SHORT COMMUNICATIONS

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An accurate calculation of $\bar{T}_\mu$ for spherical crystals.

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Abstract

A table for the calculation of $\bar{T}_\mu$ (the mean path length of X-rays weighted by absorption) has been computed using three-dimensional Gaussian integration. This table is given for μR and θ in the ranges 0–4 and 0–90°, respectively. Its accuracy is estimated as better than 0·1%.

Table 1. *Values of* $\bar{T}_{\mu R}$ *for spheres*

μR \ θ°	0	5	10	15	20	25	30	35	40
0·1	0·1485	0·1484	0·1483	0·1481	0·1478	0·1474	0·1469	0·1464	0·1458
0·2	0·2938	0·2936	0·2931	0·2922	0·2910	0·2894	0·2875	0·2853	0·2829
0·3	0·4358	0·4355	0·4342	0·4322	0·4293	0·4257	0·4213	0·4165	0·4112
0·4	0·5744	0·5737	0·5714	0·5677	0·5625	0·5559	0·5383	0·5397	0·5305
0·5	0·7094	0·7083	0·7046	0·6986	0·6903	0·6799	0·6680	0·6549	0·6408
0·6	0·8406	0·8390	0·8335	0·8246	0·8124	0·7975	0·7803	0·7618	0·7422
0·7	0·9680	0·9657	0·9580	0·9455	0·9288	0·9083	0·8852	0·8605	0·8347
0·8	1·091	1·088	1·078	1·061	1·039	1·012	0·9824	0·9509	0·9186
0·9	1·211	1·207	1·193	1·172	1·143	1·109	1·072	1·033	0·9941
1·0	1·326	1·320	1·303	1·276	1·241	1·199	1·154	1·108	1·062
1·1	1·436	1·429	1·408	1·375	1·331	1·282	1·229	1·174	1·121
1·2	1·543	1·534	1·508	1·468	1·416	1·358	1·296	1·234	1·173
1·3	1·645	1·634	1·603	1·555	1·494	1·426	1·356	1·286	1·219
1·4	1·742	1·729	1·692	1·636	1·566	1·488	1·409	1·332	1·259
1·5	1·835	1·820	1·777	1·711	1·631	1·544	1·456	1·371	1·292
1·6	1·923	1·906	1·855	1·780	1·689	1·593	1·497	1·405	1·321
1·7	2·007	1·987	1·929	1·843	1·742	1·636	1·531	1·434	1·345
1·8	2·086	2·063	1·997	1·901	1·788	1·673	1·561	1·457	1·365
1·9	2·160	2·134	2·060	1·953	1·829	1·704	1·585	1·477	1·381
2·0	2·231	2·201	2·118	1·999	1·864	1·731	1·605	1·492	1·393
2·1	2·297	2·263	2·170	2·039	1·894	1·752	1·621	1·505	1·403
2·2	2·358	2·321	2·217	2·075	1·919	1·769	1·633	1·514	1·410
2·3	2·416	2·374	2·260	2·105	1·940	1·783	1·642	1·520	1·415
2·4	2·469	2·423	2·298	2·131	1·956	1·792	1·648	1·524	1·418
2·5	2·519	2·468	2·332	2·153	1·969	1·799	1·651	1·526	1·420
2·6	2·565	2·509	2·361	2·171	1·978	1·803	1·653	1·526	1·420
2·7	2·607	2·546	2·387	2·185	1·983	1·804	1·652	1·525	1·419
2·8	2·646	2·580	2·409	2·195	1·986	1·803	1·650	1·523	1·417
2·9	2·682	2·610	2·427	2·202	1·987	1·800	1·646	1·519	1·414
3·0	2·715	2·637	2·442	2·206	1·985	1·796	1·641	1·515	1·411
3·1	2·744	2·661	2·453	2·208	1·981	1·790	1·635	1·510	1·407
3·2	2·772	2·682	2·462	2·207	1·975	1·783	1·629	1·505	1·403
3·3	2·796	2·700	2·468	2·204	1·968	1·776	1·622	1·499	1·399
3·4	2·819	2·716	2·472	2·199	1·960	1·767	1·614	1·493	1·394
3·5	2·839	2·730	2·474	2·193	1·951	1·758	1·606	1·486	1·389
3·6	2·857	2·741	2·473	2·185	1·941	1·748	1·598	1·480	1·384
3·7	2·873	2·751	2·471	2·176	1·930	1·738	1·590	1·473	1·379
3·8	2·888	2·759	2·467	2·166	1·919	1·728	1·581	1·466	1·373
3·9	2·901	2·765	2·462	2·155	1·907	1·718	1·573	1·459	1·368
4·0	2·913	2·770	2·456	2·144	1·895	1·708	1·564	1·453	1·363

