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Equi-Inclination Weissenberg Intensity Correction Factors for Absorption in Spheres and Cylinders, and for Crystal Monochromatized Radiation

BY W. L. BOND

Bell Telephone Laboratories, Inc., Murray Hill, New Jersey, U.S.A.

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Increased precision of intensity measurements through the use of counting methods calls for more careful corrections. A new absorption correction table is presented for cylinders with μR running from 0 to 8 by tenths and on to 20 by units; also a table for spheres, μR running from 0 to 10 by tenths. In both tables θ runs from 0° to 90° in 5° steps. For cylinders, the correction factor for upper levels is gotten by entering the table with $\mu R \sec \nu$ in place of μR and $\nu/2$ in place of θ , then multiply this value by $\cos \nu$. Tables are also given of the power series coefficients to be used in expanding absorption factors for very large cylinders. A combined polarization Lorentz correction factor is presented for the case of crystal monochromatized radiation.

Introduction

In recent years, there has been increasing emphasis on obtaining highly accurate structure amplitudes from single crystal X-ray data. In the course of work in these Laboratories on a single crystal automatic diffractometer (Bond, 1955; Benedict, 1955), several problems arose with regard to the conversion of intensities to structure amplitudes. These involved: (1) A Lorentz-polarization correction for monochromatized radiation; (2) expanding and improving the absorption tables for cylindrical and spherical crystals; and (3) deriving the method for absorption correction of upper level equi-inclination Weissenberg intensities. In particular, the latter has, as far as can be ascertained, been ignored. It is rather difficult to see how

even for very small crystals containing light atoms, one can claim great accuracy (some claims have been 3%) for F 's obtained say from layers with $\nu \approx 30^\circ$ when such proper correction has not been made. As an example for $\mu R = 1$, $\mu = 20^\circ$, $\nu = 10^\circ$ the absorption correction is 5.09 not 4.80 as is gotten from $\mu R = 1$, true $\theta = 20.6^\circ$.

Absorption correction tables

Consider scattering from a very small element of volume ΔV bathed in a uniform monochromatic collimated beam of X-rays. Let the beam be of intensity I watts cm.^{-2} and let the scattering power in a direction parallel to a vector \mathbf{r} be ϱ_r watts per cm.^3

per incident watt per cm.². In these terms the total power scattered parallel to \mathbf{r} is

$$P_r = I \varrho_r \Delta V \quad (1)$$

watts. This is the power entering the radiation detector RD , Fig. 1. Now consider scattering from a large body

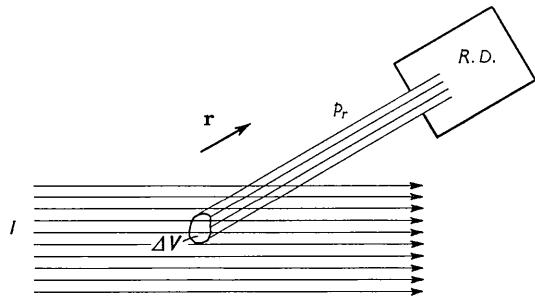


Fig. 1. Power scattered in a direction \mathbf{r} from an element of volume.

of volume V which has a linear absorption coefficient μ , Fig. 2. Choose an element of volume, ΔV in V . The

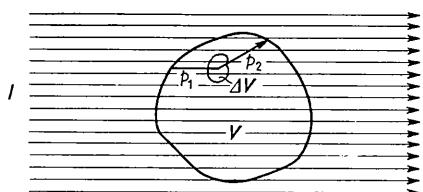


Fig. 2. Power scattered from a finite volume.

intensity I' falling on ΔV is $I' = I \exp(-\mu p_1)$ where p_1 is the path length, inside V of the incident radiation. The power leaving ΔV in the direction \mathbf{r} is therefore $\Delta P'_r = I' \varrho_r \Delta V$ but this is further reduced by absorption along the path p_2 to $\Delta P_r = \Delta P'_r \exp(-\mu p_2)$. Whence the total power received by a properly placed radiation detector is

$$P_r = I \varrho_r \sum_s \exp(-\mu p) \Delta V \quad \text{where } p = p_1 + p_2. \quad (2)$$

Cylindrical specimens

Fig. 3 shows a circular cylinder receiving rays in a direction normal to its axis and scattering in a direction \mathbf{r} also normal to this axis—the zero level case. Now let $\Delta V = w \Delta S$ where S is the cross sectional area of the cylinder, the length w being the width of the incident beam. Thus $P_r = I \varrho_r w \sum_s \exp(-\mu p) \Delta S$.

Following Claassen (1930) we now replace S by s where:

$$S = \pi R^2 s$$

whence

$$P_r = \pi R^2 I \varrho_r w \sum_s \exp(-\mu p) \Delta s, \quad (3)$$

where Δs is the fraction of the cross section in the area element which has path length p . For Bragg

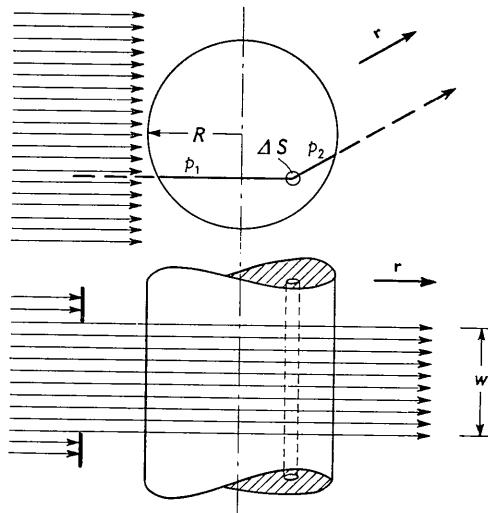


Fig. 3. Power scattered out of a cylinder.

angles θ of 0° , 22.5° , 45° , 67.5° and 90° Claassen constructed curves of equal path length in a set of circles, the path lengths being $1/5R$, $2/5R$, etc. A planimeter was then used to measure the areas between successive curves and hence compute a set of Δs 's. From this small set of Δs 's with their associated path lengths he computed values for $A(\mu, \theta) = \sum \exp(-\mu gR) \Delta s$ where gR is the effective path length associated with Δs . Now making the proper substitution in (3)

$$P_r = \pi R^2 I \varrho_r w A_\theta \quad (4)$$

or solving for ϱ_r

$$\varrho_r = P_r (\pi R^2 I w)^{-1} A_\theta^{-1}.$$

For relative values of ϱ_r the terms π , R^2 , I and w may be omitted. These relative ϱ_r 's are the intensities corrected only for absorption.

