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Debye–Waller Factors and Absorptive Scattering Factors of Elemental Crystals

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Abstract

Debye–Waller factors and absorptive scattering factors are given of 44 elemental crystals over the temperature range from 1 to 1000 K or to the melting temperature, whichever is smaller. The Debye–Waller factors are derived from the experimentally determined phonon density of states and the accuracy of these factors is typically 2 to 3%. Necessary data have also been compiled for an additional 22 elemental crystals for which the characteristic Debye temperatures are known. These data can be used to estimate the Debye–Waller factor at any temperature using the analytical Debye expression of the phonon density of states.

1. Introduction

The *Debye–Waller factor* is among the few parameters that one must know in order to perform any kind of dynamical electron diffraction calculation, including multislice calculations of high-resolution electron microscopy (HREM) images. The important role played by the Debye–Waller factor in dynamical electron diffraction calculations is twofold. The thermal vibration of the crystal lattice smears the otherwise perfectly periodic crystal potential. The real instant crystal potential is thus no longer periodic. However, in most situations, an average potential can still be defined. In general, this average crystal potential is periodic, giving rise to discrete scattered beams satisfying the *Bragg law* just for a perfect crystal. The average potential is, however, more smeared out compared with the potential of a perfect crystal. In real space and with the harmonic approximation of lattice vibrations, the effect may be described by a convolution of the perfect-crystal potential with a Gaussian function describing the statistical distribution of the lattice displacements. Alternatively, in reciprocal space, the effect is described by multiplication of the perfect-crystal structure factor with the Debye–Waller factor (James, 1965)

$$V_g = V_g^{(0)} \exp(-Bs^2), \qquad (1)$$

in which $V_g^{(0)}$ denotes the gth structure factor of a perfect crystal, $s = g/4\pi = \sin\theta/\lambda$, θ being the scattering angle and λ the electron wavelength, and $\exp(-Bs^2)$ is the usual Debye–Waller factor. The factor B is called the *temperature factor* or *Debye parameter* and sometimes simply the Debye–Waller factor. For the convenience of later discussion in this paper, we will call this parameter the Debye–Waller factor.

The deviation between the real instant crystal potential and the average potential gives rise to diffuse scattering. The diffusely scattered electrons mainly appear between the elastically scattered Bragg beams (Cowley, 1981; Hirsch, Howie, Nicholson, Pashley & Whelan, 1965) and, to a good approximation, the effect of the diffuse scattering on the elastically scattered electrons may be described by an additional imaginary part of the *optical potential* (Yoshioka, 1957; Dederichs, 1972). As we will see later, the calculation of the imaginary part of the optical potential also requires a prior knowledge of the Debye–Waller factor.

Despite the importance of the Debye–Waller factor in dynamical electron diffraction calculations, accurate values of the Debye–Waller factors are not readily available for most crystals. Experimentally, the Debye–Waller factors may be measured using such techniques as neutron and X-ray diffraction. However, the experimental results are normally published for one temperature, such as room temperature (Butt, Willis & Heger, 1988), which does not correspond exactly to the experimental situation under which an electron microscopy experiment is normally conducted. It is the aim of this paper to present tables of Debye–Waller factors for 44 elemental crystals over the full temperature range from 1 to 1000 K, or to the melting point of the crystal, whichever is smaller. For these elemental crystals, accurate data on the phonon density of states have been obtained by neutron scattering experiments (Sears & Shelley, 1991). For other elemental crystals with known Debye temperatures, all necessary data have been compiled so that an estimate of the Debye–Waller factor can be made for any temperature using the Debye formula.

Numerical evaluation of the absorptive part of the scattering factors is straightforward and these numerical data can be used directly for dynamical diffraction

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calculations. However, a more efficient and probably more widely used form of the electron scattering factor is that of Doyle & Turner (1968), who fitted the numerical elastic electron scattering factors with four Gaussians in the form

$$f(s) = \sum_{i=1}^{4} a_i \exp(-b_i s^2). \quad (2)$$

Recently, Dudarev, Peng & Whelan (1995) successfully fitted the absorptive part of the electron scattering factors using five Gaussians. Relevant parameters for some selected elements were calculated for room temperature using the Debye–Waller factors compiled by Radi (1970). Some of the Debye–Waller factors given by Radi (1970) are, however, not accurate. For example, for K, Ca, Rb, Sr, Y, Sn, Cs and Ba, the Debye–Waller factors given by Radi differ from experimental data by more than 100%. In this paper, parameterization of the absorptive part of the scattering factors for 43 elemental crystals with known phonon density of states has been made over the temperature range from 65 to 500 K or to the melting temperature, whichever is smaller. When an accurate value of the Debye–Waller factor is available, the parameterization can also be made for other crystals using the computer program developed by Peng, Ren, Dudarev & Whelan (1996).

2. The Debye–Waller factor

The Debye–Waller B factor is related to the mean square of the x component u_x of the thermal displacement of an atom from its equilibrium position

$$B = 8\pi^2 \langle u_x^2 \rangle, \quad (3)$$

where $\langle \ldots \rangle$ denotes the thermal average. In the harmonic approximation, $\langle u_x^2 \rangle$ is given by (Lovesey, 1984)

$$\langle u_x^2 \rangle = (\hbar/2m) \int_0^{\omega_m} \coth(\hbar\omega/2k_B T)[g(\omega)/\omega]\, d\omega, \quad (4)$$

in which m is the atomic mass, T the temperature, k_B the usual Boltzmann constant, $g(\omega)$ the *normalized phonon density of states* and ω_m the *maximum phonon frequency*.

Following Sears & Shelley (1991), we introduce two dimensionless quantities:

$$x = \omega/\omega_m, \qquad y = T/T_m, \quad (5)$$

where T_m is related to the maximum phonon frequency ω_m by the relation $\hbar\omega_m = k_B T_m$. The Debye–Waller factor is then given by

$$B = (4\pi^2\hbar/m\omega_m) \int_0^1 \coth(x/2y)[f(x)/x]\, dx, \quad (6)$$

where $f(x) = \omega_m g(\omega_m x)$ is the *reduced phonon density of states*. Experimentally, the reduced phonon density of states can be determined by the technique of neutron inelastic scattering. Once this function is determined, a direct numerical integration of (6) then gives the Debye–Waller factor for any temperature. In a recent paper, Sears & Shelley (1991) compiled all the relevant data and references for 46 elemental crystals in the Periodic Table with the f.c.c., b.c.c., h.c.p. and diamond structures for which the phonon densities of states have been determined from neutron inelastic scattering measurements. These data allow us to calculate the Debye–Waller factor for 44 elemental crystals over the temperature range from 1 to 1000 K or to the melting temperature of the crystal, whichever is smaller. In Table 1 are given some of the most relevant Debye–Waller factors; other factors are given in Tables 4 to 46.*

For those elements for which the data of the phonon density of states are not available, an estimate of the Debye–Waller factor may be made using the Debye formula for the reduced phonon density of states

$$f(x) = 3x^2. \quad (7)$$

Substitution of the Debye formula into (7) then gives (Willis & Pryor, 1975)

$$B = (11492/A)(T/\Theta_D^2)[\Phi(\Theta_D/T) + \tfrac{1}{4}(\Theta_D/T)](A^{-2}), \quad (8)$$

in which Θ_D is the Debye temperature, A is the atomic weight in terms of $^{12}C = 12$ and $\Phi(y)$ is the Debye integral

$$\Phi(y) = (1/y) \int_0^y [\exp(x) - 1]^{-1} x\, dx. \quad (9)$$

In Table 2, we have complied values of atomic weights and Debye temperatures for 22 elements that are not included in Table 1. The data for atomic weights and crystal melting point are taken from §2.1.2 of Kaye & Laby (1966), crystal structures and Debye temperatures are from Kittel (1971). In Table 3, the values of the Debye integral (9) for y up to 10 are given. Since this integral is a smooth function of y, values of this integral for any y not listed in Table 3 can be obtained safely by interpolation. For $y > 10.0$ and to a good approximation, this integral may be taken to be equal to $1.6454/y$. From the data listed in Tables 2 and 3 and (8), an estimate of the Debye–Waller factor can be made for any temperature.

* An extended version of Table 1 for the temperature range 1–1000 K and more extensive Tables 4–46 giving absorptive scattering factors for the temperature range 65 to 500 K have been deposited with the IUCr (Reference: ZH0008). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Debye–Waller factors of elemental crystals*

T (K)	Li (B.c.c.)	Be (H.c.p.)	C (Dia)	Na (B.c.c.)	Mg (H.c.p.)	Al (F.c.c.)	Si (Dia)	K (B.c.c.)	Ca (F.c.c.)	Ca (B.c.c.)	Sc (H.c.p.)	Ti (H.c.p.)	V (B.c.c.)	Cr (B.c.c.)
85.0	1.9009	0.3637	0.1299	1.9377	0.5263	0.3301	0.2170	3.1319	0.5805	0.7556	0.2165	0.1491	0.1660	0.1259
90.0	1.4780	0.3652	0.1300	2.0516	0.5572	0.3374	0.2201	3.3159	0.6146	0.8000	0.2292	0.1579	0.1758	0.1274
110.0	1.8063	0.3719	0.1307	2.5072	0.6810	0.2932	0.2342	4.0510	0.7511	0.9777	0.2801	0.1930	0.2148	0.0943
120.0	1.9705	0.3758	0.1311	2.7348	0.7429	0.3198	0.2423	4.4182	0.8194	1.0665	0.3056	0.2105	0.2343	0.1028
130.0	2.1347	0.3800	0.1315	2.9624	0.8048	0.3465	0.2511	4.7852	0.8876	1.1553	0.3310	0.2281	0.2539	0.1114
140.0	2.2989	0.3846	0.1320	3.1900	0.8667	0.3731	0.2607	5.1518	0.9558	1.2441	0.3565	0.2456	0.2734	0.1200
160.0	2.6272	0.3947	0.1330	3.6448	0.9904	0.4264	0.2648	5.8840	1.0922	1.4216	0.4074	0.2807	0.3124	0.1371
170.0	2.7913	0.4002	0.1336	3.8721	1.0523	0.4531	0.2814	6.2496	1.1603	1.5104	0.4328	0.2982	0.3320	0.1457
180.0	2.9554	0.4061	0.1342	4.0993	1.1141	0.4797	0.2979	6.6148	1.2285	1.5991	0.4583	0.3158	0.3515	0.1542
190.0	3.1195	0.4123	0.1349	4.3264	1.1759	0.5064	0.3145	6.9796	1.2966	1.6878	0.4837	0.3333	0.3710	0.1628
210.0	3.4477	0.3032	0.1363	4.7802	1.2996	0.5596	0.3476	7.7077	1.4328	1.8651	0.5346	0.3684	0.4100	0.1799
220.0	3.6117	0.3176	0.1370	5.0070	1.3614	0.5863	0.3641	8.0711	1.5008	1.9537	0.5600	0.3859	0.4295	0.1885
230.0	3.7758	0.3321	0.1378	5.2336	1.4232	0.6129	0.3807	8.4340	1.5688	2.0423	0.5854	0.4034	0.4490	0.1970
240.0	3.9398	0.3465	0.1386	5.4601	1.4849	0.6395	0.3972	8.7963	1.6368	2.1308	0.6109	0.4210	0.4685	0.2056
260.0	4.2678	0.3754	0.1403	5.9128	1.6085	0.6928	0.4303	9.5192	1.7728	2.3078	0.6617	0.4560	0.5075	0.2227
270.0	4.4318	0.3898	0.1412	6.1389	1.6702	0.7194	0.4469	9.8798	1.8407	2.3963	0.6871	0.4735	0.5270	0.2313
280.0	4.5958	0.4042	0.1422	6.3648	1.7319	0.7460	0.4634	10.2398	1.9086	2.4847	0.7125	0.4911	0.5465	0.2398

