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Parameterization of the temperature dependence of the Debye–Waller factors

H. X. Gao[a] and L.-M. Peng[a,b]*

[a]*Beijing Laboratory of Electron Micoscopy, Center for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, PO Box 2724, Beijing 100080, People's Republic of China, and* [b]*Department of Electronics, Peking University, Beijing 100871, People's Republic of China. E-mail: lmpeng@lmplab.blem.ac.cn*

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Abstract

Parameterization has been made for the temperature dependence of the Debye–Waller factors of 68 elemental crystals and 17 compounds with the zinc-blende structure. The Debye–Waller factors of 46 elemental crystals were calculated based on the available phonon density of states, and those of the remaining 22 elemental crystals were estimated using the Debye approximation for the phonon density of states. The Debye–Waller factors of the zinc-blende compounds were obtained from the 14-parameter shell-model calculations of Reid [*Acta Cryst.* (1983), A**39**, 1–13].

1. Introduction

The importance of the effect of thermal motion in crystallography cannot be overemphasized (Willis & Pryor, 1975). A Temperature Factor Project was indeed initiated in 1985 by the Neutron Diffraction Commission of the International Union of Crystallography [*Acta Cryst.* (1985), B**41**, 374], and compilations have been made of Debye–Waller factors of several cubic elements (Butt *et al.*, 1988), cubic compounds (Butt *et al.*, 1993) and hexagonal close packed elements (Gopi & Sirdeshmukh, 1998). The recommended values of the Debye–Waller factors are given, however, only at a fixed temperature, *i.e.* at 293 K, and these values are usually difficult to interpolate into different temperature regimes.

Previously, the Debye–Waller factors have been obtained over a temperature range from 1 to 1000 K for 17 zinc-blende-structure materials by Reid (1983) and 66 elemental crystals (Peng *et al.*, 1996). For 44 elemental crystals of the 66 studied, the Debye–Waller factors were calculated based on expansions (Sears & Shelley, 1991) which were found later to be inaccurate. It is the purpose of this article to correct this inaccuracy by avoiding the expansions and to make a parameterization of the temperature dependence of the Debye–Waller factors of 68 elemental crystals and 17 compounds with the zinc-blende structure (Reid, 1983).

2. Debye–Waller factors of elemental crystals

Debye–Waller factors are isotropic for a cubic lattice and may be calculated for all temperatures given the phonon density of states (PDS). For elemental crystals with only one atom per unit cell, the temperature-dependent Debye–Waller factors may be obtained *via* direct integration of the following equation (Bruüesch, 1987):

$$B = \frac{4\pi^2\hbar}{m}\int_0^{\omega_m} \coth\left(\frac{\hbar\omega}{2k_BT}\right)\left[\frac{g(\omega)}{\omega}\right]\mathrm{d}\omega, \qquad (1)$$

in which $g(\omega)$ is the phonon density of states (PDS), m is the mass of the atom, T is the temperature, k_B is the usual Boltzman constant and ω_m is the maximum phonon frequency. Experimentally, the phonon density of states $g(\omega)$ may be measured by inelastic neutron scattering (Bruüesch, 1987). A direct numerical integration of (1) then gives the Debye–Waller factor for any temperature.

Previously, we have calculated the Debye–Waller factors for 44 elemental crystals over the temperature range from 1 to 1000 K or the melting temperature of the crystal, whichever is smaller (Peng *et al.*, 1996).

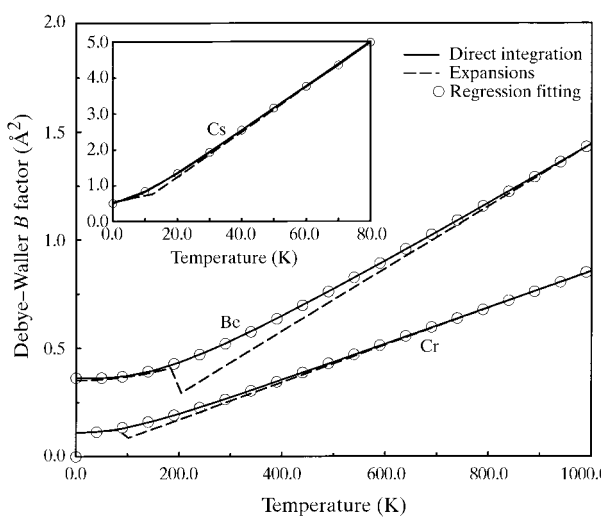

Fig. 1. Debye–Waller factors as a function of temperature for three typical elemental crystals.

Table 1. *Parameterization of the temperature dependence of the Debye–Waller factors of 46 elemental crystals*

The Debye–Waller factors were calculated based on PDS (0–80 K).

