International Tables for Crystallography (2006). Vol. C, Section 6.3.3.2, pp. 600–604.

tion in incident-beam intensity is many times larger than the sum of the squares of the individual atomic scattering powers.

An extreme case occurs in a perfect crystal, for which total reflection is possible. There is destructive interference with the incident beam producing a marked change in the index of refraction from its normal value of

$$n = 1 - \frac{\lambda^2 e^2}{2\pi mc^2} \sum_a N_a f_a(0), \qquad (6.3.1.4)$$

where e and m are the charge and mass of the electron. $f_a(0)$ is the scattering factor in the forward direction for an atom of type a and N_a is the number of atoms of that type per unit volume.

Thus, for strong reflections in near-perfect crystals, the Rayleigh scattering is affected by both crystal texture and beam direction. This reduction of primary-beam intensity due to the Rayleigh scattering is usually included, along with other specimen-dependent factors affecting diffracted-beam intensity, in the analysis of extinction.

6.3.1.4. *Attenuation (mass absorption) coefficients*

Since the reduction of intensity depends on the quantity of matter traversed by the beam, the absorption coefficient is often expressed on a mass basis by dividing by the density ρ_m. μ/ρ_m defines the attenuation coefficient.

The determination of attenuation coefficients to high precision is possible only when contributions from all different scattering processes are analysed in detail. To a level of accuracy appropriate to most experiments, however, the coefficient can be determined from the atomic cross sections for scattering and photoelectric absorption. Ideally, absorption corrections for scattering from single crystals in the absence of extinction should be evaluated using the Rayleigh cross section for a crystal in the non-reflecting position. However, as Rayleigh scattering is a minor contribution to the total absorption except for the lighter elements, no large error is made by applying the absorption correction appropriate to an assembly of isolated atoms to a single crystal.

Likewise, μ/ρ_m is, to a good approximation, given by the sum of the attenuation coefficients for each constituent element $(\mu/\rho_m)_a$, weighted by the mass fraction g_a for that element, *i.e.*

$$\frac{\mu}{\rho_m} = \sum_a g_a(\mu/\rho_m)_a, \qquad (6.3.1.5)$$

where the sum is over the elements. The atomic cross section for attenuation is given by

$$\sigma_a = (\mu/\rho_m)_a A_a/N_A = \mu/N_a, \qquad (6.3.1.6)$$

where A_a is the atomic weight and N_a is Avogadro's number. The evaluation of the attenuation coefficients is described in Section 4.2.4.

6.3.2. Dispersion

In the wavelength regime associated with anomalous scattering, where

$$f = f^0 + f' + f'', \qquad (6.3.2.1)$$

the refractive index becomes complex, its imaginary component contributing an additional term to the absorption.

f^0 is the scattering factor for ideal elastic scattering. The dispersion corrections f' and f'' are related to the absorption since (James, 1962; Wagenfeld, 1975)

$$f''(\omega) = mc\omega\sigma(\omega)/4\pi e^2, \quad \omega = 2\pi c/\lambda \qquad (6.3.2.2)$$

$$f'(\omega) = \frac{2}{\pi} \int_0^\infty [\omega' f''(\omega')/(\omega^2 - \omega'^2)]\, \mathrm{d}\omega'. \qquad (6.3.2.3)$$

That is, the dispersion corrections are determined by the absorption cross sections. The relationships (6.3.2.2) and (6.3.2.3) can be used in measuring absorption coefficients, as described in Section 4.2.4. The dispersion terms change rapidly near the absorption edge, especially on the short-wavelength side. The changes are anisotropic, sensitive to structure and to the direction of polarization. Details are given by Templeton & Templeton (1980, 1982, 1985).

In near-perfect crystals, the changes near the absorption edge are also sensitive to temperature (Karamura & Fukamachi, 1979; Fukamachi, Karamura, Hayakawa, Nakano & Koh, 1982). The effective absorption coefficient can also be altered by the Borrmann effect (Azaroff, Kaplow, Kato, Weiss, Wilson & Young, 1974).

6.3.3. Absorption corrections

The reduction in the intensity of an X-ray reflection from a uniform beam due to absorption is given by the transmission coefficient

$$A = \frac{1}{V} \int \exp(-\mu T)\, \mathrm{d}V, \qquad (6.3.3.1)$$

where the integration is over the volume of the crystal. The absorption correction

$$A^* = 1/A. \qquad (6.3.3.2)$$

T, the path length of the X-ray beam in the crystal, is the sum of the path lengths for the incident and diffracted beams. A technique for measuring crystals for absorption measurements is described in Subsection 6.3.3.6.

Any least-squares analysis involving variation of the linear absorption coefficient, or equivalently an isotropic variation in crystal size, requires the weighted mean path length

$$\bar{T} = -A^{-1}\frac{\partial A}{\partial \mu} = \frac{1}{A^*}\frac{\partial A^*}{\delta \mu}. \qquad (6.3.3.3)$$

This path length is also required in some analyses of extinction (Zachariasen, 1968; Becker & Coppens, 1974).

6.3.3.1. *Special cases*

For special cases, the integral can be solved analytically, and in some of these the expression reduces to closed form. These are listed in Table 6.3.3.1.

