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Exact evaluation of the 'interference function'. By N. GÜVEN, *Department of Geosciences, Texas Technological University, Lubbock, Texas* 79409, *U.S.A.*

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The numerical value of the function ($\sin^2 \pi Mu/M^2 \sin^2 \pi u$) has been given in terms of the variables u and M which are independent of any real or reciprocal crystal parameters. The argument u is a fractional coordinate in reciprocal space and the variable M is the number of unit cells in a given direction.

The one-dimensional 'interference function' may be given by the following expression:

$$S=\sum_{m=0}^{m=M-1} \exp\,(2\pi i m\,\mathbf{a}\,.\,\mathbf{s})=\frac{\sin \pi M\mathbf{a}\,.\,\mathbf{s}}{\sin \pi\mathbf{a}\,.\,\mathbf{s}}\,\exp\,[\pi i(M-1)\mathbf{a}\,.\,\mathbf{s}]\,,$$

where **a** and **s** are the real and reciprocal-lattice vectors respectively, and $|\mathbf{s}|=2\sin\theta/\lambda$; M is the number of unit cells in the **a** direction. The total 'interference function' is the triple product of such summations. For intensity calculations, the function $|S|^2$ is needed. The exponential term $\exp\,[\pi i(M-1)\mathbf{a}\,.\,\mathbf{s}]$ can then be disregarded as it has the unit modulus. The function $|S|^2$ can be further simplified by expressing **s** in units of $\mathbf{a}^*$:

$$\mathbf{s}=u\mathbf{a}^*$$

$$\mathbf{a}\,.\,\mathbf{s}=u\mathbf{a}^*\,.\,\mathbf{a}=u$$

$$S^2=\frac{\sin^2 \pi Mu}{\sin^2 \pi u}\,.$$

The 'interference function' in this form becomes perfectly general and it is independent of any cell parameters (real and reciprocal). The argument (u) of the function represents a fraction of the distance between two consecutive reciprocal lattice points in any direction. This is considered in increments of one-hundredths of the reciprocal spacing. The function S^2 has been exactly evaluated and normalized (*i.e.* $|S|^2/M^2$) for $M=2$ to 40. For larger values of M, the crystal can be considered as 'infinite' for most practical purposes. The numerical values of the 'normalized interference function' have been listed in Table 1. These values can now be used for any other crystal. For the special case $M=1$, the function is always unity and it is therefore not listed in the Table.

The 'interference function' has often been approximated by the expression $(\sin x)/x$ for which tables are already available (*International Tables for X-ray Crystallography*, 1959). The function $(\sin x)/x$ has the following disadvantages: The argument (x) is given in radians and unlike the argument (u) it does not directly relate to the reciprocal space. The argument (u) gives, for instance, the elongation of a reflection due to 'finite' crystal thickness as $u=1/M$. Furthermore, the function $(\sin x)/x$ only approximates the 'interference function' and it may deviate appreciably for large x values. The function ($\sin^2 \pi Mu/\sin^2 \pi u$) is symmetrical at the origin and at $u=\frac{1}{2}$. It is, therefore, completely sufficient to list the values of the function in the interval $u=0{\cdot}00$ to $0{\cdot}50$.

Table 1. *Numerical values for the normalized interference function* $(S^2/M^2)\times 10^4$ *for the crystal thickness of* 2 *to* 40 *unit cells*

The u values are given in fractions of the distance between two consecutive reciprocal-lattice points.