Element	Z	Structure	a_0	a_1	a_2	a_3	a_4	ME (%)	Reference
He	2	H.c.p.	16.03115	0.1926E−01	0.6846E−01	−0.5670E−02	0.9275E−03	0.01	[1]
He	2	F.c.c.	4.55876	−0.2830E−02	0.9170E−02	−0.1670E−02	0.1334E−03	0.01	[2]
Li	3	B.c.c.	1.20401	−0.4142E−03	0.1264E−03	−0.3584E−06	−0.5327E−09	0.03	[3]
Be	4	H.c.p.	0.36275	0.6590E−05	−0.7256E−06	0.2249E−07	−0.5366E−10	0.01	[4]
C	6	Diamond	0.11918	−0.6360E−07	0.1962E−06	0.3167E−09	−0.1858E−11	0.01	[5]
Ne	10	F.c.c.	1.66115	0.2430E−02	−0.3280E−03	0.1197E−03	−0.2696E−05	0.03	[6]
Na	11	B.c.c.	0.81176	−0.1380E−02	0.3954E−03	−0.3464E−05	0.1240E−07	0.08	[7]
Mg	12	H.c.p.	0.42425	0.1714E−03	0.2935E−04	0.1405E−06	−0.1449E−08	0.06	[4]
Al	13	F.c.c.	0.27196	−0.4254E−04	0.7433E−05	0.7042E−07	−0.4391E−09	0.02	[8]
Si	14	Diamond	0.19284	0.1670E−04	−0.7475E−06	0.1410E−06	−0.8174E−09	0.02	[5]
Ar	18	F.c.c.	0.82048	−0.2580E−02	0.9105E−03	−0.1047E−04	0.4603E−07	0.29	[9]
K	19	B.c.c.	0.78847	−0.2233E−03	0.8963E−03	−0.1055E−04	0.4711E−07	0.37	[10]
Ca	20	F.c.c.	0.31376	−0.1804E−03	0.8118E−04	−0.4502E−06	0.8299E−09	0.05	[11]
Ca	20	B.c.c.	0.37894	−0.4210E−03	0.1313E−03	−0.1006E−05	0.3204E−08	0.05	[12]
Sc	21	H.c.p.	0.20201	−0.9230E−04	0.5810E−05	0.1373E−06	−0.9440E−09	0.04	[13]
Ti	22	H.c.p.	0.16677	0.2669E−04	0.2068E−05	0.1022E−06	−0.6030E−09	0.02	[14]
V	23	B.c.c.	0.15421	0.6057E−04	0.1253E−04	−0.5130E−07	0.1305E−09	0.03	[15]
Cr	24	B.c.c.	0.11316	−0.4193E−05	0.2064E−05	−0.1451E−10	0.3307E−10	0.02	[16]
Fe	26	B.c.c.	0.12132	−0.1893E−04	0.3513E−05	0.1327E−07	−0.8533E−10	0.02	[17]
Fe	26	F.c.c.	0.15517	−0.1997E−04	0.9983E−05	0.8506E−08	−0.2064E−09	0.02	[18]
Ni	28	F.c.c.	0.12573	−0.1977E−04	0.2775E−05	0.3922E−07	−0.2291E−09	0.01	[19]
Cu	29	F.c.c.	0.14616	−0.1212E−04	0.8220E−05	0.4448E−07	−0.4132E−09	0.01	[20]
Zn	30	H.c.p.	0.20745	−0.2901E−03	0.3690E−04	−0.3618E−07	−0.8717E−09	0.24	[4]
Ge	32	Diamond	0.13367	−0.2609E−03	0.2061E−04	−0.4908E−07	−0.2569E−09	0.14	[5]
Kr	36	F.c.c.	0.52667	0.1250E−02	0.8848E−03	−0.1137E−04	0.5367E−07	0.86	[21]
Rb	37	B.c.c.	0.57468	0.7600E−02	0.1160E−02	−0.1563E−04	0.7640E−07	1.76	[22]
Sr	38	B.c.c.	0.30725	−0.1276E−03	0.2858E−03	−0.3173E−05	0.1362E−07	0.20	[23]
Y	39	H.c.p.	0.15651	−0.1590E−03	0.2634E−04	−0.3492E−07	−0.4910E−09	0.11	[24]
Zr	40	H.c.p.	0.12491	−0.6417E−04	0.1215E−04	0.3310E−07	−0.5068E−09	0.06	[25]
Nb	41	B.c.c.	0.10862	−0.4088E−04	0.1003E−04	−0.4529E−08	−0.1664E−09	0.01	[26]
Mo	42	B.c.c.	0.07620	0.3230E−04	0.1210E−05	0.2189E−07	−0.1052E−09	0.02	[27]
Pd	46	F.c.c.	0.10288	−0.1177E−03	0.1154E−04	−0.6362E−08	−0.2215E−09	0.04	[28]
Ag	47	F.c.c.	0.12932	−0.7537E−04	0.2371E−04	−0.5679E−07	−0.2679E−09	0.10	[29]
Sn	50	Diamond	0.14057	−0.8009E−03	0.9321E−04	−0.9629E−06	0.3901E−08	0.56	[30]
Xe	54	F.c.c.	0.38452	0.4820E−02	0.7547E−03	−0.1007E−04	0.4870E−07	1.23	[31]
Cs	55	B.c.c.	0.50698	0.2166E−01	0.1350E−02	−0.1933E−04	0.9769E−07	3.58	[32]
Ba	56	B.c.c.	0.23013	−0.3114E−03	0.2572E−03	−0.2981E−05	0.1314E−07	0.38	[33]
La	57	F.c.c.	0.18446	−0.6587E−03	0.1378E−03	−0.1364E−05	0.5296E−08	0.26	[34]
Tb	65	H.c.p.	0.12655	−0.2718E−03	0.5559E−04	−0.4050E−06	0.1100E−08	0.20	[35]
Ho	67	H.c.p.	0.11529	−0.2341E−03	0.4000E−04	−0.2202E−06	0.2775E−09	0.25	[36]
Ta	73	B.c.c.	0.06738	0.1172E−04	0.5384E−05	0.4135E−07	−0.4006E−09	0.07	[37]
W	74	B.c.c.	0.04702	0.3234E−04	0.9579E−06	0.2342E−07	−0.1351E−09	0.04	[38]
Pt	78	F.c.c.	0.06770	−0.4038E−04	0.1223E−04	−0.3998E−07	−0.5083E−10	0.06	[39]
Au	79	F.c.c.	0.08767	−0.2654E−03	0.3587E−04	−0.2836E−06	0.9104E−09	0.07	[29]
Pb	82	F.c.c.	0.13625	0.1480E−02	0.1297E−03	−0.1434E−05	0.6111E−08	0.19	[40]
Th	90	F.c.c.	0.08981	−0.2508E−03	0.4298E−04	−0.3296E−06	0.9576E−09	0.28	[41]