6.3.3.2. *Cylinders and spheres*

For diffraction in the equatorial plane of a cylinder of radius R within the X-ray beam, the expression for the transmission coefficient reduces to

$$A = \frac{1}{A^*} = \frac{1}{\pi R^2} \int_0^R \int_0^{2\pi} \exp\Big(-\mu\{[R^2 - r^2\sin^2(\theta+\varphi)]^{1/2} + [R^2 - r^2\sin^2(\theta-\varphi)]^{1/2}\}\Big) \times \cosh(2\mu r \sin\theta \sin\varphi) r\, \mathrm{d}r\, \mathrm{d}\varphi. \qquad (6.3.3.4)$$

Table 6.3.3.1. *Transmission coefficients*

(1) Reflection from a crystal slab with negligible transmission; the crystal planes are inclined at an angle φ to the extended face, and the normal in the plane of the incident and diffracted beams $$A = \frac{\sin(\theta - \varphi)}{\mu\{\sin(\theta - \varphi) + \sin(\theta + \varphi)\}}$$ (1*a*) $\varphi = 0$ $$A = 1/2\mu$$
(2) Reflection from a crystal slab of thickness t, with planes parallel to the extended face $$A = \{1 - \exp(-2\mu t \operatorname{cosec} \theta)\}/2\mu$$
(3) Transmission through a crystal slab of thickness t; the crystal planes are at $\pi/2 - \varphi$ to the surface, with the normal in the plane of the incident and reflected beams $$A = \frac{\exp\{-\mu t \sec(\theta + \varphi)\} - \exp\{-\mu t \sec(\theta - \varphi)\}}{\mu\left[1 - \frac{\sec(\theta + \varphi)}{\sec(\theta - \varphi)}\right]}$$ (3*a*) $\varphi = 0$ $$A = t \sec\theta \exp(-\mu t \sec\theta)$$
(4) Transmission through a sphere of radius R (*i.e.* for a uniform X-ray beam and $\theta = 0^\circ$) $$A = \frac{3}{2(\mu R)^3}[1/2 - e^{-2\mu R}\{1/2 + \mu R + (\mu R)^2\}]$$
(5) Reflection from a sphere of radius R (*i.e.* for a uniform X-ray beam, and $\theta = 90^\circ$) $$A = \frac{3}{4\mu R}\left\{1/2 - \frac{1}{16(\mu R)^2}\,[1 - (1 + 4\mu R)\,e^{-4\mu R}]\right\}$$

Values of the absorption correction A^* obtained by numerical integration by Dwiggins (1975*a*) are listed in Table 6.3.3.2.

The reduced expression for a spherical crystal of radius R is

$$A = \frac{3}{4\pi R^3} \int\limits_0^R \int\limits_{-1}^1 \int\limits_0^{2\pi} \exp\Big(-\mu\{[R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta+\varphi)]^{1/2} + [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta-\varphi)]^{1/2} - 2r\sin\theta\sin\alpha\sin\varphi\}\Big) r^2\,\mathrm{d}r\,\mathrm{d}(\cos\alpha)\,\mathrm{d}\varphi. \qquad (6.3.3.5)$$

Values of A^* obtained using numerical integration by Dwiggins (1975*b*) are listed in Table 6.3.3.3. An estimate of the accuracy of the numerical integration is given by comparison with the results for special values of θ at which equations (6.3.3.4) and (6.3.3.5) may be integrated analytically, which are included in Table 6.3.3.1. The comparison indicates a reliability for the tabulated values of better than 0.1%. Tables at finer intervals for cylinders and spheres for $\mu R < 1.0$ are given by Rouse, Cooper, York & Chakera (1970). A tabulation up to $\mu R < 5.0$ for spheres is given by Weber (1969). Interpolation for μR may be effected by the formula

$$A^*(\mu R) = \exp\left\{\sum_{m=1}^{M} K_m(\mu R)^m\right\}, \qquad (6.3.3.6)$$

where the K_m are determined, for fixed θ, from the values in Tables 6.3.3.2 and 6.3.3.3.

Subsequent interpolation as a function of θ may be effected by the interpolation formula

$$A^*\{\theta\} = \sum_{n=1}^{N} L_n \sin^{2n}(\theta). \qquad (6.3.3.7)$$

Interpolation is accurate to 0.1% with $N = M = 3$.

For cylinders and spheres, $\bar{T}$ may be obtained by means of the expression

$$\bar{T} = \frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}\mu} = R\left[\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}(\mu R)}\right] \qquad (6.3.3.8)$$

using the values listed in Tables 6.3.3.2 and 6.3.3.3.

Values of $(1/A^*)[\mathrm{d}A^*/\mathrm{d}(\mu R)]$ obtained by numerical integration by Flack & Vincent (1978) for spheres with $\mu R < 2.5$ are listed in Table 6.3.3.4. An equivalent table of $\mu(R/A^*)/[\mathrm{d}A^*/\mathrm{d}(\mu R)]$ for $\mu R < 4.0$ is given by Rigoult & Guidi-Morosini (1980).