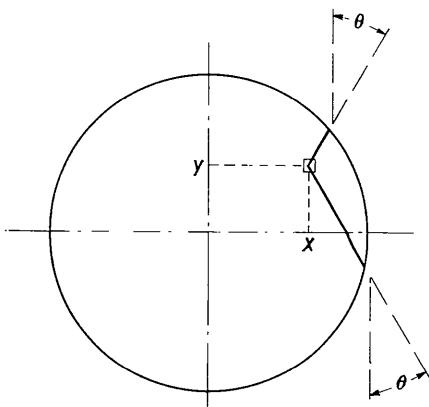


Fig. 4. Paths in a cylinder.

The accuracy of Claassen's method is limited by the necessity of drawing curves of equal path length and the measurement of areas by means of a plani-

Table 1. Areas Δs attributable to reduced paths g.

Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g	Δs	g																													
.00005	.05	.00033	.050	.00094	.050	.00119	.05	.00308	.050	.00457	.050	.0063	.05	.00888	.050	.01046	.050	.0129	.05	.0144	.05																													
.00037	.15	.00076	.150	.00164	.150	.0028	.15	.00423	.150	.00590	.150	.0076	.15	.00986	.150	.01213	.150	.0144	.15	.0144	.15																													
.00102	.25	.00135	.250	.00248	.250	.0039	.25	.00549	.250	.00732	.250	.0093	.25	.01116	.250	.01371	.250	.0160	.25	.0160	.25																													
.00203	.35	.00224	.350	.00349	.350	.0051	.35	.00689	.350	.00886	.350	.0110	.35	.01314	.350	.01539	.350	.0177	.35	.0177	.35																													
.00332	.45	.00360	.450	.00465	.450	.0065	.45	.00843	.450	.01051	.450	.01217	.45	.01489	.450	.01712	.450	.0194	.45	.0194	.45																													
.00522	.55	.00527	.550	.00660	.550	.0080	.55	.01010	.550	.01229	.550	.01445	.55	.01672	.550	.01882	.550	.0210	.55	.0210	.55																													
.00868	.75	.00868	.750	.00986	.750	.0097	.75	.01193	.750	.01419	.750	.01664	.75	.01861	.750	.02078	.750	.0227	.75	.0227	.75																													
.01273	.85	.01285	.850	.01328	.850	.0116	.75	.01623	.750	.01885	.75	.02059	.750	.02265	.750	.0244	.75	.0244	.75	.0244	.75																													
.01635	.95	.01642	.950	.01663	.950	.0160	.95	.01852	.950	.02081	.950	.02289	.950	.02483	.950	.02662	.950	.02826	.95	.02826	.95																													
.02065	1.05	.02064	1.050	.02064	1.050	.0202	1.05	.02216	1.050	.02340	1.050	.02564	1.050	.02712	1.050	.02859	1.050	.0298	1.05	.0298	1.05																													
.02577	1.15	.02568	1.150	.02568	1.150	.0250	1.15	.02911	1.150	.02623	1.150	.02820	1.150	.02953	1.150	.03174	1.150	.0317	1.15	.0317	1.15																													
.03191	1.25	.03171	1.250	.03113	1.250	.0322	1.25	.02741	1.250	.0339	1.25	.03211	1.250	.03288	1.250	.0335	1.25	.0335	1.25	.0335	1.25																													
.03939	1.35	.03905	1.350	.03836	1.350	.0366	1.35	.03333	1.350	.03848	1.350	.0341	1.35	.03488	1.350	.0353	1.350	.0355	1.35	.0355	1.35																													
.04869	1.45	.04816	1.450	.04666	1.450	.0443	1.45	.04141	1.450	.03681	1.450	.0376	1.45	.03792	1.450	.03785	1.450	.0375	1.45	.0375	1.45																													
.05068	1.55	.05099	1.550	.05071	1.550	.0541	1.55	.04979	1.550	.04144	1.550	.0415	1.55	.04123	1.550	.04754	1.550	.0396	1.55	.0396	1.55																													
.07698	1.65	.07571	1.650	.07231	1.650	.0671	1.65	.06072	1.650	.05059	1.650	.04662	1.65	.04900	1.650	.04348	1.650	.0417	1.65	.0417	1.65																													
.10347	1.75	.10342	1.750	.09588	1.750	.0878	1.75	.08250	1.750	.06561	1.750	.05919	1.75	.04944	1.750	.04678	1.750	.0440	1.75	.0440	1.75																													
.15857	1.85	.14195	1.850	.15113	1.850	.1154	1.85	.09562	1.850	.08520	1.850	.07880	1.850	.06916	1.850	.05765	1.850	.04665	1.85	.04665	1.85																													