References: [1] Reese *et al.* (1971); [2] Eckert *et al.* (1977); [3] Smith *et al.* (1968); [4] Young & Koppel (1964); [5] Dolling *et al.* (1966); [6] Skalyo *et al.* (1972); [7] Gilat & Dolling (1964); [8] Gilat & Nicklow (1966); [9] Fujii *et al.* (1974); [10] Cowley *et al.* (1966); [11] Stassis *et al.* (1983); [12] Heiroth *et al.* (1986); [13] Wakabayashi *et al.* (1971); [14] Stassis *et al.* (1979); [15] Page (1967); [16] Shaw & Muhlestein (1971); [17] Minkiewicz *et al.* (1967); [18] Zarestky & Stassis (1987); [19] Birgeneau *et al.* (1964); [20] Svensson *et al.* (1967); [21] Skalyo *et al.* (1974); [22] Copley & Brockhouse (1973); [23] Mizuki & Stassis (1985); [24] Sinha *et al.* (1970); [25] Stassis *et al.* (1978); [26] Sharp (1969); [27] Powell *et al.* (1977); [28] Miiller & Brockhouse (1971); [29] Lynn *et al.* (1973); [30] Price & Rowe (1969); [31] Lurie *et al.* (1974); [32] Nucker & Buchenau (1985); [33] Mizuki *et al.* (1985); [34] Stassis *et al.* (1982); [35] Houmann & Nicklow (1970); [36] Nicklow *et al.* (1971); [37] Woods (1964); [38] Higuera *et al.* (1985); [39] Ohrlich & Drexel (1968); [40] Stedman *et al.* (1967); [41] Reese *et al.* (1973).

These earlier calculations were however, based on two expansions at low- and high-temperature regimes. It was claimed (Sears & Shelley, 1991) that the validity of the two expansions overlap at approximately $T = 0.2T_m$ for all elemental crystals, with T_m being the Debye temperature of the crystal. Fig. 1 shows three typical curves of the Debye–Waller factors as a function of temperature. In the figure, the dashed curves were calculated based on the above mentioned expansions, and the solid curves were based on direct numerical integration of equation (1). The figure shows clearly that the expansions are indeed not accurate over a rather

Table 2. *Parameterization of the temperature dependence of the Debye–Waller factors of 46 elemental crystals*

The Debye–Waller factors were calculated based on PDS ($T > 80$ K).

