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Compilation of Temperature Factors of Cubic Compounds

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Abstract

A compilation of the isotropic temperature factors of 52 diatomic cubic compounds, determined by the diffraction method using X-rays, neutrons and γ-rays, is presented. For each compound, the recommended temperature factors of the cation B^+, the anion B^- and the mass-weighted average of B^+ and B^-, $\bar{B}$, along with the Debye temperature, Θ, are given. This represents the second stage of a temperature-factor project initiated by the Commission on Neutron Diffraction of the International Union of Crystallography [*Acta Cryst.* (1985), B**41**, 374].

Introduction

The Debye-Waller factor describes the effect of lattice vibrations on Bragg peak intensities and is denoted by $\exp(-2M)$, where

$$2M = 2B(\sin^2\theta)/\lambda^2, \qquad (1)$$

where B is the temperature factor, θ is the Bragg angle and λ is the wavelength. The temperature factor B is related to the mean square amplitude of vibration perpendicular to the lattice planes, $\langle u_s^2\rangle$, through the relation

$$B = 8\pi^2\langle u_s^2\rangle. \qquad (2)$$

For a cubic system, the mean square displacement parallel to all directions is identical. In this case, $B = (8\pi^2/3)\langle u^2\rangle$, where $\langle u^2\rangle = 3\langle u_s^2\rangle$ is the mean square of the 'total displacement' (James, 1967). B is also related to the Debye temperature Θ of the solid through the relation

$$B = (6h^2/mk)(T/\Theta^2)[\varphi(x) + x/4], \qquad (3)$$

where the symbols have their usual meanings (James, 1967).

Although accurate values of the temperature factors can be determined by both X-ray and neutron diffraction, in some cases, for a given material, large variations in the B values are found in the literature. A typical example is that of GaP, for which the quoted average temperature factor, $\bar{B}$, varies between 0.38 (3) and 0.74 (3) Å^2. It was therefore decided to compile the temperature factors of cubic elements and compounds with the aim of providing a recommended list of temperature factors for these materials. In the first phase of the work the temperature-factor data of cubic elements was published (Butt, Bashir, Willis, & Heger, 1988). In the present paper, results of a similar study carried out on 52 cubic compounds are presented.

Results and discussion

The accuracy of the temperature factors depends on the accuracy of the structure factors and hence on the measurement of the diffraction intensity. The various factors affecting the diffraction intensity are discussed in detail by Suortti & Jennings (1977). An important factor affecting the temperature factors is thermal diffuse scattering (TDS).

The consequences of neglecting the TDS correction on the structure analysis have been discussed by Willis & Pryor (1975) and Stevenson & Harada (1983). They concluded that the positional parameters are slightly affected but the temperature factors are underestimated if TDS correction is neglected. Furthermore, Stevenson & Harada (1983) showed that the relative reduction of the temperature parameters due to the neglect of the TDS is largely independent of the hardness of the material, depending mainly on the experimental conditions under which the Bragg intensities were measured: the size and shape of the counter aperture, the scan width and the wavelength of radiation used.

Unfortunately, suitable studies where all necessary experimental conditions under which the intensities were recorded, as well as the change in the derived temperature factors as a result of TDS correction, are few. Therefore, to derive maximum benefit from the published data, it was decided to include all data irrespective of whether the TDS correction was made or not. Another point in favour of retaining all the data was that a number of authors have used high-resolution diffractometers or triple-axis spectrometers. In these instruments the TDS contribution to the diffracted intensity is reduced considerably. This is experimentally confirmed by the measurements of Beg, Aslam, Butt, Khan & Rolandson (1974). However, as a check, when we considered only the TDS corrected values, the recommended values of the temperature factors were not much different from those that we calculated considering all the data, the

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Table 1. *Recommended values of temperature factors for cubic compounds at room temperature* (293 K)