.39101	1.95	.31101	1.950	.24577	1.950	.1967	1.95	.15114	1.950	.12473	1.950	.17339	1.950	.12813	1.950	.18164	1.950	.0477	1.95	.0477	1.95																													
		.38672	2.004	.17033	2.015	.2424	2.036	.07215	2.114	.18682	2.150	.1318	2.15	.08841	2.150	.06372	2.150	.0511	2.15	.0511	2.15																													
										.01292	2.233	.1468	2.35	.09953	2.250	.06641	2.350	.0512	2.35	.0512	2.35																													
										.01140	2.395	.11033	2.350	.06641	2.350	.0512	2.35	.0512	2.35	.0512	2.35																													
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Table 2. Absorption correction factors A^* for X-ray intensitiesCylinders of radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	45°	50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0	
.1	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	.1	
.2	1.40	1.40	1.40	1.40	1.40	1.40	1.39	1.39	1.39	1.39	1.38	1.38	1.38	1.38	1.38	1.37	1.37	1.37	.2	
.3	1.65	1.65	1.65	1.65	1.65	1.64	1.64	1.63	1.62	1.62	1.61	1.61	1.60	1.59	1.59	1.59	1.59	1.59	.3	
.4	1.95	1.95	1.95	1.94	1.93	1.92	1.91	1.90	1.89	1.87	1.86	1.85	1.84	1.83	1.82	1.82	1.81	1.81	.4	
.5	2.29	2.29	2.29	2.28	2.27	2.26	2.24	2.23	2.22	2.21	2.20	2.19	2.18	2.17	2.16	2.15	2.14	2.13	.5	
.6	2.62	2.62	2.62	2.61	2.61	2.60	2.59	2.58	2.57	2.56	2.55	2.54	2.53	2.52	2.51	2.50	2.49	2.49	.6	
.7	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	.7	
.8	3.70	3.70	3.70	3.68	3.68	3.68	3.66	3.66	3.66	3.65	3.65	3.65	3.65	3.65	3.65	3.65	3.65	3.65	.8	
.9	4.33	4.33	4.33	4.30	4.30	4.26	4.17	4.08	3.98	3.87	3.76	3.65	3.55	3.45	3.37	3.29	3.23	3.18	.9	
1.0	5.05	5.05	5.01	4.92	4.81	4.68	4.54	4.39	4.24	4.10	3.97	3.84	3.73	3.63	3.55	3.48	3.43	3.40	1.0	
1.1	5.90	5.98	5.81	5.69	5.54	5.36	5.16	4.94	4.76	4.58	4.40	4.24	4.00	3.79	3.59	3.33	3.09	3.06	1.1	
1.2	6.86	6.84	6.74	6.57	6.35	6.10	5.84	5.57	5.32	5.08	4.86	4.66	4.49	4.33	4.20	4.11	4.03	3.98	1.2	
1.3	7.96	7.93	7.79	7.55	7.25	6.92	6.58	6.23	5.91	5.61	5.34	5.09	4.88	4.70	4.54	4.42	4.34	4.28	1.3	
1.4	9.23	9.18	8.97	8.65	8.25	7.82	7.37	6.94	6.53	6.16	5.83	5.50	5.29	5.07	4.89	4.75	4.65	4.58	1.4	
1.5	10.7	10.6	10.3	9.88	9.35	8.79	8.22	7.62	7.09	6.74	6.35	6.00	5.65	5.32	5.03	4.79	4.57	4.37	1.5	
1.6	12.3	12.2	12.0	11.8	11.6	11.4	11.3	11.0	10.7	10.4	10.1	9.80	9.51	9.24	8.98	8.70	8.40	8.07	1.6	
1.7	13.8	13.6	13.4	13.2	13.0	12.7	12.1	11.8	11.4	11.1	10.8	10.5	10.2	9.95	9.65	9.33	9.02	8.70	1.7	
1.8	16.3	16.0	15.4	14.6	13.9	13.2	12.2	11.1	10.2	9.32	8.59	7.97	7.45	7.01	6.63	6.33	6.09	5.92	1.8	
1.9	18.6	18.3	17.3	16.8	16.4	15.5	14.8	14.2	13.5	12.2	11.1	10.1	9.25	8.76	8.24	7.75	7.23	6.69	1.9	
2.0	21.3	20.9	19.8	18.8	17.8	16.5	14.8	13.3	12.0	10.9	9.91	9.12	8.45	7.91	7.44	7.06	6.78	6.56	2.0	
2.1	24.2	23.7	22.3	20.3	18.2	16.2	14.5	12.9	11.7	10.6	9.71	8.97	8.36	7.84	7.44	7.13	6.89	6.75	2.1	
2.2	27.5	26.9	25.1	22.6	20.1	17.7	15.7	13.9	12.5	11.3	10.3	9.49	8.82	8.26	7.81	7.47	7.22	7.06	2.2	
2.3	31.2	30.4	28.1	25.1	22.0	19.3	16.9	14.9	13.3	12.0	10.9	10.0	9.29	8.67	8.19	7.82	7.54	7.38	2.3	
2.4	35.3	34.3	31.4	27.7	24.1	20.9	18.2	16.0	14.2	12.7	11.5	10.9	9.76	9.09	8.57	8.17	7.87	7.69	2.4	
2.5	39.8	38.5	34.9	30.5	26.1	22.5	19.5	17.0	15.0	13.1	12.1	11.1	10.2	9.51	8.93	8.53	8.10	7.90	2.5	
2.6	44.7	43.4	38.7	33.4	28.5	23.5	20.2	17.8	14.8	12.8	11.6	10.7	9.93	9.32	8.88	8.53	8.27	8.07	2.6	
2.7	49.1	46.1	41.8	36.8	30.8	26.0	22.2	18.2	14.8	12.8	11.2	10.4	9.72	9.23	8.87	8.54	8.28	8.07	2.7	