T (K)	Fe (B.c.c.)	Fe (F.c.c.)	Ni (F.c.c.)	Cu (F.c.c.)	Zn (H.c.p.)	Ge (Dia)	Kr (F.c.c.)	Rb (B.c.c.)	Sr (B.c.c.)	Y (H.c.p.)	Zr (H.c.p.)	Nb (B.c.c.)	Mo (B.c.c.)	Pd (F.c.c.)
85.0	0.1461	0.1619	0.1502	0.1598	0.3317	0.1670	2.8102	3.8986	1.1061	0.2486	0.1652	0.1306	0.0626	0.1294
90.0	0.1493	0.1715	0.1094	0.1692	0.3512	0.1844	2.9748	4.1269	1.1710	0.2633	0.1749	0.1383	0.0662	0.1370
110.0	0.1221	0.2095	0.1337	0.2068	0.4292	0.2254	3.6321	5.0388	1.4308	0.3217	0.2137	0.1690	0.0809	0.1674
120.0	0.1332	0.2286	0.1458	0.2256	0.4682	0.2458		5.4935	1.5606	0.3510	0.2331	0.1843	0.0883	0.1827
130.0	0.1443	0.2476	0.1580	0.2444	0.5072	0.2663		5.9475	1.6903	0.3802	0.2526	0.1997	0.0957	0.1979
140.0	0.1554	0.2667	0.1701	0.2632	0.5462	0.2868		6.4004	1.8199	0.4094	0.2720	0.2150	0.1030	0.2131
160.0	0.1775	0.3047	0.1944	0.3008	0.6242	0.3278		7.3033	2.0788	0.4678	0.3108	0.2457	0.1177	0.2435
170.0	0.1886	0.3238	0.2066	0.3196	0.6632	0.3483		7.7531	2.2082	0.4970	0.3302	0.2611	0.1251	0.2587
180.0	0.1997	0.3428	0.2187	0.3384	0.7022	0.3687		8.2016	2.3374	0.5262	0.3496	0.2764	0.1324	0.2739
190.0	0.2108	0.3618	0.2309	0.3571	0.7411	0.3892		8.6488	2.4665	0.5554	0.3690	0.2918	0.1398	0.2891
210.0	0.2330	0.3999	0.2551	0.3947	0.8190	0.4302		9.5392	2.7243	0.6137	0.4078	0.3225	0.1545	0.3196
220.0	0.2441	0.4189	0.2673	0.4135	0.8580	0.4506		9.9821	2.8530	0.6429	0.4272	0.3378	0.1619	0.3347
230.0	0.2552	0.4379	0.2794	0.4322	0.8969	0.4711		10.4235	2.9816	0.6720	0.4466	0.3531	0.1692	0.3499
240.0	0.2663	0.4570	0.2916	0.4510	0.9359	0.4915		10.8632	3.1100	0.7011	0.4660	0.3685	0.1766	0.3651
260.0	0.2884	0.4950	0.3158	0.4886	1.0137	0.5325		11.7373	3.3664	0.7594	0.5047	0.3991	0.1912	0.3955
270.0	0.2995	0.5140	0.3280	0.5073	1.0526	0.5529		12.1717	3.4944	0.7885	0.5241	0.4144	0.1986	0.4107
280.0	0.3106	0.5330	0.3401	0.5261	1.0915	0.5734		12.6041	3.6221	0.8176	0.5435	0.4297	0.2059	0.4259

T (K)	Ag (F.c.c.)	Sn (Dia)	Xe (F.c.c.)	Cs (B.c.c.)	Ba (B.c.c.)	La (F.c.c.)	Tb (H.c.p.)	Ho (H.c.p.)	Ta (B.c.c.)	W (B.c.c.)	Pt (F.c.c.)	Au (F.c.c.)	Pb (F.c.c.)	Th (F.c.c.)
85.0	0.2134	0.3290	2.5987	5.2797	0.8961	0.5419	0.2944	0.2444	0.0936	0.0464	0.1082	0.1802	0.6228	0.2125
90.0	0.2259	0.3483	2.7507	5.5878	0.9488	0.5738	0.3117	0.2588	0.0991	0.0491	0.1145	0.1908	0.6593	0.2250
110.0	0.2761	0.4257	3.3574	6.8158	1.1591	0.7010	0.3809	0.3162	0.1211	0.0600	0.1400	0.2332	0.8055	0.2750
120.0	0.3012	0.4644	3.6598	7.4268	1.2641	0.7646	0.4155	0.3449	0.1321	0.0654	0.1527	0.2544	0.8784	0.2999
130.0	0.3262	0.5031	3.9614	8.0355	1.3691	0.8281	0.4500	0.3737	0.1431	0.0709	0.1654	0.2755	0.9514	0.3249
140.0	0.3513	0.5418	4.2622	8.6418	1.4739	0.8916	0.4846	0.4023	0.1541	0.0763	0.1781	0.2967	1.0242	0.3498
160.0	0.4015	0.6191	4.8611	9.8464	1.6833	1.0185	0.5536	0.4597	0.1761	0.0872	0.2035	0.3390	1.1697	0.3997
170.0	0.4265	0.6577		10.4443	1.7878	1.0818	0.5881	0.4883	0.1871	0.0927	0.2162	0.3602	1.2423	0.4246
180.0	0.4516	0.6964		11.0390	1.8922	1.1451	0.6226	0.5170	0.1981	0.0981	0.2289	0.3813	1.3148	0.4495
190.0	0.4766	0.7350		11.6304	1.9965	1.2083	0.6570	0.5456	0.2090	0.1036	0.2416	0.4025	1.3873	0.4744
210.0	0.5267	0.8123		12.8022	2.2046	1.3345	0.7259	0.6028	0.2310	0.1145	0.2670	0.4448	1.5318	0.5241
220.0	0.5517	0.8509		13.3823	2.3085	1.3975	0.7603	0.6313	0.2420	0.1199	0.2797	0.4659	1.6040	0.5490
230.0	0.5767	0.8895		13.9583	2.4121	1.4605	0.7946	0.6599	0.2529	0.1254	0.2924	0.4870	1.6760	0.5738
240.0	0.6017	0.9281		14.5300	2.5157	1.5233	0.8290	0.6884	0.2639	0.1308	0.3051	0.5081	1.7478	0.5986
260.0	0.6517	1.0053		15.6596	2.7222	1.6488	0.8975	0.7454	0.2858	0.1417	0.3304	0.5503	1.8912	0.6482
270.0	0.6767	1.0439		16.2173	2.8251	1.7113	0.9318	0.7739	0.2968	0.1471	0.3431	0.5714	1.9627	0.6730
280.0	0.7017	1.0825		16.7698	2.9279	1.7739	0.9660	0.8023	0.3078	0.1526	0.3557	0.5925	2.0341	0.6977

It should be noted, however, that the Debye model applies strictly only for cubic lattices with one atom per primitive unit cell, and the model does not provide a good representation of the Debye–Waller factor over a wide range of temperature. Fig. 1 shows the Debye–Waller factor as a function of temperature for potassium. The two curves in the figure were calculated using the Debye model and the experimentally determined phonon density of states (denoted by PDS in the figure), respectively. It is seen that over the whole temperature range the Debye model gives excellent results. On the other hand, for Si (see Fig. 2), the chosen Debye temperature is seen to give a good fit at low temperatures but the model fails badly at high temperatures. If the Debye temperature Θ_D is taken as a fitting parameter, by equating (6) to (8), we then obtain a temperature-dependent Debye temperature $\Theta_D(T)$ and the result is plotted in the insert of Fig. 2. It should be noted that

Table 2. *Parameters relevant to the Debye model*

Element	Z	Structure	Atomic weight	Debye temperature (K)	Melting point (K)
Mn	25	Cubic	54.940	410.000	1523.150
Co	27	H.c.p.	58.930	445.000	1767.150
Ga	31	Complex	69.720	320.000	302.950
As	33	Rhomb.	74.920	282.000	886.150
Se	34	Hex.	78.960	90.000	493.150
Ru	44	H.c.p.	101.070	600.000	2583.150
Rh	45	F.c.c.	102.910	480.000	2236.150
Cd	48	H.c.p.	112.400	209.000	594.250
In	49	Tetr.	114.820	108.000	429.750
Sb	51	Rhomb.	121.750	211.000	903.890
Te	52	Hex.	127.600	153.000	723.150
Gd	64	H.c.p.	157.250	200.000	1583.150
Dy	66	H.c.p.	162.500	210.000	1683.150
Hf	72	H.c.p.	178.490	252.000	2503.150
Ta	73	B.c.c.	180.950	240.000	3273.150
Re	75	H.c.p.	186.210	430.000	3453.150
Os	76	H.c.p.	190.200	500.000	3303.150
Ir	77	F.c.c.	192.220	420.000	2720.150
Hg	80	Rhomb.	200.590	71.900	234.290
Tl	81	H.c.p.	204.370	78.500	577.150
Bi	83	Rhomb.	209.000	119.000	544.550
U	92	Complex	238.000	207.000	1408.150

for all temperatures the Debye temperature obtained this way is much smaller than the corresponding specific heat value of 647 K (Flubacher, Leadbetter & Morrison, 1959). In the high-temperature region with $T > 300.0$ K, the Debye temperature is seen to be almost temperature independent and at 1000 K a limiting value of $\Theta_D = 500$ K has been achieved that is in good agreement with that given by Batterman & Chipman (1962). In general, the Debye model can be used only for a rough estimation. More reliable data should be used whenever possible.

3. Absorptive part of the scattering factor

In general, the crystal potential is time dependent. The time dependence of the potential is caused, among other factors, by the excitation of plasmon, core electrons or the thermal vibration of the lattice. The plasmon is a collective electron excitation with, in many cases, a well defined quantum of energy. The excitation of a plasmon is thus by nature a delocalized process. The associated momentum transfer during an inelastic collision is very small. Effectively, the plasmon excitation then contributes to the absorptive scattering factor at zero angle only (Howie, 1963). But the zeroth absorptive scattering factor does not affect the overall angular dependence of the diffracted-beam intensity in transmission diffraction geometry (Spence & Zuo, 1992). For many important applications, the effect of plasmon excitation may therefore be neglected. In principle, the core excitation process is a localized process that may affect the scattering properties of the crystal at large angles. The effect is, however, typically an order of magnitude smaller than the contribution due to thermal diffuse scattering (TDS) (Radi, 1970; Whelan, 1965).

The TDS contribution to the absorptive part of the scattering factor can be readily calculated by using an Einstein model of the thermal vibration of the crystal lattice (Hall & Hirsch, 1965; Bird & King, 1990)

$$f_{\rm abs}(E,B,s) = (2h/\beta m_0 c) \times \int {\rm d}\mathbf{s}' f^{(e)}(|\mathbf{s}/2+\mathbf{s}'|) f^{(e)}(|\mathbf{s}/2-\mathbf{s}'|) \times \{1-\exp[-2B(s'^2 - s^2/4)]\}, \quad (10)$$

where β is the velocity ratio $\beta = v/c$ and $f^{(e)}(s)$ the elastic scattering factor. From (10), it is clear that the absorptive part of the scattering factor depends on the acceleration voltage E, the Debye–Waller factor B and the angle of scattering. In this study, the elastic scattering factors listed in *International Tables for Crystallography* (Cowley, 1992) have been used in evaluating (10).

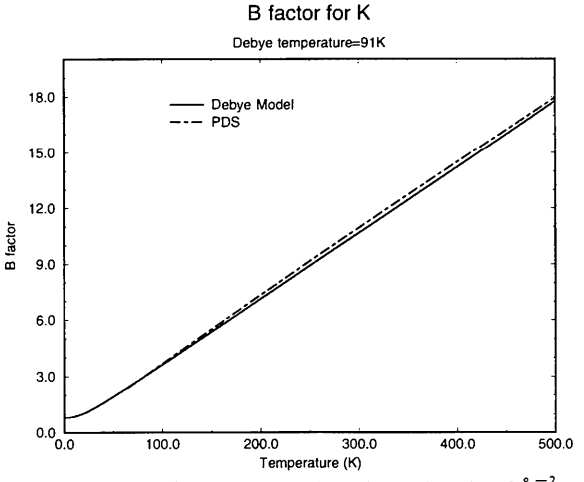

Fig. 1. Dependence of the Debye–Waller B factor (in units of Å^{-2}) on the temperature (in units of K) for potassium. The curve denoted by 'Debye model' was calculated using the Debye model and that denoted by 'PDS' was obtained using the experimentally determined phonon density of states.

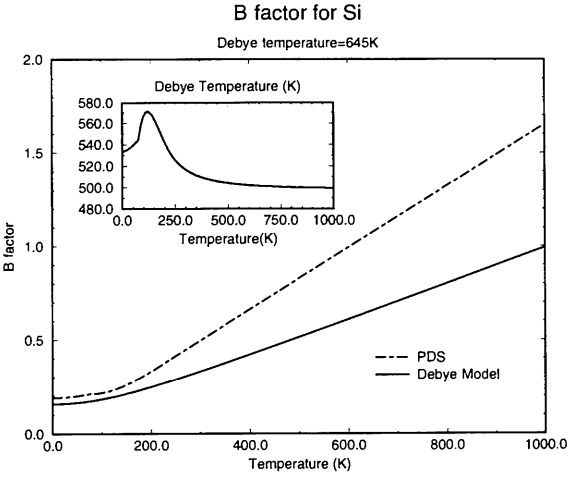

Fig. 2. Same as Fig. 1 but for Si. The insert is a plot of the Debye temperature obtained by fitting the B factor calculated using the Debye formula (8) to that using the phonon density of states (6).