Element	Z	Structure	a_0	a_1	a_2	a_3	a_4	ME (%)
Li	3	B.c.c.	0.90169	0.8780E−02	0.3039E−04	−0.5940E−07	0.4448E−10	0.33
Be	4	H.c.p.	0.35851	−0.1421E−03	0.3225E−05	−0.3136E−08	0.1139E−11	0.69
C	6	Diamond	0.12034	−0.2231E−04	0.3348E−06	−0.2108E−09	0.5320E−13	0.09
Na	11	B.c.c.	0.38531	0.1831E−01	0.2176E−04	−0.5389E−07	0.5105E−10	0.12
Mg	12	H.c.p.	0.22668	0.4830E−02	0.3239E−05	−0.3499E−08	0.1362E−11	1.00
Al	13	F.c.c.	0.18496	0.1630E−02	0.2469E−05	−0.2630E−08	0.1015E−11	1.31
Si	14	Diamond	0.14236	0.9261E−03	0.1623E−05	−0.1677E−08	0.6351E−12	0.93
K	19	B.c.c.	0.24960	0.3377E−01	0.1624E−04	−0.4263E−07	0.4262E−10	0.02
Ca	20	F.c.c.	0.12238	0.6070E−02	0.1815E−05	−0.1975E−08	0.7726E−12	0.62
Ca	20	B.c.c.	0.14441	0.8010E−02	0.2131E−05	−0.2317E−08	0.9057E−12	0.57
Sc	21	H.c.p.	0.11892	0.1650E−02	0.1665E−05	−0.1791E−08	0.6952E−12	1.06
Ti	22	H.c.p.	0.10764	0.1140E−02	0.1470E−05	−0.1573E−08	0.6088E−12	1.12
V	23	B.c.c.	0.09905	0.1370E−02	0.1334E−05	−0.1424E−08	0.5500E−12	1.02
Cr	24	B.c.c.	0.08979	0.3666E−03	0.1137E−05	−0.1198E−08	0.4588E−12	1.24
Fe	26	B.c.c.	0.08725	0.6233E−03	0.1143E−05	−0.1213E−08	0.4670E−12	1.22
Fe	26	F.c.c.	0.09411	0.1370E−02	0.1302E−05	−0.1398E−08	0.5420E−12	1.01
Ni	28	F.c.c.	0.08579	0.7271E−03	0.1152E−05	−0.1229E−08	0.4745E−12	1.24
Cu	29	F.c.c.	0.08444	0.1380E−02	0.1185E−05	−0.1276E−08	0.4956E−12	1.00
Zn	30	H.c.p.	0.10549	0.3030E−02	0.3054E−05	−0.5039E−08	0.3072E−11	0.38
Ge	32	Diamond	0.06984	0.1650E−02	0.9448E−06	−0.1010E−08	0.3904E−12	0.82
Kr	36	F.c.c.	0.21138	0.2794E−01	0.5403E−04	−0.3045E−06	0.6835E−09	0.01
Rb	37	B.c.c.	0.11346	0.4446E−01	0.6973E−05	−0.1760E−07	0.1684E−10	0.01
Sr	38	B.c.c.	0.06924	0.1227E−01	0.1052E−05	−0.1151E−08	0.4515E−12	0.20
Y	39	H.c.p.	0.06510	0.2520E−02	0.9606E−06	−0.1044E−08	0.4082E−12	0.77
Zr	40	H.c.p.	0.06133	0.1570E−02	0.8855E−06	−0.9584E−09	0.3736E−12	0.84
Nb	41	B.c.c.	0.05889	0.1190E−02	0.8383E−06	−0.9048E−09	0.3521E−12	0.88
Mo	42	B.c.c.	0.05292	0.4392E−03	0.7142E−06	−0.7625E−09	0.2946E−12	1.26
Pd	46	F.c.c.	0.05200	0.1220E−02	0.7458E−06	−0.8062E−09	0.3140E−12	0.97
Ag	47	F.c.c.	0.05358	0.2190E−02	0.7901E−06	−0.8588E−09	0.3357E−12	0.69
Sn	50	Diamond	0.13541	0.1900E−02	0.1113E−04	−0.2640E−07	0.2193E−10	1.82
Xe	54	F.c.c.	0.10655	0.2824E−01	0.1613E−04	−0.6878E−07	0.1157E−09	0.01
Cs	55	B.c.c.	0.07343	0.6136E−01	0.4538E−05	−0.1147E−07	0.1098E−10	0.01
Ba	56	B.c.c.	0.04457	0.1016E−01	0.6803E−06	−0.7445E−09	0.2922E−12	0.20
La	57	F.c.c.	0.04370	0.6040E−02	0.6646E−06	−0.7269E−09	0.2852E−12	0.24
Tb	65	H.c.p.	0.03765	0.3200E−02	0.5682E−06	−0.6205E−09	0.2432E−12	0.46
Ho	67	H.c.p.	0.03625	0.2630E−02	0.5462E−06	−0.5963E−09	0.2337E−12	0.57
Ta	73	B.c.c.	0.03159	0.9039E−03	0.4625E−06	−0.5021E−09	0.1961E−12	0.88
W	74	B.c.c.	0.02908	0.3748E−03	0.4073E−06	−0.4382E−09	0.1701E−12	1.20
Pt	78	F.c.c.	0.02938	0.1090E−02	0.4310E−06	−0.4681E−09	0.1829E−12	0.91
Au	79	F.c.c.	0.02981	0.1930E−02	0.4444E−06	−0.4842E−09	0.1895E−12	0.70
Pb	82	F.c.c.	0.03639	0.6980E−02	0.1124E−05	−0.1881E−08	0.1157E−11	0.08
Th	90	F.c.c.	0.02586	0.2330E−02	0.3902E−06	−0.4261E−09	0.1670E−12	0.35

wide range of temperatures, and that results obtained *via* direct numerical integration agree well with our earlier results at both very low and high temperatures.