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Table 1 (*cont.*)

μR \ $\theta°$	45	50	55	60	65	70	75	80	85	90
0·1	0·1451	0·1444	0·1437	0·1431	0·1424	0·1418	0·1413	0·1410	0·1408	0·1405
0·2	0·2803	0·2776	0·2750	0·2724	0·2700	0·2678	0·2660	0·2647	0·2639	0·2636
0·3	0·4055	0·3997	0·3940	0·3886	0·3835	0·3790	0·3752	0·3724	0·3708	0·3701
0·4	0·5208	0·5109	0·5013	0·4923	0·4839	0·4764	0·4701	0·4655	0·4629	0·4617
0·5	0·6262	0·6115	0·5974	0·5842	0·5720	0·5612	0·5521	0·5456	0·5417	0·5401
0·6	0·7220	0·7020	0·6830	0·6653	0·6490	0·6346	0·6227	0·6140	0·6089	0·6068
0·7	0·8085	0·7828	0·7585	0·7362	0·7159	0·6980	0·6831	0·6723	0·6660	0·6633
0·8	0·8860	0·8545	0·8250	0·7981	0·7738	0·7523	0·7346	0·7218	0·7142	0·7110
0·9	0·9551	0·9176	0·8830	0·8517	0·8236	0·7989	0·7785	0·7637	0·7550	0·7512
1·0	1·016	0·9729	0·9334	0·8980	0·8664	0·8386	0·8157	0·7991	0·7893	0·7851
1·1	1·069	1·021	0·9772	0·9373	0·9020	0·8721	0·8476	0·8291	0·8177	0·8137
1·2	1·116	1·063	1·015	0·9713	0·9331	0·9008	0·8745	0·8544	0·8421	0·8377
1·3	1·156	1·099	1·047	1·000	0·9595	0·9252	0·8972	0·8758	0·8627	0·8580
1·4	1·191	1·129	1·074	1·025	0·9819	0·9459	0·9165	0·8940	0·8801	0·8752
1·5	1·220	1·155	1·097	1·046	1·001	0·9635	0·9329	0·9095	0·8949	0·8898
1·6	1·245	1·176	1·116	1·063	1·017	0·9784	0·9469	0·9226	0·9075	0·9021
1·7	1·265	1·194	1·132	1·078	1·030	0·9911	0·9589	0·9339	0·9183	0·9127
1·8	1·282	1·209	1·146	1·090	1·042	1·002	0·9691	0·9435	0·9275	0·9218
1·9	1·296	1·221	1·157	1·100	1·052	1·011	0·9778	0·9518	0·9355	0·9296
2·0	1·306	1·230	1·165	1·109	1·060	1·019	0·9854	0·9590	0·9423	0·9364
2·1	1·315	1·238	1·172	1·115	1·067	1·025	0·9913	0·9653	0·9482	0·9422
2·2	1·321	1·244	1·178	1·121	1·072	1·031	0·9968	0·9708	0·9535	0·9474
2·3	1·325	1·248	1·182	1·126	1·077	1·036	1·002	0·9755	0·9580	0·9519
2·4	1·328	1·251	1·186	1·129	1·081	1·040	1·006	0·9796	0·9620	0·9558
2·5	1·330	1·253	1·188	1·132	1·084	1·043	1·009	0·9833	0·9656	0·9593
2·6	1·330	1·254	1·190	1·134	1·087	1·046	1·013	0·9865	0·9687	0·9624
2·7	1·330	1·255	1·191	1·136	1·089	1·049	1·015	0·9894	0·9715	0·9652
2·8	1·329	1·254	1·191	1·137	1·091	1·051	1·018	0·9919	0·9740	0·9676
2·9	1·327	1·254	1·191	1·138	1·092	1·053	1·020	0·9942	0·9763	0·9698
3·0	1·325	1·252	1·191	1·138	1·093	1·054	1·022	0·9962	0·9783	0·9718
3·1	1·322	1·251	1·190	1·138	1·094	1·055	1·023	0·9978	0·9802	0·9737
3·2	1·319	1·249	1·189	1·138	1·094	1·056	1·025	0·9994	0·9819	0·9753
3·3	1·316	1·247	1·188	1·138	1·095	1·057	1·026	1·001	0·9834	0·9768
3·4	1·312	1·244	1·187	1·137	1·095	1·058	1·027	1·002	0·9847	0·9781
3·5	1·309	1·242	1·185	1·136	1·095	1·059	1·028	1·003	0·9860	0·9794
3·6	1·305	1·239	1·183	1·136	1·095	1·059	1·029	1·004	0·9872	0·9805
3·7	1·301	1·237	1·182	1·135	1·094	1·059	1·030	1·005	0·9882	0·9816
3·8	1·297	1·234	1·180	1·134	1·094	1·060	1·030	1·006	0·9892	0·9825
3·9	1·293	1·231	1·178	1·133	1·094	1·060	1·031	1·007	0·9910	0·9834
4·0	1·289	1·228	1·176	1·132	1·093	1·060	1·031	1·008	0·9909	0·9843