Table 3. *Values of the Debye integral*

y	$\Phi(y)$	y	$\Phi(y)$	y	$\Phi(y)$	y	$\Phi(y)$	y	$\Phi(y)$
0.0500	0.9878	2.0500	0.5998	4.0500	0.3844	6.0500	0.2692	8.0500	0.2041
0.1000	0.9755	2.1000	0.5926	4.1000	0.3805	6.1000	0.2671	8.1000	0.2028
0.1500	0.9633	2.1500	0.5855	4.1500	0.3768	6.1500	0.2651	8.1500	0.2016
0.2000	0.9513	2.2000	0.5786	4.2000	0.3731	6.2000	0.2631	8.2000	0.2004
0.2500	0.9394	2.2500	0.5717	4.2500	0.3694	6.2500	0.2610	8.2500	0.1992
0.3000	0.9277	2.3000	0.5649	4.3000	0.3658	6.3000	0.2591	8.3000	0.1980
0.3500	0.9161	2.3500	0.5583	4.3500	0.3623	6.3500	0.2571	8.3500	0.1968
0.4000	0.9046	2.4000	0.5517	4.4000	0.3588	6.4000	0.2552	8.4000	0.1957
0.4500	0.8933	2.4500	0.5453	4.4500	0.3554	6.4500	0.2533	8.4500	0.1945
0.5000	0.8821	2.5000	0.5389	4.5000	0.3520	6.5000	0.2514	8.5000	0.1934
0.5500	0.8711	2.5500	0.5327	4.5500	0.3487	6.5500	0.2496	8.5500	0.1923
0.6000	0.8601	2.6000	0.5265	4.6000	0.3454	6.6000	0.2478	8.6000	0.1912
0.6500	0.8494	2.6500	0.5204	4.6500	0.3422	6.6500	0.2460	8.6500	0.1901
0.7000	0.8387	2.7000	0.5145	4.7000	0.3390	6.7000	0.2442	8.7000	0.1890
0.7500	0.8282	2.7500	0.5086	4.7500	0.3359	6.7500	0.2424	8.7500	0.1879
0.8000	0.8178	2.8000	0.5028	4.8000	0.3328	6.8000	0.2407	8.8000	0.1869
0.8500	0.8076	2.8500	0.4971	4.8500	0.3298	6.8500	0.2390	8.8500	0.1858
0.9000	0.7975	2.9000	0.4915	4.9000	0.3268	6.9000	0.2373	8.9000	0.1848
0.9500	0.7875	2.9500	0.4860	4.9500	0.3239	6.9500	0.2357	8.9500	0.1837
1.0000	0.7777	3.0000	0.4806	5.0000	0.3210	7.0000	0.2340	9.0000	0.1827
1.0500	0.7680	3.0500	0.4752	5.0500	0.3181	7.0500	0.2324	9.0500	0.1817
1.1000	0.7584	3.1000	0.4699	5.1000	0.3153	7.1000	0.2308	9.1000	0.1807
1.1500	0.7489	3.1500	0.4648	5.1500	0.3126	7.1500	0.2293	9.1500	0.1798
1.2000	0.7396	3.2000	0.4597	5.2000	0.3098	7.2000	0.2277	9.2000	0.1788
1.2500	0.7304	3.2500	0.4547	5.2500	0.3072	7.2500	0.2262	9.2500	0.1778
1.3000	0.7213	3.3000	0.4497	5.3000	0.3045	7.3000	0.2247	9.3000	0.1769
1.3500	0.7124	3.3500	0.4449	5.3500	0.3019	7.3500	0.2232	9.3500	0.1759
1.4000	0.7036	3.4000	0.4401	5.4000	0.2994	7.4000	0.2217	9.4000	0.1750
1.4500	0.6949	3.4500	0.4354	5.4500	0.2968	7.4500	0.2202	9.4500	0.1741
1.5000	0.6863	3.5000	0.4307	5.5000	0.2943	7.5000	0.2188	9.5000	0.1732
1.5500	0.6778	3.5500	0.4262	5.5500	0.2919	7.5500	0.2174	9.5500	0.1723
1.6000	0.6695	3.6000	0.4217	5.6000	0.2895	7.6000	0.2160	9.6000	0.1714
1.6500	0.6613	3.6500	0.4173	5.6500	0.2871	7.6500	0.2146	9.6500	0.1705
1.7000	0.6532	3.7000	0.4129	5.7000	0.2847	7.7000	0.2132	9.7000	0.1696
1.7500	0.6452	3.7500	0.4087	5.7500	0.2824	7.7500	0.2119	9.7500	0.1687
1.8000	0.6374	3.8000	0.4044	5.8000	0.2802	7.8000	0.2105	9.8000	0.1679
1.8500	0.6296	3.8500	0.4003	5.8500	0.2779	7.8500	0.2092	9.8500	0.1670
1.9000	0.6220	3.9000	0.3962	5.9000	0.2757	7.9000	0.2079	9.9000	0.1662
1.9500	0.6145	3.9500	0.3922	5.9500	0.2735	7.9500	0.2066	9.9500	0.1654
2.0000	0.6071	4.0000	0.3883	6.0000	0.2714	8.0000	0.2053	10.0000	0.1645

The dependence of f_{abs} on the acceleration voltage can be factored out and results can be converted easily from one voltage (for example 100 keV) to any other voltage

$$f_{abs}(E) = [\beta(100\,\text{keV})/\beta(E)]f_{abs}(100\,\text{keV}), \qquad (11)$$

in which $\beta = (1 - \gamma^{-2})^{-1}$, $\gamma = (m/m_0) = 1.0 + 1.9569341 \times 10^{-3}E$ and the acceleration voltage E is in keV.

The dependence of the absorptive part of the scattering factor on the angle of scattering or s can also be expressed more effectively by fitting the curve with five Gaussians, as Doyle & Turner did for the elastic scattering factor (Doyle & Turner, 1968)

$$f_{abs}(s)\exp(-Bs^2/2) = \sum_{i=1}^{5} a_i \exp(-b_i s^2). \qquad (12)$$

The inclusion of the factor $\exp(-Bs^2/2)$ on the left-hand side of (12) is because the absorptive part of the scattering factors increases with s as $-\exp(Bs^2/2)$ at large angles of scattering, while the fitted quantity $f_{abs}(s)\exp(-Bs^2/2)$ converges with increasing s. In general, the crystal structure factor V_g is given by

$$V_g = (\hbar^2/2m_0)(4\pi/\Omega)\sum_n \exp(-i\mathbf{g}\cdot\mathbf{r}_n) \times \sum_{i=1}^{5}\{a_{i,n}^{(\text{Re})}\exp[-(b_{i,n}^{(\text{Re})} + B_n)s^2] + ia_{i,n}^{(\text{Im})}\exp[-(b_{i,n}^{(\text{Im})} + B_n/2)s^2]\}, \qquad (13)$$

in which n labels the atoms within a unit cell with position vector $\mathbf{r}_n$, Ω is the unit-cell volume, and the superscripts Re and Im refer to the real and imaginary coefficients, respectively.

In Tables 4 to 46, we list the parameters for 43 elemental crystals of Table 1 (except for Ne) over the temperature range 75 to 275 K or to the melting point of the crystal, whichever is smaller.* The fitting was performed using a combined simulated annealing and least-squares method. Details of this method and its application to fit elastic and absorptive scattering factors of some important materials with zinc blende structure have been published separately (Peng *et al.*, 1996). Also listed in these tables is the root mean square of the

* See deposition footnote.

Table 4. *Absorptive scattering factors for Li and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	1.7479	−0.0001	−0.0007	0.0044	0.0018	0.0009	0.0718	0.3220	1.5240	5.2007	32.2820	0.2419E−05
77.0	1.7770	−0.0001	−0.0008	0.0044	0.0019	0.0009	0.0755	0.3334	1.5257	5.0272	31.1176	0.2696E−05
80.0	1.8220	−0.0001	−0.0007	0.0046	0.0018	0.0009	0.0727	0.3296	1.5973	5.6081	34.3960	0.2239E−05
100.0	1.6422	−0.0001	−0.0007	0.0043	0.0018	0.0008	0.0657	0.2996	1.4550	5.1049	32.3323	0.2245E−05
150.0	2.4630	−0.0001	−0.0009	0.0054	0.0020	0.0011	0.0956	0.4442	2.0467	6.6381	34.1771	0.1588E−05
200.0	3.2836	−0.0001	−0.0011	0.0064	0.0022	0.0014	0.1215	0.5824	2.6091	7.9076	35.7732	0.1628E−05
250.0	4.1038	−0.0001	−0.0012	0.0072	0.0023	0.0016	0.1477	0.7128	3.1856	9.5236	38.1815	0.1472E−05
290.0	4.7597	−0.0001	−0.0012	0.0079	0.0024	0.0016	0.1649	0.8019	3.6908	11.7402	41.7849	0.1179E−05
293.0	4.8089	−0.0001	−0.0013	0.0078	0.0024	0.0017	0.1694	0.8223	3.6744	10.9027	40.0126	0.1380E−05
295.0	4.8417	−0.0001	−0.0013	0.0080	0.0024	0.0016	0.1661	0.8112	3.7554	12.0014	42.1248	0.1177E−05

Table 5. *Absorptive scattering factors for Be and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.3610	−0.0004	0.0024	0.0014	0.0004	0.0006	0.0599	0.3877	1.5707	5.6472	14.0525	0.2700E−05
77.0	0.3615	−0.0004	0.0024	0.0015	0.0006	0.0003	0.0592	0.3943	1.6877	8.6158	19.1383	0.2720E−05
80.0	0.3623	−0.0004	0.0024	0.0014	0.0007	0.0003	0.0600	0.3893	1.5913	7.8296	22.5571	0.2295E−05
100.0	0.3684	−0.0004	0.0024	0.0015	0.0007	0.0003	0.0609	0.3957	1.6259	7.9839	21.9215	0.2319E−05
150.0	0.3894	−0.0004	0.0024	0.0015	0.0008	0.0003	0.0650	0.4058	1.5305	6.9546	24.6217	0.2068E−05
200.0	0.2888	−0.0003	0.0019	0.0012	0.0007	0.0003	0.0493	0.3101	1.1708	5.4594	24.3437	0.2180E−05
250.0	0.3609	−0.0004	0.0022	0.0014	0.0008	0.0004	0.0620	0.3671	1.2383	4.7992	19.8094	0.1818E−05
290.0	0.4187	−0.0004	0.0025	0.0015	0.0007	0.0006	0.0698	0.4275	1.4891	5.0565	17.2977	0.1442E−05
293.0	0.4230	−0.0004	0.0025	0.0015	0.0009	0.0004	0.0707	0.4287	1.4847	5.9267	22.2474	0.1853E−05
295.0	0.4259	−0.0004	0.0026	0.0016	0.0008	0.0003	0.0704	0.4392	1.6364	7.2607	24.6900	0.1920E−05

Table 6. *Absorptive scattering factors for C and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1296	−0.0003	0.0019	0.0012	0.0011	0.0007	0.0183	0.1493	0.4962	1.7662	6.9381	0.1613E−05
77.0	0.1296	−0.0003	0.0019	0.0012	0.0011	0.0007	0.0190	0.1471	0.4778	1.6958	6.7581	0.1632E−05
80.0	0.1297	−0.0003	0.0019	0.0012	0.0011	0.0007	0.0192	0.1467	0.4748	1.6866	6.7462	0.1663E−05
100.0	0.1303	−0.0003	0.0020	0.0013	0.0011	0.0006	0.0184	0.1507	0.5096	1.8262	7.1149	0.1525E−05
150.0	0.1325	−0.0003	0.0020	0.0013	0.0011	0.0006	0.0179	0.1549	0.5326	1.8897	7.2316	0.1433E−05
200.0	0.1355	−0.0003	0.0019	0.0013	0.0012	0.0007	0.0221	0.1473	0.4610	1.6504	6.7582	0.1447E−05
250.0	0.1394	−0.0003	0.0020	0.0013	0.0012	0.0007	0.0218	0.1548	0.5022	1.7798	7.1356	0.1183E−05
290.0	0.1432	−0.0003	0.0021	0.0014	0.0012	0.0006	0.0212	0.1627	0.5573	2.0070	7.8300	0.9269E−06
293.0	0.1435	−0.0003	0.0021	0.0014	0.0012	0.0007	0.0215	0.1621	0.5506	1.9735	7.7289	0.9114E−06
295.0	0.1437	−0.0003	0.0021	0.0014	0.0012	0.0007	0.0216	0.1622	0.5516	1.9776	7.7313	0.9111E−06

Table 7. *Absorptive scattering factors for Na and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	1.7099	−0.0010	−0.0099	0.0396	0.0270	0.0030	0.0814	0.3667	1.2598	2.8514	23.7104	0.5227E−04
77.0	1.7554	−0.0068	0.0569	0.0251	−0.0211	0.0055	0.2277	1.7152	9.4654	13.1051	32.9902	0.8048E−04
80.0	1.8238	−0.0008	−0.0092	0.0483	0.0199	0.0024	0.0758	0.3547	1.4727	3.5641	39.3003	0.3560E−04
100.0	2.2794	−0.0008	−0.0101	0.0601	0.0151	0.0014	0.0853	0.4160	1.8558	4.7842	40.3841	0.9110E−05
150.0	3.4174	−0.0010	−0.0126	0.0753	0.0128	0.0020	0.1172	0.5871	2.5708	6.2995	37.9184	0.9693E−05
200.0	4.5533	−0.0012	−0.0141	0.0824	0.0142	0.0032	0.1521	0.7466	3.1796	6.5522	32.4184	0.1213E−04
250.0	5.6865	−0.0014	−0.0144	0.0886	0.0133	0.0044	0.1814	0.8694	3.8320	7.0012	30.0097	0.1450E−04
290.0	6.5906	−0.0015	−0.0145	0.0939	0.0124	0.0042	0.2070	0.9707	4.3378	8.3210	35.5237	0.1232E−04
293.0	6.6583	−0.0015	−0.0145	0.0953	0.0113	0.0041	0.2083	0.9749	4.3959	8.7251	36.0870	0.1214E−04
295.0	6.7034	−0.0015	−0.0143	0.0975	0.0093	0.0040	0.2088	0.9729	4.4626	9.5466	36.2160	0.1156E−04

