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Compilation of temperature factors of hexagonal close packed elements

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Abstract

The Commission on Neutron Diffraction has initiated a project for compiling accurate temperature factors [International Union of Crystallography (1985). *Acta Cryst.* B**41**, 374]. Recommended values of the temperature factors of 14 hexagonal close packed (h.c.p.) elements are presented in this compilation.

1. Introduction

The Commission on Neutron Diffraction of the International Union of Crystallography initiated a project on the compilation of data on accurate temperature factors (International Union of Crystallography, 1985). Compilations of data on temperature factors of cubic elements and cubic compounds have been presented by Butt *et al.* (1988) and Butt *et al.* (1993), respectively. Data on temperature factors of 14 h.c.p. elements are presented in this compilation.

2. Results and discussion

Recommended values of the temperature factors and Debye temperatures are given in Table 1 along with the sources; sources of data not included in the table are also mentioned. Several authors have reported values of the mean square amplitudes of vibrations along the a and c directions ($\langle u_a^2\rangle$ and $\langle u_c^2\rangle$) rather than the Debye–Waller factors B_a and B_c. In such cases, B_a and B_c have been calculated from the relation

$$B_a = 8\pi^2\langle u_a^2\rangle, \quad B_c = 8\pi^2\langle u_c^2\rangle. \tag{1}$$

Where the mean Debye–Waller factor B is not given directly, it has been calculated from the relation

$$\overline{B} = \tfrac{1}{3}(2B_a + B_c). \tag{2}$$

Where the Debye temperature θ_M is not given in the original source, it has been calculated from the mean Debye–Waller factor $\overline{B}$ (and *vice versa*) from the relation

$$\overline{B} = (6h^2/mk)(T/\theta_M^2)[\varphi(x) + (x/4)], \tag{3}$$

the symbols having the usual meaning (James, 1967). Where more than a single report was available, the most recent/most accurate values are recommended. With the exception of (α)Ti and Ru, all recommended values are TDS corrected. In general, the temperature factor in the c direction is larger than that in the a direction. Watanabe *et al.* (1971) pointed out that the ratio ($\langle u_c^2\rangle/\langle u_a^2\rangle$) lies on a smooth curve when plotted against the axial ratio (c/a).

Table 1. *Recommended values of the temperature factors of h.c.p. elements at room temperature (295±3 K)*

Element	B_a (Å^2)	B_c (Å^2)	B (Å^2)	θ_M (K)	Source references†
Be	0.599 (9)	0.541 (8)	0.580 (9)	897 (8)	[*e*], [*t*]
Cd	1.15 (2)	3.04 (2)	1.78 (2)	131 (7)	[*d*], [*m*], [*q*], [*r*]
Dy	0.81 (8)	0.89 (7)	0.84 (8)	160 (8)	[*h*]
Er	0.57 (7)	0.73 (7)	0.62 (7)	182 (10)	[*g*]
Gd	0.80 (1)	0.88 (2)	0.83 (1)	165 (1)	[*h*]
Ho	0.96 (16)	0.97 (4)	0.96 (12)	147 (9)	[*n*]
Lu	0.86 (6)	0.97 (6)	0.90 (6)	148 (5)	[*h*]
Mg	1.34	1.58	1.42	321	[*a*], [*c*], [*f*], [*r*]
Ru			0.29	350	[*a*]
Sc	0.72 (1)	0.73 (1)	0.72 (1)	330 (2)	[*i*]
Tb	0.67 (4)	0.71 (4)	0.68 (4)	178 (7)	[*i*]
(α)Ti			1.00 (21)	270 (30)	[*p*]
Y	0.83 (2)	0.80 (3)	0.82 (2)	219 (3)	[*h*]
Zn	0.82 (5)	2.04 (6)	1.23 (5)	208 (4)	[*b*], [*j*], [*k*], [*l*], [*o*], [*s*]

† The source reference for recommended values is indicated by an underline. Source references: [*a*] Brill & Chopra (1962); [*b*] Brindley (1936); [*c*] Brindley & Ridley (1938); [*d*] Brindley & Ridley (1939); [*e*] Brown (1972); [*f*] Germanov & Shivrin (1970); [*g*] Gopikrishna (1985); [*h*] Gopikrishna *et al.* (1986); [*i*] Gopikrishna *et al.* (1988); [*j*] Jauncey & Bruce (1937); [*k*] Merisalo & Larsen (1977); [*l*] Rossmanith (1977); [*m*] Rossmanith (1978); [*n*] Skelton (1969); [*o*] Skelton & Katz (1968); [*p*] Spreadborough & Christian (1959); [*q*] Walford *et al.* (1968); [*r*] Watanabe *et al.* (1971); [*s*] Wollan & Harvey (1937); [*t*] Yang & Coppens (1978).

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