Diffractometer detector aperture system with independently controlled jaws

Recently I have drawn attention to the presence of a significant error source in the conventional procedure for the measurement of X-ray integrated intensity from a small single crystal (Mathieson, 1982) and have subsequently suggested (Mathieson, 1983) a modification by which this error source can be eliminated when using a standard scintillation detector. The modified procedure involves no greater expenditure of time than the conventional procedure once the main parameters of the experiment are determined (Mathieson, 1984).

To put this improved procedure into practice requires an aperture system in front of the detector consisting of two jaws, each being capable of independent adjustment so that both the width of the aperture and its relative position can be varied during the measurement of a single reflection. With this arrangement, it is possible to integrate within a designated \( \Delta \theta, \Delta 2\theta \) domain. To carry out this function, the jaw positions have to be accurately and reliably reproducible and must be capable of being established in angular units which match those of the crystal specimen displacement units, \( \Delta \theta \) (usually 001 or 0005). In the device which has been built for this purpose, a direct drive has been used, each jaw being displaced by a screw (from a micrometer) which is fixed effectively directly to the shaft of a stepping motor. The locations of the two jaws are set from the computer control, the aperture settings being adjusted with each step in \( \Delta \theta \) during the measurement of each reflection — in order to follow the appropriate boundary in \( \Delta \theta, \Delta 2\theta \) space (see Mathieson, 1983 for terminology). Fig. 1(a) shows the structure of the device which is to be mounted in front of the detector on the rail of the detector arm of the diffractometer. In Fig. 1(b) is shown the aperture as viewed from the specimen.

The approximate match of jaw step \( (\Delta 2\theta) \) to the specimen crystal step \( (\Delta \theta) \) is determined at the design stage by selecting the pitch of the micrometer thread and the number of steps of the motor for a complete cycle. Fine tuning is by adjustment of the distance of the unit from the diffractometer centre along the detector rail.

While the device shown here was designed for use with X-rays to follow the outline of a six-sided figure, corresponding to the ranges of mosaic spread, source size and wavelength distribution (see Mathieson, 1983), it can be programmed to follow, to a close approximation, the boundary of an area of virtually any shape in \( \Delta \theta, \Delta 2\theta \) space, e.g. an ellipsoid. A device of this type is therefore applicable in neutron diffractometry.

It should be noted that this procedure does not of course have the resolution capabilities nor does it yield the information content associated with point-by-point determination of intensity in \( \Delta \theta, \Delta 2\theta \) space feasible with a fine slit (or a linear position-sensitive detector) as outlined by Mathieson (1982).

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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 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 I. Nitta, Emeritus Professor at Osaka University, Japan, died on 16 January. Professor Nitta was a Member of the Japan Academy of Science and a former Vice-President of the International Union of Crystallography. A full obituary will be published in Acta Crystallographica, Section A.

International Union of Crystallography


Acta Crystallographica

Journal of Applied Crystallography

Appreciation of Co-editors’ Service

The Co-editors of Acta Crystallographica and the Journal of Applied Crystallography serve the crystallographic community with great devotion and distinction, and it is appropriate that the Executive Committee of the Union records its sincere appreciation for the work of all present and past Co-editors from time to time. The Executive Committee particularly wishes to express its appreciation and gratitude, on behalf of the Union and the international crystallographic community, to Professor G. A. Jeffrey for his 10 years of outstanding service as a Co-editor of Acta Crystallographica. On his retirement as a Co-editor on 1 September 1983 Professor Jeffrey had handled nearly 1300 papers. He has been succeeded by Professor C. E. Nordman and Professor J. A. Ibers.

References