Table 8. *Absorptive scattering factors for Mg and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.4644	−0.0036	0.0228	0.0136	−0.0027	0.0050	0.0753	0.4861	1.6083	4.6335	7.0508	0.1988E−04
77.0	0.4768	−0.0037	0.0231	0.0133	0.0000	0.0029	0.0773	0.4957	1.5823	4.9542	8.8279	0.1861E−04
80.0	0.4953	−0.0039	0.0234	0.0124	0.0018	0.0026	0.0802	0.5093	1.5055	2.9095	9.7799	0.1893E−04
100.0	0.6191	−0.0001	−0.0050	0.0288	0.0146	0.0031	0.0001	0.1128	0.6089	1.9055	11.3436	0.1994E−04
150.0	0.9286	−0.0005	−0.0069	0.0392	0.0160	0.0036	0.0358	0.1801	0.8445	2.5088	13.7782	0.2228E−04
200.0	1.2378	−0.0009	−0.0089	0.0463	0.0181	0.0046	0.0612	0.2537	1.0323	2.8026	13.9662	0.2727E−04
250.0	1.5467	−0.0010	−0.0104	0.0518	0.0200	0.0056	0.0740	0.3127	1.2168	3.0648	14.7109	0.4018E−04
290.0	1.7936	−0.0010	−0.0106	0.0612	0.0172	0.0038	0.0782	0.3372	1.4521	4.4379	24.4504	0.2811E−04
293.0	1.8122	−0.0010	−0.0105	0.0620	0.0168	0.0036	0.0765	0.3347	1.4771	4.6238	25.3124	0.2671E−04
295.0	1.8245	−0.0010	−0.0106	0.0620	0.0170	0.0037	0.0769	0.3372	1.4811	4.5950	25.2689	0.2661E−04

Table 9. *Absorptive scattering factors for Al and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.3167	−0.0032	0.0188	0.0124	0.0019	0.0024	0.0528	0.3256	1.1173	3.6669	9.5939	0.1839E−04
77.0	0.3193	−0.0035	0.0154	0.0104	0.0073	0.0028	0.0561	0.2938	0.6960	1.7533	9.4904	0.1488E−04
80.0	0.3232	−0.0035	0.0163	0.0104	0.0067	0.0028	0.0563	0.3034	0.7543	1.8431	9.5694	0.1469E−04
100.0	0.2666	−0.0029	0.0147	0.0105	0.0047	0.0021	0.0468	0.2595	0.7610	2.0968	10.1535	0.1404E−04
150.0	0.3998	−0.0039	0.0214	0.0132	0.0045	0.0020	0.0666	0.3888	1.1191	3.5063	15.6665	0.1325E−04
200.0	0.5330	−0.0047	0.0275	0.0068	0.0107	0.0038	0.0834	0.5226	1.0807	2.1732	13.1130	0.3671E−04
250.0	0.6662	−0.0002	−0.0060	0.0347	0.0165	0.0049	0.0022	0.1194	0.6271	2.0250	12.8574	0.4138E−04
290.0	0.7726	−0.0002	−0.0065	0.0398	0.0163	0.0047	0.0020	0.1335	0.7291	2.4528	15.3907	0.3868E−04
293.0	0.7806	−0.0002	−0.0065	0.0404	0.0162	0.0046	0.0006	0.1337	0.7393	2.5271	16.1100	0.3847E−04
295.0	0.7860	−0.0001	−0.0064	0.0412	0.0159	0.0042	0.0001	0.1325	0.7543	2.7030	18.1124	0.3863E−04

Table 10. *Absorptive scattering factors for Si and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2113	−0.0028	0.0127	0.0108	0.0058	0.0024	0.0382	0.2025	0.5845	1.7728	10.6593	0.1677E−04
77.0	0.2124	−0.0028	0.0129	0.0108	0.0056	0.0023	0.0381	0.2058	0.6035	1.8379	10.8728	0.1641E−04
80.0	0.2141	−0.0028	0.0132	0.0111	0.0054	0.0022	0.0383	0.2087	0.6238	1.9607	11.7245	0.1503E−04
100.0	0.2268	−0.0029	0.0136	0.0113	0.0058	0.0024	0.0407	0.2181	0.6275	1.9000	11.1498	0.1569E−04
150.0	0.2709	−0.0032	0.0182	0.0132	0.0036	0.0020	0.0457	0.2815	0.9440	3.5756	13.4231	0.1336E−04
200.0	0.3310	−0.0039	0.0204	0.0146	0.0051	0.0021	0.0570	0.3259	0.9670	3.4619	15.0027	0.8599E−05
250.0	0.4138	−0.0044	0.0269	0.0156	0.0030	0.0026	0.0678	0.4239	1.3762	5.5655	12.0619	0.1424E−04
290.0	0.4799	−0.0050	0.0285	0.0131	0.0070	0.0042	0.0777	0.4729	1.1851	2.6479	11.6520	0.1715E−04
293.0	0.4849	−0.0050	0.0288	0.0108	0.0087	0.0047	0.0783	0.4792	1.1336	2.2353	10.7654	0.1918E−04
295.0	0.4882	−0.0050	0.0298	0.0110	0.0076	0.0048	0.0785	0.4873	1.2383	2.2678	10.6100	0.1978E−04

Table 11. *Absorptive scattering factors for Ar and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	2.7913	−0.0025	−0.0258	0.1443	0.0555	0.0148	0.1008	0.5011	2.1233	5.3459	11.8827	0.2027E−04
77.0	2.8656	−0.0026	−0.0266	0.1372	0.0542	0.0261	0.1038	0.5183	2.1182	4.5036	10.0236	0.2408E−04
80.0	2.9770	−0.0026	−0.0273	0.1332	0.0562	0.0319	0.1071	0.5383	2.1594	4.1569	9.5383	0.2695E−04

Table 12. *Absorptive scattering factors for K and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	2.7639	−0.0028	−0.0289	0.1594	0.0623	0.0167	0.1016	0.4999	2.0886	5.3022	15.1615	0.3505E−04
77.0	2.8376	−0.0028	−0.0289	0.1654	0.0622	0.0132	0.1030	0.5074	2.1639	5.7842	17.2215	0.3101E−04
80.0	2.9480	−0.0028	−0.0293	0.1703	0.0620	0.0123	0.1048	0.5220	2.2511	6.0799	18.0644	0.3105E−04
100.0	3.6836	−0.0032	−0.0330	0.1887	0.0654	0.0150	0.1258	0.6399	2.7196	6.6621	18.2230	0.4004E−04
150.0	5.5181	−0.0040	−0.0392	0.2291	0.0710	0.0146	0.1793	0.9192	3.8836	8.5134	22.9742	0.4482E−04
200.0	7.3439	−0.0045	−0.0426	0.2606	0.0664	0.0196	0.2277	1.1674	5.0440	9.6230	23.7013	0.5055E−04
250.0	9.1581	−0.0050	−0.0455	0.2483	0.0970	0.0262	0.2747	1.4144	5.9770	8.9968	24.5994	0.5301E−04
290.0	10.5991	−0.0053	−0.0467	0.3204	0.0546	0.0122	0.3108	1.5957	7.1026	14.0801	36.4298	0.4496E−04
293.0	10.7067	−0.0054	−0.0473	0.2969	0.0725	0.0194	0.3146	1.6213	7.0177	11.4978	30.7452	0.4897E−04
295.0	10.7785	−0.0055	−0.0477	0.2978	0.0757	0.0164	0.3188	1.6406	7.0282	11.9413	33.3542	0.4756E−04

Table 13. *Absorptive scattering factors for Ca (f.c.c.) and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.5122	−0.0094	0.0577	0.0344	0.0258	−0.0108	0.0767	0.4889	1.6549	7.1203	8.7518	0.7277E−04
77.0	0.5259	−0.0095	0.0587	0.0348	0.0191	−0.0037	0.0784	0.5009	1.6734	6.8178	10.5510	0.7593E−04
80.0	0.5464	−0.0096	0.0619	0.0363	0.0231	−0.0103	0.0803	0.5283	1.8719	9.0557	12.9014	0.7765E−04
100.0	0.6829	−0.0111	0.0711	0.0377	0.0230	−0.0059	0.0972	0.6480	1.9934	7.6162	14.2376	0.1395E−03
150.0	1.0240	−0.0028	−0.0222	0.0691	0.0636	0.0360	0.0588	0.2470	0.7016	1.5913	5.4306	0.1882E−03
200.0	1.3647	−0.0025	−0.0225	0.0893	0.0570	0.0453	0.0652	0.2830	1.0230	1.9396	5.6388	0.2420E−03
250.0	1.7048	−0.0024	−0.0263	0.0449	0.1101	0.0598	0.0702	0.3375	1.0698	1.6925	5.6722	0.2586E−03
290.0	1.9765	−0.0024	−0.0258	0.6386	−0.4834	0.0726	0.0773	0.3633	1.7381	1.7726	5.5723	0.3144E−03
293.0	1.9968	−0.0020	−0.0184	−0.0112	0.1586	0.0734	0.0690	0.3182	0.5675	1.6255	5.5660	0.3210E−03
295.0	2.0104	−0.0028	−0.0284	0.1422	0.0726	0.0212	0.0830	0.3924	1.5569	4.0690	12.4817	0.5227E−04

standard variation

$$\sigma = \left\{(1/m)\sum_{j=1}^{m}\left[f(s_j) - \sum_i a_i \exp(-b_i s_j^2)\right]^2\right\}^{-1/2}. \quad (14)$$

These tables clearly show that for all elemental crystals considered and all temperatures the fitting is quite satisfactory. Fig. 3 shows a typical example of the numerical data of $f_{abs}(s)$ for Ag at 77 K and the fitted curve using the parameter given in Table 33. It is seen that for the full range of s up to 6 Å^{-1} the fitting is almost perfect.

Table 14. *Absorptive scattering factors for Ca (b.c.c.) and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.6667	−0.0108	0.0721	0.0387	0.0241	−0.0108	0.0947	0.6441	2.1758	9.8308	15.6214	0.1223E−03
77.0	0.6845	−0.0109	0.0735	0.0390	0.0246	−0.0113	0.0966	0.6614	2.2227	10.0838	16.2374	0.1310E−03
80.0	0.7111	−0.0113	0.0740	0.0382	0.0234	−0.0070	0.1003	0.6783	2.1095	8.2036	15.5291	0.1500E−03
100.0	0.8889	−0.0128	0.0914	0.0434	0.0278	−0.0173	0.1210	0.8612	2.9597	14.2379	21.7774	0.1697E−03
150.0	1.3329	−0.0164	0.1245	0.0502	0.0294	−0.0241	0.1729	1.2719	4.4483	24.3120	35.3721	0.2274E−03
200.0	1.7764	−0.0199	0.1479	0.0409	0.0265	−0.0067	0.2264	1.6382	4.4544	11.1285	48.0849	0.2833E−03
250.0	2.2193	−0.0023	−0.0269	0.1713	0.0683	0.0045	0.0777	0.3882	1.8654	6.3191	38.8251	0.4262E−04
290.0	2.5731	−0.0027	−0.0307	0.1805	0.0748	0.0079	0.0929	0.4625	2.0600	6.1808	25.6697	0.3012E−04
293.0	2.5996	−0.0027	−0.0310	0.1807	0.0755	0.0086	0.0939	0.4683	2.0709	6.1207	24.3882	0.3094E−04
295.0	2.6173	−0.0028	−0.0312	0.1814	0.0755	0.0086	0.0944	0.4713	2.0837	6.1493	24.3777	0.3110E−04

Table 15. *Absorptive scattering factors for Sc and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1910	−0.0054	0.0275	0.0183	0.0117	0.0051	0.0327	0.1826	0.5819	1.7889	6.3360	0.2372E−04
77.0	0.1961	−0.0053	0.0290	0.0195	0.0112	0.0038	0.0325	0.1922	0.6572	2.2118	7.7030	0.2299E−04
80.0	0.2037	−0.0059	0.0277	0.0186	0.0133	0.0061	0.0362	0.1868	0.5486	1.6277	6.1553	0.1857E−04
100.0	0.2547	−0.0069	0.0332	0.0224	0.0146	0.0060	0.0441	0.2320	0.6835	2.0405	7.7872	0.2168E−04
150.0	0.3819	−0.0087	0.0491	0.0279	0.0109	0.0097	0.0608	0.3624	1.1302	2.4705	7.1901	0.4072E−04
200.0	0.5091	−0.0103	0.0612	0.0180	0.0259	0.0109	0.0770	0.4844	1.1628	2.2363	8.6311	0.5677E−04
250.0	0.6363	−0.0004	−0.0134	0.0745	0.0440	0.0152	0.0009	0.1131	0.5780	1.9114	7.8619	0.4450E−04
290.0	0.7379	−0.0009	−0.0152	0.0814	0.0475	0.0173	0.0208	0.1394	0.6473	2.0124	7.6586	0.4136E−04
293.0	0.7455	−0.0010	−0.0152	0.0824	0.0475	0.0171	0.0216	0.1408	0.6554	2.0459	7.7646	0.4083E−04
295.0	0.7506	−0.0009	−0.0152	0.0834	0.0475	0.0166	0.0203	0.1402	0.6636	2.0983	7.9758	0.3967E−04