Introduction

The usual theory of extinction corrections for mosaic absorbing crystals (Becker & Coppens, 1974) makes use of the mean path length weighted by absorption, $\bar{T}_\mu$, defined by:

$$\bar{T}_\mu = A^{*-1}\frac{\partial A^*}{\partial \mu} = -A^{-1}\frac{\partial A}{\partial \mu}, \quad (1)$$

where $A = A^{*-1}$ is the transmission factor.

$\bar{T}_\mu$ also appears in a least-squares treatment of any diffraction effect involving variation of the linear absorption coefficiei Indeed, if F_k^2 and F^2 are the kinematical diffracted intensities without and with absorption ($F^2 = A\ F_k^2$), the derivative of F^2 for an arbitrary parameter α describing this effect will be:

$$\frac{\partial F^2}{\partial \alpha} = A\frac{\partial F_k^2}{\partial \alpha} + F_k^2\frac{\partial A}{\partial \mu}\frac{\partial \mu}{\partial \alpha}$$

$$= A\frac{\partial F_k^2}{\partial \alpha} - F^2\,\bar{T}_\mu\frac{\partial \mu}{\partial \alpha}.$$

In particular, the treatment of the Borrmann effect in mosaic crystals needs such a calculation (Becker, 1978).

These examples show the importance of the quantity $\bar{T}_\mu$ in all diffraction data processing.

Weber (1969) has carried out an accurate calculation of A^* for spheres up to a value of μR of 31·5. The same calculation limited to the μR range of 0–2·5 was reproduced later by Dwiggins (1975). The accuracy of these tables was estimated to be around 0·1%.

The common procedure for computing $\bar{T}_\mu$ is thus the numerical differentiation of the A^* values. Although the step in μR is small for Weber's table (0·1 up to μR = 10), this numerical method may give large errors in particular where A^* varies rapidly and at the ends of the table where it is difficult to estimate the derivative. It is therefore necessary to have a better knowledge of $\bar{T}_\mu$ for spherical crystals.

Direct calculation of $\bar{T}$

Let us define the quantity $\bar{T}_{\mu R}$ which is related to $\bar{T}_\mu$:

$$\bar{T}_{\mu R} = \int_v \mu t \exp(-\mu t)\,dv \Big/ \int_v \exp(-\mu t)\,dv, \quad (2)$$

$$\bar{T}_\mu = \mu^{-1}\,\bar{T}_{\mu R} \quad (3)$$

In (2), t is the path length of the rays in the crystal.

For a sphere, considering the usual spherical coordinates r, α, φ (the polar axis z is normal to the diffraction plane), t is calculated as follows:

$$t(r,\alpha,\varphi) = -2r\sin\theta\sin\alpha\sin\varphi + [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta-\varphi)]^{1/2} + [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta+\varphi)]^{1/2}, \quad (4)$$

with θ = Bragg angle, R = radius of the sphere.