Alternatively, one can differentiate the interpolation formula (6.3.3.6), yielding

$$\bar{T}(\mu R, \theta) = \frac{1}{\mu}\sum_{m=1}^{M} mK_m(\mu R)^m. \qquad (6.3.3.9)$$

In this case, however, the maximum index $M = 7$ is required to obtain convergence for $\mu R \leq 2.5$. Numerical values of the coefficients K_m for cylinders and spheres evaluated by Tibballs (1982) are listed in Table 6.3.3.5.

Interpolation between the tabulated θ values is obtained from the θ interpolation formula, noting that

$$L_m = \sum_{j=1}^{7} (C^{-1})_{mj} A_j^*, \qquad (6.3.3.10)$$

where

$$C_{mj} = \sin^{2m}\theta_j. \qquad (6.3.3.11)$$

The elements $(C^{-1})_{mj}$ and the $K_m(\theta_j)$ for θ_j at 15° intervals in the range $0 < \theta_j < 90^\circ$ are listed in Table 6.3.3.5. Differentiating (6.3.3.7) yields

$$A^*(\mu R, \theta)\bar{T}(\mu R, \theta) = \sum_{m=0}^{M} P_m \sin^{2m}\theta, \qquad (6.3.3.12)$$

where

$$P_m = R\frac{\partial L_m}{\partial(\mu R)} = \sum_{j=1}^{7}(C^{-1})_{mj} A_j^* \bar{T}_j. \qquad (6.3.3.13)$$

Equation (6.3.3.12) for path lengths is the analogue of equation (6.3.3.7) for the transmission factors. It provides the basis for an interpolation formula.

In the case of a cylindrical crystal much larger than the X-ray beam, the absorption correction has been determined by Coyle (1972), in an extension of earlier work by Coyle & Schroeder (1971). The absorption correction for the case of the cylinder axis coincident with the φ axis of a Eulerian cradle, shown in Fig. 6.3.3.1, reduces to the line integral

$$\frac{1}{2\tau}\int\limits_0^{2\tau} \exp\{-\mu[(z) + T(z)]\}\,\mathrm{d}z, \qquad (6.3.3.14)$$

