Acta Cryst. (1965). **19**, 68

The Integrated Intensities of Perfect Crystals

BY J. J. DEMARCO AND R. J. WEISS

U.S. Army Materials Research Agency, Watertown, Massachusetts, U.S.A.

(*Received* 16 *October* 1964)

The absorption correction R_H^y to Bragg reflections from perfect crystals, evaluated on the IBM 1620 computer, is presented in tabular form as a function of g and k to an interpolated accuracy of 0·1 % (the notation is that of Zachariasen, *Theory of X-ray Diffraction in Crystals,* 1945).

Values of the integrals involved in the expressions for R_H^y and R_T^y (Laue case) are tabulated.

Expressions are given which enable one to determine the thermal diffuse scattering correction to the integrated intensity of a perfect crystal.

For $g>0·85$ where $k \simeq |g|$, we find the unusual case that the ratio of the integrated intensity of a mosaic to a perfect crystal becomes less than unity.

1. Introduction

The expressions for the integrated intensities from perfect absorbing crystals are available only in integral form since the expressions are not soluble in terms of simple fuctions (Zachariasen, 1945; Kato, 1955; Hirsch & Ramachandran, 1950; Hirsch, 1952). For the Bragg case (reflection from a perfect crystal) we have evaluated the so-called 'Prins' correction and present it in tabular form so that linearly interpolated values are accurate to ~0·1%. In the Laue case (transmission through a plane parallel perfect crystal slab) the solutions are given partially in tabular form and partially in convenient power series, the only limitation being that $k<0·1$; $|g|<0·1$ for the diffracted beams. These conditions are generally met in transmission [($|g|$ and k are defined in equations (2) and (3)].

2. The Bragg case

Thick crystal $|g|A>4$

The integral reflecting power, E, for X-rays is given by

$$\frac{E\omega}{I} = \frac{K\lambda^2 e^2 |F'_H| e^{-M}}{\pi\sqrt{|b|}mc^2 V \sin 2\theta_B} R_H^y(\text{Bragg})$$

$$R_H^y(\text{Bragg}) = \int_{-\infty}^{\infty} (L-\sqrt{L^2-1})\,dy$$

$$L=\{y^2+g^2 + |\sqrt{(y^2-g^2-1+k^2)^2+4(gy-k)^2}|\}/(1+k^2) \quad (1)$$

where θ_B is the Bragg angle, e^{-M} the Debye–Waller factor, K the polarization factor ($|\cos 2\theta|$ and unity respectively for π and σ polarization), ω the angular velocity of the crystal, I the incident beam power (photons . sec^{-1}), V the volume of the unit cell, F_H the structure factor for the unit cell, b the ratio of the direction cosines of the incident and emergent beams relative to the crystal surface ($b=-1$ for symmetrical reflection), and R_H^y(Bragg) is the Prins correction which is given in Table 1 as a function of the two parameters g and k ($|g|$, 0 to 3·0; k, 0 to 1·0).

$$g=-\frac{(1-b)mc^2\mu V\sqrt{1+k^2}}{4\sqrt{|b|}e^2\lambda|F_H|Ke^{-M}} \quad (2)$$

$$k=\frac{F''_H}{F'_H} \equiv \frac{\varepsilon F''_0}{F'_H} \quad (3)^*$$

where μ is the measured linear absorption coefficient, F''_H the imaginary part of the strcture factor, F'_H the real part of the structure factor ($F''_H+F'_H=F_H$), and ε the ratio of the imaginary part of the structure factor for a given Bragg peak relative to its value in the forward direction ($\varepsilon=F''_H/F''_0$). At the present writing this quantity is undergoing theoretical investigation and its precise value is rarely known (Wagenfeld, 1962). Fortunnately, it is generally close to unity. Since k is generally small compared with unity and since R_H^y varies $\sim(1+k^2)$, precise values of ε are generally not required in the Bragg case in order to evaluate equation (1) to 0·1%. Table 1 may be interpolated between g values and between k values. [For values of $|g|$ and k larger than 1·0, R_H^y(Bragg) can be obtained from values of the enhancement factor Γ [equation (15)] given in Table 4; *cf.* § 5 and § 6.]

3. The Laue case

(*a*) *Diffracted beam,* $k<0·1$; $g<0·1$

The integrated intensity for X-rays diffracted by a plane parallel plate (Kato, 1955) is given by equation (1) except that R_H^y(Bragg) is replaced by R_H^y(Laue) where for $|g|<0·1$, $k<0·1$

* For non-centrosymmetric reflections such as the odd index reflection in the diamond structure, $k=\psi_H\bar{\psi}_H-|\psi_H'|^2/2i|\psi_H'|^2$. See Zachariasen (1945, p. 137) for notation. For a general treatment of the non-centrosymmetric case, see Cole & Stemple (1962).

Table 1. *Values of R^y_H for the Bragg reflection from infinitely thick perfect crystals* ($A>4$) *where*

$$R_H{}^y(\text{Bragg}) = \int_{-\infty}^{\infty} L - \sqrt{L^2-1}\, dy$$

$$L = \{y^2+g^2+|[(y^2-g^2-1+k^2)^2+4(gy-k^2)]^{\frac{1}{2}}|\}/(1+k^2)\ .$$

Interpolated values are accurate to $\sim 0{\cdot}1\,\%$. From the definitions of k and g, $|k|<|g|$. For $|g|<0{\cdot}1$ we have the approximation

$$R_H{}^y(\text{Bragg}) \simeq \tfrac{8}{3}[1-2{\cdot}4|g|+5{\cdot}3g^2+2{\cdot}1k^2]$$

which is accurate to about $\frac{1}{2}\,\%$.

The subsidiary table gives values of $R_H{}^y(\text{Bragg})$ for $|g|=k$ and these are useful for interpolation when values of k are only slightly smaller than $|g|$.