U	M=2	M=3	M=4	M=5	M=6	M=7	M=8	M=9	M=10	M=11	M=12	M=13	M=14	M=15	M=16	M=17	M=18	M=19	M=20
0.0	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000
0.01	9990	9974	9951	9921	9885	9843	9794	9740	9678	9611	9538	9459	9375	9284	9189	9088	8981	8870	8754
0.02	9961	9895	9804	9688	9548	9384	9198	8990	8763	8517	8254	7975	7883	7378	7063	6739	6409	6074	5735
0.03	9911	9765	9563	9309	9005	8656	8267	7843	7390	6914	6420	5915	5405	4896	4393	3903	3430	2979	2553
0.04	9843	9585	9234	8798	8287	7713	7091	6434	5758	5076	4403	3752	3134	2559	2036	1570	1167	826	550
0.05	9755	9358	8824	8173	7429	6621	5775	4921	4086	3295	2567	1920	1365	908	551	291	120	28	0
0.06	9649	9086	8341	7456	6477	5453	4433	3461	2576	1807	1174	685	337	121	17	4	54	143	246
0.07	9524	8771	7798	6673	5476	4284	3168	2185	1375	760	339	97	4	23	111	230	345	431	475
0.08	9382	8419	7204	5850	4474	3164	2068	1185	559	181	18	15	112	248	375	458	482	446	366
0.09	9222	8032	6574	5013	3513	2208	1192	501	123	1	55	197	348	453	484	441	343	222	111
0.10	9045	7616	5920	4189	2631	1399	565	123	0	83	251	406	483	465	370	237	112	28	0
0.11	8853	7174	5256	3401	1859	778	185	1	83	271	431	491	438	308	160	48	1	19	75
0.12	8645	6713	4594	2670	1217	350	18	56	255	435	494	421	268	113	18	4	53	121	167
0.13	8423	6236	3947	2013	716	101	16	203	415	499	425	257	93	7	15	82	150	174	143
0.14	8187	5750	3327	1444	356	4	117	362	499	449	273	94	4	23	101	165	170	117	48
0.15	7939	5259	2743	970	129	24	262	476	485	318	116	7	24	108	171	164	98	28	0
0.16	7679	4769	2205	595	19	119	400	513	390	167	19	16	103	173	162	89	18	2	37
0.17	7409	4284	1719	318	4	249	494	472	253	50	4	86	170	167	90	15	4	47	87
0.18	7129	3809	1292	133	60	378	525	372	120	1	56	158	177	101	18	4	50	91	79
0.19	6841	3350	927	31	159	479	493	244	30	20	130	186	124	29	2	48	92	78	27
0.20	6545	2909	625	0	278	534	409	123	0	83	182	155	51	0	39	91	81	28	0
0.21	6243	2491	386	26	393	538	297	38	25	150	184	89	5	24	85	88	33	0	23
0.22	5937	2100	208	94	487	494	180	1	85	191	140	26	8	72	96	45	1	20	56
0.23	5627	1738	88	189	549	413	83	13	150	187	74	0	47	99	64	6	13	53	52
0.24	5314	1408	21	295	572	310	21	61	193	144	20	17	89	86	19	5	47	57	18
0.25	5000	1111	0	400	556	204	0	123	200	83	0	59	102	44	0	35	62	28	0
0.26	4686	850	18	493	504	110	18	178	170	28	18	96	79	8	17	61	41	2	16
0.27	4373	626	69	564	427	42	64	209	116	1	58	105	37	2	49	57	10	8	40
0.28	4063	434	143	609	334	5	123	207	58	9	96	82	5	26	66	27	1	33	38
0.29	3757	281	232	625	234	3	178	175	15	42	111	41	3	57	51	3	20	44	14
0.30	3455	162	330	611	147	30	216	123	0	83	96	9	27	68	21	5	43	28	0
0.31	3159	77	428	570	74	77	228	68	14	111	60	1	57	52	1	28	42	5	13
0.32	2871	24	520	508	24	139	211	23	48	115	23	19	71	22	7	47	20	2	32
0.33	2591	1	601	429	1	188	173	1	88	94	1	50	60	1	31	45	1	21	31
0.34	2321	6	666	341	6	230	121	6	118	57	6	72	31	6	49	18	5	36	11
0.35	2061	34	712	252	33	231	70	32	116	21	30	75	10	28	25	1	25	26	0
0.36	1813	84	737	169	79	248	26	71	110	2	60	32	6	49	16	25	28	0	11
0.37	1597	151	739	98	134	223	3	109	78	5	80	22	17	51	3	26	28	0	27
0.38	1355	233	720	44	191	161	3	134	40	27	78	42	3	51	3	39	8	13	26
0.39	1147	325	681	11	241	130	24	139	11	58	56	3	57	10	21	33	0	29	10
0.40	955	424	625	0	278	78	60	123	0	83	27	23	51	0	39	13	12	28	0
0.41	778	527	555	11	296	35	101	92	10	90	5	48	29	10	41	0	29	11	9
0.42	618	629	475	41	295	8	136	53	37	76	1	62	7	31	25	7	32	0	24
0.43	476	728	390	87	274	0	158	20	69	49	17	57	0	46	6	25	17	8	24
0.44	351	821	304	143	236	13	161	2	94	20	43	36	12	42	1	36	2	24	9
0.45	245	904	221	205	186	43	145	3	103	2	64	13	34	23	14	28	3	28	0
0.46	157	976	147	266	132	84	113	23	92	3	70	0	50	4	32	10	19	15	9
0.47	89	1034	85	320	80	129	74	54	66	22	57	7	48	1	39	0	31	1	23
0.48	39	1076	39	363	38	168	36	88	35	49	33	28	30	15	28	8	25	4	23
0.49	10	1102	10	391	10	195	10	114	10	73	9	50	9	35	9	26	9	19	9
0.50	0	1111	0	400	0	204	0	123	0	83	0	59	0	44	0	35	0	28	0