Table 16. *Absorptive scattering factors for Ti and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1940	−0.0061	0.0289	0.0196	0.0142	0.0061	0.0340	0.1795	0.5382	1.6122	6.2392	0.2461E−04
77.0	0.1955	−0.0061	0.0291	0.0200	0.0145	0.0058	0.0343	0.1804	0.5422	1.6638	6.5646	0.2314E−04
80.0	0.1978	−0.0062	0.0295	0.0203	0.0143	0.0057	0.0347	0.1828	0.5549	1.7036	6.6529	0.2287E−04
100.0	0.1755	−0.0053	0.0277	0.0184	0.0126	0.0054	0.0295	0.1692	0.5406	1.6489	6.1867	0.2480E−04
150.0	0.2632	−0.0077	0.0355	0.0242	0.0174	0.0070	0.0456	0.2352	0.6528	1.8716	7.1105	0.3225E−04
200.0	0.3509	−0.0091	0.0469	0.0278	0.0169	0.0086	0.0574	0.3235	0.9102	2.2355	6.9813	0.3621E−04
250.0	0.4385	−0.0103	0.0551	0.0221	0.0267	0.0108	0.0687	0.4058	0.9239	2.0103	7.4068	0.5831E−04
290.0	0.5086	−0.0111	0.0654	0.0246	0.0259	0.0093	0.0769	0.4827	1.1961	2.5047	9.3129	0.7190E−04
293.0	0.5138	−0.0110	0.0698	0.0359	0.0098	0.0103	0.0771	0.4994	1.6166	3.1651	8.5373	0.7584E−04
295.0	0.5173	−0.0112	0.0685	0.0318	0.0180	0.0082	0.0780	0.4968	1.4459	3.0713	9.9956	0.7190E−04

Table 17. *Absorptive scattering factors for V and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2242	−0.0067	0.0394	0.0268	0.0134	0.0020	0.0358	0.2233	0.8177	3.0821	12.8874	0.2202E−04
77.0	0.2277	−0.0068	0.0395	0.0270	0.0139	0.0022	0.0367	0.2248	0.8087	2.9998	12.8524	0.2072E−04
80.0	0.1562	−0.0042	0.0306	0.0204	0.0112	0.0011	0.0206	0.1701	0.6739	2.7704	13.3147	0.4253E−04
100.0	0.1953	−0.0051	0.0377	0.0250	0.0101	0.0007	0.0265	0.2128	0.9048	3.9739	12.1415	0.4100E−04
150.0	0.2929	−0.0091	0.0408	0.0265	0.0219	0.0086	0.0502	0.2573	0.6466	1.7650	6.4375	0.3805E−04
200.0	0.3905	−0.0105	0.0566	0.0322	0.0203	0.0071	0.0625	0.3620	1.0150	2.5842	8.2118	0.3164E−04
250.0	0.4880	−0.0118	0.0720	0.0379	0.0165	0.0061	0.0741	0.4686	1.4591	3.5432	10.4872	0.5382E−04
290.0	0.5660	−0.0129	0.0813	0.0360	0.0209	0.0061	0.0837	0.5452	1.6000	3.4733	12.1168	0.6995E−04
293.0	0.5718	−0.0127	0.0866	0.0473	0.0089	0.0022	0.0832	0.5678	2.1089	7.9312	13.9743	0.7672E−04
295.0	0.5757	−0.0130	0.0825	0.0384	0.0198	0.0051	0.0849	0.5543	1.6589	3.8334	13.6824	0.7008E−04

Table 18. *Absorptive scattering factors for Cr and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1230	−0.0057	0.0223	0.0152	0.0145	0.0074	0.0248	0.1090	0.2951	0.8730	3.0480	0.1113E−03
77.0	0.1235	−0.0065	0.0213	0.0164	0.0152	0.0074	0.0271	0.1017	0.2728	0.8566	3.0731	0.1102E−03
80.0	0.1244	−0.0032	0.0279	0.0183	0.0095	0.0015	0.0116	0.1448	0.5918	2.1468	5.2786	0.1106E−03
100.0	0.0857	−0.0016	0.0217	0.0140	0.0082	−0.0007	0.0003	0.1134	0.5275	2.3678	5.4313	0.1415E−03
150.0	0.1285	−0.0061	0.0231	0.0161	0.0148	0.0073	0.0262	0.1125	0.3103	0.9218	3.2146	0.1039E−03
200.0	0.1714	−0.0066	0.0297	0.0195	0.0176	0.0069	0.0305	0.1560	0.4287	1.2003	4.3749	0.7410E−04
250.0	0.2142	−0.0080	0.0351	0.0234	0.0199	0.0073	0.0383	0.1906	0.5151	1.3853	5.0865	0.6029E−04
290.0	0.2484	−0.0089	0.0396	0.0273	0.0206	0.0069	0.0435	0.2206	0.6014	1.6222	5.9456	0.5389E−04
293.0	0.2510	−0.0080	0.0459	0.0320	0.0086	0.0074	0.0406	0.2459	0.8741	2.3184	5.2140	0.6096E−04
295.0	0.2527	−0.0089	0.0403	0.0255	0.0213	0.0081	0.0439	0.2260	0.5989	1.4973	5.4251	0.5511E−04

Table 19. *Absorptive scattering factors for Fe (b.c.c.) and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1403	−0.0069	0.0279	0.0216	0.0159	0.0093	0.0263	0.1265	0.3289	0.9940	3.1217	0.5696E−04
77.0	0.1414	−0.0063	0.0301	0.0211	0.0155	0.0078	0.0245	0.1356	0.3716	1.1443	3.4518	0.5515E−04
80.0	0.1431	−0.0060	0.0320	0.0208	0.0146	0.0073	0.0233	0.1431	0.4122	1.2429	3.5566	0.5189E−04
100.0	0.1110	−0.0023	0.0315	0.0188	0.0119	−0.0023	0.0011	0.1467	0.6213	2.9501	6.0682	0.1126E−03
150.0	0.1665	−0.0061	0.0398	0.0250	0.0161	0.0014	0.0245	0.1768	0.6075	2.2500	10.3790	0.4110E−04
200.0	0.2219	−0.0086	0.0496	0.0304	0.0185	0.0017	0.0364	0.2219	0.7380	2.5078	11.9202	0.2402E−04
250.0	0.2773	−0.0102	0.0616	0.0370	0.0157	0.0011	0.0449	0.2784	1.0175	3.3850	12.4782	0.3428E−04
290.0	0.3217	−0.0121	0.0638	0.0370	0.0238	0.0024	0.0539	0.3014	0.8954	2.6337	9.4988	0.3617E−04
293.0	0.3250	−0.0121	0.0652	0.0378	0.0225	0.0020	0.0541	0.3070	0.9447	2.7902	10.2683	0.3681E−04
295.0	0.3272	−0.0121	0.0666	0.0386	0.0208	0.0020	0.0541	0.3120	0.9950	2.9238	9.2577	0.3683E−04

Table 20. *Absorptive scattering factors for Fe (f.c.c.) and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1429	−0.0038	0.0389	0.0233	0.0371	−0.0269	0.0116	0.1764	0.7638	3.8989	4.2329	0.6387E−04
77.0	0.1467	−0.0072	0.0295	0.0227	0.0166	0.0083	0.0278	0.1324	0.3531	1.1129	3.4793	0.4724E−04
80.0	0.1524	−0.0072	0.0309	0.0229	0.0170	0.0081	0.0281	0.1397	0.3726	1.1668	3.6336	0.4261E−04
100.0	0.1905	−0.0088	0.0360	0.0264	0.0208	0.0085	0.0350	0.1691	0.4240	1.3062	4.1039	0.3179E−04
150.0	0.2857	−0.0113	0.0554	0.0323	0.0253	0.0054	0.0491	0.2628	0.7061	2.0155	6.4573	0.2280E−04
200.0	0.3809	−0.0123	0.0833	0.0496	0.0437	−0.0376	0.0584	0.3897	1.6791	13.3470	14.8292	0.8339E−04
250.0	0.4760	−0.0146	0.0970	0.0557	0.0151	−0.0088	0.0718	0.4732	1.9106	12.9783	17.6435	0.7484E−04
290.0	0.5520	−0.0161	0.1067	0.0591	0.0197	−0.0122	0.0817	0.5390	2.0372	11.2090	13.1529	0.7854E−04
293.0	0.5577	−0.0165	0.1045	0.0435	0.0171	0.0094	0.0832	0.5344	1.7458	2.4735	7.1758	0.7596E−04
295.0	0.5615	−0.0005	−0.0185	0.1033	0.0619	0.0125	0.0001	0.1001	0.5111	1.7802	6.3991	0.3904E−04

Table 21. *Absorptive scattering factors for Ni and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1445	−0.0212	0.0328	0.0307	0.0242	0.0115	0.0424	0.0798	0.2351	0.7781	2.5696	0.7918E−04
77.0	0.1456	−0.0115	0.0293	0.0266	0.0232	0.0107	0.0339	0.1054	0.2698	0.8317	2.6741	0.7622E−04
80.0	0.1472	−0.0081	0.0349	0.0229	0.0202	0.0090	0.0270	0.1328	0.3634	0.9889	2.9162	0.7262E−04
100.0	0.1215	−0.0063	0.0274	0.0150	0.0204	0.0128	0.0202	0.1120	0.2346	0.6222	2.0611	0.1342E−03
150.0	0.1823	−0.0106	0.0352	0.0277	0.0271	0.0114	0.0355	0.1461	0.3404	0.9492	3.0204	0.5592E−04
200.0	0.2430	−0.0105	0.0588	0.0417	0.0083	0.0106	0.0396	0.2347	0.8138	2.0434	3.5060	0.4193E−04
250.0	0.3037	−0.0134	0.0590	0.0290	0.0364	0.0134	0.0513	0.2664	0.5720	1.2399	3.7105	0.5691E−04
290.0	0.3522	−0.0145	0.0724	0.0499	0.0261	0.0019	0.0579	0.3189	0.8903	2.5064	9.2624	0.7151E−04
293.0	0.3559	−0.0141	0.0793	0.0549	0.0169	−0.0003	0.0572	0.3373	1.1080	3.7726	12.5556	0.6571E−04
295.0	0.3583	−0.0144	0.0770	0.0531	0.0208	0.0007	0.0581	0.3327	1.0167	3.0895	10.8183	0.6683E−04

Table 22. *Absorptive scattering factors for Cu and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1410	−0.0059	0.0437	0.0304	0.0148	−0.0018	0.0174	0.1550	0.6253	2.3393	5.1971	0.1379E−03
77.0	0.1448	−0.0060	0.0443	0.0303	0.0150	−0.0008	0.0180	0.1583	0.6206	2.1568	5.3096	0.1304E−03
80.0	0.1504	−0.0067	0.0443	0.0301	0.0169	0.0004	0.0209	0.1578	0.5757	1.8571	5.2003	0.1210E−03
100.0	0.1880	−0.0085	0.0536	0.0387	0.0149	−0.0008	0.0282	0.1930	0.7363	2.5877	11.8466	0.1130E−03
150.0	0.2820	−0.0132	0.0685	0.0508	0.0202	−0.0007	0.0470	0.2625	0.8458	2.6346	6.1339	0.1198E−03
200.0	0.3759	−0.0161	0.0851	0.0586	0.0317	−0.0108	0.0608	0.3468	1.0183	3.0896	3.7482	0.1531E−03
250.0	0.4698	−0.0009	−0.0215	0.0976	0.0715	0.0217	0.0050	0.0918	0.4012	1.1248	3.1799	0.1142E−03
290.0	0.5448	−0.0019	−0.0245	0.1068	0.0796	0.0227	0.0209	0.1144	0.4488	1.1988	3.4363	0.8661E−04
293.0	0.5505	−0.0012	−0.0238	0.1126	0.0780	0.0183	0.0118	0.1080	0.4707	1.3082	3.8109	0.8479E−04
295.0	0.5542	−0.0015	−0.0241	0.1119	0.0786	0.0194	0.0156	0.1104	0.4697	1.2869	3.7227	0.8431E−04

Table 23. *Absorptive scattering factors for Zn and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2927	−0.0147	0.0682	0.0462	0.0309	0.0049	0.0496	0.2598	0.6881	1.7014	6.2841	0.1999E−04
77.0	0.3005	−0.0140	0.0797	0.0652	−0.0290	0.0356	0.0486	0.2885	1.0418	2.0840	2.7919	0.5227E−04
80.0	0.3122	−0.0149	0.0782	0.0562	0.0196	0.0015	0.0514	0.2901	0.9087	2.6275	11.9538	0.2118E−04
100.0	0.3902	−0.0170	0.0964	0.0644	0.0149	0.0012	0.0618	0.3690	1.1572	3.4770	11.7670	0.3398E−04
150.0	0.5852	−0.0006	−0.0232	0.1430	0.0755	0.0052	0.0003	0.0994	0.5551	1.8383	13.1226	0.7901E−04
200.0	0.7801	−0.0021	−0.0308	0.1673	0.0876	0.0088	0.0257	0.1487	0.6774	1.9195	8.1717	0.3688E−04
250.0	0.9748	−0.0046	−0.0389	0.1836	0.1039	0.0131	0.0513	0.2087	0.7738	1.9449	7.8071	0.5795E−04
290.0	1.1304	−0.0042	−0.0407	0.2187	0.0937	0.0080	0.0522	0.2251	0.9263	2.4425	13.3162	0.5231E−04
293.0	1.1420	−0.0043	−0.0412	0.2194	0.0946	0.0083	0.0533	0.2288	0.9312	2.4349	12.8539	0.5249E−04
295.0	1.1498	−0.0043	−0.0412	0.2208	0.0941	0.0082	0.0532	0.2289	0.9390	2.4568	13.1568	0.5167E−04