-g	k = 0	0.025	0.050	0.075	0.100	0.125	0.150	0.175	0.200	0.250	0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000
0.000	2.6667																	
.005	2.6357																	
.010	2.6059																	
.015	2.5769																	
.020	2.5487																	
.025	2.5207	2.5278																
.030	2.4937	2.4998																
.035	2.4674	2.4730																
.040	2.4415	2.4468																
.045	2.4162	2.4212																
.050	2.3913	2.3959	2.4113															
.055	2.3669	2.3713	2.3855															
.060	2.3430	2.3472	2.3606															
.065	2.3195	2.3236	2.3364															
.070	2.2964	2.3004	2.3126															
.075	2.2738	2.2775	2.2893	2.3106														
.080	2.2515	2.2552	2.2664	2.2864														
.085	2.2296	2.2332	2.2440	2.2631														
.090	2.2081	2.2115	2.2220	2.2404														
.095	2.1870	2.1903	2.2005	2.2182														
.100	2.1662	2.1694	2.1793	2.1961	2.2230													
.105	2.1457	2.1488	2.1584	2.1748	2.1994													
.110	2.1256	2.1286	2.1380	2.1538	2.1774													
.115	2.1058	2.1088	2.1178	2.1332	2.1557													
.120	2.0863	2.0892	2.0980	2.1130	2.1347													
.125	2.0671	2.0700	2.0785	2.0931	2.1142	2.1442												
.130	2.0483	2.0510	2.0594	2.0736	2.0941	2.1224												
.135	2.0297	2.0324	2.0405	2.0544	2.0743	2.1016												
.140	2.0114	2.0140	2.0220	2.0355	2.0549	2.0810												
.145	1.9934	1.9960	2.0037	2.0169	2.0358	2.0611												
.150	1.9757	1.9781	1.9858	1.9986	2.0170	2.0416	2.0773											
.155	1.9582	1.9606	1.9681	1.9806	1.9986	2.0225	2.0540											
.160	1.9410	1.9434	1.9506	1.9629	1.9804	2.0038	2.0339											
.165	1.9240	1.9264	1.9335	1.9455	1.9626	1.9854	2.0145											
.170	1.9073	1.9096	1.9166	1.9283	1.9450	1.9672	1.9956											
.175	1.8909	1.8931	1.8999	1.9114	1.9278	1.9494	1.9771	2.0129										
.180	1.8746	1.8768	1.8835	1.8948	1.9107	1.9320	1.9589	1.9930										
.185	1.8586	1.8608	1.8673	1.8783	1.8940	1.9147	1.9410	1.9740										
.190	1.8429	1.8450	1.8514	1.8622	1.8776	1.8978	1.9234	1.9555										
.195	1.8273	1.8294	1.8357	1.8463	1.8614	1.8812	1.9062	1.9373										
.200	1.8120	1.8140	1.8202	1.8306	1.8454	1.8648	1.8893	1.9196	1.9576									
.210	1.7820	1.7840	1.7899	1.7999	1.8141	1.8328	1.8562	1.8849	1.9202									
.220	1.7529	1.7547	1.7605	1.7701	1.7838	1.8017	1.8242	1.8516	1.8851									
.230	1.7244	1.7263	1.7319	1.7411	1.7544	1.7716	1.7932	1.8195	1.8512									
.240	1.6969	1.6986	1.7040	1.7130	1.7257	1.7424	1.7632	1.7885	1.8187									
.250	1.6700	1.6717	1.6769	1.6856	1.6979	1.7140	1.7341	1.7584	1.7874	1.8637								
.260	1.6438	1.6455	1.6505	1.6589	1.6709	1.6864	1.7058	1.7292	1.7571	1.8290								
.270	1.6183	1.6199	1.6248	1.6330	1.6446	1.6596	1.6783	1.7010	1.7278	1.7964								
.280	1.5935	1.5951	1.5998	1.6077	1.6190	1.6335	1.6517	1.6735	1.6994	1.7652								
.290	1.5693	1.5708	1.5754	1.5831	1.5940	1.6082	1.6257	1.6469	1.6719	1.7350								
.300	1.5457	1.5472	1.5516	1.5592	1.5697	1.5835	1.6005	1.6210	1.6452	1.7059	1.7886							
.310	1.5227	1.5242	1.5285	1.5358	1.5461	1.5594	1.5760	1.5959	1.6192	1.6779	1.7561							
.320	1.5003	1.5017	1.5059	1.5130	1.5230	1.5360	1.5521	1.5714	1.5941	1.6507	1.7256							
.330	1.4784	1.4798	1.4839	1.4908	1.5006	1.5132	1.5288	1.5476	1.5695	1.6244	1.6963							
.340	1.4571	1.4584	1.4625	1.4692	1.4787	1.4910	1.5062	1.5244	1.5458	1.5989	1.6681							
.350	1.4363	1.4376	1.4415	1.4481	1.4573	1.4693	1.4841	1.5019	1.5227	1.5742	1.6409							
.360	1.4160	1.4172	1.4211	1.4275	1.4365	1.4482	1.4626	1.4799	1.5001	1.5502	1.6147							
.370	1.3962	1.3974	1.4011	1.4074	1.4162	1.4276	1.4417	1.4585	1.4782	1.5268	1.5893							
.380	1.3768	1.3780	1.3816	1.3877	1.3964	1.4075	1.4212	1.4376	1.4568	1.5041	1.5647							
.390	1.3578	1.3591	1.3626	1.3886	1.3770	1.3879	1.4013	1.4173	1.4360	1.4821	1.5409							
.400	1.3394	1.3406	1.3441	1.3499	1.3581	1.3687	1.3818	1.3975	1.4157	1.4606	1.5178	1.6816						
.410	1.3213	1.3225	1.3259	1.3316	1.3397	1.3500	1.3628	1.3781	1.3960	1.4397	1.4953	1.6524						
.420	1.3037	1.3048	1.3082	1.3138	1.3216	1.3318	1.3443	1.3592	1.3767	1.4194	1.4735	1.6252						
.430	1.2865	1.2876	1.2909	1.2963	1.3040	1.3139	1.3262	1.3408	1.3578	1.3995	1.4523	1.5990						
.440	1.2697	1.2707	1.2739	1.2793	1.2868	1.2965	1.3085	1.3228	1.3394	1.3802	1.4317	1.5739						
.450	1.2532	1.2542	1.2574	1.2626	1.2700	1.2795	1.2913	1.3052	1.3215	1.3613	1.4116	1.5496						
.460	1.2371	1.2381	1.2412	1.2463	1.2536	1.2629	1.2744	1.2881	1.3040	1.3430	1.3920	1.5261						
.470	1.2213	1.2223	1.2253	1.2304	1.2375	1.2466	1.2579	1.2713	1.2869	1.3250	1.3730	1.5035						
.480	1.2059	1.2069	1.2098	1.2148	1.2218	1.2307	1.2418	1.2549	1.2702	1.3075	1.3544	1.4815						
.490	1.1909	1.1918	1.1947	1.1996	1.2064	1.2152	1.2260	1.2389	1.2539	1.2904	1.3363	1.4602						
.500	1.1761	1.1770	1.1799	1.1847	1.1913	1.2000	1.2106	1.2233	1.2379	1.2737	1.3186	1.4396	1.6178					
.525	1.1406	1.1415	1.1442	1.1488	1.1551	1.1634	1.1735	1.1856	1.1996	1.2337	1.2763	1.3903	1.5540					
.550	1.1069	1.1078	1.1103	1.1148	1.1209	1.1287	1.1384	1.1500	1.1634	1.1959	1.2365	1.3444	1.4969					
.575	1.0749	1.0758	1.0783	1.0824	1.0883	1.0959	1.1052	1.1162	1.1290	1.1601	1.1988	1.3014	1.4446					
.600	1.0446	1.0453	1.0477	1.0517	1.0574	1.0646	1.0735	1.0841	1.0964	1.1262	1.1633	1.2610	1.3962	1.5852				
