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DECA-ZONAX: a program for indexing zone-axis patterns of decagonal quasicrystals

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The crystallographic problem: When doing electron diffraction on decagonal quasicrystals one often faces the problem of having to identify the indices of a given zone axis. This is rather difficult, since the zone axes in the decagonal quasicrystals are not at discrete positions but are spread all along the twofold directions. This is because the reciprocal vectors that are parallel to each other in a crystal or icosahedral quasicrystal are not so in the decagonal quasicrystal. The pseudo-fivefold zone axis, for example, consists of more than one zone axis close to each other. Furthermore the choice of lattice constants for quasicrystal lattices is ambiguous, thus making a standardization of the indexing procedures more difficult. A method for identifying important zone axes for several decagonal phases with varying periodicities along their tenfold axes was proposed recently (Singh & Ranganathan, 1996*a*,*b*, 1997). This method uses five coplanar reciprocal vectors and a sixth one perpendicular to them for the indexing. *DECA-ZONAX* is meant as a suite to the papers by Singh and Ranganathan, in order to provide the interested reader with the means to use this method for analyzing electron diffraction patterns (or Kikuchi patterns). *DECA-ZONAX* is intended to promote the use of indices instead of labels, in order to facilitate the exchange of data between the different scientists working in this field.

Method of solution: For finding the indices of a zone axis, a defined area of the stereogram is chosen, which is formed by the tenfold axis *A* [000001] and the twofold axes *G* [−110000] and *H* [0000−10]. The indices found in this way could be applied to other areas of the stereogram by simple permutation rules. Since they would be equivalent, only the indices derived from the specified region are displayed. *DECA-ZONAX* draws the traces of reciprocal vectors (selected by the user) on the stereogram, using spherical trigonometric formulae. The positions of the zone axes created by these vectors with the twofold vectors together with their indices are written into an output file. An on-screen indexing is possible by using the mouse to click at any zone-axis pole. For some zone axes, the program may suggest several possible sets of indices corresponding to varying degrees of accuracy (due to the inflation/deflation property in the quasiperiodic plane). Since the angular position of a zone axis obtained from the indices is compared to the angular values obtained by spherical trigonometry calculations, the resulting difference (delta) serves as indicator for the accuracy of the proposed set of indices. The indices chosen for a particular axis should be consistent with those of the others, as proposed by Singh & Ranganathan (1996*a*,*b*).

Program specification: An integrated input file editor allows one to create input data for different phases and different choices of traces with a few mouse clicks. The traces of up to nine reciprocal vectors can be drawn in one diagram, whereby different colors may be assigned to each trace. A PostScript (PS) (Adobe Systems Incorporated, 1986) file is automatically generated with the zone axis pattern for the chosen section of the stereogram. This 18° section is displayed with doubled *y* coordinates, thus turning it into a 36° pie-slice in order to make the pattern more easily accessible. This is done both on-screen and for the PS graphics. Furthermore the program features a simple ASCII-file viewer, which allows the user to check the generated output file without quitting the program.

Documentation: Instructions are given in a read.me file and in an on-screen help file. On-screen figures explain schematically the specified region of the stereogram as well as the components of a given reciprocal vector $V(Q,P)$. Four example input files are provided, which reproduce the patterns given in Fig. 3 of Singh & Ranganathan (1996*b*).

Software environment: The source code is written in Turbo Pascal 7.0 for the DOS real mode. The program offers a user-friendly graphical user interface (GUI), which is fully mouse-controlled.

Hardware environment: The program runs on IBM-compatible PC-ATs under MSDOS 6.0 and higher or in a DOS window of Windows95. The program uses standard VGA graphics and an IBM-compatible mouse.

Availability: *DECA-ZONAX* can be obtained in form of a self-extracting archive by anonymous ftp from ftp.nirim.go.jp/pub/education/dos/zonax/zonax!.exe (67 Kbytes) or by downloading from the author's homepage at http://www.nirim.go.jp/~weber/.

Keywords: decagonal quasicrystal; zone-axis patterns; PostScript; GUI.

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Notes and News

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The **International Centre for Diffraction Data** announces the following Officers and Directors for 1998: Chairman – Robert L. Snyder; Vice Chairman – R. A. Young; Treasurer – Julian Messick; General Manager – Ron Jenkins; Chairman, Technical Committee – Camden R. Hubbard; Members-at-Large, Board of Directors – James A. Kaduk, Brian H. O'Connor, Jeffrey E. Post, Charles T. Prewitt, David F. Rendle.

Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

J. Appl. Cryst. (1998). **31**, 828

Inorganic materials, 2nd ed. Edited by D. W. BRUCE and M. O'HARE. Pp. xvi + 593. Chichester: John Wiley & Sons Ltd, 1997. Price £29.95, US $55.00 (paper). ISBN 0 471 96036 5. The first edition of this book was reviewed in this journal by B. A. Averill [*J. Appl. Cryst.* (1993). **26**, 625–626]. In this second edition 'six chapters have been substantially revised or updated, while another contains updated reference material'.