Table 24. *Absorptive scattering factors for Ge and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1597	−0.0099	0.0506	0.0343	0.0244	0.0049	0.0267	0.1513	0.4689	1.3187	5.0758	0.2382E−04
77.0	0.1611	−0.0099	0.0514	0.0351	0.0238	0.0044	0.0267	0.1536	0.4845	1.3795	5.4966	0.2234E−04
80.0	0.1632	−0.0099	0.0523	0.0355	0.0233	0.0044	0.0268	0.1566	0.4993	1.4088	5.4880	0.2188E−04
100.0	0.2049	−0.0133	0.0560	0.0403	0.0324	0.0066	0.0369	0.1776	0.4749	1.2870	5.2629	0.4376E−04
150.0	0.3073	−0.0171	0.0790	0.0515	0.0356	0.0066	0.0517	0.2715	0.6888	1.6476	7.0253	0.4577E−04
200.0	0.4097	−0.0199	0.1043	0.0341	0.0547	0.0100	0.0647	0.3758	0.7795	1.5093	6.4112	0.6347E−04
250.0	0.5120	−0.0007	−0.0245	0.1386	0.0829	0.0110	0.0002	0.0903	0.4719	1.4956	7.6944	0.8427E−04
290.0	0.5938	−0.0008	−0.0278	0.1551	0.0868	0.0109	0.0004	0.1058	0.5377	1.6436	8.5279	0.7905E−04
293.0	0.6000	−0.0008	−0.0281	0.1559	0.0873	0.0110	0.0002	0.1071	0.5417	1.6461	8.4617	0.7724E−04
295.0	0.6041	−0.0008	−0.0283	0.1558	0.0879	0.0115	0.0003	0.1078	0.5433	1.6336	8.1604	0.7718E−04

Table 25. *Absorptive scattering factors for Kr and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	2.4806	−0.0087	−0.0750	0.4399	0.1167	0.0392	0.0922	0.4253	1.7556	4.0000	9.9823	0.6051E−04
77.0	2.5466	−0.0087	−0.0752	0.4498	0.1158	0.0354	0.0933	0.4326	1.8061	4.2378	10.5075	0.5949E−04
80.0	2.6455	−0.0089	−0.0766	0.4516	0.1189	0.0393	0.0964	0.4489	1.8560	4.1621	10.3264	0.6563E−04
100.0	3.3037	−0.0090	−0.0796	0.5075	0.0951	0.0526	0.1084	0.5252	2.3014	4.7710	10.0530	0.8533E−04

Table 26. *Absorptive scattering factors for Rb and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	3.4413	−0.0092	−0.0875	0.5303	0.1442	0.0302	0.1112	0.5575	2.3791	5.1488	15.9551	0.1276E−03
77.0	3.5328	−0.0094	−0.0892	0.4853	0.1778	0.0486	0.1139	0.5729	2.3652	4.2524	12.8135	0.1578E−03
80.0	3.6700	−0.0082	−0.0821	0.6037	0.0804	0.0273	0.1078	0.5471	2.6852	7.3866	14.4820	0.1761E−03
100.0	4.5832	−0.0108	−0.0950	0.5924	0.1509	0.0302	0.1428	0.7169	3.0561	6.0831	19.6224	0.1262E−03
150.0	6.8524	−0.0128	−0.1016	0.6454	0.1783	0.0416	0.1987	1.0033	4.3357	6.8444	22.0424	0.1323E−03
200.0	9.0947	−0.0115	−0.0110	−0.0906	0.8601	0.0608	0.2273	0.6889	1.2839	5.9676	22.5266	0.1329E−03
250.0	11.3011	−0.0152	−0.1014	0.4018	0.5128	0.0522	0.2974	1.4849	6.6299	7.7152	27.9224	0.1153E−03
290.0	13.0344	−0.0164	−0.1043	0.8627	0.1117	0.0239	0.3379	1.7166	7.8460	13.8430	46.3280	0.1132E−03
293.0	13.1632	−0.0165	−0.1022	0.9009	0.0681	0.0290	0.3425	1.7134	8.0510	15.1920	40.4558	0.9758E−04
295.0	13.2489	−0.0170	−0.1046	0.8898	0.0964	0.0159	0.3496	1.7583	7.9994	16.2880	58.4469	0.1013E−03

Table 27. *Absorptive scattering factors for Sr and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.9761	−0.0061	−0.0524	0.2965	0.1205	0.0278	0.0452	0.1879	0.7816	2.3293	10.6330	0.1853E−03
77.0	1.0021	−0.0051	−0.0515	0.3104	0.1152	0.0223	0.0411	0.1833	0.8224	2.6350	13.1493	0.1686E−03
80.0	1.0411	−0.0065	−0.0539	0.3107	0.1212	0.0268	0.0487	0.1996	0.8313	2.4981	11.5240	0.1885E−03
100.0	1.3009	−0.0074	−0.0612	0.3549	0.1272	0.0266	0.0582	0.2456	1.0102	2.9653	12.7561	0.1704E−03
150.0	1.9494	−0.0090	−0.0766	0.4241	0.1485	0.0355	0.0787	0.3565	1.4061	3.5457	13.7300	0.2368E−03
200.0	2.5955	−0.0096	−0.0845	0.4813	0.1541	0.0417	0.0940	0.4475	1.8145	4.1515	13.8859	0.1492E−03
250.0	3.2383	−0.0100	−0.0902	0.5303	0.1599	0.0423	0.1079	0.5333	2.2159	4.8307	16.0217	0.1576E−03
290.0	3.7498	−0.0106	−0.0923	0.5867	0.1482	0.0336	0.1204	0.5975	2.5724	5.9654	20.1987	0.1344E−03
293.0	3.7880	−0.0104	−0.0915	0.5993	0.1399	0.0306	0.1201	0.5969	2.6212	6.3281	21.2154	0.1281E−03
295.0	3.8135	−0.0106	−0.0927	0.5934	0.1479	0.0316	0.1221	0.6064	2.6149	6.1477	21.2802	0.1291E−03

Table 28. *Absorptive scattering factors for Y and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2194	−0.0200	0.0876	0.0630	0.0384	0.0117	0.0385	0.1905	0.5141	1.3760	6.3134	0.7014E−04
77.0	0.2253	−0.0200	0.0921	0.0657	0.0351	0.0108	0.0390	0.1989	0.5595	1.5254	6.9315	0.6460E−04
80.0	0.2340	−0.0200	0.0984	0.0689	0.0309	0.0100	0.0395	0.2119	0.6249	1.7477	7.6464	0.6069E−04
100.0	0.2925	−0.0239	0.1088	0.0690	0.0457	0.0151	0.0492	0.2542	0.6175	1.4799	6.9123	0.9205E−04
150.0	0.4386	−0.0297	0.1644	0.0832	0.0404	0.0126	0.0677	0.3990	0.9889	2.4923	12.5403	0.1343E−03
200.0	0.5846	−0.0331	0.2461	1.1528	−1.1294	0.0796	0.0827	0.5782	3.1617	3.3578	6.5337	0.3033E−03
250.0	0.7303	−0.0029	−0.0463	0.2576	0.1157	0.0289	0.0209	0.1359	0.6241	1.8064	8.8064	0.1545E−03
290.0	0.8466	−0.0043	−0.0512	0.2869	0.1190	0.0293	0.0325	0.1612	0.7085	2.0386	9.8045	0.1538E−03
293.0	0.8553	−0.0054	−0.0523	0.2843	0.1235	0.0314	0.0389	0.1697	0.7031	1.9658	9.3338	0.1648E−03
295.0	0.8612	−0.0048	−0.0519	0.2902	0.1201	0.0293	0.0360	0.1665	0.7168	2.0634	9.9825	0.1534E−03

4. Conclusions

Debye–Waller factors for 44 elemental crystals are given over a temperature range from 1 to 1000 K or to the melting temperature, whichever is smaller. These values are calculated using the experimentally determined phonon density of states and the typical error associated with these data is 2 to 3%. A compilation has also been given of all the necessary data for an additional 22 elemental crystals for which the Debye temperature is known but

Table 29. *Absorptive scattering factors for Zr and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1457	−0.0202	0.0601	0.0492	0.0413	0.0158	0.0314	0.1115	0.2769	0.7941	3.1062	0.2410E−03
77.0	0.1496	−0.0157	0.0716	0.0456	0.0337	0.0135	0.0265	0.1353	0.3729	0.9722	3.4905	0.2241E−03
80.0	0.1554	−0.0121	0.0865	0.0559	0.0153	0.0067	0.0202	0.1645	0.6226	2.2125	4.0622	0.2231E−03
100.0	0.1943	−0.0170	0.0978	0.0644	0.0205	0.0096	0.0308	0.1883	0.6352	1.9344	4.8161	0.1685E−03
150.0	0.2914	−0.0218	0.1457	0.0834	0.0202	−0.0036	0.0438	0.2920	1.1144	7.2844	21.5561	0.1527E−03
200.0	0.3884	−0.0278	0.1782	0.0932	0.0228	−0.0025	0.0589	0.3742	1.3074	7.3452	19.9550	0.1226E−03
250.0	0.4854	−0.0319	0.2124	0.0965	0.0216	0.0005	0.0714	0.4639	1.5741	7.7738	17.9331	0.1238E−03
290.0	0.5628	−0.0353	0.2295	0.0913	0.0303	0.0083	0.0814	0.5244	1.5164	4.3714	17.0544	0.1577E−03
293.0	0.5686	−0.0345	0.2471	0.0970	0.0354	−0.0191	0.0806	0.5501	2.0322	15.8582	20.2532	0.2036E−03
295.0	0.5725	−0.0349	0.2450	0.0971	0.0284	−0.0088	0.0814	0.5490	1.9300	11.2196	13.7825	0.1839E−03

Table 30. *Absorptive scattering factors for Nb and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1152	−0.0105	0.0662	0.0333	0.0246	0.0166	0.0159	0.1184	0.3619	0.7551	2.5038	0.4340E−03
77.0	0.1183	−0.0087	0.0709	0.0418	0.0141	0.0144	0.0114	0.1306	0.4623	1.0945	2.6775	0.4275E−03
80.0	0.1229	−0.0101	0.0701	0.0379	0.0224	0.0157	0.0148	0.1290	0.4013	0.9007	2.7047	0.4174E−03
100.0	0.1536	−0.0114	0.0908	0.0575	0.0112	0.0095	0.0177	0.1677	0.6655	2.6174	3.7423	0.3731E−03
150.0	0.2304	−0.0213	0.1081	0.0640	0.0338	0.0183	0.0383	0.2099	0.5874	1.3670	4.6361	0.3713E−03
200.0	0.3071	−0.0268	0.1241	0.0608	0.0575	0.0245	0.0508	0.2667	0.5755	1.2526	4.6987	0.3851E−03
250.0	0.3838	−0.0294	0.1757	0.0975	−0.0149	0.0436	0.0597	0.3587	1.1637	3.4585	4.4712	0.3923E−03
290.0	0.4451	−0.0013	−0.0349	0.1935	0.1067	0.0321	0.0057	0.0799	0.3968	1.2427	5.3263	0.3933E−03
293.0	0.4496	−0.0320	0.2007	0.0225	0.0790	0.0276	0.0676	0.4224	1.0781	1.4718	5.8832	0.3964E−03
295.0	0.4527	−0.0317	0.2088	0.1179	−0.2197	0.2235	0.0674	0.4331	1.6065	3.6732	4.0841	0.4027E−03

Table 31. *Absorptive scattering factors for Mo and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.0885	−0.0082	0.0458	0.0336	0.0279	0.0157	0.0106	0.0894	0.2100	0.5674	2.2588	0.3285E−03
77.0	0.0567	−0.0104	0.0407	0.0280	0.0170	0.0096	0.0164	0.0566	0.2009	0.5957	2.3943	0.2281E−03
80.0	0.0589	−0.0029	0.0475	0.0301	0.0132	−0.0006	0.0007	0.0849	0.3838	2.1191	3.9080	0.2460E−03
100.0	0.0736	−0.0126	0.0329	0.0395	0.0272	0.0143	0.0153	0.0543	0.1532	0.4855	2.0886	0.3107E−03
150.0	0.1104	−0.0112	0.0553	0.0376	0.0333	0.0180	0.0165	0.1069	0.2398	0.6236	2.5570	0.2848E−03
200.0	0.1471	−0.0152	0.0823	0.0548	0.0269	0.0122	0.0239	0.1453	0.4198	1.3241	4.4581	0.1715E−03
250.0	0.1839	−0.0184	0.1027	0.0634	0.0291	0.0086	0.0302	0.1808	0.5444	1.9282	6.3599	0.1460E−03
290.0	0.2133	−0.0176	0.1334	0.0672	0.0245	−0.0047	0.0298	0.2325	0.9406	5.5286	10.1692	0.1851E−03
293.0	0.2155	−0.0170	0.1371	0.0669	0.0292	−0.0122	0.0288	0.2399	1.0232	7.1497	10.7942	0.2104E−03
295.0	0.2169	−0.0192	0.1294	0.0680	0.0248	0.0020	0.0327	0.2261	0.8136	3.6071	10.0469	0.1431E−03