.625	1.0156	1.0164	1.0187	1.0226	1.0280	1.0350	1.0436	1.0537	1.0655	1.0941	1.1296	1.2229	1.3511	1.5257				
.650	0.9881	0.9889	0.9911	0.9948	1.0000	1.0067	1.0150	1.0248	1.0361	1.0636	1.0977	1.1871	1.3091	1.4726				
.675	0.9619	0.9626	0.9648	0.9683	0.9734	0.9798	0.9878	0.9972	1.0082	1.0346	1.0674	1.1531	1.2696	1.4238				
.700	0.9369	0.9376	0.9396	0.9431	0.9479	0.9542	0.9619	0.9710	0.9815	1.0071	1.0386	1.1210	1.2324	1.3786	1.5759			
.725	0.9130	0.9137	0.9157	0.9191	0.9238	0.9298	0.9372	0.9460	0.9562	0.9808	1.0113	1.0905	1.1974	1.3365	1.5198			
.750	0.8902	0.8909	0.8928	0.8961	0.9006	0.9065	0.9136	0.9221	0.9320	0.9558	0.9852	1.0616	1.1642	1.2972	1.4695			
.775	0.8685	0.8691	0.8710	0.8741	0.8785	0.8842	0.8911	0.8993	0.9089	0.9319	0.9603	1.0341	1.1329	1.2620	1.4234			
.800	0.8476	0.8482	0.8500	0.8531	0.8573	0.8628	0.8696	0.8776	0.8868	0.9091	0.9366	1.0079	1.1032	1.2253	1.3806	1.5844		
.825	0.8277	0.8282	0.8300	0.8330	0.8371	0.8424	0.8490	0.8567	0.8657	0.8873	0.9140	0.9830	1.0749	1.1924	1.3407	1.5309		
.850	0.8086	0.8091	0.8108	0.8137	0.8178	0.8229	0.8293	0.8368	0.8455	0.8665	0.8923	0.9591	1.0480	1.1612	1.3032	1.4828		
.875	0.7903	0.7908	0.7925	0.7953	0.7992	0.8042	0.8104	0.8177	0.8261	0.8465	0.8716	0.9364	1.0224	1.1317	1.2680	1.4387		
.900	0.7727	0.7732	0.7749	0.7776	0.7814	0.7863	0.7922	0.7993	0.8075	0.8274	0.8517	0.9147	0.9980	1.1036	1.2348	1.3976	1.6069	
.925	0.7558	0.7564	0.7579	0.7606	0.7643	0.7690	0.7749	0.7818	0.7898	0.8090	0.8327	0.8938	0.9747	1.0769	1.2034	1.3593	1.5553	
.950	0.7396	0.7401	0.7416	0.7443	0.7478	0.7525	0.7582	0.7649	0.7727	0.7914	0.8145	0.8739	0.9525	1.0514	1.1736	1.3233	1.5090	
.975	0.7240	0.7245	0.7260	0.7286	0.7321	0.7366	0.7421	0.7487	0.7563	0.7745	0.7970	0.8548	0.9311	1.0271	1.1453	1.2894	1.4663	
1.000	0.7091	0.7096	0.7110	0.7135	0.7169	0.7213	0.7267	0.7331	0.7405	0.7583	0.7802	0.8366	0.9107	1.0040	1.1184	1.2573	1.4266	1.6402
1.050	0.6808	0.6813	0.6826	0.6850	0.6882	0.6924	0.6976	0.7037	0.7107	0.7277	0.7485	0.8021	0.8724	0.9605	1.0682	1.1981	1.3544	1.5452
1.100	0.6546	0.6550	0.6563	0.6585	0.6617	0.6657	0.6706	0.6764	0.6831	0.6993	0.7192	0.7702	0.8371	0.9207	1.0225	1.1446	1.2902	1.4649
1.150	0.6301	0.6306	0.6318	0.6339	0.6369	0.6407	0.6455	0.6510	0.6574	0.6729	0.6919	0.7407	0.8044	0.8840	0.9805	1.0958	1.2324	1.3944
1.200	0.6073	0.6078	0.6090	0.6110	0.6139	0.6176	0.6221	0.6274	0.6335	0.6484	0.6666	0.7133	0.7741	0.8500	0.9419	1.0512	1.1800	1.3314
1.250	0.5861	0.5865	0.5877	0.5896	0.5924	0.5959	0.6003	0.6053	0.6112	0.6254	0.6429	0.6877	0.7460	0.8185	0.9062	1.0101	1.1321	1.2746
1.300	0.5662	0.5666	0.5677	0.5696	0.5722	0.5756	0.5798	0.5847	0.5904	0.6041	0.6209	0.6638	0.7198	0.7892	0.8730	0.9722	1.0881	1.2228
1.350	0.5474	0.5479	0.5490	0.5508	0.5534	0.5566	0.5606	0.5654	0.5708	0.5840	0.6000	0.6415	0.6953	0.7620	0.8422	0.9370	1.0476	1.1755
1.400	0.5300	0.5304	0.5314	0.5332	0.5356	0.5388	0.5426	0.5472	0.5525	0.5651	0.5807	0.6205	0.6723	0.7365	0.8135	0.9044	1.0100	1.1318
1.450	0.5136	0.5139	0.5149	0.5166	0.5190	0.5220	0.5257	0.5302	0.5353	0.5475	0.5624	0.6004	0.6508	0.7126	0.7867	0.8740	0.9751	1.0915
1.500	0.4980	0.4983	0.4993	0.5010	0.5033	0.5062	0.5098	0.5141	0.5190	0.5308	0.5454	0.5824	0.6306	0.6902	0.7616	0.8455	0.9427	1.0541
1.550	0.4834	0.4837	0.4847	0.4862	0.4885	0.4913	0.4948	0.4989	0.5037	0.5151	0.5290	0.5651	0.6116	0.6691	0.7380	0.8189	0.9123	1.0193
1.600	0.4696	0.4698	0.4708	0.4723	0.4744	0.4772	0.4806	0.4846	0.4892	0.5003	0.5139	0.5486	0.5937	0.6493	0.7158	0.7938	0.8839	0.9868
1.700	0.4440	0.4443	0.4452	0.4467	0.4487	0.4513	0.4545	0.4582	0.4625	0.4730	0.4858	0.5184	0.5607	0.6129	0.6752	0.7481	0.8321	0.9277
1.800	0.4211	0.4214	0.4222	0.4235	0.4254	0.4279	0.4309	0.4344	0.4386	0.4484	0.4605	0.4913	0.5311	0.5803	0.6389	0.7074	0.7861	0.8755
1.900	0.4003	0.4006	0.4014	0.4026	0.4045	0.4068	0.4096	0.4130	0.4169	0.4262	0.4376	0.4668	0.5045	0.5510	0.6063	0.6709	0.7449	0.8290
2.000	0.3815	0.3817	0.3824	0.3837	0.3854	0.3876	0.3903	0.3935	0.3972	0.4060	0.4169	0.4446	0.4804	0.5244	0.5767	0.6379	0.7079	0.7872
2.100	0.3642	0.3645	0.3652	0.3664	0.3680	0.3701	0.3727	0.3757	0.3792	0.3877	0.3980	0.4244	0.4584	0.5003	0.5501	0.6081	0.6744	0.7495
2.200	0.3485	0.3487	0.3494	0.3505	0.3521	0.3541	0.3566	0.3594	0.3628	0.3708	0.3807	0.4059	0.4383	0.4782	0.5257	0.5809	0.6440	0.7152
2.300	0.3341	0.3343	0.3349	0.3359	0.3374	0.3394	0.3418	0.3445	0.3477	0.3554	0.3648	0.3889	0.4199	0.4580	0.5034	0.5560	0.6161	0.6840
2.400	0.3207	0.3209	0.3216	0.3225	0.3240	0.3258	0.3281	0.3307	0.3338	0.3412	0.3502	0.3732	0.4029	0.4395	0.4828	0.5331	0.5906	0.6554
2.500	0.3084	0.3086	0.3092	0.3102	0.3115	0.3133	0.3155	0.3180	0.3210	0.3280	0.3367	0.3588	0.3873	0.4223	0.4639	0.5121	0.5671	0.6291
2.600	0.2970	0.2971	0.2977	0.2987	0.3000	0.3017	0.3038	0.3062	0.3091	0.3158	0.3242	0.3454	0.3728	0.4064	0.4464	0.4927	0.5455	0.6049
2.700	0.2863	0.2865	0.2871	0.2880	0.2892	0.2909	0.2929	0.2952	0.2980	0.3045	0.3126	0.3330	0.3594	0.3917	0.4301	0.4746	0.5254	0.5825
2.800	0.2764	0.2766	0.2771	0.2780	0.2792	0.2808	0.2828	0.2850	0.2877	0.2940	0.3017	0.3215	0.3469	0.3780	0.4150	0.4579	0.5067	0.5617
2.900	0.2672	0.2674	0.2679	0.2687	0.2699	0.2714	0.2733	0.2755	0.2780	0.2842	0.2916	0.3106	0.3352	0.3653	0.4009	0.4423	0.4894	0.5423
3.000	0.2586	0.2587	0.2592	0.2600	0.2612	0.2626	0.2644	0.2666	0.2690	0.2749	0.2821	0.3006	0.3243	0.3533	0.3878	0.4277	0.4732	0.5242