U	M=21	M=22	M=23	M=24	M=25	M=26	M=27	M=28	M=29	M=30	M=31	M=32	M=33	M=34	M=35	M=36	M=37	M=38	M=39	M=40
0.0	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000	10000
0.01	8634	8509	8379	8246	8108	7967	7823	7675	7524	7371	7215	7056	6895	6733	6568	6403	6236	6068	5899	5730
0.02	5396	5056	4719	4386	4058	3737	3425	3122	2829	2549	2282	2028	1789	1564	1355	1162	985	823	678	548
0.03	2157	1791	1460	1164	903	679	489	334	212	120	56	17	1	4	23	54	95	142	192	244
0.04	335	178	74	17	0	15	54	110	176	244	310	369	417	451	470	474	463	439	404	360
0.05	23	81	159	245	327	396	445	471	474	454	415	361	298	231	167	109	62	27	7	0
0.06	343	419	465	477	456	407	338	259	180	109	54	17	1	4	22	51	85	117	144	161
0.07	472	427	352	260	168	89	33	4	2	22	57	96	132	157	167	162	142	112	78	45
0.08	261	157	71	17	0	15	51	97	137	162	168	152	122	83	46	17	2	2	14	35
0.09	33	1	12	52	103	146	168	163	135	93	50	17	1	4	22	46	70	83	84	73
0.10	23	75	130	164	168	140	94	46	12	0	10	35	63	82	85	73	50	25	7	0
0.11	135	169	163	124	70	23	1	7	33	63	84	85	67	40	15	1	3	17	36	49
0.12	167	125	65	17	0	15	47	77	87	74	46	17	1	4	21	41	52	49	35	16
0.13	81	24	0	15	51	81	87	66	33	7	1	14	36	51	50	35	15	2	2	14
0.14	4	7	42	78	88	67	31	4	2	21	44	54	44	22	4	1	12	27	36	31
0.15	23	66	89	76	39	7	2	21	46	54	40	16	1	4	20	34	35	22	7	0
0.16	80	89	58	17	0	15	42	55	42	17	1	6	23	36	32	16	2	2	13	24
0.17	83	42	6	4	31	54	49	23	2	4	23	36	31	14	1	4	18	26	21	8
0.18	32	1	12	43	56	37	9	1	17	35	34	16	1	4	19	27	20	6	0	8
0.19	0	19	50	53	25	2	7	29	38	23	4	2	16	27	21	6	0	9	19	18
0.20	23	54	49	17	0	15	36	33	12	0	10	26	24	9	0	8	19	18	7	0
0.21	56	48	13	1	21	39	27	5	2	19	28	15	1	4	17	20	9	0	6	15
0.22	48	12	2	25	39	22	1	7	25	25	7	0	12	21	13	1	3	14	15	5
0.23	13	2	27	40	18	0	12	28	20	2	4	18	19	6	0	10	17	8	0	5
0.24	1	26	40	17	0	15	29	16	0	8	21	15	1	4	16	13	2	2	11	12
0.25	23	41	19	0	16	30	14	0	12	22	10	0	9	17	8	0	7	14	7	0
0.26	42	23	0	15	30	13	0	14	22	7	1	13	16	4	1	12	12	2	2	11
0.27	30	1	13	31	14	0	15	22	5	2	16	14	1	4	14	8	0	7	12	4
0.28	5	8	31	17	0	15	22	5	3	17	12	0	7	15	5	1	10	10	1	4
0.29	3	29	22	0	13	23	6	3	18	12	0	9	14	3	3	12	7	0	7	9
0.30	23	29	3	9	24	8	2	18	12	0	10	13	1	5	12	4	1	10	7	0
0.31	33	9	4	24	12	1	17	13	0	11	13	1	6	12	2	3	11	4	1	8
0.32	19	0	22	17	0	15	16	0	10	14	1	6	12	2	4	11	2	2	9	3
0.33	1	15	24	1	11	19	1	8	15	1	6	13	1	5	11	1	4	9	1	3
0.34	5	27	7	5	21	4	5	17	3	5	13	2	5	11	1	5	9	1	5	7
0.35	23	17	1	20	10	2	17	6	3	14	3	4	11	1	5	9	0	6	7	0
0.36	27	2	14	17	0	15	10	1	14	5	3	12	2	5	9	0	6	6	0	7
0.37	12	4	22	3	9	15	0	12	8	1	12	3	4	10	0	7	6	0	7	3
0.38	0	20	12	3	19	2	8	12	0	12	5	3	10	1	6	6	0	8	2	2
0.39	8	22	0	16	9	3	15	1	9	8	1	11	2	5	7	0	8	2	3	6
0.40	23	8	7	17	0	15	5	5	12	0	10	4	4	9	0	8	3	3	7	0
0.41	22	0	20	4	9	12	1	14	1	8	7	1	10	0	7	4	2	7	0	6
0.42	7	10	15	1	17	1	11	6	4	11	0	10	2	5	6	1	8	0	6	2
0.43	0	21	2	13	8	4	13	0	12	1	8	5	3	8	0	8	1	6	3	2
0.44	11	15	3	17	0	15	2	9	6	4	9	1	9	0	8	2	4	4	2	6
0.45	23	2	15	6	8	10	3	12	0	11	0	9	2	6	4	3	6	1	7	0
0.46	18	3	18	0	16	0	13	2	9	4	6	6	3	7	1	8	0	7	0	6
0.47	4	16	6	10	8	6	9	3	10	1	10	0	9	0	8	0	7	1	5	2
0.48	1	20	0	17	0	15	0	12	1	10	1	8	2	6	3	5	3	3	4	2
0.49	14	8	11	8	8	8	6	8	4	7	3	7	2	7	2	6	1	6	1	6
0.50	23	0	19	0	16	0	14	0	12	0	10	0	9	0	8	0	7	0	7	0

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