We have recalculated the Debye–Waller factors for 46 elemental crystals with known phonon density of states. The phonon density of states was obtained *via* either direct measurements using neutron inelastic scattering or calculations based on experimentally measured phonon-dispersion curves. For all elemental crystals and compounds to be discussed below, we found that the temperature dependence of the Debye–Waller factors is rather smooth and may be fitted excellently using fourth-degree polynomial regression fitting, *i.e.*

$$B(T) = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4, \qquad (2)$$

where T is measured in Kelvin, B is given in Å^2 and a_i are fitting parameters. The goodness of fit is measured by the maximum-error (ME) indicator of all data points, *i.e.*

$$\text{ME} = \max\left\{ \frac{B^{(i)} - B^{(i)}_{\text{fit}}}{(B^{(i)} + B^{(i)}_{\text{fit}})/2}, \quad i = 1, \dots \right\} \times 100\%.$$

For the 46 elemental crystals with known phonon density of states, the temperature dependence of the Debye–Waller factors has been parameterized, and the fitting parameters are given in Tables 1 and 2 together with the ME for the fit and references to the phonon density of states. Tables 1 and 2 show clearly that the polynomial fit to the $B(T)$ curves is in general excellent,

Table 3. *Polynomial regression fitting parameters of the Debye–Waller factors of 22 elemental crystals estimated using Debye theory (0–80 K)*

Element	Z	a_0	a_1	a_2	a_3	a_4	ME (%)
Mn	25	0.12754	0.2818E−05	0.4722E−05	0.8580E−08	−0.8769E−10	0.01
Co	27	0.10955	0.1879E−05	0.3467E−05	0.5237E−08	−0.5071E−10	0.01
Ga	31	0.12877	0.2241E−05	0.7940E−05	0.1539E−07	−0.2170E−09	0.01
As	33	0.13599	−0.2725E−05	0.1122E−04	0.1326E−07	−0.3003E−09	0.02
Se	34	0.40458	−0.5352E−03	0.4310E−03	−0.4870E−05	0.2103E−07	0.20
Ru	44	0.04738	0.1585E−06	0.8522E−06	0.3805E−09	−0.3294E−11	0.01
Rh	45	0.05816	0.7334E−06	0.1596E−05	0.1919E−08	−0.1786E−10	0.01
Cd	48	0.12239	−0.4091E−04	0.2150E−04	−0.5408E−07	−0.2069E−09	0.06
In	49	0.23229	−0.4124E−03	0.1821E−03	−0.1839E−05	0.7271E−08	0.17
Sb	51	0.11192	−0.3555E−04	0.1918E−04	−0.4560E−07	−0.1995E−09	0.06
Te	52	0.14748	−0.1611E−03	0.5615E−04	−0.3793E−06	0.9330E−09	0.12
Gd	64	0.09144	−0.3805E−04	0.1799E−04	−0.5673E−07	−0.1073E−09	0.07
Dy	66	0.08425	−0.2745E−04	0.1462E−04	−0.3576E−07	−0.1464E−09	0.06
Hf	72	0.06389	−0.5951E−05	0.6949E−05	0.1648E−09	−0.1566E−09	0.03
Ta	73	0.06618	−0.9267E−05	0.8144E−05	−0.4773E−08	−0.1609E−09	0.04
Re	75	0.03588	0.7034E−06	0.1212E−05	0.2006E−08	−0.1980E−10	0.01
Os	76	0.03021	0.3114E−06	0.7675E−06	0.7978E−09	−0.7300E−11	0.01
Ir	77	0.03559	0.7481E−06	0.1257E−05	0.2188E−08	−0.2193E−10	0.02
Hg	80	0.19812	0.2056E−03	0.2895E−03	−0.3592E−05	0.1657E−07	0.55
Tl	81	0.17865	−0.3461E−04	0.2324E−03	−0.2793E−05	0.1260E−07	0.36
Bi	83	0.11585	−0.1975E−03	0.7561E−04	−0.7050E−06	0.2596E−08	0.16
U	92	0.05836	−0.2049E−04	0.1051E−04	−0.2789E−07	−0.9295E−10	0.06

Table 4. *Polynomial regression fitting parameters of the Debye–Waller factors of 22 element crystals estimated using Debye theory ($T > 80$ K)*