Table 6.3.3.2. *Values of A^* for cylinders*

μR	$\theta = 0°$	$\theta = 5°$	$\theta = 10°$	$\theta = 15°$	$\theta = 20°$	$\theta = 25°$	$\theta = 30°$	$\theta = 35°$	$\theta = 40°$	$\theta = 45°$	$\theta = 50°$	$\theta = 55°$	$\theta = 60°$	$\theta = 65°$	$\theta = 70°$	$\theta = 75°$	$\theta = 80°$	$\theta = 85°$	$\theta = 90°$
0.0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.1	1.1843	1.1843	1.1842	1.1840	1.1838	1.1835	1.1832	1.1828	1.1823	1.1818	1.1813	1.1808	1.1802	1.1798	1.1793	1.1790	1.1787	1.1785	1.1785
0.2	1.4009	1.4007	1.4002	1.3995	1.3984	1.3970	1.3953	1.3934	1.3912	1.3889	1.3865	1.3841	1.3818	1.3796	1.3777	1.3761	1.3749	1.3741	1.3739
0.3	1.6548	1.6544	1.6531	1.6510	1.6481	1.6443	1.6398	1.6347	1.6290	1.6230	1.6169	1.6108	1.6049	1.5994	1.5946	1.5906	1.5876	1.5857	1.5851
0.4	1.9522	1.9513	1.9485	1.9439	1.9376	1.9296	1.9201	1.9094	1.8979	1.8857	1.8733	1.8611	1.8495	1.8388	1.8293	1.8215	1.8157	1.8121	1.8108
0.5	2.2996	2.2979	2.2926	2.2840	2.2721	2.2572	2.2398	2.2204	2.1996	2.1781	2.1564	2.1352	2.1152	2.0969	2.0809	2.0677	2.0579	2.0518	2.0497
0.6	2.7047	2.7017	2.6926	2.6775	2.6570	2.6317	2.6023	2.5701	2.5359	2.5010	2.4662	2.4327	2.4012	2.3728	2.3480	2.3277	2.3126	2.3033	2.3001
0.7	3.1762	3.1712	3.1561	3.1315	3.0982	3.0575	3.0111	2.9607	2.9081	2.8549	2.8028	2.7530	2.7068	2.6653	2.6295	2.6003	2.5786	2.5651	2.5606
0.8	3.7236	3.7157	3.6919	3.6532	3.6015	3.5392	3.4691	3.3941	3.3169	3.2400	3.1656	3.0953	3.0307	2.9732	2.9239	2.8839	2.8542	2.8359	2.8297
0.9	4.3578	4.3456	4.3093	4.2507	4.1733	4.0812	3.9792	3.8718	3.7629	3.6560	3.5538	3.4584	3.3717	3.2951	3.2299	3.1772	3.1383	3.1142	3.1061
1.0	5.0907	5.0724	5.0185	4.9323	4.8196	4.6877	4.5439	4.3948	4.2461	4.1022	3.9664	3.8413	3.7286	3.6298	3.5462	3.4790	3.4295	3.3990	3.3886
1.1	5.9356	5.9089	5.8305	5.7065	5.5466	5.3624	5.1649	4.9636	4.7660	4.5776	4.4022	4.2424	4.0998	3.9759	3.8717	3.7882	3.7269	3.6891	3.6763
1.2	6.907	6.869	6.757	6.582	6.360	6.109	5.8436	5.5782	5.3219	5.0811	4.8598	4.6604	4.4842	4.3322	4.2051	4.1038	4.0295	3.9838	3.9682
1.3	8.021	7.967	7.810	7.568	7.266	6.929	6.581	6.238	5.9125	5.6110	5.3376	5.0938	4.8805	4.6976	4.5456	4.4248	4.3365	4.2821	4.2636
1.4	9.294	9.219	9.003	8.674	8.268	7.826	7.376	6.942	6.536	6.166	5.8341	5.5413	5.2873	5.0711	4.8922	4.7506	4.6471	4.5835	4.5619
1.5	10.746	10.643	10.349	9.907	9.372	8.800	8.230	7.689	7.192	6.744	6.348	6.002	5.7036	5.4516	5.2441	5.0804	4.9609	4.8875	4.8625
1.6	12.397	12.257	11.862	11.276	10.581	9.852	9.141	8.477	7.877	7.344	6.877	6.473	6.128	5.8385	5.6007	5.4136	5.2773	5.1935	5.1650
1.7	14.267	14.080	13.555	12.788	11.897	10.982	10.106	9.304	8.589	7.963	7.420	6.955	6.561	6.231	5.961	5.7499	5.5960	5.5014	5.4691
1.8	16.379	16.131	15.441	14.450	13.323	12.189	11.125	10.168	9.327	8.600	7.976	7.446	7.000	6.628	6.326	6.089	5.9166	5.8107	5.7746
1.9	18.76	18.43	17.53	16.267	14.858	13.470	12.194	11.066	10.089	9.253	8.544	7.946	7.444	7.030	6.693	6.430	6.239	6.121	6.081
2.0	21.43	21.00	19.84	18.24	16.50	14.824	13.311	11.995	10.871	9.921	9.122	8.452	7.895	7.435	7.063	6.773	6.562	6.433	6.389
2.1	24.41	23.87	22.39	20.38	18.25	16.247	14.472	12.953	11.673	10.602	9.709	8.965	8.349	7.843	7.436	7.118	6.887	6.745	6.697
2.2	27.74	27.04	25.17	22.69	20.11	17.74	15.675	13.938	12.493	11.295	10.304	9.484	8.808	8.255	7.810	7.464	7.213	7.059	7.006
2.3	31.44	30.55	28.20	25.16	22.07	19.29	16.92	14.947	13.328	11.999	10.906	10.008	9.271	8.669	8.187	7.812	7.540	7.372	7.315
2.4	35.54	34.41	31.49	27.79	24.13	20.90	18.19	15.978	14.177	12.711	11.515	10.537	9.736	9.086	8.565	8.161	7.868	7.687	7.625
2.5	40.06	38.65	35.05	30.59	26.28	22.56	19.50	17.03	15.040	13.433	12.130	11.069	10.205	9.505	8.945	8.511	8.196	8.002	7.935