2.8	56.1	53.5	47.9	39.3	32.2	27.8	21.6	17.7	13.1	11.7	10.8	10.1	9.59	9.20	8.96	8.69	8.40	8.18	2.8	
2.9	62.5	59.1	51.8	43.1	35.7	29.6	25.0	21.4	18.6	16.4	14.6	13.2	12.1	11.2	10.5	9.95	9.53	9.28	2.9	
3.0	69.5	65.8	56.7	46.6	38.2	31.5	26.4	22.5	19.5	17.1	15.3	13.8	12.6	11.6	10.9	10.3	9.85	9.60	9.53	3.0
3.1	77.2	72.6	61.8	50.3	40.8	33.4	27.9	23.7	20.4	17.9	15.9	14.3	13.1	12.1	11.3	10.7	10.2	9.92	9.81	3.1
3.2	85.4	79.9	67.3	54.0	43.5	35.4	29.3	24.8	21.4	18.7	16.6	14.9	13.6	12.5	11.7	11.0	10.5	10.2	3.2	
3.3	94.2	87.6	72.9	57.7	46.2	37.3	30.8	26.0	22.3	19.4	17.2	15.5	14.1	12.9	12.0	11.1	10.9	10.6	3.3	
3.4	104	95.9	78.9	61.9	48.9	39.3	32.3	27.1	23.2	20.2	17.9	16.0	14.6	13.4	12.4	11.7	11.2	10.9	3.4	
3.5	114	105	85.0	65.1	51.7	41.3	33.8	28.3	24.2	21.0	18.5	16.6	15.1	13.8	12.8	12.1	11.7	11.1	3.5	
3.6	125	114	91.4	70.1	54.6	43.3	35.3	29.5	25.1	21.7	19.3	17.1	15.6	14.2	13.1	12.1	11.5	11.4	3.6	
3.7	136	124	90.0	76.0	60.8	51.6	39.4	32.0	27.7	23.4	20.5	17.7	15.6	14.1	12.9	12.0	11.7	11.7	3.7	
3.8	146	135	105	76.4	70.4	60.4	51.0	39.9	32.0	27.0	23.5	20.5	18.5	16.4	15.1	13.9	12.8	12.1	3.8	
3.9	155	145	112	83.1	63.3	59.2	39.9	31.1	28.0	24.1	21.2	18.8	17.1	15.6	14.4	13.6	12.5	12.4	3.9	
4.0	175	156	119	87.6	66.3	51.6	41.5	34.3	28.9	24.9	21.8	17.6	16.0	14.8	13.9	12.8	12.7	12.0	4.0	
4.1	190	168	127	92.1	69.3	53.8	43.1	35.5	29.9	25.7	22.5	19.6	17.1	15.3	13.6	12.5	11.7	11.0	4.1	
4.2	206	180	134	96.7	72.3	55.9	44.6	37.3	30.8	26.5	23.2	20.6	18.6	16.9	15.6	14.6	13.9	13.5	4.2	
4.3	222	193	142	101	75.4	58.0	46.2	37.9	31.8	27.3	23.8	21.1	19.1	17.3	16.0	15.0	14.3	13.8	4.3	
4.4	239	206	150	106	78.6	65.2	57.8	40.2	32.8	28.1	24.5	21.7	19.6	17.8	16.4	15.4	14.6	14.0	4.4	
4.5	257	220	158	111	81.6	62.3	59.4	40.4	33.8	28.9	25.2	22.3	20.1	18.2	16.8	15.7	14.9	14.3	4.5	
4.6	275	234	166	126	84.7	64.9	51.0	41.6	34.8	29.3	25.0	22.0	19.7	17.6	16.7	15.8	14.8	4.6		
4.7	295	249	175	135	87.0	66.7	52.6	42.8	35.8	30.5	26.5	22.6	20.1	18.1	16.7	15.7	14.7	4.7		
4.8	315	265	182	142	91.0	70.7	55.2	42.7	35.9	30.2	26.0	21.6	18.6	16.9	15.0	14.5	13.8	4.8		
4.9	337	280	192	151	92.8	71.1	55.8	45.3	37.7	32.1	27.9	22.4	20.0	18.4	17.2	16.3	15.7	4.9		
5.0	359	295	200	135	97.4	73.3	57.5	46.6	38.7	32.9	28.6	25.2	22.6	20.5	18.8	17.6	16.1	15.9	5.0	
5.1	383	313	209	140	101	75.5	59.1	47.8	39.7	33.7	29.2	25.8	23.1	20.9	19.2	18.0	17.0	16.4	5.1	
5.2	407	330	218	145	107	77.8	60.7	59.1	40.7	34.5	29.9	26.3	23.6	21.4	19.6	18.3	17.3	16.6	5.2	
5.3	432	348	228	150	107	80.0	62.4	50.3	41.7	35.3	30.6	26.9	24.1	21.8	20.0	18.7	17.7	17.1	5.3	
5.4	458	366	237	156	110	82.3	64.0	51.6	42.7	36.1	31.3	27.5	24.6	22.3	20.4	19.1	18.0	17.4	5.4	
5.5	485	384	246	161	114	84.5	65.7	52.9	43.7	37.0	32.0	28.1	25.2	22.7	20.9	19.5	18.4	5.5		
5.6	513	503	255	166	118	86.8	68.1	54.1	44.7	37.6	32.7	29.2	25.7	22.8	20.9	19.8	18.7	5.6		
5.7	542	522	255	176	124	91.0	69.0	52.2	45.4	38.2	33.4	29.8	26.8	23.6	21.5	20.7	19.5	5.7		
5.8	562	542	255	182	127	97.9	73.5	63.3	52.8	45.3	39.5	35.1	31.5	28.7	25.7	22.1	20.6	19.1	5.8	
5.9	582	572	267	182	127	103	99.8	78.9	64.3	53.7	46.0	40.1	35.6	31.9	29.2	25.7	22.6	21.5	5.9	
6.0	602	610	277	185	126	105	102	98.0	71.3	60.1	53.7	43.1	37.6	33.5	29.6	25.1	22.7	21.5	6.0	
6.1	620	625	282	187	127	107	101	98.7	74.2	63.0	54.3	45.2	37.6	33.5	29.7	25.5	22.8	21.8		

