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Rapid calculation of X-ray absorption correction factors for spheres to an accuracy of 0.05%.

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X-ray absorption factors A^* for spherical samples were calculated in the range of the product of sphere radius R and linear absorption coefficient μ of $0 \le \mu R \le 2{\cdot}5$ and in the range of Bragg angle θ of $0° \le \theta \le 90°$. A new method that requires numerical integration over only one variable using high-accuracy values of A^* recently calculated for cylinders was developed. A table of values of A^* was tabulated. A full-range, curve-fitting procedure that is accurate to 0·05% also was developed for routine calculation of A^*.

Introduction

X-ray intensities can be measured to a precision of one percent, or slightly better, in some cases. To make full use of precise intensities, various corrections should be made more carefully than in the past so that any errors in data result from experimental observables and not from calculations. If the error in the absorption correction factor A^* can be reduced to about 0·1 % or less, then any error caused by this source can be neglected for most purposes. Also, it is desirable to have a full-range, curve-fitting procedure for A^* for routine use so that values of A^* can be calculated rapidly without storage of massive tables of A^* as a function of both θ and μR.

A table of values of A^* for spheres prepared by W. L. Bond is given in *International Tables for X-ray Crystallography* (1959). These values of A^* were obtained by interpolation from a table of values of $A \equiv 1/A^*$. The limited number of A values were obtained by numerical integration over three variables. Also, equations for exact calculation of A at values of θ of 0° and 90° are given. Values of A^* and A taken from tables in the mentioned reference will be called IT values.

The IT A^* table can have errors up to 0·5% owing to round-off and possibly interpolation errors. To reduce the error to 0·1 % or lower, it was decided that new values of A^* should be calculated directly in increments of 0·1 in μR and 5° in θ and not in the much larger increments used in the IT A table from which the IT A^* table was obtained by interpolation.

Even using modern computers, many hundred numerical integrations over three variables require more time than desirable. Thus another, more rapid method for calculation of A^* was sought. Because accurate values of A^* for cylinders have recently been calculated (Dwiggins, 1975), it was decided to attempt use of these values to calculate A^* values for spheres using numerical integration over only a single variable.

Theory

The basic equations for calculation of A^* values are given in *International Tables for X-ray Crystallography* (1959).

To make use of data for cylinders, the sphere is considered to be made up of cylinders of infinitesimal length with their axes in the direction of a normal to the plane defined by the incident and scattered X-ray beam. If R_c is

Table 1. *Values of A* for spheres*

μR	$\theta=0°$	$\theta=5°$	$\theta=10°$	$\theta=15°$	$\theta=20°$	$\theta=25°$	$\theta=30°$	$\theta=35°$	$\theta=40°$	$\theta=45°$
0·0	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
0·2	1·3457	1·3456	1·3452	1·3447	1·3439	1·3428	1·3415	1·3400	1·3383	1·3366
0·3	1·5574	1·5571	1·5561	1·5546	1·5525	1·5497	1·5463	1·5426	1·5383	1·5339
0·4	1·7994	1·7988	1·7968	1·7935	1·7891	1·7833	1·7765	1·7689	1·7604	1·7515
0·5	2·0755	2·0743	2·0706	2·0647	2·0565	2·0462	2·0340	2·0204	2·0056	1·9901
0·6	2·3897	2·3877	2·3816	2·3715	2·3578	2·3406	2·3206	2·2984	2·2746	2·2500
0·7	2·7467	2·7434	2·7336	2·7177	2·6959	2·6691	2·6382	2·6042	2·5683	2·5316
0·8	3·1511	3·1461	3·1312	3·1069	3·0740	3·0339	2·9882	2·9386	2·8869	2·8347
0·9	3·6082	3·6009	3·5789	3·5431	3·4952	3·4374	3·3723	3·3026	3·2308	3·1592
1·0	4·1237	4·1131	4·0815	4·0304	3·9625	3·8816	3·7917	3·6966	3·6001	3·5048
1·1	4·7035	4·6886	4·6442	4·5729	4·4790	4·3686	4·2474	4·1211	3·9945	3·8710
1·2	5·3542	5·3335	5·2722	5·1747	5·0476	4·9001	4·7404	4·5761	4·4137	4·2571
1·3	6·082	6·054	5·9710	5·8399	5·6710	5·4776	5·2711	5·0617	4·8573	4·6625
1·4	6·895	6·857	6·746	6·573	6·352	6·102	5·8400	5·5774	5·3244	5·0862
1·5	7·801	7·750	7·604	7·377	7·092	6·775	6·447	6·123	5·8143	5·5273
1·6	8·806	8·740	8·549	8·256	7·894	7·497	7·092	6·697	6·326	5·9849
1·7	9·920	9·834	9·587	9·214	8·759	8·268	7·774	7·299	6·859	6·458
1·8	11·151	11·040	10·725	10·254	9·689	9·088	8·492	7·928	7·411	6·946
1·9	12·507	12·366	11·967	11·380	10·685	9·957	9·246	8·583	7·982	7·447
2·0	13·998	13·819	13·320	12·593	11·746	10·873	10·034	9·262	8·570	7·961
2·1	15·632	15·408	14·788	13·895	12·874	11·837	10·855	9·964	9·175	8·486
2·2	17·419	17·141	16·376	15·290	14·067	12·847	11·708	10·688	9·795	9·023
2·3	19·369	19·025	18·089	16·778	15·327	13·902	12·592	11·433	10·429	9·569
2·4	21·489	21·069	19·931	18·361	16·652	15·000	13·504	12·198	11·077	10·125
2·5	23·791	23·280	21·907	20·040	18·041	16·142	14·445	12·982	11·738	10·690

Table 1 (*cont.*)

