Method of solution: For conventional crystal systems, the reciprocal-lattice matrices are set up from the unit-cell parameters. For the quasicrystal systems, the corresponding user-defined matrices (rank 5 or 6) are read in from a matrix data file. A loop then generates possible Miller indices and maps the corresponding reflection lines on a stereographic hemisphere. It is also possible to specify a list of desired reflections. The overall distribution can be viewed by choosing the whole range of the hemisphere. After finding an area of interest, one can zoom in on that particular area of the pattern. The reflections may be indexed by a mouse click. Unidentified reflections from the experiment can be searched for. Lattice parameters can be changed interactively, in order to view the resulting change in the pattern.

Software environment: The source code is written in Turbo Pascal 7.0. The executable file is compiled for the protected DOS mode. The program offers a user-friendly graphical user interface (GUI) that is fully mouse-controlled.

Hardware environment: The program runs on IBM-compatible PCs under MSDOS 6.0 and higher. The program uses VGA graphics and an IBM-compatible mouse. Output is in the form of PostScript files, which then can be sent to a PostScript printer or viewed with the public-domain software *GhostScript*.

Program specification: For conventional crystals, it is possible to specify the space group, in order to ensure that the extinction rules are obeyed. Since the reflections are plotted in a stereographic projection, all lines appear as circles on a hemisphere. For small wavelengths and a small angle range, these circles become almost straight lines. This is especially the case for channeling and Kikuchi patterns. The program was modified to use line-drawing routines instead of circle routines for these cases, in order to avoid errors. Among other things, *KOQUA*2.0 can be used to identify Kikuchi patterns from icosahedral quasicrystal phases. One may specify a maximum internal space component of the possible wave vectors, in order to allow only strong reflections. This criterion allows one to keep the number of reflections within a reasonable range. The program furthermore features a built-in input-file editor and a data-file viewer. It is also possible to simulate Laue diffraction patterns for the transmission and back-reflection modes; however, without intensity calculation. Also here the reflections are indexable by a mouse-click.

Documentation: A manual is provided in form of a MS-Word document as well as in PostScript format.

Availability: *KOQUA*2.0 can be obtained by anonymous FTP from ftp.nirim.go.jp/pub/education/dos/kossel/koqua2.exe or by downloading from the author's homepage at http://www.nirim.go.jp/~weber/.

Keywords: Kossel patterns, channeling patterns, Kikuchi patterns, PostScript output, graphical user interface

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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 Co-editors, should be sent to The Executive Secretary, 2 Abbey Square, Chester CH1 2HU, England.

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Peder Kierkegaard 1928–1996

Professor Peder Kierkegaard, Swedish crystallographer and chemist, was born in 1928 and suddenly passed away on 29 January 1996. He spent his entire academic career at Stockholm University where he obtained his PhD in 1955. In 1962 he obtained his DSc and was appointed Assistant Professor of Inorganic and Physical Chemistry. In 1970 he became the first holder of the newly established chair of structural chemistry. He remained in that position until his emeritus retirement in 1994.

Research at the Laboratory of General and Inorganic Chemistry at the University had, since the pioneering work by Arne Westgren in the 1920s, been directed towards X-ray crystallographic studies of alloys and inorganic compounds. For his DSc thesis he chose a field not previously treated at the Laboratory, *viz.* transition metal oxide phosphates. That this was a wise choice was very clearly demonstrated by his excellent thesis in 1962. Among several subsequent papers in the field is the much quoted article on the structure of a sodium zirconium phosphate, known to everybody interested in solid electrolytes as the Nasicon structure.

Over the years Kierkegaard retained an interest in metal phosphates and similar inorganic compounds but his scientific curiosity soon drove him to explore other fields of structural chemistry. Thus, with young co-workers, studies were undertaken of metal complexes, organic molecules and substances of biochemical interest. X-ray diffraction studies were also made of glasses and liquids. In research on equilibria in solutions the diffraction studies were complemented with potentiometric measurements. New apparatus was developed and constructed for collecting accurate diffraction data for non-crystalline specimens.

In the late 1960s Kierkegaard and his co-workers took an active part in an international collaboration involving systematic studies of a series of flavin derivatives with the aim to provide detailed structural information on the reactions of flavoenzymes. Other areas of study included structural characterization of sugar derivatives and investigations of molecular complexes of host–guest type.

Over the years a large number of students and co-workers gathered around Kierkegaard. He was generous with ideas and advice. He put indefatigable effort into acquiring modern high-standard research facilities for his staff. He was successful in transmitting his enthusiasm for research and created a very positive collaborative atmosphere in the laboratory.

Kierkegaard possessed exceptional organizing skills which he used in the service of the University at many posts including its board of directors. He was active for the Royal Swedish Academy of Sciences, of which he became a member in 1982, and for the National Committee for Crystallography . He was an organizer of several international conferences. Since 1987 he had served as secretary of the Nobel Committee for Chemistry. The day before his death he was at his office at the Academy recording nomination letters for the 1996 Nobel Prize.

Openness and naturalness were genuine with Kierkegaard. He treated everybody alike. He was a strong leader, but one who preferred to lead by cooperation. He loved to solve problems over daily morning coffee at the laboratory. He had an unusual talent for friendship and will be missed and remembered by many.

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A. MAGNELI