From the symmetries of t in α and φ, the integration of (2) can be reduced to a quarter of the sphere:

$$\int_{\text{sphere}} dv = 4\int_0^R dr \int_0^{\pi/2} d\alpha \int_{-\pi/2}^{\pi/2} d\varphi\, r^2\sin^2\alpha. \quad (5)$$

This three-dimensional integration cannot be performed exactly in the general case, but can be accurately carried out by the numerical Gauss method. This calculation was done on an IRIS 80 (CII H-B) computer with 10^3 to 32^3 grid points of integration for the range 0·1–4·0 of μR, which is that over which the Becker–Coppens extinction theory is valid and covers most practical situations with accurate data. The results of this computation are given in Table 1.

For $\theta = 0$ and 90°, $\bar{T}_{\mu R}$ can be exactly known from (1) and the exact values of A for these angles (*International Tables for X-ray Crystallography*, 1959):

$$\theta = 0°,\quad \bar{T}_{\mu R} = 3 - 2(\mu R)^3/[1/2\exp(2\mu R) - 1/2 - \mu R - (\mu R)^2];$$

$$\theta = 90°,\quad \bar{T}_{\mu R} = 1 + \{2[1 + 4\mu R + 8(\mu R)^2]\times\exp(-4\mu R) - 2\}/[(1+4\mu R)\exp(-4\mu R) - 1 + 8(\mu R)^2].$$

These functions provide a good check of the accuracy of the previous computation and we found that the root-mean-square error based on them is less than 0·0005 for all of Table 1 (these exact values are given in Table 1 instead of the computed ones). The accuracy of this table is therefore better than 0·1%.

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Polarization states of dynamically diffracted X-ray beams.

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Abstract

A phase difference between the coherent σ and π components of dynamically diffracted X-rays was observed in the Laue case. The incident X-ray beam was linearly polarized Cu $K\alpha$ radiation. A Si single crystal was used to produce the phase difference. The Ge 333 reflexion was used to polarize the incident beam and also to examine the polarization state of the diffracted beam in the 220 Laue-case reflexion from a Si crystal. For comparison, the polarization state in the Bragg case was also analysed.

Polarization phenomena of X-rays are one of the basic problems in X-ray scattering. Recently, changes in the polarization states of X-ray beams were reported for Laue-case diffraction (Skalicky & Malgrange, 1972; Sauvage, Petroff & Skalicky, 1977) and for simple transmission through a (110) Si crystal (Cohen & Kuriyama, 1978). In the former case it was shown that the phase difference between the σ and π components was produced in a similar way to linearly polarized visible light.

According to the dynamical theory of X-ray diffraction for the two-beam case (Kohra, 1961; Batterman & Cole, 1964), two diffracted waves with different wave vectors are produced which correspond to the two branches (I, II) of the dispersion surfaces and thus in the Laue case the *Pendellösung* fringes can be observed. Furthermore, for the same branch, *e.g.* branch I with wave vector $\mathbf{k}_{h1}$, there are two different wave vectors, $\mathbf{k}^{\sigma}_{h1}$ and $\mathbf{k}^{\pi}_{h1}$ corresponding to the σ and π dispersion surfaces. At the exact Bragg condition and for the symmetrical Laue case the phase difference φ between the σ and π components for the branch I is given by

$$\varphi = 2\pi(\mathbf{k}^{\sigma}_{h1} - \mathbf{k}^{\pi}_{h1})\cdot\mathbf{r}, \quad (1)$$

where $\mathbf{r}$ denotes the position vector. Equation (1) can be rewritten using the real part of the Fourier coefficient of the susceptibility of the crystal ψ'_H

$$\varphi = \pi|\mathbf{k}|\psi'_H|(1 - |\cos 2\theta|)\, t_0/\cos\theta, \quad (2)$$

where $\mathbf{k}$, t_0 and θ are the wave vector of the incident X-ray beam, the thickness of the specimen and the Bragg angle, respectively. In this communication we report some experimental results for the change of the polarization state in the

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