Element	Z	a_0	a_1	a_2	a_3	a_4	ME (%)
Mn	25	0.09004	0.7491E−03	0.1187E−05	−0.1261E−08	0.4858E−12	1.17
Co	27	0.08122	0.5452E−03	0.1045E−05	−0.1104E−08	0.4238E−12	1.16
Ga	31	0.11303	0.3962E−03	0.6605E−05	−0.1772E−07	0.1854E−10	0.05
As	33	0.07665	0.1450E−02	0.1268E−05	−0.1500E−08	0.6424E−12	1.02
Se	34	0.07777	0.1750E−01	0.1177E−05	−0.1277E−08	0.4974E−12	0.18
Ru	44	0.04068	0.1125E−03	0.4621E−06	−0.4754E−09	0.1793E−12	1.02
Rh	45	0.04497	0.2454E−03	0.5634E−06	−0.5922E−09	0.2265E−12	1.12
Cd	48	0.06319	0.1830E−02	0.1861E−05	−0.3082E−08	0.1883E−11	0.27
In	49	0.08212	0.7660E−02	0.4795E−05	−0.1169E−07	0.1066E−10	0.08
Sb	51	0.04974	0.1810E−02	0.8538E−06	−0.1017E−08	0.4378E−12	0.61
Te	52	0.05164	0.3490E−02	0.1075E−05	−0.1424E−08	0.6835E−12	0.29
Gd	64	0.03722	0.1610E−02	0.5511E−06	−0.5995E−09	0.2344E−12	0.64
Dy	66	0.03579	0.1390E−02	0.5278E−06	−0.5736E−09	0.2242E−12	0.83
Hf	72	0.03167	0.8288E−03	0.4584E−06	−0.4965E−09	0.1936E−12	0.89
Ta	73	0.03150	0.9178E−03	0.4586E−06	−0.4972E−09	0.1940E−12	0.86
Re	75	0.02607	0.1917E−03	0.3390E−06	−0.3591E−09	0.1381E−12	1.17
Os	76	0.02386	0.1160E−03	0.2944E−06	−0.3084E−09	0.1177E−12	1.11
Ir	77	0.02550	0.1993E−03	0.3339E−06	−0.3542E−09	0.1363E−12	1.16
Hg	80	0.05788	0.1026E−01	0.5610E−05	−0.1853E−07	0.2364E−10	0.03
Tl	81	0.03756	0.8810E−02	0.1170E−05	−0.1957E−08	0.1204E−11	0.07
Bi	83	0.03610	0.3580E−02	0.1111E−05	−0.1855E−08	0.1140E−11	0.19
U	92	0.02449	0.9819E−03	0.3617E−06	−0.3933E−09	0.1538E−12	0.71

with ME being typically less than 0.5%. The worst ME occurs for Cs at zero temperature. Shown in the insert of Fig. 1 are the numerical and fitted $B(T)$ curves for Cs. It is seen that even for the worst case the fit is excellent for all temperatures above zero.

When the phonon density of states is not available, the Debye–Waller factors of elemental crystals with cubic lattice may be estimated using the Debye theory assuming that the phonon density of states is given by

$$g(\omega) = \begin{cases} 3\omega^2/\omega_m^3 & \text{for } 0 < \omega < \omega_m \\ 0 & \text{for } \omega_m < \omega, \end{cases} \tag{3}$$

where ω_m is the maximum phonon frequency and is related to the usual Debye temperature T_m *via* the relation $kT_m = \hbar\omega_m$. For 22 elemental crystals, the Debye–Waller factors have been estimated this way (Peng *et al.*, 1996). The temperature dependence of these factors has been parameterized using polynomial

Table 5. *Polynomial regression fitting parameters of the Debye–Waller factors of 17 zinc-blende-structure crystals (0–80 K)*

