in a paper being returned to its authors, care should be taken to ensure that the final tables and results presented in the manuscript correspond accurately to the primary data.

Anisotropic Thermal Parameters

Anisotropic thermal parameters are to be published only if the table of values is very short, or they are necessary for understanding the paper, or they possess unusual features or cast doubt on the structure but do not lead to rejection of the paper. In all other cases, the table of values is to be deposited: a brief discussion of deposited values should instead be presented, including the maximum and minimum values found and the presence of any nonpositive-definite coefficients determined. In addition, the equivalent values of the Debye–Waller factor should be given for publishing with the list of atomic coordinates.

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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Request for donations of publications and geological specimens

On 18 March 1978 a fire destroyed a large part of the University of Lisbon, namely the building where the Faculty of Science and the Natural History Museum were located. The Mineralogical and Geological Museums were almost completely destroyed, together with all records and specimens, as was the Library belonging to the Geological Society of Portugal, entrusted to the Department, and all its books, maps, *etc.* were lost in the fire.

Under these circumstances, teaching and research activities are almost impossible, and the Department is making an appeal for international assistance, requesting donations of books, magazines and geological specimens (including minerals, rocks and fossils).

Offers of assistance should be sent to Professor C. A. de Matos Alves, Head of the Department of Mineralogy and Geology, Faculty of Science, University of Lisbon, Lisbon, Portugal.

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).

Professor **E. F. Bertaut** has been elected to the Académie des Sciences de l'Institut de France. Professor Bertaut is head of the Laboratoire de Cristallographie de CNRS in Grenoble and is a member of the Executive Committee of the International Union of Crystallography.

Professor **J. M. Cowley**, of the Department of Physics, Arizona State University, and Professor **D. W. J. Cruickshank**, of the Department of Chemistry, University of Manchester Institute of Science and Technology, have been elected Fellows of the Royal Society.

Dr **Jenny P. Glusker**, a member of the Department of Molecular Structure of the Institute for Cancer Research at Philadelphia, Pennsylvania, and Research Associate Professor of Physical Biochemistry at the University of Pennsylvania, has been awarded the Garvan Medal of the American Chemical Society. Dr Glusker also received the Philadelphia Section Award in October 1978. She is currently President of the American Crystallographic Association.

Professor **James A. Ibers**, Professor of Chemistry at Northwestern University, Evanston, Illinois, has been awarded the American Chemical Society Award in Inorganic Chemistry.

Professor **George A. Jeffrey**, Chairman of the Department of Crystallography at the University of Pittsburgh, Pennsylvania, received the Pittsburgh Section Award of the American Chemical Society in December 1978.

At the time of his death on 23 August 1978 Professor **Sergio Quareni** was only 49 years of age. It is a great sorrow to see a scientist pass away at the height of his career. For the last two years, he had been in and out of hospital. But, during the brief moments when he returned to the Laboratory, he still found the strength to work and teach.

Sergio Quareni was Professor of Mineralogy at the University of Padova (Italy). His scientific interests had always been directed towards crystallography. His contributions to the study of feldspars were outstanding. So too was his attitude towards perfecting equipment – particularly high-temperature apparatus for Weissenberg and precession cameras – which permitted him to carry out his experiments.

For many years, he was the Treasurer of the Italian Crystallographic Association.

Clearly, it is impossible to do justice to a scientist like Professor Quareni in such a limited space. But, above all, his warm humanity towards his students and colleagues will be remembered; also his attachment to his family. These great gifts of his, together with his scientific talents, will be greatly missed.

Professor **Harold W. Wyckoff**, of the Department of Molecular Biophysics and Biochemistry, Yale University, has been elected Vice-President of the American Crystallographic Association for 1979 and will become President in 1980. Dr **K. Ann Kerr**, of the Department of Chemistry and Physics, University of Calgary, has been elected Secretary, and Professor **Charles N. Caughlan**, of the Department of Chemistry, Montana State University, continues as Treasurer.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Multicomponent alloy constitution bibliography. By *Alan Prince*. Pp. xxxviii + 1105. London: The Metals Society, 1978. Price £30.00, $90.00.

Since *The Constitutional Diagrams for Alloys: A Bibliography* (J. L. Haughton &