Computer Program


A program for the evaluation of weighting functions used in small-angle X-ray scattering*. By MARY G. BUCHANAN† and ROBERT W. HENDRICKS, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, U.S.A.

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In a previous paper, Hendricks & Schmidt (1967) have derived a general equation for evaluating the slit-width and slit-length weighting functions which are necessary for correcting small-angle X-ray scattering data for the smearing effects of the collimation system. Their result, for slit widths, is

\[ W_u(u) = L_0 L_d A_u(L_0 + L_d)^{-1} \int_{x_d(u)}^{x_d(x,u)} dx \int_{z_d(x,u)}^{z_d(x,u)} dz f_w(z). \]

The limits of integration are given by

\[ z_b(x,u) = \min(z_{2i-1}; z_{2j-1}) \]
\[ z_a(x,u) = \max(z_i; z_j) \]

in which

\[ z_i = \frac{(L_0 - d_i)(L_x - x) + (-1)^i+1 (L + L_d) h_i}{L + d_i} \]
\[ z_j = \frac{(L_0 + d_j)x + (-1)^j (L + L_d) h_j}{L - d_j} \]

and

\[ x_b(u) = \min(x_{2i-1}; x_{2i-1}; w_c) \]
\[ x_a(u) = \max(x_{2i-1}; x_{2i-1}; - w_c) \]

with

\[ x_{ii} = \frac{L(d_i - d_j)u + (-1)^i h_i(L + d_i) + (-1)^{i+1} h_j(L + d_j)}{d_i - d_j} \]
\[ x_{ii} = \frac{(L_0 - d_j)(L_x - x) + (-1)^i h_i(L + d_i) + (-1)^{i+1} h_j(L + d_j)}{L + d_i} \].

The weighting function is non-zero only in the range

\[ u_{aaa} \leq u \leq u_{bbb} \]

where

\[ u_{bbb} = \min[u_{2i-1, 2j}(w_c); u_{2i-1, z}(w_c)] \]
\[ u_{aaa} = \max[u_{2i-1, 2j}(w_c); u_{2i-1, z}(w_c)] \]

and

\[ u^{ii} = \frac{x(d_i + d_j) + (-1)^{i+1} h_i(L - d_i) + (-1)^j h_j(L + d_j)}{d_i(L - d_i)}. \]

In this derivation, the variables have the following meanings: \( L \) is the distance from the sample plane to the detector plane, \( L_0 \) is the distance from the sample plane to the plane containing the X-ray focal spot, \( d_i \) is the distance from the sample plane to the \( i \)th collimation edge between the sample plane and the tube plane, \( h_i \) is the distance from the \( i \)th collimation edge to the camera axis, and \( d_i \) and \( h_i \) are similarly defined for edges between the sample plane and the detector plane (not including the slit at the detector). The width of the detector slit is \( 2w_c \), \( e_w(x) \) describes the sensitivity of the detector in a direction parallel to the slit width, \( f_w(z) \) describes the intensity of the focal spot in the direction of the slit width, and \( A_u \) is a normalization constant which ensures that the area under the weighting function is unity. [The physical significance of \( A_u \) is discussed by Hendricks (1971)]. The weighting function for slit lengths has the same form and can be evaluated from equations (1) through (5) by making the appropriate changes in notation.

The slit-width collimation correction procedures outlined by Kratky, Porod & Skala (1960) and Sauder (1966) require only knowledge of the \( k \)th moment of the weighting function about either the origin or the mean. These moments are readily computed from the relationships

\[ M_k = \int_{u_{aaa}}^{u_{bbb}} u^k W_u(u) du \]

and

\[ M_k(\bar{u}) = \int_{u_{aaa}}^{u_{bbb}} (u - \bar{u})^k W_u(u) du. \]

The practical evaluation of equations (1) and (6) is tedious except for geometries having a high degree of symmetry. However, they are ideally suited to computer evaluation. We have prepared a FORTRAN IV computer code which may be used to calculate the weighting functions and their moments for any small-angle X-ray geometry which can be constructed with slit-edges (e.g. Beeman four-slit, Rigaku-Denki or Kratky collimation systems). This code is described in detail by Buchanan & Hendricks (1970) including instructions for use, flow charts, program listings and test examples. We give here only a brief summary and a typical result.

The input to the program consists of the positions of all slit-edges and the spatial sensitivity of the focal spot and detector (if they are not uniform). The printed output consists of the input data, including the values of \( z \), \( f_w(z) \), \( x \) and \( e_w(x) \) if they are not uniform; the normalization factor; the \( u \) values and corresponding \( W_u(u) \) values; the moments...
of the function, if they were calculated; and the theoretical limit of resolution* of the collimation system under consideration. Punched output, if requested, contains only \( u \) and \( W_\theta(u) \) values. Plotting routines (for the CALCOMP mechanical plotters) are provided to produce a graphical representation of the weighting function. A typical example of a CALCOMP plot produced during the evaluation of the slit-width weighting function for a Kratky collimation system is shown in Fig. 1. The reader is referred to the original derivation (Hendricks & Schmidt, 1967) for a complete discussion of the approximations which limit the validity of the application of equation (1) and hence the usefulness of this program. Copies of our report (Buchanan & Hendricks, 1970) and a punched deck of the program may be obtained from R. W. Hendricks.

References