SUBSIDIARY

k = g	R^y_H	k = g	R^y_H	k = g	R^y_H
0.000	2.6667	0.195	1.9681	0.700	1.5759
0.005	2.6366	0.200	1.9576	0.725	1.5765
0.010	2.6098	0.210	1.9371	0.750	1.5782
0.015	2.5801	0.220	1.9175	0.775	1.5809
0.020	2.5535	0.230	1.8988	0.800	1.5844
0.025	2.5278	0.240	1.8809	0.825	1.5889
0.030	2.5030	0.250	1.8637	0.850	1.5941
0.035	2.4790	0.260	1.8474	0.875	1.6001
0.040	2.4558	0.270	1.8317	0.900	1.6069
0.045	2.4332	0.280	1.8167	0.925	1.6143
0.050	2.4113	0.290	1.8023	0.950	1.6223
0.055	2.3901	0.300	1.7886	0.975	1.6310
0.060	2.3694	0.310	1.7755	1.000	1.6402
0.065	2.3493	0.320	1.7630	1.050	1.6603
0.070	2.3297	0.330	1.7511	1.100	1.6824
0.075	2.3106	0.340	1.7397	1.150	1.7062
0.080	2.2920	0.350	1.7288	1.200	1.7316
0.085	2.2739	0.360	1.7184	1.250	1.7585
0.090	2.2563	0.370	1.7085	1.300	1.7867
0.095	2.2391	0.380	1.6991	1.350	1.8161
0.100	2.2230	0.390	1.6902	1.400	1.8466
0.105	2.2059	0.400	1.6816	1.450	1.8781
0.110	2.1899	0.410	1.6736	1.500	1.9105
0.115	2.1743	0.420	1.6659	1.550	1.9438
0.120	2.1590	0.430	1.6586	1.600	1.9779
0.125	2.1442	0.440	1.6517	1.700	2.0481
0.130	2.1297	0.450	1.6452	1.800	2.1208
0.135	2.1154	0.460	1.6390	1.900	2.1957
0.140	2.1016	0.470	1.6332	2.000	2.2724
0.145	2.0880	0.480	1.6277	2.100	2.3507
0.150	2.0773	0.490	1.6226	2.200	2.4305
0.155	2.0618	0.500	1.6178	2.300	2.5115
0.160	2.0492	0.525	1.6071	2.400	2.5937
0.165	2.0368	0.550	1.5981	2.500	2.6768
0.170	2.0247	0.575	1.5909	2.600	2.7608
0.175	2.0129	0.600	1.5852	2.700	2.8457
0.180	2.0013	0.625	1.5809	2.800	2.9313
0.185	1.9900	0.650	1.5780	2.900	3.0175
0.190	1.9789	0.675	1.5763	3.000	3.1044

