International Tables for Crystallography (2006). Vol. C, Figure 6.3.3.3, p. 605.

The crystal is divided into polygons *ADC*, *AFD*, *CDE*, and *BEDF* as shown. The radiation incident on each polygon enters through one face of the crystal, and is either absorbed or emerges through another. Within each polygon, the loci of constant absorption are the straight lines dotted in Fig. 6.3.3.3. It is convenient to subdivide *BEDF* into the triangles *BEF* and *EDF*. By the derivation of an expression for the contribution of a triangular crystal to the scattering, including allowance for absorption, and with the sum taken over the component triangles *ADC*, *AFD*, *CDE*, *BEF*, and *EDF*, the correction for absorption can be calculated.

A three-dimensional crystal is divided into polyhedra, for each of which the radiation enters through one crystal face and leaves through another. Corners for the polyhedra are of five types, namely,

(1) Crystal vertex.

(2) An intersection of a ray through a lit vertex with an opposite face.

(3) An intersection of an incident ray through a lit (i) vertex with a plane of diffracted (d) rays through a lit (d) edge, and the corresponding intersection with incident and diffracted beams interchanged.

(4) An intersection of a plane of incident rays through a lit (i) edge with an opposite edge, and its equivalent.

(5) An intersection on a shaded face of planes of incident and diffracted rays through (i) and (d) edges.

For each vertex x, y, z, the sum of the path lengths to each of the crystal faces is calculated, and multiplied by the absorption coefficient μ to give the optical path length using the equation

$$\mu r_j = \mu(d_j - a_j x - b_j y - c_j z)/(a_j u + b_j v + c_j w),$$

where u, v, w are the direction cosines for the beam direction, and $a_j x + b_j y + c_j z = d_j$ is the equation for the crystal face. The minimum for all j is the path length to the surface.

The analytical expression for the scattering power for each polyhedron, including the effect of absorption, can be expressed in a convenient form by subdividing the polyhedra into tetrahedra. The auxiliary points define the corners of the tetrahedra.

The total diffracted intensity is proportional to the sum of contributions, one from each tetrahedron, of the form

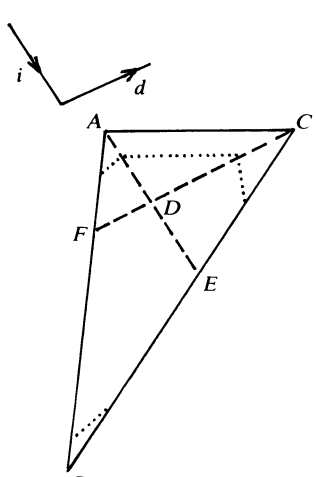

Fig. 6.3.3.3. The crystal *ABC* divided into polygons by the dashed lines *AE* and *CF* parallel to the incident (i) and diffracted (d) beams, respectively. A locus of constant absorption is shown dotted.

$$\begin{aligned} R_t &= 6V_t e^{-g} H(1) \\ &= \frac{6V_t}{(b+c)} e^{-g} \left\{ \frac{h(a) - h(a+b)}{b} - \frac{h(a+b) - h(a+b+c)}{c} \right\}, \end{aligned} \qquad (6.3.3.20)$$

where

$$h(x) = \frac{1 - e^{-x}}{x}. \qquad (6.3.3.21)$$

V_t is the volume of the tetrahedron. For a crystal with Cartesian coordinate vertices 1, 2, 3, and 4,

$$V_t = \tfrac{1}{6} \begin{vmatrix} x_1 - x_2 & x_1 - x_3 & x_1 - x_4 \\ y_1 - y_2 & y_1 - y_3 & y_1 - y_4 \\ z_1 - z_2 & z_1 - z_3 & z_1 - z_4 \end{vmatrix}. \qquad (6.3.3.22)$$

The g_i are optical path lengths (*i.e.* path lengths rescaled by the absorption coefficient) ordered so that

$$g_1 < g_2 < g_3 < g_4$$

and

$$g = g_1, \quad a = g_2 - g_1, \quad b = g_3 - g_2, \quad c = g_4 - g_3. \qquad (6.3.3.23)$$

The transmission factor for the crystal is the sum of the scattering powers for all the tetrahedra $\sum R_t$ divided by the volume $\sum V_t$. The equality of the total volume to the sum of the V_t values for the component tetrahedra provides a useful check on the accuracy of the calculations, since the total volume is independent of the beam directions, and must be the same for all reflections.

When any of a, b, and c are small, asymptotic forms are required for the expressions in (6.3.3.20). For $\varepsilon < 0.3 \times 10^{-2}$, and

$$\begin{array}{ll}
a < \varepsilon & h(a) = 1 - a/2 + a^2/3! \\
 & h(b+a) = h(b) + a h_1(b) + a^2 h_2(b)/2; \\
b < \varepsilon & h(a+b) = h(a) + b h_1(a) + b^2 h_2(a)/2 \\
 & [h(a) - h(a+b)]/b \\
 & \quad = -h_1(a) - b h_2(a)/2 - b^2 h_3(a)/3!; \\
c < \varepsilon & [h(a+b) - h(a+b+c)]/c \\
 & \quad = -h_1(a+b) - c h_2(a+b)/2 \\
 & \quad\quad -c^2 h_3(a+b)/3!; \\
b, c < \varepsilon & H(1) = h_2(a)/2 + (2b+c) h_3(a)/3! \\
 & \quad\quad + (3b^2 + 3bc + c^2) h_4(a)/4!; \\
a, c < \varepsilon & h(a) = 1 - a/2 + a^2/3! \\
 & [h(a+b) - h(a+b+c)]/c \\
 & \quad = -h_1(a+b) - c h_2(a+b)/2 \\
 & \quad\quad -c^2 h_3(a+b)/3!; \\
a, b < \varepsilon & h(a+b) = 1 - (a+b)/2 + (a+b)^2/3! \\
 & [h(a) - h(a+b)]/b \\
 & \quad = 1/2 - a/3 - b/3! + a^2/8 + ab/8 + b^2/4!; \\
a, b, c < \varepsilon & H(1) = \dfrac{1}{3!} - \dfrac{a+b}{8} + (b-c)/4! \\
 & \quad\quad + [(a+b+c)(4a+3b) \\
 & \quad\quad + 2a^2 + ab + c^2]/5!;
\end{array} \qquad (6.3.3.24)$$