Compound	B^+ (Å^2)	B^- (Å^2)	$\bar{B}$ (Å^2)	Θ (K)	Source references
AgBr	2.42	1.89	2.20	128	[42], [115]
AgCl	2.14 (5)	2.08 (2)	2.13 (5)	149 (2)	[65], [66], [115], [130]
BaF_2	0.64 (1)	0.99 (1)	0.72 (1)	287 (2)	[38], [15], [117]
BaO	0.79 (2)	1.19 (3)	0.83 (4)	232 (6)	[129]
CaF_2	0.55 (5)	0.76 (7)	0.65 (9)	452 (31)	[31], [35], [44], [118], [123], [134], [138]
CaO	0.35 (1)	0.44 (1)	0.38 (1)	596 (8)	[9], [129]
CdTe	1.70 (1)	1.42 (1)	1.55 (1)	135 (1)	[55], [56], [99], [102], [125], [133], [139]
CeO_2	-	-	0.49 (4)	354 (15)	[120]
CsBr	2.00 (9)	2.24 (12)	2.09 (15)	123 (4)	[12], [48]
CsCl	1.83 (2)	1.89 (5)	1.84 (5)	148 (2)	[2], [10], [12]
CsI	2.27 (11)	2.19 (12)	2.24 (16)	108 (4)	[2], [12], [24], [67]
CuBr	2.57 (15)	2.47 (4)	2.51 (16)	137 (4)	[29], [54], [57], [102]
CuCl	4.18 (4)	2.29 (2)	3.50 (4)	140 (1)	[49], [97], [102], [105], [126]
CuI	2.74 (6)	1.58 (6)	1.97 (9)	135 (3)	[85], [102]
GaAs	0.69 (1)	0.68 (1)	0.68 (1)	264 (2)	[4], [22], [78], [90], [102], [111], [124]
GaP	0.53 (1)	0.66 (1)	0.57 (1)	347 (3)	[21], [22], [90], [96], [102], [111]
GaSb	0.90 (1)	0.70 (1)	0.77 (1)	215 (1)	[4], [22], [86], [90], [102], [111], [122]
HgSe	3.65 (2)	0.98 (1)	2.90 (2)	92 (1)	[102], [132]
InAs	0.97 (1)	0.78 (1)	0.89 (1)	200 (1)	[22], [90], [102], [111], [122]
InP	0.84 (1)	0.88 (1)	0.85 (1)	235 (1)	[22], [90], [102], [111]
InSb	1.24 (1)	1.04 (1)	1.14 (1)	160 (1)	[4], [6], [17], [22], [69], [90], [102], [111]
KBr	2.36 (4)	2.38 (4)	2.37 (6)	155 (2)	[5], [7], [8], [26], [77], [79], [92], [98], [116]
KCl	2.17 (1)	2.16 (1)	2.17 (1)	206 (1)	[15], [20], [28], [36], [39], [62], [77], [92], [94], [121], [128], [131]
KF	-	-	1.21 (2)	316 (3)	[16], [23]
KI	3.52 (22)	2.80 (15)	2.97 (27)	117 (5)	[5], [14], [91], [95]
LiF	1.05 (1)	0.65 (1)	0.76 (1)	594 (4)	[60], [77], [81], [135], [137]
MgO	0.37 (1)	0.33 (1)	0.35 (1)	697 (10)	[9], [13], [25], [32], [70], [100], [104], [106], [107], [129]
Mg_2Si	0.76	0.55	0.66	461	[34]
NaCl	1.72 (2)	1.41 (1)	1.53 (2)	278 (2)	[1], [20], [27], [52], [71], [72], [77], [82], [108], [131]
NaF	0.91 (1)	0.91 (1)	0.91 (1)	426 (2)	[59], [80], [93], [110]
NbC	0.18 (1)	0.25 (1)	0.19 (1)	618 (16)	[46], [68], [84]
PbS	1.36 (10)	0.78 (3)	1.28 (10)	149 (6)	[89], [112]
PbTe	2.13 (3)	1.60 (3)	1.73 (4)	102 (1)	[19], [51], [63]
RbBr	-	-	2.24 (16)	135 (5)	[93], [114], [116], [119]
RbCl	2.14 (7)	2.27 (7)	2.18 (10)	161 (4)	[50], [61], [64], [92], [114]
RbF	-	-	1.40 (25)	216 (19)	[16]
RbI	-	-	3.36 (40)	95 (5)	[14], [61], [91]
SiC	0.22	0.23	0.22	983	[102]
$SrCl_2$	1.28 (4)	1.46 (4)	1.36 (6)	218 (5)	[41], [73]
SrF_2	0.56 (1)	0.84 (2)	0.65 (2)	358 (6)	[37], [43], [76]
SrO	0.43 (2)	1.93 (6)	0.66 (6)	318 (14)	[129]
TaC	0.19 (1)	0.47 (1)	0.21 (1)	421 (10)	[68]
ThC	0.32 (8)	0.68 (8)	0.34 (11)	290 (47)	[83]
TiC	0.20 (1)	0.19 (1)	0.20 (1)	871 (22)	[30], [58], [127]
TiN	0.31 (2)	0.30 (2)	0.31 (3)	630 (30)	[47], [58], [127]
TlCl	3.28 (7)	2.00 (7)	3.10 (10)	95 (2)	[53], [75], [88]
UC	-	-	0.21 (1)	366 (7)	[33]
UO_2	0.22 (1)	0.43 (1)	0.25 (1)	400 (8)	[3], [45], [103]
V_3Si	0.48	0.67	0.51	388	[113]
ZnS	0.87 (1)	0.71 (1)	0.82 (1)	295 (2)	[18], [37], [87], [102]
ZnSe	1.00 (3)	0.74 (1)	0.86 (3)	235 (4)	[40], [74], [101], [102], [109], [133]
ZnTe	1.31 (2)	0.77 (1)	0.95 (2)	193 (2)	[11], [18], [37], [102], [136]