$$R^y_H(\text{Laue}) \simeq e^{-\mu t/\gamma_0} \int_{-\infty}^{\infty} [\sin^2(A\sqrt{1+y^2})$$

$$+\sinh^2(A\sqrt{k+yg}/\sqrt{1+y^2})]dy/(1+y^2)$$

$$\simeq \frac{\pi}{2} e^{-\mu t/\gamma_0}[J_0(2iA\sqrt{k^2+g^2}) + \int_0^{2A} J_0(x)dx - 1] \quad (4)$$

$$A = \frac{e^2\lambda|F'_H|tKe^{-M}}{mc^2V\sqrt{|\gamma_0\gamma_H|}} \quad (5)$$

where t is the crystal thickness and γ_0 and γ_H are the direction cosines of the incident and emergent beams relative to the surface. For symmetrical transmission $b=\gamma_0/\gamma_H=+1$ and $g=0$. Equation (4) has been derived by dropping terms of order k^2 and g^2 (compared with unity). The first order correction to equation (4) for symmetrical transmission is $\sim(1+7k^2/16)$ so that the maximum error in equation (4) is $\sim\frac{1}{2}\%$ for $k\sim0{\cdot}1$.

The integral of the zero order Bessel function appearing in equation (4) can be evaluated as follows:

(1) For $A<5$
See Table 2.

(2) For $A>5$

$$\int_0^{2A} J_0(x)dx = 1-(2A)^{-\frac{1}{2}}\left[P(A)\cos\left(2A+\frac{\pi}{4}\right) + Q(A)\sin\left(2A+\frac{\pi}{4}\right)\right]$$

$$P(A) = 0{\cdot}7979 - \frac{0{\cdot}2010}{A^2} + \frac{0{\cdot}4575}{A^4}$$

$$Q(A) = \frac{0{\cdot}2493}{A} - \frac{0{\cdot}2586}{A^3} + \frac{1{\cdot}0332}{A^5}. \quad (6)$$

The modified Bessel functions (imaginary argument, equations (4) and (8)]are tabulated by Jahnke & Emde (1945) up to values of 10 in the argument; for $x>10$

$$J_0(ix) \simeq \frac{e^x}{\sqrt{2\pi x}}\left(1+\frac{1}{8x}+\frac{9}{128x^2}\right). \quad (7)$$

(*b*) *Forward diffracted beam*, $k<0{\cdot}1$, $g<0{\cdot}1$

The integrated intensity is also given by equation (1) except that we replace $R^y_H(\text{Bragg})$ by $R^y_T(\text{Laue})$ (Kato, 1955). For $A\sqrt{k^2+g^2}<3$ we have

$$R^y_T(\text{Laue}) = 2\pi e^{-\mu t/\gamma_0} A\sqrt{k^2+g^2}\left[iJ_1(2iA\sqrt{k^2+g^2}) - \frac{|g|}{\sqrt{k^2+g^2}} J_0(2iA\sqrt{k^2+g^2}) + \frac{k^2e^{2|g|A}}{k^2+g^2}\int_0^{2A\sqrt{k^2+g^2}} J_0(ix)e^{-|g|x/\sqrt{g^2+k^2}}\,dx\right] - R^y_H(\text{Laue}) \quad (8)$$

where $R^y_H(\text{Laue})$ is given by equation (4) and the integral of the modified Bessel function is given in Table 3. For the symmetric case ($b=+1$, $g=0$) equation (8) becomes

$$R^y_T(\text{Laue}) \simeq 4\pi e^{-\mu t/\gamma_0} Ak\left[\sum_{n=0}^{\infty} \frac{(Ak)^{2n+1}}{(2n+1)(2n+2)(n!)^2}\right] - R^y_H(\text{Laue}), \quad (9)$$

which converges quite rapidly.

For $A\sqrt{k^2+g^2}>3$ we can use an expression derived by Kato (1955):

$$R^y_T(\text{Laue}) \simeq \pi e^{-\mu t/\gamma_0} \frac{\exp(2A\sqrt{k^2+g^2})}{(4\pi A\sqrt{k^2+g^2})^{\frac{1}{2}}}\left[D_0 + \frac{D_1}{2A\sqrt{k^2+g^2}} + \frac{D_2}{(2A\sqrt{k^2+g^2})^2} + \ldots + \frac{D_n}{(2A\sqrt{k^2+g^2})^n}\right] - R^y_H(\text{Laue}), \quad (10)$$

where

$$D_0 = \tfrac{1}{2}\left[\frac{1+(|g|/\sqrt{k^2+g^2})}{1-(|g|/\sqrt{k^2+g^2})}\right] + \tfrac{1}{2}$$

$$D_1 = \tfrac{3}{4}\left[1+\tfrac{1}{4}[1-(|g|)/\sqrt{k^2+g^2})]\right]\frac{1+(|g|/\sqrt{k^2+g^2})}{[1-(|g|/\sqrt{k^2+g^2})]^2} + \tfrac{3}{16} \quad (11)$$

$$D_n = \frac{1{\cdot}3{\cdot}5\ldots2n+1}{2^{n+1}}\left[\left(\frac{1+(|g|/\sqrt{k^2+g^2})}{[1-(|g|/\sqrt{k^2+g^2})]^{n+1}}\right)\times\left(1+\sum_{r=1}^{n}\frac{[1-(|g|/\sqrt{g^2+k^2})]^r[1{\cdot}3{\cdot}5\ldots2r-1]}{r!4^r}\right) + \frac{1{\cdot}3{\cdot}5\ldots2n-1}{n!4^n}\right]$$

$$n \le 2A\sqrt{k^2+g^2}-1\,.$$

Table 2. *Table of values of the integral of the Bessel function*, $\int_0^{2A} J_0(x)dx$, *appearing in equation* (4)

