A Stored-Image Method for Calculating Absorption Corrections

We propose here a procedure for computing absorption corrections for X-ray diffraction intensity measurements. It is based on storing an image of the crystal in the form of a bit pattern in a block of a computer memory which we can treat as an 'image space'. The incident and diffracted beams for selected diffracting points are traced in image space, using an algorithm to estimate their lengths.

The steps in the procedure are: (a) read the image into memory, together with the scale constant in image space (mm/div), and the linear absorption coefficient; (b) choose a reflection, and determine the direction cosines of the incident and diffracted beams in image space; (c) choose a 'diffracting point' lying within the crystal image, i.e. a bit tested and found to be unity; (d) trace the incident and diffracted beams from the diffracting point, and determine the total lengths τ_i and τ_d of each lying within the crystal image; (e) calculate the attenuation exp $[-\mu(\tau_i+\tau_d)]$ for the chosen point, and add to a running sum; (f) return to (c) until finished, then calculate the absorption correction by dividing the number of points by the sum of attenuation values.

The success of the procedure depends on the algorithm used in step (d) to estimate the length of a beam. We have found an effective compromise between speed and accuracy of interpolation in the following method: (d_1) take a unit jump along the beam to an 'absorbing point' to be tested by adding the respective beam direction cosines to the current coordinates; (d_2) take a poll of the vertices of the cell in image space surrounding the absorbing point to determine whether it lies within the crystal, and add the number of yea votes to a running total; (d_3) return to (d_1) until a boundary of image space is reached, then divide the sum of yea votes in the running total by eight to estimate the beam length.

This method is distinguished from many absorption-correction programs developed successfully heretofore in that the latter have treated the crystal shape analytically in terms of the parameters of the bounding planes. This method has been applied in several variants by BUSING and LEVY[1], BURNHAM[2], WUENSCH and PREWITT[3], ALBERTI and GOTTARDI[4] and COPPENS, DE MEULENAER and TOMPA[5]. One drawback of these methods is that re-entrant angles present a special problem requiring subdivision of the crystal into a set of convex polyhedra. In contrast, the stored-image method involves no special difficulties in handling any shape, but has a limitation in accuracy occasioned by the graininess of the image.

We have investigated the feasibility and accuracy of this procedure by writing and testing a program for the PDP-7 computer (Digital Equipment Corporation, Maynard, Massachusetts, USA, 8192 words of 18-bit length). The program operates with an image space having an $18 \times 18 \times 18$ grid (324 words of computer memory). The general flow of the program follows the logic of the WUENSCH-PREWITT program, differing primarily in using the stored-image method. Especially, we have followed WUENSCH and PREWITT in the formulas for the beam directions, for which they give a thorough discussion. To test the accuracy of the program, we used an object in the form of the image of a sphere tangent to the boundaries of image space. The values of μR and 2θ were varied, as well as the orientation of the diffraction vector with respect to the axes of image space. Since the absorption correction should be independent of orientation for a sphere, any variations with different orientations give a measure of the errors arising from graininess of the image. The Table gives some calculated values of the absorption correction, in comparison with the correct tabulated values from the *International Tables for X-ray Crystallography*[6]. Several calculated values are entered at some places in the Table for cases in which the calculation was repeated for different orientations. The results of the test suggest that the current version of the program begins to show serious errors in the vicinity of $\mu R = 1.0$. The computing time per reflection was 49 sec, comparing favorably with other programs[1].

The test shows that the procedure is quite practicable, but refinements are required if applied for general use. Two evident possible improvements come to mind. First, a finer-grained image would be quite feasible on a larger computer, and should extend the range of μR values for which the procedure is valid. Second, whereas the current program tests all possible diffracting points in image space, a Monte-Carlo procedure for choosing diffracting points[4] should speed up the program greatly, and might become quite necessary when working with a fine-grained image[7].

Zusammenfassung. Eine Methode wird entwickelt, welche die Berechnung der Absorptionskorrekturen bei Messungen von Röntgendiffraktionsintensitäten von Kristallen beliebiger Form möglich macht. Dabei wird der Strahlengang auf einer elektronischen Rechenanlage simuliert, in der das Kristallabbild als Binärmuster gespeichert ist.

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R	2θ	Correct value of the absorption correction	Calculated values
0.1	any	1.16	1.1549, 1.1422, 1.1503
0.2	0°	1.35	1.3311
0.2	90°	1.34	1.2984
0.5	0°	2.08	2.0096
0.5	90°	1.99	1.8514
1.0	0°	4.12	3.7854, 3.5032, 3.7808
1.0	90°	3.50	3.0409

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