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discrepancy being less than 5% for most of the compounds. The notable exceptions were GaAs, GaP, InP, LiF and TiC but in these cases there was a large spread among the individual temperature factors (47% for GaP).

From the considered data, the recommended values of the temperature factors B^+ and B^- for a given compound are obtained by the weighted average of the individual values given by the different authors, the weight w_i being $1/\sigma_i^2$, where σ_i is the error for an individual observation. In all cases for which the author did not give the error in the B value, the error assigned to this B is defined as $\sigma_i = B_i\rho$, where ρ is the maximum percentage error found in a given set of data and B_i is the temperature factor without the error. The recommended values of the average temperature factors $\bar{B}$ are obtained from the recommended values of B^+ and B^- using the relation

$$\bar{B} = (m^+B^+ + m^-B^-)/(m^+ + m^-), \tag{4}$$

where m^+ and m^- are the masses of the cation and anion, respectively. The recommended value of the corresponding Debye temperature was calculated using (3) with T the room temperature. The recommended values of the temperature factors B^+, B^- and $\bar{B}$ and the Debye temperature Θ for the 52 compounds are given in Table 1.

It is expected that the heavier of the two atoms in a compound should have a smaller B value. This is indeed the case for most of the compounds. However, for certain compounds (*e.g.* AgBr, CuCl, HgSe, InAs, TlCl, PbS, PbTe and ZnS) it is observed that the heavier atom has a larger B value than that of the lighter atom. This is not surprising because, in the harmonic approximation and for $T > \Theta$, the mean square displacements are independent of the atomic masses (Huiszoon & Groenewegen, 1972; Jex, Mullner & Dyck, 1974). In such cases, the mass dependence of the temperature factors may not be observed.

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X-ray Integrated Intensities from Semiconductor Substrates and Epitaxic Layers – a Comparison of Kinematical and Dynamical Theories with Experiment

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Abstract

X-ray integrated intensities have been collected from extended-face specimens as a function of azimuthal angle ψ (rotation angle about the scattering vector) with a four-circle diffractometer for a number of semiconductor substrate materials and epitaxic layers. The Bragg reflections (and X-ray wavelengths) have been chosen so that as wide a range of asymmetry as possible is encompassed. It is shown that the interpretation of these results, in terms of kinematical and perfect-crystal dynamical X-ray diffraction theories, provides a measure of the perfection of the crystal being investigated. The interpretation of some results requires consideration of extinction effects and their dependence on asymmetry. Such

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