2A	∫	2A	∫	2A	∫
0.00	0.00000	3.40	1.26056	6.80	0.89512
0.10	0.09991	3.50	1.22330	6.90	0.92470
0.20	0.19933	3.60	1.18467	7.00	0.95464
0.30	0.29775	3.70	1.14509	7.10	0.98462
0.40	0.39469	3.80	1.10496	7.20	1.01435
0.50	0.48968	3.90	1.06471	7.30	1.04354
0.60	0.58224	4.00	1.02473	7.40	1.07190
0.70	0.67193	4.10	0.98541	7.50	1.09917
0.80	0.75834	4.20	0.94712	7.60	1.12508
0.90	0.84106	4.30	0.91021	7.70	1.14941
1.00	0.91973	4.40	0.87502	7.80	1.17192
1.10	0.99399	4.50	0.84186	7.90	1.19243
1.20	1.06355	4.60	0.81100	8.00	1.21074
1.30	1.12813	4.70	0.78271	8.10	1.22671
1.40	1.18750	4.80	0.75721	8.20	1.24021
1.50	1.24144	4.90	0.73468	8.30	1.25112
1.60	1.28982	5.00	0.71531	8.40	1.25939
1.70	1.33249	5.10	0.69920	8.50	1.26494
1.80	1.36939	5.20	0.68647	8.60	1.26777
1.90	1.40048	5.30	0.67716	8.70	1.26787
2.00	1.42577	5.40	0.67131	8.80	1.26528
2.10	1.44528	5.50	0.66891	8.90	1.26005
2.20	1.45912	5.60	0.66992	9.00	1.25226
2.30	1.46740	5.70	0.67427	9.10	1.24202
2.40	1.47029	5.80	0.68187	9.20	1.22946
2.50	1.46798	5.90	0.69257	9.30	1.21473
2.60	1.46069	6.00	0.70622	9.40	1.19799
2.70	1.44871	6.10	0.72263	9.50	1.17944
2.80	1.43231	6.20	0.74160	9.60	1.15927
2.90	1.41181	6.30	0.76290	9.70	1.13772
3.00	1.38756	6.40	0.78628	9.80	1.11499
3.10	1.35992	6.50	0.81147	9.90	1.09134
3.20	1.32928	6.60	0.83820	10.00	1.06701
3.30	1.29602	6.70	0.86618		

4. Anomalous transmission

In the range of anomalous transmission ($Ak>10$), equations (4) and (10) for the symmetric case ($b=+1$, $g=0$) and for $K=1$ become

$$R_H^y(\text{Laue}) \simeq \left[\frac{\pi}{2}\exp\left(-\mu t/\gamma_0\right)(1-\varepsilon e^{-M})\right] \times \frac{\left[1+\dfrac{1}{16Ak}\right]}{\sqrt{4\pi Ak}}$$

$$R_T^y(\text{Laue}) \simeq \left(1+\frac{1}{Ak}+\frac{410}{128A^2k^2}\right) R_H^y(\text{Laue})\,. \qquad (12)$$

Thus we see that R_H^y(Laue) and R_T^y(Laue) are very sensitive to the deviations from unity of ε and e^{-M}.

5. Thermal diffuse scattering correction and enhancement factor

If one integrates a peak over an angular range of Δ (2θ scale), then one has included a certain amount of thermal diffuse scattering. In order to determine the true coherent intensity, the observed X-ray integrated intensity must be reduced by the factor (Nilsson, 1957; Chipman & Batterman, 1963):

$$1+\alpha\Gamma \qquad (13)$$

$$\alpha=\frac{4\pi kT}{3\lambda^3}\sin 2\theta_B \sin^2\theta_B \mathscr{K}\Delta$$

Table 3. *Table of values of*

$$\int_0^{2A\sqrt{g^2+k^2}} J_0(ix)\exp\left(-gx/\sqrt{g^2+k^2}\right)dx$$

appearing in equation (8)