Crystal	Atom	a_0	a_1	a_2	a_3	a_4	ME (%)
GaP	Ga	0.12919	−0.2611E−04	0.4277E−05	0.1318E−06	−0.9790E−09	0.11
	P	0.19714	−0.4786E−04	0.4958E−05	0.1507E−06	−0.1144E−08	0.10
GaSb	Ga	0.16223	−0.4262E−03	0.4610E−04	−0.3021E−06	0.6715E−09	0.30
	Sb	0.12072	−0.3684E−03	0.4148E−04	−0.2710E−06	0.5895E−09	0.35
GaAs	Ga	0.13890	−0.1719E−03	0.1738E−04	0.8267E−08	−0.5764E−09	0.20
	As	0.14029	−0.2267E−03	0.2059E−04	−0.1258E−08	−0.6303E−09	0.23
InP	In	0.14043	−0.3528E−03	0.3512E−04	−0.9239E−07	−0.4990E−09	0.34
	P	0.17317	−0.1375E−03	0.2216E−04	−0.1676E−06	0.5101E−09	0.11
InSb	In	0.15730	−0.8061E−03	0.1070E−03	−0.1097E−05	0.4394E−08	0.51
	Sb	0.13590	−0.6231E−03	0.8837E−04	−0.9244E−06	0.3805E−08	0.46
InAs	In	0.13955	−0.4468E−03	0.4965E−04	−0.3152E−06	0.6372E−09	0.35
	As	0.12433	−0.1992E−03	0.3181E−04	−0.2601E−06	0.8854E−09	0.16
ZnO	Zn	0.14263	0.1850E−04	0.9258E−06	0.1791E−06	−0.1174E−08	0.07
	O	0.21643	−0.1364E−04	0.4672E−05	0.2922E−07	−0.3009E−09	0.03
ZnS	Zn	0.17311	−0.1457E−03	0.1957E−04	0.7536E−07	−0.1091E−08	0.16
	S	0.20061	−0.1104E−03	0.1876E−04	−0.3090E−07	−0.3146E−09	0.09
ZnSe	Zn	0.18397	−0.3260E−03	0.3395E−04	−0.6329E−07	−0.6199E−09	0.25
	Se	0.13154	−0.1820E−03	0.2496E−04	−0.1169E−06	0.8580E−10	0.15
ZnTe	Zn	0.20473	−0.5841E−03	0.7675E−04	−0.6235E−06	0.2023E−08	0.32
	Te	0.12583	−0.3925E−03	0.6072E−04	−0.5412E−06	0.1937E−08	0.30
CdTe	Cd	0.19189	−0.1110E−02	0.1689E−03	−0.1886E−05	0.8109E−08	0.51
	Te	0.13937	−0.5429E−03	0.1052E−03	−0.1182E−05	0.5163E−08	0.33
HgSe	Hg	0.21070	−0.5317E−03	0.4040E−03	−0.5438E−05	0.2651E−07	1.59
	Se	0.15574	0.1412E−03	0.1214E−03	−0.1608E−05	0.7951E−08	0.75
HgTe	Hg	0.22918	0.2620E−02	0.5125E−03	−0.7157E−05	0.3573E−07	2.46
	Te	0.12889	0.7283E−03	0.1402E−03	−0.1894E−05	0.9419E−08	1.18
CuCl	Cu	0.36726	−0.2360E−02	0.3149E−03	−0.3370E−05	0.1392E−07	0.65
	Cl	0.31459	−0.1090E−02	0.1879E−03	−0.2122E−05	0.9284E−08	0.33
CuBr	Cu	0.23794	−0.6525E−03	0.1545E−03	−0.1725E−05	0.7561E−08	0.24
	Br	0.28486	−0.1550E−02	0.2473E−03	−0.2714E−05	0.1150E−07	0.51
CuI	Cu	0.29083	−0.1490E−02	0.1944E−03	−0.1993E−05	0.8041E−08	0.52
	I	0.15310	−0.5973E−03	0.1059E−03	−0.1107E−05	0.4561E−08	0.38
SiC	Si	0.12859	0.2243E−05	0.6939E−06	0.3985E−09	0.2158E−10	0.02
	C	0.16771	−0.8428E−05	0.9532E−06	−0.1570E−08	0.6547E−11	0.01

regression fitting and the fitting parameters are given in Tables 3 and 4.

3. Debye–Waller factors of compounds

For compounds, both the phonon frequency $\omega(\mathbf{q}j)$ and the complex displacement eigenvector $U_k(\mathbf{q}j)$ for the kth atom and phonon state $(\mathbf{q}j)$ ($\mathbf{q}$ being the phonon wavevector and j the branch index) may be obtained using one of the proper models of the lattice dynamics. The model parameters may be obtained by refining the model against experimentally measured phonon-dispersion curves. Given the phonon frequencies and displacement eigenvectors for all phonon states, the Debye–Waller factors can be calculated for the kth atom as follows:

$$B_k = \frac{8\pi^2}{3m_k N} \sum_{\mathbf{q}j} \left(\frac{\overline{E}}{\omega^2} \right)_{\mathbf{q}j} \left| U_k(\mathbf{q}j) \right|^2, \qquad (4)$$

where $\overline{E}_{\mathbf{q}j}$ is the mean energy of the phonon in the mode $(\mathbf{q}j)$,

$$\overline{E}_{\mathbf{q}j} = \hbar\omega_{\mathbf{q}j}(\overline{n}_{\mathbf{q}j} + 1/2),$$

and $\overline{n}_{\mathbf{q}j}$ is the mean occupation number of the mode and is given by the Bose–Einstein distribution:

$$\overline{n}_{\mathbf{q}j} = 1/[\exp(\hbar\omega_{\mathbf{q}j}/k_B T) - 1],$$

in which N is the number of wavevectors in the first Brillouin zone.

In a separate publication (Gao *et al.*, 1999), we have presented results on the lattice dynamics of 19 compounds with the sodium chloride structure and the parameterization of the temperature dependence of the Debye–Waller factors of these compounds. The Debye–Waller factors have also been calculated for a wide range of temperatures for 17 compounds with the zinc-blende structure by Reid (1983). Parameterization of these Debye–Waller factors has been made and the results are listed in Tables 5 and 6.