Table 6.3.3.3. *Values of A^* for spheres*

μR	$\theta = 0°$	$\theta = 5°$	$\theta = 10°$	$\theta = 15°$	$\theta = 20°$	$\theta = 25°$	$\theta = 30°$	$\theta = 35°$	$\theta = 40°$	$\theta = 45°$	$\theta = 50°$	$\theta = 55°$	$\theta = 60°$	$\theta = 65°$	$\theta = 70°$	$\theta = 75°$	$\theta = 80°$	$\theta = 85°$	$\theta = 90°$
0.0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.1	1.1609	1.1609	1.1609	1.1607	1.1606	1.1603	1.1600	1.1597	1.1593	1.1589	1.1586	1.1582	1.1579	1.1575	1.1572	1.1570	1.1568	1.1567	1.1567
0.2	1.3457	1.3456	1.3452	1.3447	1.3439	1.3428	1.3415	1.3400	1.3383	1.3366	1.3348	1.3331	1.3313	1.3297	1.3282	1.3271	1.3262	1.3256	1.3254
0.3	1.5574	1.5571	1.5561	1.5546	1.5525	1.5497	1.5463	1.5426	1.5383	1.5339	1.5293	1.5248	1.5204	1.5162	1.5126	1.5096	1.5074	1.5059	1.5055
0.4	1.7994	1.7988	1.7968	1.7935	1.7891	1.7833	1.7765	1.7689	1.7604	1.7515	1.7425	1.7335	1.7249	1.7169	1.7099	1.7041	1.6997	1.6970	1.6961
0.5	2.0755	2.0743	2.0706	2.0647	2.0565	2.0462	2.0340	2.0204	2.0056	1.9901	1.9745	1.9592	1.9445	1.9311	1.9194	1.9097	1.9024	1.8979	1.8964
0.6	2.3897	2.3877	2.3816	2.3715	2.3578	2.3406	2.3206	2.2984	2.2746	2.2500	2.2255	2.2015	2.1789	2.1583	2.1403	2.1257	2.1145	2.1076	2.1063
0.7	2.7467	2.7434	2.7336	2.7177	2.6959	2.6691	2.6382	2.6042	2.5683	2.5316	2.4952	2.4602	2.4274	2.3977	2.3719	2.3508	2.3351	2.3253	2.3220
0.8	3.1511	3.1461	3.1312	3.1069	3.0740	3.0339	2.9882	2.9386	2.8869	2.8347	2.7835	2.7346	2.6892	2.6484	2.6133	2.5845	2.5632	2.5499	2.5454
0.9	3.6082	3.6009	3.5789	3.5431	3.4952	3.4374	3.3723	3.3026	3.2308	3.1592	3.0898	3.0241	2.9637	2.9098	2.8634	2.8258	2.7979	2.7805	2.7747
1.0	4.1237	4.1131	4.0815	4.0304	3.9625	3.8816	3.7917	3.6966	3.6001	3.5048	3.4135	3.3280	3.2499	3.1807	3.1216	3.0738	3.0383	3.0163	3.0090
1.1	4.7035	4.6886	4.6442	4.5729	4.4790	4.3686	4.2474	4.1211	3.9945	3.8710	3.7540	3.6455	3.5470	3.4605	3.3870	3.3276	3.2838	3.2566	3.2474
1.2	5.3542	5.3335	5.2722	5.1747	5.0476	4.9001	4.7404	4.5761	4.4137	4.2571	4.1104	3.9756	3.8542	3.7483	3.6586	3.5866	3.5334	3.5005	3.4894
1.3	6.082	6.054	5.9710	5.8399	5.6710	5.4776	5.2711	5.0617	4.8573	4.6625	4.4819	4.3175	4.1706	4.0432	3.9360	3.8500	3.7868	3.7477	3.7344
1.4	6.895	6.857	6.746	6.573	6.352	6.102	5.8400	5.5774	5.3244	5.0862	4.8676	4.6703	4.4955	4.3447	4.2183	4.1174	4.0432	3.9974	3.9819
1.5	7.801	7.750	7.604	7.377	7.092	6.775	6.447	6.123	5.8143	5.5273	5.2666	5.0333	4.8281	4.6520	4.5052	4.3883	4.3024	4.2495	4.2315
1.6	8.806	8.740	8.549	8.256	7.894	7.497	7.092	6.697	6.326	5.9849	5.6780	5.4057	5.1678	4.9647	4.7961	4.6622	4.5641	4.5036	4.4830
1.7	9.920	9.834	9.587	9.214	8.759	8.268	7.774	7.299	6.859	6.458	6.101	5.7867	5.5140	5.2823	5.0907	4.9390	4.8279	4.7595	4.7361
1.8	11.151	11.040	10.725	10.254	9.689	9.088	8.492	7.928	7.411	6.946	6.535	6.176	5.8662	5.6045	5.3888	5.2184	5.0936	5.0170	4.9908
1.9	12.507	12.366	11.967	11.380	10.685	9.957	9.246	8.583	7.982	7.447	6.978	6.572	6.224	5.9308	5.6900	5.5001	5.3613	5.2760	5.2468
2.0	13.998	13.819	13.320	12.593	11.746	10.873	10.034	9.262	8.570	7.961	7.431	6.975	6.587	6.261	5.9942	5.7842	5.6307	5.5365	5.5041
2.1	15.632	15.408	14.788	13.895	12.874	11.837	10.855	9.964	9.175	8.486	7.893	7.385	6.955	6.595	6.301	6.070	5.9017	5.7982	5.7627
2.2	17.419	17.141	16.376	15.290	14.067	12.847	11.708	10.688	9.795	9.023	8.362	7.800	7.327	6.932	6.610	6.358	6.174	6.061	6.022
2.3	19.369	19.025	18.089	16.778	15.327	13.902	12.592	11.433	10.429	9.569	8.839	8.220	7.702	7.272	6.922	6.648	6.448	6.325	6.282
2.4	21.489	21.069	19.931	18.361	16.652	15.000	13.504	12.198	11.077	10.125	9.322	8.645	8.081	7.614	7.235	6.938	6.722	6.589	6.543
2.5	23.791	23.280	21.907	20.040	18.041	16.142	14.445	12.982	11.738	10.690	9.810	9.074	8.462	7.957	7.548	7.229	6.996	6.853	6.803