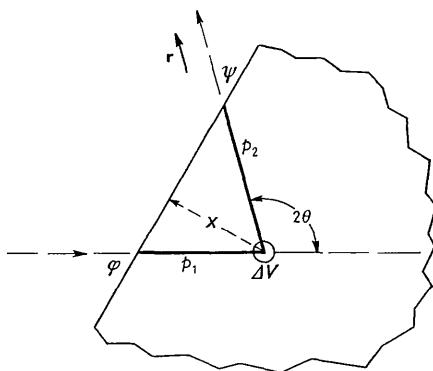


Fig. 5. Path lengths in a semi-infinite solid.

next few coefficients may be found empirically. Consider scattering from an element of volume ΔV inside a semi infinite solid, Fig. 5,

$$\Delta P_r = I\varrho_r \exp [-\mu(p_1 + p_2)] \Delta V$$

but $x = p_1 \sin \Phi = p_2 \sin (2\theta - \Phi)$ so

$$\Delta P_r = I\varrho_r \exp \left[-\mu p_1 \left\{ 1 + \frac{\sin \Phi}{\sin (2\theta - \Phi)} \right\} \right] \Delta V .$$

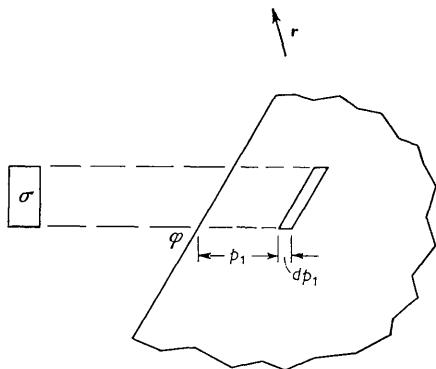


Fig. 6. Scattering from an element of volume in a semi-infinite solid.

A beam of cross sectional area σ (see Fig. 6) sends power

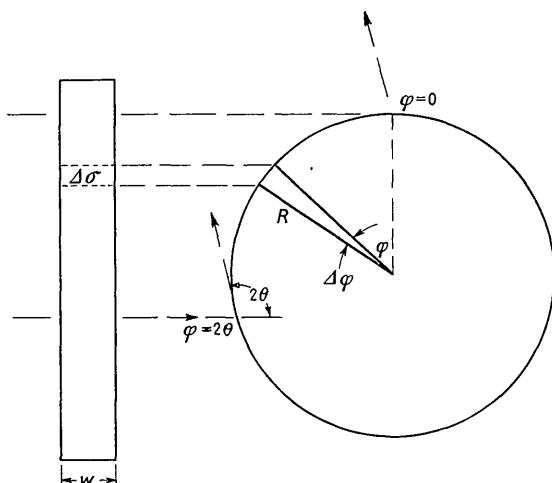
$$P_r = I\varrho_r \sigma \int_{-\infty}^{\infty} \exp \left[-\mu p_1 \left\{ 1 + \frac{\sin \Phi}{\sin (2\theta - \Phi)} \right\} \right] dp_1$$

in the direction r .

Integrating:

$$P_r = \frac{I\varrho_r \sigma \sin (2\theta - \Phi)}{\mu [\sin \Phi + \sin (2\theta - \Phi)]} .$$

Now consider the effective scattering section, of the cylinder, Fig. 7, the part between $\Phi = 0$ and $\Phi = 2\theta$. We can compute the power sent parallel to r by an infinity of blocks of length $R\Delta\Phi$. Here σ of the preceding equation is replaced by $\Delta\sigma = wR \sin \Phi \Delta\Phi$ so that the power increment is

Fig. 7. Scattering from a cylinder of large μ .

$$\Delta P_v = \frac{I\varrho_r w R}{\mu} \cdot \frac{\sin \Phi \sin (2\theta - \Phi)}{\sin \Phi + \sin (2\theta - \Phi)} \Delta\Phi$$

and

$$P_v = \frac{I\varrho_r w R}{\mu} \int_{\Phi=0}^{2\theta} \frac{\sin \Phi \sin (2\theta - \Phi)}{\sin \Phi + \sin (2\theta - \Phi)} d\Phi .$$

Integrating

$$P_r = \frac{I\varrho_r w R}{\mu} \left\{ 1 - \frac{\cos^2 \theta}{\sin \theta} \ln \tan \left(\frac{\pi}{4} + \frac{\theta}{2} \right) \right\} .$$

Comparing this with equation (4)

$$A_\theta = \frac{1}{\pi \mu R} \left\{ 1 - \frac{\cos^2 \theta}{\sin \theta} \ln \tan \left(\frac{\pi}{4} + \frac{\theta}{2} \right) \right\} \text{ for } \mu R \text{ large.}$$

Hence the coefficient of $(\mu R)^{-1}$ is

$$\pi^{-1} \left\{ 1 - \frac{\cos^2 \theta}{\sin \theta} \ln \tan \left(\frac{\pi}{4} + \frac{\theta}{2} \right) \right\} .$$

Table 3. Coefficients for 5° intervals of θ

θ	α	2β	6γ	248	120ε	5040η
0	0	0	0.3183	0	0.955	0 7·1
5	0.001615	0.0314	0.0648	0.835	0.14	
10	0.00642	0.053	0.179	0.057		
15	0.01442	0.086	0.061	0.33		
20	0.0254	0.105	0.080	0.13		
25	0.0394	0.123	0.073	-0.16		
30	0.0560	0.139	0			
35	0.0752	0.150	-0.022			
40	0.0966	0.159	-0.10			
45	0.1199	0.164	-0.16			
50	0.1448	0.16	-0.20			
55	0.1741	0.13	-0.30			
60	0.1984	0.11	-0.21			
65	0.226	0.10	-0.33			
70	0.250	0.105	-0.48			
75	0.274	0.08	-0.52			
80	0.295	0.064	-0.64			
85	0.3107	0.03	-0.5			
90	0.3183	0	-0.53			

For small θ , $\alpha = 2\theta^2/(3\pi)$. $A = \alpha/(\mu R) + 2\beta/(\mu^2 R^2) \dots$

Table 3 gives the values of the coefficients for 5° intervals of θ . We can find A and hence A^* for intermediate values of θ by plotting A against $\sin^2 \theta$ (Bradley, 1935).