$2A\sqrt{g^2+k^2}$ \ $g/\sqrt{g^2+k^2}$	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.100	0.100	0.100	0.100	0.099	0.098	0.098	0.097	0.097	0.096	0.096	0.095
0.200	0.201	0.199	0.197	0.195	0.193	0.191	0.189	0.187	0.185	0.184	0.182
0.300	0.302	0.298	0.293	0.289	0.285	0.281	0.277	0.273	0.269	0.265	0.261
0.400	0.405	0.397	0.389	0.382	0.374	0.367	0.360	0.353	0.347	0.340	0.334
0.500	0.510	0.498	0.486	0.474	0.462	0.451	0.440	0.430	0.420	0.410	0.401
0.600	0.618	0.600	0.582	0.565	0.549	0.532	0.519	0.503	0.489	0.476	0.463
0.700	0.729	0.704	0.679	0.656	0.634	0.613	0.593	0.574	0.555	0.538	0.521
0.800	0.844	0.810	0.778	0.748	0.719	0.692	0.666	0.641	0.618	0.596	0.575
0.900	0.963	0.919	0.878	0.840	0.804	0.770	0.737	0.707	0.678	0.651	0.626
1.000	1.087	1.032	0.981	0.933	0.888	0.847	0.807	0.771	0.736	0.704	0.674
1.100	1.216	1.149	1.086	1.028	0.974	0.923	0.876	0.832	0.792	0.754	0.719
1.200	1.352	1.270	1.154	1.124	1.059	1.000	0.945	0.894	0.846	0.803	0.762
1.300	1.495	1.396	1.305	1.222	1.246	1.076	1.012	0.953	0.899	0.849	0.803
1.400	1.646	1.528	1.421	1.323	1.234	1.153	1.079	1.012	0.950	0.894	0.842
1.500	1.806	1.666	1.540	1.426	1.324	1.231	1.146	1.070	1.000	0.937	0.880
1.600	1.976	1.812	1.665	1.533	1.415	1.309	1.213	1.127	1.050	0.979	0.916
1.700	2.156	1.965	1.795	1.643	1.508	1.388	1.280	1.184	1.098	1.020	0.950
1.800	2.349	2.126	1.930	1.757	1.604	1.468	1.348	1.241	1.145	1.060	0.984
1.900	2.555	2.297	2.072	1.875	1.702	1.550	1.416	1.297	1.192	1.099	1.016
2.000	2.775	2.478	2.221	1.998	1.803	1.633	1.484	1.353	1.238	1.137	1.048
2.100	3.011	2.671	2.378	2.125	1.907	1.718	1.553	1.410	1.284	1.174	1.078
2.200	3.265	2.876	2.543	2.259	2.014	1.804	1.623	1.466	1.330	1.211	1.107
2.300	3.538	3.093	2.717	2.397	2.125	1.893	1.693	1.522	1.375	1.247	1.136
2.400	3.831	3.326	2.901	2.543	2.240	1.983	1.765	1.579	1.419	1.282	1.164
2.500	4.148	3.574	3.095	2.694	2.359	2.076	1.838	1.636	1.464	1.317	1.192
2.600	4.490	3.838	3.300	2.854	2.482	2.172	1.312	1.693	1.509	1.352	1.218
2.700	4.860	4.122	3.517	3.020	2.610	2.270	1.987	1.751	1.553	1.386	1.244
2.800	5.259	4.426	3.748	3.196	2.743	2.371	2.064	1.809	1.597	1.419	1.270
2.900	5.692	4.751	3.993	3.380	2.881	2.475	2.142	1.868	1.641	1.453	1.295
3.000	6.161	5.100	4.253	3.573	3.026	2,582	2.222	1.928	1.686	1.486	1.319
3.100	6.669	5.475	4.529	3.777	3.176	2.693	2.304	1.988	1.730	1.518	1.344
3.200	7.221	5.877	4.823	3.991	3.332	2.807	2.387	2.049	1.774	1.551	1.367
3.300	7.820	6.310	5.135	4.217	3.455	2.925	2.472	2.110	1.819	1.583	1.390
3.400	8.471	6.776	5.468	4.455	3.666	3.047	2.559	2.173	1.863	1.615	1.413
3.500	9.179	7.277	5.823	4.707	3.844	3.173	2.649	2.236	1.908	1.647	1.436
3.600	9.949	7.817	6.202	4.972	4.030	3.304	2.740	2.300	1.953	1.678	1.458
3.700	10.787	8.398	6.606	5.252	4.224	3.439	2.834	2.365	1.998	1.709	1.480
3.800	11.699	9.025	7.036	5.548	4.428	3.579	2.930	2.431	2.044	1.741	1.501
3.900	12.692	9.701	7.496	5.861	4.641	3.723	3.029	2.498	2.089	1.772	1.522
4.000	13.775	10.431	7.988	6.192	4.864	3.874	3.130	2.566	2.135	1.803	1.543
4.100	14.956	11.218	8.513	6.542	5.097	4.029	3.234	2.638	2.182	1.833	1.564
4.200	16.243	12.068	9.074	6.913	5.342	4.191	3.340	2.706	2.228	1.864	1.584
4.300	17.648	12.986	9.674	7.305	5.599	4.359	3.450	2.778	2.275	1.895	1.604
4.400	19.181	13.979	10.317	7.721	5.868	4.533	3.563	2.851	2.322	1.925	1.624
4.500	20.854	15.051	11.004	8.161	6.150	4.714	3.679	2.925	2.370	1.956	1.643
4.600	22.682	16.210	11.739	8.628	6.446	4.901	3.798	3.001	2.418	1.986	1.663
4.700	24.678	17.464	12.527	9.123	6.756	5.097	3.920	3.078	2.466	2.017	1.682
4.800	26.859	18.820	13.370	9.647	7.083	5.299	4.047	3.156	2.515	2.047	1.700
4.900	29.243	20.288	14.274	10.203	7.425	5.510	4.176	3.236	2.564	2.077	1.719
5.000	31.849	21.876	15.242	10.794	7.785	5.730	4.310	3.317	2.614	2.108	1.738
5.100	34.698	23.596	16.280	11.420	8.163	5.958	4.448	3.400	2.664	2.138	1.756
5.200	37.815	25.458	17.392	12.084	8.560	6.195	4.589	3.485	2.714	2.168	1.774
5.300	41.224	27.474	18.585	12.790	8.977	6.442	4.735	3.572	2.766	2.198	1.792
5.400	44.954	29.659	19.864	13.539	9.416	6.699	4.886	3.660	2.817	2.229	1.809
5.500	49.036	32.026	21.237	14.335	9.877	6.966	5.041	3.750	2.869	2.259	1.827
5.600	53.505	34.591	22.709	15.180	10.363	7.245	5.201	3.841	2.922	2.289	1.844
5.700	58.397	37.371	24.289	16.078	10.873	7.535	5.366	3.935	2.975	2.319	1.862
5.800	63.754	40.385	25.985	17.032	11.410	7.837	5.536	4.031	3.029	2.350	1.879
5.900	69.620	43.653	27.806	18.047	11.975	8.152	5.711	4.128	3.084	2.380	1.896
6.000	76.046	47.197	29.760	19.125	12.569	8.480	5.892	4.228	3.139	2.410	1.912

$$\mathscr{K}=\frac{(C_{11}+C_{12})(C_{11}-C_{12}-2C_{44})/5+C_{44}(2C_{11}+C_{44})}{C_{11}C_{44}^2+(C_{11}-C_{12}-2C_{44})^2(C_{11}+2C_{12}+C_{44})/105+(C_{11}-C_{12}-2C_{44})(C_{11}+C_{12})C_{44}/5}\,, \qquad (14)$$

where T is the absolute temperature, k the Boltzman constant, C_{11}, C_{12}, and C_{44} the elastic constants, and Γ is the enhancement factor which takes into account that the thermal diffuse scattering obeys the mosaic crystal formula. Thus, Γ is the ratio of the integrated intensity of a mosaic to aperfect crystal.