Table 32. *Absorptive scattering factors for Pd and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1142	−0.0187	0.0543	0.0540	0.0482	0.0227	0.0219	0.0878	0.1921	0.5893	2.3558	0.2929E−03
77.0	0.1172	−0.0083	0.0952	0.0765	−0.5719	0.5718	0.0050	0.1420	0.6715	1.4985	1.5569	0.2848E−03
80.0	0.1218	−0.1050	0.1297	0.0694	0.0501	0.0234	0.0424	0.0576	0.1922	0.6141	2.4638	0.2598E−03
100.0	0.1522	−0.0144	0.1114	0.0704	−0.2310	0.2574	0.0181	0.1639	0.6327	2.4666	2.5105	0.1390E−03
150.0	0.2283	−0.0292	0.1106	0.0782	0.0610	0.0281	0.0406	0.1860	0.4116	1.0250	3.7162	0.9520E−04
200.0	0.3043	−0.0322	0.1710	0.0612	0.0544	0.0394	0.0493	0.2755	0.7067	1.0613	3.5871	0.1452E−03
250.0	0.3803	−0.0368	0.2091	0.0043	0.1105	0.0458	0.0594	0.3469	0.6474	1.0416	3.7371	0.1902E−03
290.0	0.4411	−0.0385	2.4856	−2.3590	0.2202	0.0529	0.0655	0.5060	0.5273	0.9333	3.8399	0.1726E−03
293.0	0.4456	−0.0016	−0.0453	0.2291	0.1289	0.0522	0.0027	0.0822	0.3817	1.0753	3.8769	0.1544E−03
295.0	0.4487	−0.0015	−0.0458	0.2298	0.1296	0.0526	0.0003	0.0826	0.3833	1.0761	3.8808	0.1539E−03

Table 33. *Absorptive scattering factors for Ag and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1883	−0.0222	0.1266	0.0812	0.0389	0.0042	0.0296	0.1799	0.5897	2.1163	6.8871	0.2231E−03
77.0	0.1933	−0.0222	0.1318	0.0837	0.0372	0.0019	0.0298	0.1874	0.6389	2.4460	8.6206	0.2144E−03
80.0	0.2008	−0.0236	0.1329	0.0855	0.0395	0.0037	0.0319	0.1902	0.6215	2.2595	7.4091	0.2046E−03
100.0	0.2510	−0.0295	0.1523	0.0969	0.0461	0.0066	0.0415	0.2267	0.6804	2.2520	7.6309	0.1527E−03
150.0	0.3764	−0.0378	0.2137	0.1162	0.0476	0.0034	0.0587	0.3410	1.0072	3.2100	9.9019	0.1650E−03
200.0	0.5016	−0.0015	−0.0489	0.2713	0.1418	0.0390	0.0001	0.0883	0.4392	1.3799	5.0740	0.1002E−03
250.0	0.6267	−0.0020	−0.0575	0.3164	0.1553	0.0389	0.0027	0.1107	0.5345	1.6246	5.7536	0.7387E−04
290.0	0.7267	−0.0091	−0.0677	0.3271	0.1773	0.0572	0.0395	0.1561	0.5673	1.5060	4.8475	0.1209E−03
293.0	0.7341	−0.0087	−0.0677	0.3310	0.1765	0.0562	0.0383	0.1552	0.5759	1.5350	4.9221	0.1194E−03
295.0	0.7391	−0.0085	−0.0674	0.3349	0.1754	0.0545	0.0381	0.1550	0.5831	1.5677	5.0225	0.1159E−03

Table 34. *Absorptive scattering factors for Sn and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2903	−0.0364	0.1913	0.1175	0.0495	0.0106	0.0475	0.2634	0.7570	2.4145	8.3029	0.7156E−04
77.0	0.2980	−0.0352	0.2115	0.1209	0.0329	0.0070	0.0469	0.2849	0.9514	3.6701	6.3861	0.1300E−03
80.0	0.3096	−0.0372	0.2091	0.1207	0.0405	0.0113	0.0496	0.2871	0.8718	2.8002	6.8065	0.9576E−04
100.0	0.3870	−0.0429	0.2539	0.1296	0.0451	0.0046	0.0601	0.3593	1.0925	3.6720	12.1349	0.1054E−03
150.0	0.5804	−0.0019	−0.0615	0.3448	0.1622	0.0418	0.0005	0.1023	0.5054	1.5685	6.2277	0.1665E−03
200.0	0.7737	−0.0071	−0.0754	0.4141	0.1841	0.0443	0.0321	0.1498	0.6357	1.8730	6.9246	0.1233E−03
250.0	0.9667	−0.0108	−0.0871	0.4767	0.2036	0.0416	0.0476	0.1929	0.7657	2.2183	8.8646	0.1957E−03
290.0	1.1210	−0.0109	−0.0929	0.5324	0.2076	0.0326	0.0515	0.2149	0.8867	2.6600	12.1564	0.2038E−03
293.0	1.1326	−0.0107	−0.0930	0.5371	0.2071	0.0316	0.0514	0.2157	0.8973	2.7056	12.5885	0.2024E−03
295.0	1.1403	−0.0112	−0.0941	0.5356	0.2098	0.0338	0.0529	0.2196	0.8970	2.6568	11.9321	0.2078E−03

Table 35. *Absorptive scattering factors for Xe and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	2.2942	−0.0170	−0.1519	0.8309	0.2812	0.0981	0.0854	0.4055	1.6186	3.4951	9.2747	0.1477E−03
77.0	2.3551	−0.0171	−0.1539	0.8260	0.2906	0.1062	0.0867	0.4147	1.6466	3.4154	9.1173	0.1576E−03
80.0	2.4465	−0.0160	−0.1478	0.9454	0.2559	0.0300	0.0854	0.4104	1.8038	5.1293	15.9377	0.1047E−03
100.0	3.0544	−0.0178	−0.1662	0.8985	0.3095	0.1335	0.1014	0.5066	2.0789	3.7026	9.5320	0.2009E−03
150.0	4.5621	−0.0209	−0.1833	1.1302	0.2648	0.1327	0.1392	0.7065	3.0525	5.1159	11.7726	0.1992E−03

Table 36. *Absorptive scattering factors for Cs and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	4.6623	−0.0206	−0.1886	1.3030	0.2111	0.0810	0.1403	0.7118	3.2527	6.8877	15.4559	0.2767E−03
77.0	4.7859	−0.0217	−0.1951	1.2723	0.2771	0.0650	0.1464	0.7446	3.2619	6.6914	18.0739	0.2424E−03
80.0	4.9711	−0.0218	−0.1971	1.2078	0.3170	0.1081	0.1499	0.7669	3.3264	5.6105	14.8949	0.2877E−03
100.0	6.2027	−0.0243	−0.2054	1.4231	0.2188	0.0985	0.1820	0.9246	4.1429	7.2820	17.6615	0.2632E−03
150.0	9.2455	−0.0282	−0.2172	0.3890	1.4165	0.1206	0.2520	1.2846	5.2035	6.3865	21.7231	0.2470E−03
200.0	12.2181	−0.0326	−0.2256	1.7034	0.2905	0.0587	0.3251	1.6567	7.4117	11.6803	36.5708	0.2083E−03
250.0	15.0971	−0.0312	−0.1884	−0.0807	2.0513	0.1250	0.3656	1.7604	4.4643	9.1430	29.0648	0.2098E−03
290.0	17.3172	−0.0312	−0.1523	−0.0794	2.0855	0.1047	0.4017	1.8233	3.3339	10.4541	34.6402	0.2033E−03
293.0	17.4803	−0.0314	−0.0827	−0.1396	2.0856	0.0988	0.4061	1.6180	2.5843	10.5874	35.9707	0.2066E−03
295.0	17.5888	−0.0320	−0.0465	−0.1683	2.0896	0.0904	0.4123	1.5189	2.3413	10.6998	38.1667	0.2051E−03

Table 37. *Absorptive scattering factors for Ba and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.7909	−0.0032	−0.0809	0.5240	0.2189	0.0427	0.0074	0.1283	0.6848	2.4466	18.8316	0.9803E−03
77.0	0.8119	−0.0025	−0.0813	0.5404	0.2162	0.0386	0.0005	0.1281	0.7103	2.6358	23.6764	0.9104E−03
80.0	0.8435	−0.0037	−0.0852	0.5461	0.2247	0.0426	0.0100	0.1383	0.7225	2.5757	20.7286	0.9902E−03
100.0	1.0540	−0.0081	−0.0981	0.6242	0.2440	0.0454	0.0342	0.1826	0.8705	2.9780	25.8556	0.1038E−02
150.0	1.5787	−0.0160	−0.1349	0.7502	0.3095	0.0590	0.0667	0.3005	1.1742	3.4074	26.4013	0.1223E−02
200.0	2.1005	−0.0152	−0.1437	0.9161	0.2816	0.0281	0.0751	0.3591	1.5874	4.7956	23.4110	0.1178E−03
250.0	2.6190	−0.0166	−0.1590	1.0133	0.2911	0.0339	0.0884	0.4365	1.9206	5.3501	22.7584	0.1436E−03
290.0	3.0305	−0.0175	−0.1678	1.0927	0.2905	0.0298	0.0983	0.4940	2.1939	6.0457	27.9429	0.1600E−03
293.0	3.0612	−0.0185	−0.1767	0.9751	0.3619	0.0893	0.1019	0.5151	2.0967	4.3404	13.8303	0.3163E−03
295.0	3.0817	−0.0184	−0.1748	1.0178	0.3358	0.0740	0.1020	0.5138	2.1438	4.7346	15.4081	0.2829E−03

Table 38. *Absorptive scattering factors for La and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.4783	−0.0562	0.4117	0.1784	0.2055	−0.1761	0.0675	0.4673	1.8980	16.3321	17.1646	0.4527E−03
77.0	0.4910	−0.0570	0.4208	0.1792	0.2592	−0.2308	0.0690	0.4801	1.9625	17.7404	18.4512	0.4704E−03
80.0	0.5101	−0.0580	0.4353	0.1797	0.2406	−0.2141	0.0710	0.5002	2.0832	19.9264	20.7243	0.4914E−03
100.0	0.6374	−0.0666	0.5077	0.1885	0.0421	−0.0166	0.0861	0.6131	2.5066	19.6899	25.6551	0.5163E−03
150.0	0.9551	−0.0843	0.6548	0.1998	0.0176	0.0120	0.1216	0.8780	3.3568	11.7563	30.4042	0.8107E−03
200.0	1.2714	−0.0978	0.7803	0.2087	0.0057	0.0162	0.1550	1.1350	4.3630	14.3061	31.9952	0.1099E−02
250.0	1.5861	−0.1085	0.8880	0.2180	−0.0400	0.0517	0.1861	1.3842	5.4926	20.8542	30.9696	0.1302E−02
290.0	1.8363	−0.1158	0.9609	0.2128	−0.0559	0.0719	0.2103	1.5762	6.0757	31.6774	37.7721	0.1420E−02
293.0	1.8550	−0.1158	0.9693	0.2109	−0.0111	0.0251	0.2113	1.5952	6.2646	22.9250	48.6640	0.1429E−02
295.0	1.8674	−0.1164	0.9797	0.2377	−0.3448	0.3246	0.2133	1.6095	7.0319	20.9928	23.6393	0.1437E−02

not the phonon density of states. These data allow a rapid estimate of the Debye–Waller factor at any temperature within the Debye model of lattice vibration.

For 43 elemental crystals with known phonon density of states, parameterization has been made of the absorptive part of the electron scattering factors over the temperature range from 65 to 500 K or to the melting temperature, whichever is smaller. For other materials with known Debye–Waller factors, parameterization can be performed by using the computer program developed

Table 39. *Absorptive scattering factors for Tb and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2598	−0.0544	0.2678	0.1737	0.0870	0.0141	0.0425	0.2215	0.6500	1.9896	13.3812	0.5819E−03
77.0	0.2667	−0.0537	0.2800	0.1755	0.0806	0.0132	0.0426	0.2323	0.7010	2.1533	14.1624	0.5699E−03
80.0	0.2771	−0.0562	0.2827	0.1819	0.0853	0.0128	0.0448	0.2374	0.6977	2.1760	15.9000	0.5431E−03
100.0	0.3463	−0.0628	0.3384	0.1991	0.0850	0.0136	0.0536	0.3003	0.8586	2.4921	16.7642	0.4368E−03
150.0	0.5191	−0.0759	0.4547	0.1322	0.1755	0.0278	0.0735	0.4593	0.9082	2.0580	15.8050	0.8163E−03
200.0	0.6915	−0.0031	−0.0984	0.6265	0.2663	0.0310	0.0002	0.1126	0.6068	2.0604	16.4883	0.7049E−03
250.0	0.8633	−0.0083	−0.1161	0.7147	0.2874	0.0353	0.0249	0.1516	0.7237	2.2789	15.6202	0.7464E−03
290.0	1.0002	−0.0110	−0.1275	0.7897	0.2947	0.0315	0.0349	0.1783	0.8233	2.5880	22.7332	0.6909E−03
293.0	1.0104	−0.0091	−0.1255	0.8076	0.2817	0.0279	0.0298	0.1730	0.8454	2.7510	29.4410	0.6158E−03
295.0	1.0173	−0.0101	−0.1267	0.8079	0.2861	0.0284	0.0329	0.1769	0.8461	2.7290	28.9903	0.6211E−03