Optimum size of cylinders for the zero level

Equation (4) indicates that the power received by the radiation detector is proportional to $(\mu R)^2 A \theta$. Plots of $(\mu R)^2 / A^*$ show that for $\theta = 0^\circ$ the optimum size is $\mu R = 1.35$, for $\theta = 10^\circ$ it is $\mu R = 1.45$ and for $\theta = 20^\circ$ it is $\mu R = 1.9$. Above $\theta = 25^\circ$ there is no optimum since $(\mu R)^2 / A^*$ rises continuously from $\mu R = 0$ to $\mu R = \infty$ if $\theta > 25^\circ$. Hence a practical optimum for cylinders is $\mu R = 1.5$.

Absorption corrections for upper levels of the equi-inclination Weissenberg-cylindrical specimens

In the equi-inclination case, Fig. 8 both the on coming and the departing rays make an angle $90^\circ - \nu$ with the cylinder axis. Hence the path lengths p_1 and p_2 of Fig. 3 become $p_1 \sec \nu$ and $p_2 \sec \nu$ in Fig. 8.

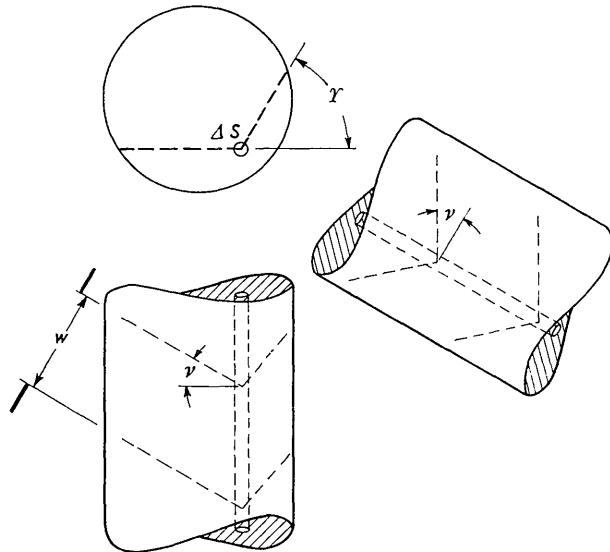


Fig. 8. Path lengths and angles for upper levels.

Also the volume element is $w \sec \nu \Delta S$. Hence the power received by a properly placed radiation detector is from equation (2):

$$P_r = I \varrho_r \sum_v \exp(-\mu \sec \nu \cdot p) \Delta V$$

or

$$P_r = \pi R^2 I \varrho_r w \sec \nu \sum_s \exp [(-\mu \sec \nu) \varrho] \Delta s. \quad (6)$$

Setting $\mu' = \mu \sec \nu$ it is seen that the function under the summation is $A(\mu' R, \gamma/2)$. If ν goes to zero $\gamma/2$ becomes θ and μ' becomes μ so that $A(\mu' R, \gamma/2)$ goes to $A(\mu R, \theta)$. To compare reflections in the same level it is necessary only to compare the respective values

of $P_v A^*(\mu' R, \gamma/2) = \varrho_v \times \text{const.}$ However if we wish to compare reflections in different levels we must use

$$\varrho_r \times \text{const.} = P_r \cos \nu A^*(\mu R \sec \nu, \gamma/2).$$

Spherical specimens

If we take $V = 4/3\pi R^3 v$ we may re-write equation (2) as

$$P_r = 4/3\pi R^3 I \varrho_r \sum_v \exp(-\mu p) \Delta v.$$

A machine integration of $\sum_v \exp(-\mu p) \Delta v$ gives the data of Table 4. It is worth noting that for $\theta = 0$ and $\theta = 90^\circ$ the equation is integrable. For $\theta = 0$ the absorption factor is

$$A = \frac{3}{2(\mu R)^3} \left\{ \frac{1}{2} - \exp(-2\mu R)[\frac{1}{2} + \mu R + (\mu R)^2] \right\}.$$

While for $\theta = 90^\circ$:

$$A = \frac{3}{4\mu R} \left[\frac{1}{2} - \frac{1}{16(\mu R)^2} [1 - (1+4\mu R) \exp(-4\mu R)] \right].$$

Optimum size for spheres

Plotting $(\mu R)^3 / A^*$ shows that there is no optimum size for spheres, the total reflected energy rises continuously from $\mu R = 0$ to $\mu R = \infty$ for all values of θ .

The concept of 'optimum size' is misleading. The desirable condition is that the correction factor for $\theta = 0$ be not too different from the correction factor for $\theta = 90^\circ$. This is met if $\mu R < 2$, when the ratio of front to back factors is less than 2.6.

The polarization correction

The polarization correction using a monochromator (Whittaker, 1952) can be combined with the Lorentz factor as follows: Whittakers result for the equi-inclination case may be written as a correction factor as

$$P = (1 + \cos^2 2e)^{-1} \{ \cos^2 2e (1 - \cos^2 \nu \sin^2 \gamma) + 1 - \sin^2 \nu \cos^2 \nu (1 + \cos \gamma)^2 \},$$

where e is the Bragg angle for the monochromator.

