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Absorption correction A^* for cylindrical and spherical samples with extended range and high accuracy calculated by the Thorkildsen and Larsen analytical method

Hua-Chen Hu,[a]* Chao Yang[b]* and Kai Zhao[a]

[a]China Institute of Atomic Energy, PO Box 275 (18), Beijing, 102413, People's Republic of China, and [b]Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. Correspondence e-mail: hchu3310@gmail.com, cyang@lbl.gov

Tables of the absorption correction A^* for cylindrical and spherical crystals were calculated by the Thorkildsen & Larsen [*Acta Cryst.* (1998), A**54**, 186–190] analytical method in the range of $0 \le \mu R \le 30$ and $0 \le \theta \le 90^\circ$ with accuracies of 10^{-6} for cylindrical crystals and 2.0×10^{-6} for spherical crystals. Bivariate Chebyshev polynomial fitting formulae for A^* are also provided for both cases. The maximum fitting error for spherical crystals is 6×10^{-3} and the average error ranges from 7×10^{-5} to 3×10^{-4}. All the important tables and the fitting program are provided in the supplementary material.

1. Introduction

An accurate absorption correction of the individual integrated reflection power ratio (or integrated reflectivity) is an essential step in the analysis of X-ray and neutron diffraction data for obtaining the observed structure factor and extinction factor of the sample and also for analysis of powder diffraction profiles. A table of $A^* = 1/A$ for spheres with 0.5% accuracy for $\mu R \le 5$ has been given by Weber (1969) and similar data for A^* in the range of $0 \le \mu R \le 2.5$ with 0.1% accuracy have been calculated by Dwiggins (1975*a*,*b*), Tibballs (1982) and Maslen based on the formulae (6.3.3.4) and (6.3.3.5) in Volume C of *International Tables for Crystallography* (Maslen, 2004), where μ is the linear absorption coefficient or absorption cross section per unit volume for X-rays. For neutrons, μ is the attenuation coefficient, which is composed of nuclear absorption, bound coherent and incoherent scattering cross sections per unit volume. However, for many cases, *e.g.* in the case of neutron diffraction, particularly in investigations of magnetic properties, the sample involved may contain very strong absorption (lanthanides and some other elements such as Cd, B *etc.*), while the sample size cannot be reduced much because of the neutron intensity requirement, *i.e.* the $\mu R \le 2.5$ restriction is too small. Based on this consideration and the successful solution of the Darwin equations for cylindrical crystals (Hu, 2003; Hu & Yang, 2004), several sets of precise secondary extinction factor tables with much extended μR range (up to 30) for cylindrical and spherical crystals have been constructed and prepared for publication in *Acta Crystallographica* Section A. In accordance with this, two accurate A^* tables with a comparable range of μR are recalculated by Thorkildsen & Larsen's (1998*a*,*b*) analytical method; the related polynomial fitting formulae are also provided.

2. Method

In this work, the authors first compute A for a cylinder in the range of $0 \le \mu R \le 30$ and for Bragg angles $0 \le \theta \le 90^\circ$, based on the expressions A for a cylinder (5) and (6) in Thorkildsen & Larsen (1998*b*) as expressed by the following:

$$A = \int_{\psi=0}^{2\theta} \int_{\varphi=0}^{\pi-2\theta} (2/\pi) \exp[-2\mu R \cos(\psi - \theta) \sin\varphi \sec\theta] \times \sin(\varphi + \psi) \sin(\varphi - \psi + 2\theta) / \sin 2\theta \, d\varphi \, d\psi. \quad (1)$$

The parameter A for a sphere was computed by considering the half sphere as a stack of 60000 cylindrical slices at a distance Z perpendicular to the diffraction plane from the center of the sphere with a radius $(R^2 - Z^2)^{1/2}$ (where R is the radius of the sphere), and with the same thickness and μ. The final A is then evaluated by using Simpson's formula to sum up the A's associated with different slices with different radii multiplied by its volume. The sum is then divided by the total volume. Tables I and II in the supplementary material[1] show the results for A^* for cylinders and spheres, respectively. The accuracy of the calculation is better than 10^{-6} for cylinders and better than 2.0×10^{-6} for spheres. The present result is much better than that in *International Tables* (1959) for spherical crystals in the range $0 \le \mu R \le 10$, where the error of A^* is 2% at $\mu R = 10$ compared with our 0.001% error at the same μR as an example.

[1] Supplementary material for this paper including all the tables and the fitting program is available from the IUCr electronic archives (Reference: WL5160). Services for accessing these data are described at the back of the journal.

Six regions were defined for the fitting:
(1, 1) region: $0 \le \theta \le 10^\circ$, $0 \le \mu R \le 3$;
(1, 2) region: $10 \le \theta \le 90^\circ$, $0 \le \mu R \le 3$;
(2, 1) region: $0 \le \theta \le 10^\circ$, $3 \le \mu R \le 10$;
(2, 2) region: $10 \le \theta \le 90^\circ$, $3 \le \mu R \le 10$;
(3, 1) region: $0 \le \theta \le 10^\circ$, $10 \le \mu R \le 30$;
(3, 2) region: $10 \le \theta \le 90^\circ$, $10 \le \mu R \le 30$.
Define $x = \sin\theta$ and $y = \mu R$.

A bivariate Chebyshev polynomial has been used for the fitting of $\ln A^*$ in each region:

$$\ln A_{\rm f}^*(x, y) = \sum_{i=0}^{k} \sum_{j=0}^{l} \alpha_{ij} T_i(x) T_j(y), \qquad (2)$$

where $A_{\rm f}^*$ is the fitting value of A^*, and $T_i(x)$ and $T_j(y)$ are the ith and jth degree of shifted Chebyshev polynomials that are bounded between -1 and 1 on fitting intervals.

Note that the labels k and l in equation (2) are replaced by pdegx11 and pdegy11 in the (1, 1) region of the bivariate Chebyshev polynomial fitting program in the supplementary material. Similarly, the k and l labels are also replaced by pdegx12, 21, 22 ... and pdegy12, 21, 22 ... *etc*. accordingly.

The number of data samples used for fitting is much larger than that shown in Tables I and II in the supplementary material; the fine sampling of the data greatly improves the accuracy of three-dimensional fitting and avoids the 'wiggles' appearing on the fitting curves. Thus, in the fitting tables, sampling intervals of 0.5 and 2.5° were used instead of 5° in the range $0 \le \theta \le 10^\circ$ and $10 \le \theta \le 90^\circ$, respectively.

In order to keep things consistent, we adopt the same three ranges of μR in the fitting program for extinction of cylindrical and spherical crystals prepared for publication.

The fitting error for each point is defined as $|A^*(x, y) - A_{\rm f}^*(x, y)|/A^*(x, y)$ and the average error for each region is defined as $\sum |A^*(x, y) - A_{\rm f}^*(x, y)|/\sum A^*(x, y)$ for (x, y) in the region.

The maximum fitting error for spherical crystals is 2×10^{-4} for the (1, 1) and (2, 1) regions. It is less than 1×10^{-3} for other regions. The average error ranges from 7×10^{-5} to 3×10^{-4}.

MATLAB was used for this calculation.

All the important tables and the bivariate Chebyshev polynomial fitting program are provided in the supplementary material.

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