4. Concluding remarks

Parameterization has been made for the temperature dependence of the Debye–Waller factors of 68 elemental crystals and 17 compounds with the zinc-

Table 6. *Polynomial regression fitting parameters of the Debye–Waller factors of 17 zinc-blende-structure crystals ($T > 80$ K)*

Crystal	Atom	a_0	a_1	a_2	a_3	a_4	ME (%)
GaP	Ga	0.07258	0.1270E−02	0.9754E−06	−0.1042E−08	0.4030E−12	1.10
	P	0.13578	0.1350E−02	0.1554E−05	−0.1607E−08	0.6090E−12	0.97
GaSb	Ga	0.07923	0.2600E−02	0.1271E−05	−0.1496E−08	0.6388E−12	0.50
	Sb	0.04830	0.2350E−02	0.8070E−06	−0.9583E−09	0.4115E−12	0.50
GaAs	Ga	0.07394	0.1690E−02	0.1003E−05	−0.1074E−08	0.4159E−12	0.96
	As	0.06972	0.1880E−02	0.9534E−06	−0.1021E−08	0.3954E−12	0.83
InP	In	0.05059	0.2660E−02	0.7411E−06	−0.8060E−09	0.3151E−12	0.62
	P	0.13490	0.1170E−02	0.1539E−05	−0.1584E−08	0.5972E−12	0.70
InSb	In	0.05476	0.4180E−02	0.1093E−05	−0.1441E−08	0.6892E−12	0.21
	Sb	0.05115	0.3450E−02	0.1012E−05	−0.1330E−08	0.6348E−12	0.34
InAs	In	0.05013	0.2880E−02	0.7275E−06	−0.7896E−09	0.3084E−12	0.56
	As	0.06880	0.1740E−02	0.9253E−06	−0.9870E−09	0.3809E−12	0.78
ZnO	Zn	0.08025	0.1310E−02	0.1107E−05	−0.1189E−08	0.4612E−12	1.12
	O	0.19457	0.5300E−03	0.1662E−05	−0.1595E−08	0.5746E−12	0.44
ZnS	Zn	0.08237	0.2370E−02	0.1152E−05	−0.1242E−08	0.4827E−12	0.71
	S	0.13763	0.1670E−02	0.1656E−05	−0.1728E−08	0.6579E−12	0.79
ZnSe	Zn	0.08353	0.2810E−02	0.1175E−05	−0.1267E−08	0.4926E−12	0.72
	Se	0.06725	0.1830E−02	0.9242E−06	−0.9912E−09	0.3841E−12	0.72
ZnTe	Zn	0.08544	0.3970E−02	0.1215E−05	−0.1312E−08	0.5105E−12	0.66
	Te	0.04544	0.2930E−02	0.6712E−06	−0.7409E−09	0.2943E−12	0.54
CdTe	Cd	0.05219	0.6150E−02	0.7666E−06	−0.8345E−09	0.3264E−12	0.31
	Te	0.04582	0.4060E−02	0.6645E−06	−0.7218E−09	0.2821E−12	0.32
HgSe	Hg	0.04160	0.1254E−01	0.1645E−05	−0.3253E−08	0.2390E−11	0.05
	Se	0.09039	0.4220E−02	0.3197E−05	−0.6104E−08	0.4364E−11	0.11
HgTe	Hg	0.04118	0.1832E−01	0.1588E−05	−0.3081E−08	0.2223E−11	0.03
	Te	0.05916	0.5360E−02	0.2153E−05	−0.4117E−08	0.2942E−11	0.09
CuCl	Cu	0.10769	0.1143E−01	0.2610E−05	−0.3835E−08	0.2058E−11	0.16
	Cl	0.16536	0.6700E−02	0.3588E−05	−0.5151E−08	0.2723E−11	0.25
CuBr	Cu	0.10301	0.6030E−02	0.2420E−05	−0.3538E−08	0.1893E−11	0.27
	Br	0.08651	0.9060E−02	0.2106E−05	−0.3101E−08	0.1667E−11	0.17
CuI	Cu	0.10593	0.7530E−02	0.2555E−05	−0.3750E−08	0.2011E−11	0.23
	I	0.05425	0.4260E−02	0.1321E−05	−0.1947E−08	0.1047E−11	0.17
SiC	Si	0.12047	0.7436E−04	0.1168E−05	−0.1163E−08	0.4301E−12	0.91
	C	0.16536	0.3385E−04	0.7346E−06	−0.5648E−09	0.1713E−12	0.21

blende structure. For 46 elemental crystals with known phonon density of states, the present results provide an improvement over our earlier results (Peng *et al.*, 1996), which were made based on two inaccurate expansions proposed by Sears (Sears & Shelley, 1991).

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