μR	$\theta=50°$	$\theta=55°$	$\theta=60°$	$\theta=65°$	$\theta=70°$	$\theta=75°$	$\theta=80°$	$\theta=85°$	$\theta=90°$
0·0	1	1	1	1	1	1	1	1	1
0·1	1·1586	1·1582	1·1579	1·1575	1·1572	1·1570	1·1568	1·1567	1·1567
0·2	1·3348	1·3331	1·3313	1·3297	1·3282	1·3271	1·3262	1·3256	1·3254
0·3	1·5293	1·5248	1·5204	1·5162	1·5126	1·5096	1·5074	1·5059	1·5055
0·4	1·7425	1·7335	1·7249	1·7169	1·7099	1·7041	1·6997	1·6970	1·6961
0·5	1·9745	1·9592	1·9445	1·9311	1·9194	1·9097	1·9024	1·8979	1·8964
0·6	2·2255	2·2015	2·1789	2·1583	2·1403	2·1256	2·1145	2·1076	2·1053
0·7	2·4952	2·4602	2·4274	2·3977	2·3719	2·3508	2·3351	2·3253	2·3220
0·8	2·7835	2·7346	2·6892	2·6484	2·6133	2·5845	2·5632	2·5499	2·5454
0·9	3·0898	3·0241	2·9637	2·9098	2·8634	2·8258	2·7979	2·7805	2·7747
1·0	3·4135	3·3280	3·2499	3·1807	3·1216	3·0738	3·0383	3·0163	3·0090
1·1	3·7540	3·6455	3·5470	3·4605	3·3870	3·3276	3·2838	3·2566	3·2474
1·2	4·1104	3·9756	3·8542	3·7483	3·6586	3·5866	3·5334	3·5005	3·4894
1·3	4·4819	4·3175	4·1706	4·0432	3·9360	3·8500	3·7868	3·7477	3·7344
1·4	4·8676	4·6703	4·4955	4·3447	4·2183	4·1174	4·0432	3·9974	3·9819
1·5	5·2666	5·0333	4·8281	4·6520	4·5052	4·3883	4·3024	4·2495	4·2315
1·6	5·6780	5·4057	5·1678	4·9647	4·7961	4·6622	4·5641	4·5036	4·4830
1·7	6·101	5·7867	5·5140	5·2823	5·0907	4·9390	4·8279	4·7595	4·7361
1·8	6·535	6·176	5·8662	5·6045	5·3888	5·2184	5·0936	5·0170	4·9908
1·9	6·978	6·572	6·224	5·9308	5·6900	5·5001	5·3613	5·2760	5·2468
2·0	7·431	6·975	6·587	6·261	5·9942	5·7842	5·6307	5·5365	5·5041
2·1	7·893	7·385	6·955	6·595	6·301	6·070	5·9017	5·7982	5·7627
2·2	8·362	7·800	7·327	6·932	6·610	6·358	6·174	6·061	6·022
2·3	8·839	8·220	7·702	7·272	6·922	6·648	6·448	6·325	6·282
2·4	9·322	8·645	8·081	7·614	7·235	6·938	6·722	6·589	6·543
2·5	9·810	9·074	8·462	7·957	7·548	7·229	6·996	6·853	6·803

the radius of a cylinder, then, to a very good approximation, the term A at fixed θ is (Dwiggins, 1975):

$$A\{\mu R_c\}=\exp\left[-\sum_{i=0}^{5} K_i(\mu R_c)^i\right]. \qquad (1)$$

The K terms in equation (1) are constants at fixed θ. Thus, K terms are obtained for each value of θ of interest using the A^* values that are available for cylinders (Dwiggins, 1975).

Making use of equation (1), an equation for A for spheres can be written as:

$$A=\tfrac{3}{2}\int_{x=0}^{1}\{\exp\left[-\sum_{i=0}^{5} K_i(\mu R\sqrt{1-x^2})^i\right]\}\{1-x^2\}\mathrm{d}x. \qquad (2)$$

Direct calculation of absorption correction factors

A double-precision computer program was written in Fortran IV, H-level, for evaluating equation (2) using Simpson's rule for the numerical integration. Increments in x of 0·01 were sufficient for the range of μR of interest. Increasing the number of increments by a factor of two resulted in no significant change in A^* values. The time required to calculate a complete table of A^* values was only a matter of seconds using an IBM 370/165 computer. Copies of the computer program are available.

Results and discussion of direct calculations

Table 1 gives values of A^* calculated at the same values of μR and θ as given in the IT table of A^* values.

At $\theta=0°$ and $\theta=90°$ where A^* can be calculated exactly, the maximum deviation in A^* values calculated using the new method from exact A^* values was 0·038%. For the same conditions, the maximum deviation of the IT A^* values was 0·43%.

If one converts the IT A values to A^* for the few points at which these data are available and compares them with the values of A^* given in Table 1, the maximum deviation between the old and new results is only 0·028%. Thus, the old and new methods of obtaining A^* directly give nearly the same results, and it is thus confirmed that the error in the A^* table is caused by interpolation, roundoff, or both.

The two comparisons just made indicate that it is reasonable to claim a maximum error of 0·05% in the values of A^* given in Table 1.

Interpolation and curve fitting

To use values of A^* given in Table 1 for routine purposes, accurate curve-fitting and interpolation methods are needed. The methods for doing this are exactly the same as in the case of cylinders (Dwiggins, 1975).

The same computer subprogram that is available for cylinders can be used for spheres for curve fitting to obtain A^* as a function of θ at fixed μR. It is necessary to change only constants in the subprogram to use it for spheres. The subprogram with constants for either cylinders or spheres is available from the author.

Values of A^* were calculated for all points of Table 1 using the full-range, curve-fitting method. The maximum deviation found between these values of A^* and those given in Table 1, calculated using equation (2), was 0·029%.

References

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