Table 40. *Absorptive scattering factors for Ho and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.2157	−0.0503	0.2400	0.1471	0.1010	0.0216	0.0358	0.1842	0.5128	1.3774	6.4539	0.3936E−03
77.0	0.2214	−0.0514	0.2456	0.1516	0.0992	0.0218	0.0368	0.1889	0.5317	1.4174	6.6003	0.4137E−03
80.0	0.2301	−0.0537	0.2491	0.1634	0.1010	0.0179	0.0386	0.1935	0.5441	1.5472	8.8290	0.4041E−03
100.0	0.2875	−0.0608	0.2923	0.1818	0.1087	0.0211	0.0466	0.2422	0.6458	1.6854	9.3328	0.4838E−03
150.0	0.4310	−0.0735	0.4133	0.1580	0.1528	0.0279	0.0640	0.3781	0.8569	1.7966	11.1300	0.6862E−03
200.0	0.5742	−0.0030	−0.0938	0.5645	0.2822	0.0381	0.0002	0.0965	0.5037	1.6380	11.7978	0.9349E−03
250.0	0.7169	−0.0036	−0.1092	0.6650	0.2896	0.0342	0.0012	0.1198	0.6197	1.9447	13.6466	0.7003E−03
290.0	0.8307	−0.0076	−0.1202	0.7398	0.2957	0.0314	0.0210	0.1450	0.7047	2.1921	17.5116	0.6562E−03
293.0	0.8393	−0.0064	−0.1201	0.7483	0.2919	0.0301	0.0169	0.1431	0.7158	2.2433	19.1826	0.6394E−03
295.0	0.8449	−0.0080	−0.1220	0.7451	0.2984	0.0329	0.0224	0.1483	0.7127	2.1882	16.4230	0.6722E−03

Table 41. *Absorptive scattering factors for Ta and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.0826	−0.0127	0.1653	0.1034	0.0457	−0.0138	0.0005	0.1014	0.4423	2.2445	5.4587	0.9120E−03
77.0	0.0848	−0.0134	0.1678	0.1052	0.0456	−0.0123	0.0012	0.1029	0.4416	2.1802	5.8015	0.9097E−03
80.0	0.0881	−0.0133	0.1741	0.1081	0.0486	−0.0171	0.0005	0.1078	0.4677	2.4432	5.2809	0.9081E−03
100.0	0.1101	−0.0177	0.2044	0.1244	0.0434	−0.0076	0.0038	0.1293	0.5269	2.3669	9.2827	0.7539E−03
150.0	0.1651	−0.0417	0.2540	0.1621	0.0636	0.0112	0.0241	0.1595	0.5192	1.6022	4.6964	0.3140E−03
200.0	0.2200	−0.0602	0.2901	0.1934	0.0940	0.0158	0.0368	0.1921	0.5301	1.5141	6.4706	0.2139E−03
250.0	0.2749	−0.0669	0.3744	0.2154	0.0592	0.0228	0.0437	0.2507	0.7563	1.9362	5.5907	0.3071E−03
290.0	0.3187	−0.0759	0.3952	0.2018	0.1082	0.0261	0.0509	0.2800	0.7023	1.5848	5.7912	0.2076E−03
293.0	0.3220	−0.0769	0.3898	0.1911	0.1243	0.0305	0.0516	0.2801	0.6630	1.4428	5.2743	0.2206E−03
295.0	0.3242	−0.0755	0.4180	0.2114	0.0787	0.0287	0.0511	0.2909	0.7991	1.7252	5.3364	0.2213E−03

Table 42. *Absorptive scattering factors for W and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.0409	0.1217	0.0616	−21.2992	25.5318	−4.4397	0.0765	0.6427	37.6643	38.7966	47.1865	0.6079E−02
77.0	0.0420	0.1253	0.0622	−4.2825	9.0207	−4.9497	0.0789	0.6822	35.4273	40.0169	46.6157	0.6188E−02
80.0	0.0436	0.1282	0.0638	−26.2513	33.1742	−7.1397	0.0811	0.6764	38.2457	39.4827	45.9307	0.6344E−02
100.0	0.0545	0.1522	0.0692	0.1664	−0.4040	0.2411	0.0992	0.7505	33.0940	43.4556	50.9045	0.1074E−02
150.0	0.0818	0.2121	0.0783	0.0174	−0.0190	0.0014	0.1465	1.0320	17.7493	37.0966	58.4213	0.3270E−02
200.0	0.1090	0.2702	0.0815	0.0198	−0.0167	−0.0035	0.1948	1.4148	21.7972	25.5764	62.9588	0.5893E−02
250.0	0.1362	−0.0100	0.3619	0.7037	−1.2951	0.6520	0.0001	0.2427	18.2078	27.7415	38.8487	0.7753E−02
290.0	0.1580	−0.0130	0.3990	0.9782	−1.5869	0.6762	0.0000	0.2682	19.7433	27.6488	40.2422	0.7748E−02
293.0	0.1596	−0.0127	0.4044	1.1727	−2.2491	1.1411	0.0000	0.2740	23.6882	32.8214	42.9957	0.8060E−02
295.0	0.1607	−0.0128	0.4064	0.5556	−19.7675	19.2764	0.0000	0.2758	21.2594	41.0190	41.6127	0.8066E−02

Table 43. *Absorptive scattering factors for Pt and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.0954	−0.0548	0.1495	0.1218	0.0977	0.0419	0.0224	0.0702	0.1844	0.5134	1.8552	0.5529E−03
77.0	0.0980	−0.1288	0.2100	0.1399	0.0999	0.0412	0.0322	0.0567	0.1810	0.5292	1.9257	0.5308E−03
80.0	0.1018	−0.0197	0.2099	0.1277	0.0199	0.0333	0.0044	0.1173	0.4337	1.2194	2.0584	0.4877E−03
100.0	0.1272	−0.0184	0.2792	0.1465	0.2875	−0.2670	0.0000	0.1609	0.7431	8.4404	8.9410	0.4707E−03
150.0	0.1908	−0.0408	0.3724	0.1875	0.0350	−0.0055	0.0206	0.2113	0.8797	6.3759	11.4900	0.5830E−03
200.0	0.2543	−0.0678	0.4214	0.2261	0.0554	0.0112	0.0389	0.2429	0.7924	2.8509	11.8465	0.4166E−03
250.0	0.3177	−0.0849	0.4702	0.2465	0.0841	0.0119	0.0505	0.2849	0.7971	2.4810	11.6157	0.1611E−03
290.0	0.3684	−0.0939	0.5052	0.2267	0.1250	0.0238	0.0576	0.3229	0.7631	1.9016	8.1125	0.2372E−03
293.0	0.3722	−0.0940	0.5172	0.2271	0.1175	0.0233	0.0579	0.3284	0.7989	1.9768	8.2127	0.2397E−03
295.0	0.3747	−0.0933	0.5454	0.2476	0.0820	0.0124	0.0579	0.3375	0.9457	2.7549	12.9454	0.2021E−03

Table 44. *Absorptive scattering factors for Au and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1590	−0.0518	0.2821	0.1783	0.0736	0.0226	0.0255	0.1505	0.4393	1.2971	3.7171	0.2960E−03
77.0	0.1632	−0.0516	0.2935	0.1787	0.0679	0.0241	0.0256	0.1567	0.4656	1.3466	3.5727	0.2893E−03
80.0	0.1696	−0.0631	0.2624	0.1864	0.1014	0.0373	0.0307	0.1446	0.3623	0.9590	3.1118	0.2821E−03
100.0	0.2120	−0.0750	0.2852	0.2048	0.1341	0.0480	0.0377	0.1729	0.3715	0.9319	3.1993	0.2142E−03
150.0	0.3179	−0.0911	0.4764	0.1298	0.1583	0.0718	0.0513	0.2801	0.6105	0.9979	3.1553	0.3827E−03
200.0	0.4236	−0.1046	0.6436	0.5196	−0.2696	0.0772	0.0639	0.3822	1.2532	1.3832	3.7619	0.2931E−03
250.0	0.5292	−0.0043	−0.1336	0.7342	0.3057	0.0670	0.0001	0.0930	0.4442	1.3103	4.9862	0.1708E−03
290.0	0.6135	−0.0046	−0.1445	0.8199	0.3117	0.0577	0.0002	0.1052	0.5108	1.5401	6.0433	0.2030E−03
293.0	0.6198	−0.0084	−0.1484	0.8069	0.3240	0.0708	0.0134	0.1127	0.5041	1.4362	5.3111	0.2139E−03
295.0	0.6240	−0.0105	−0.1499	0.8048	0.3296	0.0742	0.0184	0.1165	0.5029	1.4115	5.1805	0.2164E−03

Table 45. *Absorptive scattering factors for Pb and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.5496	−0.1177	0.8833	0.6636	−0.5062	0.1310	0.0757	0.5201	2.5055	3.2721	6.2867	0.8121E−03
77.0	0.5642	−0.1224	0.8699	0.2832	−0.0168	0.0536	0.0787	0.5202	1.7932	5.5020	8.7850	0.7493E−03
80.0	0.5862	−0.1252	0.8863	0.2723	0.0138	0.0396	0.0812	0.5366	1.7592	3.3679	9.6383	0.7652E−03
100.0	0.7324	−0.0118	−0.1681	0.9686	0.3438	0.0679	0.0216	0.1326	0.5975	1.7013	6.4400	0.1680E−03
150.0	1.0970	−0.0295	−0.2191	1.1984	0.4051	0.0766	0.0537	0.2159	0.8142	2.1260	8.0782	0.4259E−03
200.0	1.4596	−0.0324	−0.2502	1.3498	0.4392	0.0958	0.0650	0.2740	1.0303	2.4104	8.1624	0.4716E−03
250.0	1.8196	−0.0342	−0.2705	1.4518	0.4822	0.1093	0.0745	0.3265	1.2375	2.6390	8.7671	0.5706E−03
290.0	2.1053	−0.0320	−0.2632	1.7173	0.3634	0.0407	0.0775	0.3468	1.4915	4.0579	13.8245	0.1592E−03
293.0	2.1266	−0.0323	−0.2637	1.7322	0.3655	0.0309	0.0783	0.3499	1.5072	4.2205	16.9595	0.1661E−03
295.0	2.1408	−0.0311	−0.2601	1.7545	0.3479	0.0256	0.0770	0.3460	1.5304	4.4481	18.5275	0.1767E−03

Table 46. *Absorptive scattering factors for Th and s up to 6.0 Å^{-1}*

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
75.0	0.1875	−0.0778	0.3752	0.2375	0.1178	0.0456	0.0310	0.1623	0.4379	1.1517	3.7725	0.6720E−03
77.0	0.1925	−0.0901	0.3216	0.2503	0.1658	0.0614	0.0348	0.1488	0.3394	0.8861	3.2901	0.6475E−03
80.0	0.2000	−0.0859	0.3726	0.2471	0.1361	0.0552	0.0343	0.1658	0.4156	1.0523	3.5728	0.6003E−03
100.0	0.2500	−0.0902	0.5086	0.2920	0.0879	0.0256	0.0391	0.2253	0.6822	2.2435	5.7600	0.4317E−03
150.0	0.3748	−0.1188	0.6628	0.2202	0.1872	0.0728	0.0570	0.3266	0.7263	1.4091	4.7177	0.4470E−03
200.0	0.4993	−0.1351	0.9068	0.3233	0.0510	0.0436	0.0709	0.4508	1.4350	3.5135	8.4970	0.4520E−03
250.0	0.6234	−0.0058	−0.1746	1.0282	0.3973	0.0811	0.0003	0.1052	0.5218	1.6314	7.4657	0.4186E−03
290.0	0.7224	−0.0057	−0.1834	1.1654	0.3894	0.0542	0.0002	0.1163	0.6107	2.0851	10.8935	0.3674E−03
293.0	0.7298	−0.0056	−0.1825	1.1829	0.3850	0.0470	0.0004	0.1163	0.6209	2.1872	12.5741	0.4423E−03
295.0	0.7348	−0.0057	−0.1842	1.1831	0.3876	0.0504	0.0002	0.1175	0.6223	2.1582	11.7314	0.3989E−03

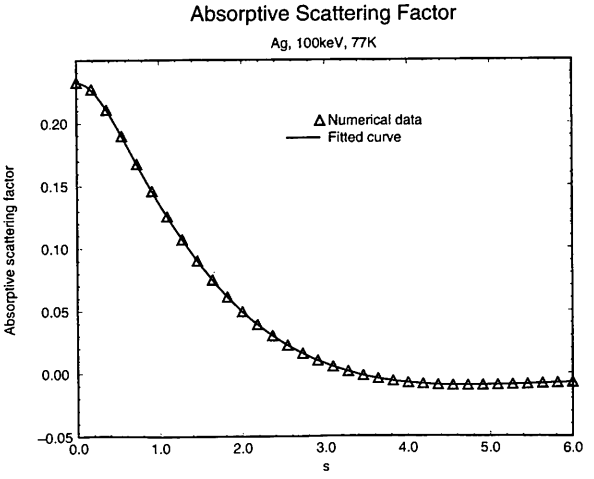

Fig. 3. Numerical and fitted absorptive scattering factors (in units of Å) as a function of s (in units of Å^{-1}) for 100 keV for a single crystal of Ag at 77 K.

by Peng *et al.* (1996). The program can be obtained free of charge by contacting Lian-Mao Peng at the following e-mail address: lmpeng@lmplab.blem.ac.cn.

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