Table 6.3.3.4. *Values of* $(1/A^*)(dA^*/d\mu R)$ *for spheres*

μR	$\theta = 0°$	$\theta = 5°$	$\theta = 10°$	$\theta = 15°$	$\theta = 20°$	$\theta = 25°$	$\theta = 30°$	$\theta = 35°$	$\theta = 40°$	$\theta = 45°$	$\theta = 50°$	$\theta = 55°$	$\theta = 60°$	$\theta = 65°$	$\theta = 70°$	$\theta = 75°$	$\theta = 80°$	$\theta = 85°$	$\theta = 90°$
0.0	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000
0.1	1.4845	1.4842	1.4829	1.4809	1.4782	1.4739	1.4690	1.4634	1.4569	1.4504	1.4439	1.4375	1.4309	1.4248	1.4191	1.4152	1.4117	1.4096	1.4089
0.2	1.4692	1.4682	1.4650	1.4611	1.4548	1.4472	1.4374	1.4268	1.4145	1.4019	1.3879	1.3748	1.3615	1.3491	1.3385	1.3292	1.3228	1.3180	1.3168
0.3	1.4527	1.4515	1.4476	1.4400	1.4309	1.4186	1.4044	1.3886	1.3708	1.3517	1.3327	1.3128	1.2947	1.2773	1.2624	1.2494	1.2397	1.2340	1.2321
0.4	1.4360	1.4341	1.4283	1.4190	1.4058	1.3898	1.3709	1.3492	1.3265	1.3018	1.2773	1.2531	1.2296	1.2089	1.1903	1.1748	1.1628	1.1560	1.1533
0.5	1.4186	1.4161	1.4090	1.3969	1.3803	1.3598	1.3360	1.3093	1.2812	1.2522	1.2231	1.1946	1.1678	1.1434	1.1218	1.1044	1.0910	1.0825	1.0797
0.6	1.4011	1.3980	1.3890	1.3742	1.3538	1.3289	1.3006	1.2693	1.2365	1.2033	1.1700	1.1382	1.1087	1.0816	1.0577	1.0383	1.0239	1.0147	1.0115
0.7	1.3830	1.3792	1.3683	1.3507	1.3264	1.2973	1.2643	1.2286	1.1918	1.1549	1.1184	1.0839	1.0516	1.0250	0.9978	0.9767	0.9615	0.9518	0.9484
0.8	1.3641	1.3600	1.3473	1.3262	1.2984	1.2650	1.2275	1.1879	1.1473	1.1071	1.0684	1.0314	0.9976	0.9674	0.9409	0.9195	0.9034	0.8931	0.8898
0.9	1.3451	1.3401	1.3253	1.3013	1.2696	1.2321	1.1908	1.1474	1.1038	1.0608	1.0198	0.9815	0.9465	0.9152	0.8880	0.8663	0.8495	0.8391	0.8359
1.0	1.3255	1.3198	1.3029	1.2758	1.2401	1.1987	1.1535	1.1070	1.0608	1.0157	0.9733	0.9340	0.8978	0.8661	0.8392	0.8167	0.8001	0.7897	0.7859
1.1	1.3058	1.2993	1.2800	1.2497	1.2103	1.1651	1.1165	1.0670	1.0185	0.9720	0.9286	0.8886	0.8522	0.8205	0.7931	0.7709	0.7542	0.7437	0.7400
1.2	1.2851	1.2780	1.2566	1.2228	1.1799	1.1312	1.0796	1.0278	0.9777	0.9299	0.8858	0.8455	0.8093	0.7776	0.7506	0.7285	0.7120	0.7017	0.6981
1.3	1.2645	1.2563	1.2324	1.1961	1.1494	1.0967	1.0430	0.9892	0.9377	0.8895	0.8451	0.8048	0.7691	0.7378	0.7113	0.6895	0.6733	0.6631	0.6596
1.4	1.2449	1.2349	1.2090	1.1684	1.1180	1.0628	1.0068	0.9517	0.8990	0.8504	0.8064	0.7666	0.7315	0.7009	0.6749	0.6539	0.6377	0.6278	0.6243
1.5	1.2231	1.2133	1.1845	1.1398	1.0867	1.0295	0.9711	0.9145	0.8615	0.8133	0.7696	0.7308	0.6964	0.6665	0.6414	0.6209	0.6055	0.5957	0.5922
1.6	1.2015	1.1908	1.1585	1.1118	1.0555	0.9957	0.9358	0.8782	0.8261	0.7778	0.7350	0.6970	0.6638	0.6349	0.6105	0.5907	0.5758	0.5663	0.5628
1.7	1.1806	1.1681	1.1339	1.0836	1.0244	0.9621	0.9005	0.8435	0.7912	0.7444	0.7027	0.6659	0.6334	0.6057	0.5822	0.5632	0.5484	0.5394	0.5361
1.8	1.1586	1.1456	1.1087	1.0558	0.9939	0.9294	0.8669	0.8101	0.7579	0.7121	0.6711	0.6359	0.6053	0.5787	0.5561	0.5376	0.5236	0.5148	0.5117
1.9	1.1370	1.1226	1.0835	1.0275	0.9625	0.8964	0.8341	0.7774	0.7262	0.6817	0.6420	0.6078	0.5791	0.5535	0.5321	0.5144	0.5010	0.4924	0.4892
2.0	1.1152	1.0996	1.0584	0.9982	0.9318	0.8646	0.8019	0.7457	0.6962	0.6527	0.6160	0.5830	0.5550	0.5305	0.5098	0.4927	0.4799	0.4717	0.4687
2.1	1.0932	1.0772	1.0327	0.9703	0.9014	0.8340	0.7712	0.7157	0.6678	0.6259	0.5899	0.5588	0.5322	0.5088	0.4886	0.4726	0.4603	0.4523	0.4494
2.2	1.0719	1.0543	1.0074	0.9427	0.8719	0.8039	0.7421	0.6874	0.6402	0.6003	0.5658	0.5353	0.5098	0.4884	0.4699	0.4548	0.4426	0.4347	0.4311
2.3	1.0498	1.0316	0.9822	0.9150	0.8434	0.7744	0.7133	0.6605	0.6147	0.5758	0.5433	0.5141	0.4896	0.4692	0.4518	0.4363	0.4252	0.4175	0.4149
2.4	1.0275	1.0118	0.9583	0.8889	0.8147	0.7482	0.6870	0.6340	0.5918	0.5507	0.5212	0.4937	0.4699	0.4500	0.4328	0.4187	0.4076	0.4003	0.3986
2.5	1.0108	0.9691	0.9297	0.8562	0.7904	0.7074	0.6554	0.6194	0.5618	0.5289	0.4980	0.4776	0.4554	0.4315	0.4142	0.4028	0.3921	0.3883	0.3783

