Simulated Weissenberg Photograph

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We have written a program WEISS which generates simulated Weissenberg photographs. The pictures are fullsize,representing a crystal rotation of 270° for a camera of diameter 57.13 mm. Despite the increased availability of diffractometers there are many laboratories where crystal structures are still determined by photographic methods. In the United Kingdom the Science and Engineering Research Council provide a microdensitomer service [1] which measures intensities from Weissenberg photographs and returns the data on magnetic tape ready for input to the SHELEX 76 family of crystallographic computer programs [2]. We have found that the simulations useful in indexing films for this service, in unitcell measurement and in teaching.

With unitcells of orthorhombic or higher symmetry it is a simple matter to measure the unitcell and index the spots of a Weissenberg photograph. However with low symmetry lattices it can be very difficult to index upper-level photographs. Fig.1 shows the simulations for the layer hk0 and hk9 for a triclinic unitcell. The pseudo-axial nows ho9 and ok9 are not obvious on the hk9 film and could be found only with difficulty. This problem is entirely removed by superimposing the film on the simulation.

The program can also be used to complete sets of cell dimensions for example, where the β angle of a monoclinic crystal is inaccessible*.β makes no contribution to the hkO Weissenberg but is involved in the equations for the spot positions on upper level photographs. If the photograph of, say, 3kl is compared with simulations calculated for various values of β, the best fit can be found with a precision of 0.5° in β. We have found that this value is within 1.0° of that eventually refined by least-squares analysis during microdensitometery; quite accurate enough as an initial estimate. Both precision

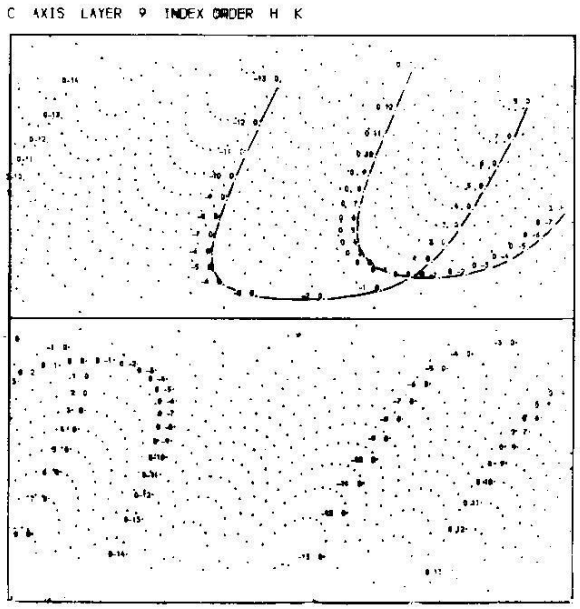

Fig.1 Simulated Weissenberg photographs for the layers hk0 and hk9 for a triclinic unitcell with a = 12.71, b = 15.91, c = 10.07 A, α = 96.50, β = 103.47 and γ = 72.54°, for CuKα radiation.

* For instance a monoclinic crystal which is air sensitive and thus must be mounted in a Lindemann glass capillary, where the crystal is needle shaped with a as the needle axis, so that it is not practicable to mount a crystal on the b axis. The other common case is the triclinic crystal where only two axes are accessible.

and accuracy could be improved by replacing the "ideal"radius of the Weissenberg camera in the calculation by the measured effective radius of a given camera loaded with a particular number of sheets of a specified film but,since we use several cameras and a variety of loading patterns, it is more convenient to use only the standard radius.

The simulations are also useful in teaching. Genuine Weissenberg photographs are difficult for beginners because of variations of background intensity, because of the fall in average intensity of the spots with increasing and because of white radiation streaks and other artifacts. All of these distractors are enhanced in printing or photocopying the original for class use, but do not occur in the simulations.

The program WEISS uses equations from Buerger [3]. It is written in FORTRAN (160 statements)and implemented on the Dundee University DEC 10 computer using the plotting post-processor GHOST. Copies of the program are available from the authors.

References

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