For the Bragg case the enhancement factor is

$$\Gamma=\frac{\pi(1+k^2)}{4|g|R_H^y(\text{Bragg})}\,. \qquad (15)^*$$

For the Laue case (diffracted beam) the enhancement factor is for $g^2 \ll 1$, $k^2 \ll 1$,

$$\Gamma=\frac{2A}{\left[J_0(2iA\sqrt{g^2+k^2})+\int_0^{2A}J_0(x)dx-1\right]}\,. \qquad (16)$$

For the forward diffracted beam in the Laue case there is essentially no thermal diffuse scattering contribution.

* For $|g|>1$ and $k<1$, $\Gamma \simeq 1+[(1-k^2)/\pi^2g^2]$. Thus the mosaic formula is applicable to a perfect crystal when $(1-k^2)/\pi^2g^2 < 0{\cdot}01$. This is not the case for $|g|$ and k both large (*cf.* § 7).

6. Asymmetric reflection (Bragg case)

If the diffracting planes are not parallel to the surface of the crystal ($b \neq -1$), then an independent measurement of the direction cosines must be made. This may be contrasted with the mosaic crystal for which the average integrated intensities obtained by reversing the incident and diffracted rays cancel any effect due to asymmetry. A method for determining the direction cosines can be performed by measuring the integrated intensity for various values of Φ, the angle of crystal rotation about an axis normal to the reflecting planes, always ensuring that the diffracted beam enters the center of the counter window. One should obtain a smooth 'sinusoidal' curve when integrated intensity is plotted against Φ over a reasonable representation of 360°, with a maxima and minima 180° apart. Situations other than this may suggest departures from crystal perfection and/or effects due to 'Umweganregung'. By averaging over Φ the correction is reduced to second order in the angle of miscut.

7. 'Anomalous' reflection

In Fig. 1 we have plotted the values of Γ [equation (15)] as a function of g for $k=|g|$ and we observe an interesting phenomenon in that the values can be less than unity for $k > 0{\cdot}85$. Thus we can obtain more integrated intensity for the Bragg reflection from a perfect crystal than from a mosaic crystal. Analogous to the case of anomalous transmission where Γ [equation (16)] can also fall below unity (for $Ak \gg 1$), we propose the term 'anomalous' reflection for the Bragg case. One does occasionally encounter such cases. For example, in neutron diffraction a perfect crystal of gadolinium gives $g = 5$ and a value of $\Gamma \simeq 0{\cdot}83$. Table 4 gives values of Γ for $|g|$ and $k > 1$.

Table 4. *Table of the enhancement factor Γ for large values of g and k* [equation (15)]

For $|g| > 1$ and $k < 0$ see footnote to equation (15). Interpolation is best done by plotting curves of *Γ versus k* for constant $|g|$.

g \ k	1	2	3	4	5	6	7	8	9	10
1	0.9577									
2	0.9977	0.8641								
3	0.9989	0.9526	0.8440							
4	0.9997	0.9734	0.9283	0.8366						
5	0.9999	0.9842	0.9566	0.9137	0.8330					
6	1.0000	0.9890	0.9705	0.9422	0.9005	0.8310				
7	1.0000	0.9915	0.9785	0.9586	0.9308	0.8918	0.8300			
8	1.0000	0.9935	0.9834	0.9687	0.9484	0.9215	0.8854	0.8292		
9	1.0000	0.9944	0.9867	0.9752	0.9597	0.9397	0.9137	0.8799	0.8287	
10	1.0000	0.9952	0.9889	0.9797	0.9674	0.9517	0.9320	0.9078	0.8754	0.8282

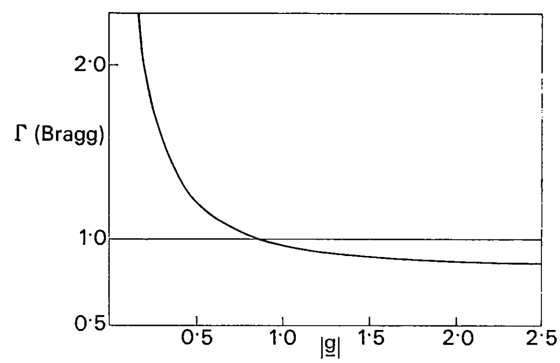

Fig. 1. The enhancement factor Γ as a function of $|g|$ for $|g| = k$. The enhancement factor (equation (15)] represents the ratio of the integrated intensity of a perfect crystal to an imperfect crystal, both in Bragg reflection. For $|g| > 0{\cdot}85$ we have the range of 'anomalous' reflection since the perfect crystal gives more integrated intensity than the imperfect crystal.

8. Discussion

For measurements of absolute scattering factors the Bragg case is considerably more accurate than the Laue case. This arises from three causes: (i) the appreciably higher intensities (sometimes several orders of magnitude) in the Bragg case; (ii) the large effect uncertainties in ε and e^{-M} can have on the diffracted intensities in the Laue case when $kA > 5$; (iii) the oscillatory nature of equation (6) which for $kA < 5$ requires a rather precise knowledge of t (the crystal thickness). Furthermore, these oscillations lead to a multiplicity of F_H values each yielding identical values for the reflecting power. In all previous work (Zachariasen, 1954; Kato, 1955; Hirsch, 1952) the authors have averaged out these oscillations by taking the limiting value of equation (6) for $A = \infty$ but this can lead to errors of $\sim 10\%$ or more. (In the Bragg case R_H^y is a monotonic function of F_H).

We wish to acknowledge the help and advice of Dr L. Jennings and the work of Mrs Athena Harvey, who programmed the calculations.

References

CHIPMAN, D. R. & BATTERMAN, B. W. (1963). *J. Appl. Phys.* **34**, 912.
COLE, H. & STEMPLE, N. R. (1962). *J. Appl. Phys.* **33**, 2227.
HIRSCH, P. B. (1952). *Acta Cryst.* **5**, 176.
HIRSCH, P. B. & RAMACHANDRAN, G. N. (1950). *Acta Cryst.* **3**, 187.
JAHNKE, E. & EMDE, F. (1945). *Tables of Functions*, p. 226. Dover Publications.
KATO, N. (1955). *J. Phys. Soc., Japan*, **10**, 46.
NILSSON, N. (1957). *Ark. Fys.* **12**, 247.
WAGENFELD, H. (1962). *J. Appl. Phys.* **33**, 2907. [ε corresponds to $\tau_{2\theta}/\tau$].
ZACHARIASEN, W. H. (1945). *Theory of X-ray Diffraction in Crystals*. New York: John Wiley.