Short Communications

Contributions intended for publication under this heading should not exceed 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.


Strategies for collecting screen-less oscillation data. By SANJEEV K. MUNSHI and MATHUR R. N. MURTHY, Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012, India

(Received 15 May 1985; accepted 9 September 1985)

Abstract

Screen-less oscillation photography is the method of choice for recording three-dimensional X-ray diffraction data for crystals of biological macromolecules. The geometry of an oscillation camera is extremely simple. However, the manner in which the reciprocal lattice is recorded in any experiment is fairly complex. This depends on the Laue symmetry of the reciprocal lattice, the lattice type, the orientation of the crystal on the camera and to a lesser extent on the unit-cell dimensions. Exploring the relative efficiency of collecting X-ray diffraction data for different crystal orientations prior to data collection might lead to strategies that reduce the number of films required to record most of the unique data and the consequent amount of time required for processing these films. Here algorithms are presented suitable for this purpose and results are reported for the 11 Laue groups, different lattice types and crystal orientations often employed in data collection.

The screen-less oscillation method of recording X-ray diffraction data is widely used for collecting data from crystals of biological macromolecules (Arndt & Wonacott, 1977). Three different sets of computer programs have been described and extensively used for processing screen-less oscillation films (Nyborg & Wonacott, 1977; Schwager, Bartels & Jones, 1975; Rossmann, 1979). A program suitable for somewhat smaller unit-cell dimensions has been described by Schmidt et al. (1983). It has been realized that exploring the relative merits of different schemes of data collection might lead to strategies that reduce the number of films required to record an asymmetric unit and hence the subsequent reduction in the computer time required for processing and scaling these films (Schutt & Winkler, 1977; Arnold et al., 1984).

Such a scheme might be devised if the following information is available: (a) unique and total reflections in arbitrary oscillation intervals; (b) the total oscillation required to record an asymmetric unit of reciprocal space; and (c) the maximum permissible interval that avoids overlap of reflections on the film. The latter information depends on the Bravais lattice and the crystal orientation, while the former two depend on crystal orientation and Laue group. All three, however, will also depend on the cell parameters. Efficient algorithms are presented in this paper to obtain these data. Model calculations were carried out for idealized cells in 11 Laue groups, different lattice types and corresponding to certain crystal orientations often used by crystallographers.

The definitions of axial directions and notations used here are identical to those used by Rossmann (1979).

Using the symmetry operators of the Laue group, the reflections corresponding to an asymmetric unit are generated and stored. Bins are set up and initialized to zero corresponding to oscillation ranges nθl to mθl, where n and m are arbitrary integers and θ is a user-specified interval. Reflections from the stored list are analysed sequentially. For each reflection, the indices of other reflections related by Laue symmetry are generated. The Miller indices are transformed to reciprocal coordinates in Å⁻¹ by multiplication with the crystal orientation matrix (Rossmann, 1979). Denoting the reciprocal coordinates by x, y, z, the point x', y', z' at which it intersects the Ewald sphere is given by

\[
y' = y \\
x' = \pm \frac{d^2}{2} \\
z' = -\frac{\lambda d^2}{2}.
\]

The two values of x' correspond to entry and exit of the reciprocal-lattice point. The rotation angle at which the reciprocal-lattice point intersects the Ewald sphere is then obtained from

\[
\cos \theta = \frac{(xx' + zz')}{(x^2 + z^2)} \\
\sin \theta = \frac{(xx' - zz')}{(x^2 + z^2)}.
\]

The independent and total reflections recorded in the bins corresponding to these θ values are suitably incremented. After exhaustive analysis of the stored list, the percentage of unique reflections in each bin is computed and printed out.

The maximum size of oscillation angle that is possible without overlaps depends on the mosaicity of the crystal, beam divergence, lattice type, resolution required and cell dimensions. In order to examine this, the film coordinates X, Y (Rossmann, 1979) and the oscillation angle θ at which reciprocal-lattice points enter or exit the Ewald sphere are computed. X, Y and θ are packed into a single computer word and sorted on X. The reflections corresponding to any desired oscillation interval are selected from this list. The new shorter list is examined if two reflections occur within the distance used for overlap test (0.6 mm at a crystal-to-film distance of 60 mm).

The results of analysis for the 11 Laue groups and certain standard orientations are recorded in Table 1. In each case, the reciprocal cell edge was set to 0.02 Å⁻¹ and reciprocal angles to 90° except for trigonal and hexagonal groups.
oscillation ranges in the 11 Laue groups about certain crystal axis midway between any two twofold axes offers maximal choice of the non-unique axis about which the crystal is oscillated (Table 2). In tetragonal rotation about an axis is far more efficient and required for recording all unique data. In monoclinic groups, rotation about a non-unique axis is far more efficient and requires 90° rotation in contrast to the unique axis where the situation is triclinic. In centred monoclinic cells, the size of the maximum interval that avoids overlap depends on the choice of the non-unique axis about which the crystal is oscillated (Table 2). In orthorhombic, rotation about an axis midway between any two twofold axes offers maximal advantage. In tetragonal 4/m, but not in 4/m2/m2/m, it is advantageous to avoid the use of the unique axis for crystal

where it is 60°. Calculations included reflection between 5 and 50 Å. The maximum value of the oscillation interval that does not result in overlap of reflections depends on crystal orientation and to an extent on spindle setting. The average sizes of the intervals for different crystal orientations and lattice types of the model cell for a resolution of 3 Å are shown in Table 2. The variation of this angle with spindle setting is minimal for primitive cells and larger for centred cells (data not shown). Also, larger oscillation intervals are shown in Table 2. The variation of this angle with spindle setting is also large for the former two directions.

The most important conclusions of the present analysis are the following. In the triclinic system, 180° oscillation is permissible when the [110] or [111] directions are set along the spindle when compared to [010]. However, variation of this interval with spindle setting is minimal for primitive cells and larger for centred cells.

This work was supported by the Department of Science and Technology (India). We thank the referees for their constructive criticism.

### References