The Lorentz factor as adapted to the equi-inclination Weissenberg by Tunnel (1939) is $L = \cos^2 \nu \sin \gamma/2$. Since $\cos \theta = \cos \nu \cos \gamma/2$ we can write the combined correction factor as

$$P_L = T \sin 2\theta \left/ \left\{ 1 + \left(\frac{q - \sin^2 \nu}{(1+q) \cos^2 \nu} \right) \times (1 + \cos 2\theta)^2 - \frac{2q}{1+q} (1 + \cos 2\theta) \right\} \right.,$$

where $q = \cos^2 2e$

and

$$T = (\sin^2 \theta - \sin^2 \nu)^{1/2} / \sin \theta.$$

Table 4. Absorption correction factors A^* for X-ray intensities
Spheres of radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	45°	50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0	
1	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.1	
2	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.2	
3	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.56	1.3	
4	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.80	1.4	
5	2.08	2.07	2.07	2.06	2.06	2.05	2.03	2.02	2.01	1.99	1.97	1.96	1.94	1.92	1.91	1.90	1.90	1.90	1.5	
6	2.39	2.39	2.38	2.37	2.36	2.34	2.32	2.30	2.27	2.25	2.23	2.20	2.18	2.16	2.14	2.13	2.11	2.11	1.6	
7	2.75	2.75	2.73	2.72	2.70	2.67	2.64	2.60	2.57	2.53	2.50	2.46	2.43	2.40	2.37	2.35	2.33	2.32	1.7	
8	3.15	3.15	3.13	3.11	3.07	3.03	2.99	2.94	2.89	2.83	2.78	2.73	2.69	2.63	2.58	2.56	2.55	2.55	1.8	
9	3.61	3.60	3.58	3.54	3.50	3.44	3.37	3.30	3.23	3.16	3.09	3.02	2.96	2.86	2.82	2.80	2.78	2.77	1.7	
1.0	4.12	4.11	4.08	4.03	3.96	3.88	3.79	3.70	3.63	3.50	3.41	3.33	3.25	3.17	3.07	3.02	3.02	3.01	1.0	
1.1	4.70	4.69	4.64	4.57	4.58	4.37	4.25	4.12	3.99	3.87	3.75	3.52	3.42	3.33	3.23	3.16	3.15	3.25	1.1	
1.2	5.33	5.33	5.27	5.1	5.05	4.90	4.74	4.54	4.34	4.11	3.97	3.75	3.59	3.42	3.29	3.19	3.19	3.19	1.2	
1.3	6.03	6.03	5.97	5.84	5.67	5.47	5.27	5.06	4.85	4.66	4.48	4.2	4.17	4.04	3.94	3.85	3.75	3.73	1.3	
1.4	6.76	6.76	6.76	6.76	6.76	6.56	6.33	6.11	5.87	5.65	5.32	5.1	4.9	4.74	4.54	4.34	4.22	4.12	1.4	
1.5	7.50	7.75	7.60	7.38	7.09	6.77	6.44	6.11	5.81	5.52	5.26	5.03	4.83	4.62	4.41	4.39	4.31	4.26	1.5	
1.6	8.81	8.74	8.55	8.25	8.09	7.79	7.08	6.69	6.32	5.98	5.67	5.0	5.17	4.97	4.80	4.67	4.57	4.51	1.6	
1.7	9.92	9.83	9.59	9.21	9.76	8.26	7.76	7.29	6.85	6.45	6.10	5.78	5.51	5.28	5.09	4.94	4.83	4.77	1.7	
1.8	11.2	11.0	10.7	10.3	9.69	9.08	8.48	7.92	7.40	6.94	6.53	6.17	5.87	5.56	5.39	5.22	5.10	5.02	1.8	
1.9	12.5	12.4	12.0	11.4	10.7	9.95	9.24	8.58	7.98	7.44	6.97	6.57	6.22	5.92	5.59	5.30	5.27	5.25	1.9	
2.0	14.0	13.8	13.3	12.6	11.8	10.9	10.0	9.26	8.57	7.96	7.43	6.97	6.59	6.26	5.99	5.78	5.63	5.54	2.0	
2.1	15.6	15.4	14.8	13.9	12.9	11.8	10.9	9.97	9.18	8.49	7.89	7.38	6.95	6.56	6.30	6.07	5.90	5.76	2.1	
2.2	17.4	17.1	16.4	15.3	14.1	12.9	11.7	10.7	9.30	8.36	7.80	7.30	6.91	6.63	6.36	6.17	6.06	6.02	2.2	
2.3	19.4	19.0	18.1	16.8	15.3	13	12.6	11.2	10.4	9.57	8.68	8.23	7.82	7.43	7.03	6.64	6.33	6.28	2.3	
2.4	21.5	21.1	19.5	18.4	17.1	15.0	13.5	12.2	11.1	10.2	9.61	9.07	8.46	7.95	7.54	7.23	6.99	6.85	2.4	
2.5	23.6	22.6	21.0	21.8	19.5	17.3	15.4	13.0	11.7	10.3	9.51	8.85	8.30	7.86	7.52	7.27	7.12	7.06	2.5	
2.6	25.0	24.2	22.1	21.0	19.8	17.8	15.4	13.8	12.4	11.3	10.3	9.84	8.61	8.17	7.81	7.54	7.38	7.27	2.6	
2.7	27.0	26.2	23.7	21.0	18.6	16.4	14.6	13.1	11.8	10.8	9.94	9.23	8.61	8.17	7.81	7.54	7.38	7.27	2.7	
2.8	31.9	30.9	28.6	25.6	22.6	19.8	17.4	15.4	13.8	12.4	11.3	10.4	9.62	8.95	8.49	8.10	7.82	7.65	2.8	