Table 6.3.3.5. *Coefficients for interpolation of* A^* *and* $\bar{T}$

θ_j	0°	15°	30°	45°	60°	75°	90°	Units
K_1 (sphere)	3/2	3/2	3/2	3/2	3/2	3/2	3/2	
K_2	−7.5234	−9.4320	−15.109	−24.3812	−35.219	−44.042	−47.745	10^{-2}
K_3	−7.0935	−10.737	−18.027	−11.088	14.265	40.021	61.084	10^{-3}
K_4	−2.3096	−2.1332	−1.4693	7.4205	24.832	44.308	37.394	10^{-3}
K_5	1.8323	1.1711	4.6784	3.0970	−10.284	−27.987	−25.879	10^{-3}
K_6	−5.1259	−1.2652	−14.491	−16.740	21.910	77.007	71.458	10^{-4}
K_7	6.0265	0.7932	16.489	21.774	−22.391	−85.570	−78.812	10^{-5}
K_1 (cylinder)	$16/3\pi$	$16/3\pi$	$16/3\pi$	$16/3\pi$	$16/3\pi$	$16/3\pi$	$16/3\pi$	
K_2	−5.7832	−8.1900	−15.651	−27.048	−40.317	−51.497	−55.837	10^{-2}
K_3	−14.737	−19.551	−22.883	−27.345	−8.807	26.637	41.420	10^{-3}
K_4	5.2399	1.2934	−12.301	6.844	40.689	61.371	68.963	10^{-3}
K_5	−4.0958	−2.8349	9.6249	7.503	−11.295	−29.397	−36.556	10^{-3}
K_6	13.178	12.731	−19.881	−30.211	9.4468	60.356	80.965	10^{-4}
K_7	−14.500	−14.846	14.414	34.222	3.1492	−49.206	−70.573	10^{-5}
$(C^{-1})_{0j}$	3	0	0	0	0	0	0	All values multiplied by 3 to eliminate fractions
$(C^{-1})_{1j}$	−73	$48+24\sqrt{3}$	−24	12	−8	$48-24\sqrt{3}$	−3	
$(C^{-1})_{2j}$	518	$-496-200\sqrt{3}$	488	−268	184	$-496+200\sqrt{3}$	70	
$(C^{-1})_{3j}$	−1600	$1920+560\sqrt{3}$	−2192	1536	−1136	$1920-560\sqrt{3}$	−448	
$(C^{-1})_{4j}$	2432	$-3520-640\sqrt{3}$	4032	−3328	2752	$-3520+640\sqrt{3}$	1152	
$(C^{-1})_{5j}$	−1792	$3072+256\sqrt{3}$	−3328	3072	−2816	$3072-256\sqrt{3}$	−1280	
$(C^{-1})_{6j}$	512	−1024	1024	−1024	1024	−1024	512	

where z and $T(z)$ are the path lengths for the incident and diffracted beams, respectively. τ is the radius, along the line of the incident beam, of the ellipse described by the cross section of the crystal in the plane of diffraction, shown in Fig. 6.3.3.2. The equation for the ellipse is

$$\tau = R(1 - \sin^2\theta \sin^2\chi)^{-1/2}. \qquad (6.3.3.15)$$

The outgoing elliptical radius v satisfies

$$Av^4 + Bv^2 + C = 0, \qquad (6.3.3.16)$$

where

$$\begin{aligned} A &= [1 - \sin^2\theta \sin^2\chi]^2 \\ B &= -2R^2[1 - \sin^2\theta \sin^2\chi] \\ &\quad - 2(\tau - z)^2[\cos^2\theta - \sin^2\theta \cos^2\chi]\sin^2 2\theta \sin^2\chi \\ C &= R^4 + 2R^2(\tau - z)^2 \sin^2 2\theta \sin^2\chi \cos 2\theta \\ &\quad + (\tau - z)^4 \sin^4 2\theta \sin^4\chi. \end{aligned}$$

In the case where the cylinder axis is inclined at an angle Γ to the φ axis, these equations become

$$\begin{aligned} A &= [1 - \sin^2(\theta + \beta)\sin^2\chi_1]^2 \\ B &= -2R^2[1 - \sin^2(\theta + \beta)\sin^2\chi_1] \\ &\quad - 2(\tau - z)^2[\cos^2(\theta + \beta) \\ &\quad - \sin^2(\theta + \beta)\cos^2\chi_1]\sin^2 2\theta \sin^2\chi_1 \\ C &= R^4 + 2R^2(\tau - z)^2 \sin^2 2\theta \sin^2\chi_1 \cos 2(\theta + \beta) \\ &\quad + (\tau - z)^4 \sin^4 2\theta \sin^4\chi_1, \end{aligned}$$

where

$$\tan\beta = \sin\Gamma \sin\varphi / [\sin\Gamma \cos\chi \cos\varphi + \sin\chi \cos\Gamma].$$

The roots of the quadratic equation (6.3.3.16) for v^2 are real and positive for reflection from within the crystal. The convergent path length T is given by the positive root of the triangle formula

$$T^2 - 2T(\tau - z)\cos 2\theta + (\tau - z)^2 - v^2 = 0. \qquad (6.3.3.17)$$

It should be noted that the volume of the specimen irradiated changes with the angular settings of the diffractometer. Normalization to constant volume requires that the absorption correction be multiplied by the volume-correction factor $[1 - \sin^2(\theta - \beta)\sin^2\chi_1]^{-1/2}$.

The method readily extends to the case of a cylindrical window or sheath, such as used for mounting an unstable crystal of conventional size. The correction in this case is

$$\begin{aligned} &\exp[-\mu(\tau_2 - \tau_1 + v_2 - v_1)] \\ &\quad = \exp\Big(- \mu(R_2 - R_1)\{[1 - \sin^2(\theta - \beta)\sin^2\chi_1]^{-1/2} \\ &\qquad + [1 - \sin^2(\theta + \beta)\sin^2\chi_1]^{-1/2}\}\Big), \end{aligned} \qquad (6.3.3.18)$$

where the subscripts 1 and 2 apply to the inner and outer radii, respectively.

The integral in equation (6.3.3.14) may be evaluated by Gaussian quadrature, *i.e.* by approximation as a weighted sum of the values of the function at the N zeros X_i of the Legendre polynomial of degree N in the interval $[-1, +1]$. The weights w_i for the points are tabulated by Abramowitz & Stegun (1964). Further details are given in Subsection 6.3.3.4. The emergent path lengths $T(z_1)$ and $T(z_2)$ for the case of the sheath are calculated as functions of the Gaussian variable X_i using the linear transformation

$$z_i = \tau_1 X_i + \tau_2, \quad i = 1, 2, \ldots, N. \qquad (6.3.3.19)$$

This transformation converts the Gaussian variable X into the beam coordinate z for each i of the N summation points.

6.3.3.3. *Analytical method for crystals with regular faces*

For a crystal with regular faces, (6.3.3.1) may be integrated exactly, giving the correction in analytical form. In its simplest form, the analytical method applies to specimens with no re-entrant angles. It is efficient for crystals with a small number of faces. Its accuracy does not depend on the size of the absorption coefficient. The principles can be illustrated by reference to the two-dimensional case of a triangular crystal shown in Fig. 6.3.3.3.

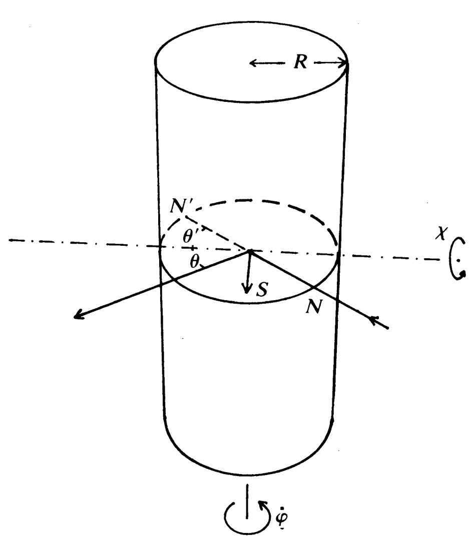

Fig. 6.3.3.1. Geometry of the Eulerian cradle with the axis of a cylindrical specimen coincident with the φ axis.

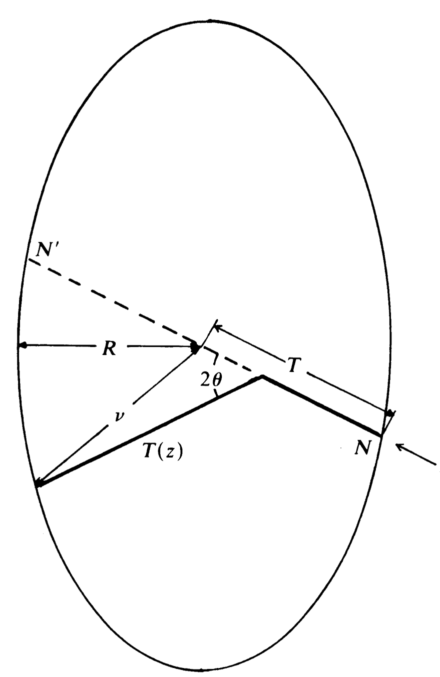

Fig. 6.3.3.2. Cross section of the plane of diffraction for a cylindrical specimen coincident with the φ axis.