2.9	35.0	33.9	31.2	27.7	24.2	21.1	18.5	16.3	13.0	11.8	10.8	10.0	9.31	8.81	8.40	8.10	7.92	7.85	2.9	
3.0	38.4	37.0	33.9	29.9	25.9	22.4	19.5	17.1	15.2	13.6	12.3	11.3	10.4	9.76	9.13	8.70	8.38	8.18	3.0	
3.1	42.0	40.4	36.7	34.1	27.7	22.8	20.6	18.0	15.9	14.2	12.8	11.7	10.8	10.0	9.45	8.99	8.66	8.45	3.1	
3.2	45.8	43.9	39.7	34.4	29.5	25.2	21.7	18.9	16.6	14.8	13.4	12.2	11.2	10.4	9.91	9.29	8.94	8.69	3.2	
3.3	49.9	47.7	42.8	36.8	31.1	26.6	22.9	19.8	17.4	15.4	13.4	12.2	11.1	10.1	9.49	9.81	9.41	9.09	3.3	
3.4	54.4	51.2	46.0	39.3	33.2	28.1	23.9	20.6	18.4	16.4	14.4	12.4	11.1	10.4	9.88	9.29	8.93	8.61	3.4	
3.5	58.9	52.0	45.6	39.1	33.2	28.1	23.9	20.6	18.4	16.4	14.4	12.4	11.1	10.7	9.97	9.52	9.13	8.75	3.5	
3.6	60.4	55.0	44.6	37.1	31.0	26.2	22.5	19.6	17.3	15.5	14.5	12.8	11.1	10.5	10.1	9.79	9.69	9.36	8.98	
3.7	69.0	65.1	56.8	51.3	39.2	32.6	27.4	23.4	20.4	17.9	16.0	14.5	13.2	11.4	10.3	10.1	9.96	9.77	9.37	
3.8	74.6	70.1	60.6	50.2	41.2	34.1	28.6	24.4	21.1	18.6	16.5	14.9	12.6	11.7	11.1	10.6	10.3	10.2	3.8	
3.9	80.4	75.3	64.6	51.1	43.3	35.7	29.8	25.3	21.9	17.1	15.4	14.0	12.9	12.0	11.4	10.9	10.6	10.5	3.9	
4.0	86.5	80.7	68.8	56.0	45.5	37.2	31.0	26.3	22.7	19.8	17.6	15.8	14.4	13.3	12.4	11.7	11.2	10.9	4.0	
4.1	93.0	86.4	73.1	59.1	47.6	38.8	32.2	27.2	23.4	20.5	18.2	16.3	14.8	13.1	12.7	12.0	11.5	11.1	4.1	
4.2	99.8	92.4	77.5	62.2	49.9	40.5	34.4	28.2	24.2	21.1	18.7	16.8	15.2	14.0	13.0	12.3	11.7	11.4	4.2	
4.3	10.7	98.6	82.1	65.3	52.1	42.1	34.7	29.2	25.0	21.8	19.3	17.2	15.7	14.1	13.4	12.6	12.0	11.7	4.3	
4.4	11.4	10.5	86.8	68.6	54.4	43.7	35.9	30.1	25.8	22.4	19.8	17.6	16.1	14.7	13.7	12.9	12.3	11.9	4.4	
4.5	12.0	11.2	91.7	71.9	56.7	55.4	37.2	31.1	26.6	21.1	20.3	18.2	16.5	15.1	14.0	13.2	12.6	12.2	4.5	
4.6	13.0	12.6	96.7	75.0	59.0	57.0	41.1	34.8	29.0	25.9	22.9	20.6	18.6	16.9	15.3	14.3	13.9	13.6	4.6	
4.7	14.9	12.6	10.2	78.6	60.9	48.8	40.1	33.8	29.0	25.2	22.7	20.4	18.7	17.1	16.2	15.4	14.9	14.5	4.7	
4.8	17.7	15.8	12.4	92.7	71.0	55.6	44.8	37.1	31.3	27.0	23.7	21.0	19.0	17.3	16.0	15.0	14.3	13.8	5.1	
4.9	18.8	16.7	12.9	96.4	73.4	57.4	46.1	38.1	32.2	27.7	24.5	21.5	19.4	17.7	16.3	15.3	14.6	14.1	5.2	
5.0	19.9	17.6	13.5	10.0	75.9	59.2	47.4	39.1	33.0	28.3	24.8	22.0	19.8	18.0	16.7	15.6	14.9	14.2	5.3	
5.1	21.0	18.5	14.1	10.4	78.1	60.9	48.8	40.1	33.8	29.0	25.5	20.2	18.4	17.0	15.9	15.1	14.6	14.5	5.4	
5.2	22.2	19.4	14.7	10.8	80.9	62.7	50.1	41.1	34.6	29.7	25.9	20.6	18.6	17.3	16.2	15.1	14.9	14.7	5.5	
5.3	23.4	20.4	12.9	87.5	68.0	52.4	45.5	39.5	32.4	26.1	23.4	19.1	17.0	15.5	14.5	13.5	13.2	13.0	5.6	
5.4	24.7	21.0	11.5	86.0	60.0	52.4	45.5	39.5	32.4	26.1	23.4	19.1	17.0	15.5	14.5	13.5	13.2	13.0	5.7	
5.5	26.0	22.4	16.6	88.6	68.1	52.1	47.0	39.7	32.6	27.0	24.9	21.9	18.8	17.6	16.5	15.5	15.3	15.0	5.8	
5.6	27.4	23.5	17.3	91.2	71.8	57.8	47.8	40.5	34.9	30.7	27.3	24.7	21.1	20.0	19.9	19.0	18.7	18.4	5.9	
5.7	28.8	24.6	17.9	86.4	73.2	58.9	48.7	41.2	35.0	31.5	27.8	25.1	23.0	21.4	20.3	19.2	19.0	18.7	6.0	
5.8	30.0	28.0	20.0	13.9	10.2	77.2	70.6	60.8	49.4	42.1	35.0	30.4	26.8	24.0	21.7	20.0	18.7	18.4	6.1	
5.9	31.8	29.3	20.7	14.3	10.4	79.1	71.9	64.5	51.0	45.3	39.4	33.7	29.4	26.1	23.1	20.9	19.7	19.4	6.2	
6.0	35.0	30.9	27.5	18.2	12.9	90.0	77.4	71.7	65.9	50.1	42.9	36.1	31.6	28.2	25.5	22.8	20.5	19.2	6.3	
6.1	37.1	34.1	21.																	