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X-ray determination of Debye–Waller factors and Debye temperatures of h.c.p. elements Ti, Zr, Ru, Tm, Hf

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Debye–Waller factors of five h.c.p. elements (Ti, Zr, Ru, Tm, Hf) have been determined from X-ray diffraction intensities. Within the limits of experimental errors, the Debye–Waller factors associated with the two principal directions are equal. The Debye temperatures (θ_M) have been evaluated. The energy of formation of vacancies (E_f) has been estimated from a semi-empirical relation between E_f and θ.

1. Introduction

Gopi Krishna & Sirdeshmukh (1998) recently published a compilation of the Debye–Waller factors and Debye temperatures of h.c.p. elements. From this compilation, it is observed that:

(i) The Debye–Waller factors B_c and B_a associated with the c and a directions are significantly different only in h.c.p. elements having a c/a ratio significantly different from the ideal value of 1.63.

(ii) There are no X-ray data on the Debye–Waller factors and Debye temperatures (θ_M) of Zr, Tm and Hf.

(iii) While the Debye temperatures of Ti and Ru have been determined from the temperature variation of X-ray diffraction intensities, there is no explicit attempt to determine the Debye–Waller factors.

The purpose of this communication is to report the results of an X-ray investigation to determine the Debye–Waller factors and Debye temperatures of Ti, Zr, Ru, Tm and Hf.

2. Experimental

3*N* purity powders of grain size < 350 μm were used. Ru and Tm were supplied by Strem Chem, USA, and Ti, Zr and Hf were obtained from the Nuclear Fuel Complex, Hyderabad, India.

Integrated intensities were recorded using a JEOL JDX-8P powder X-ray diffractometer fitted with an NaI (Tl) scintillation counter; filtered Cu radiation was employed. The number of reflections recorded ranged from 12 to 16. The procedure for sample preparation, instrumental conditions for recording intensities and the details of the various corrections applied are given in earlier papers (Gopi Krishna *et al.*, 1986; Geeta Krishna *et al.*, 1998).

The procedure for the determination of Debye–Waller factors and θ_M from the intensity data and the estimation of associated errors is as discussed by Gopi Krishna *et al.* (1986).

3. Results and discussion

The values of the directional Debye–Waller factor (B_c, B_a) and the mean Debye–Waller factor ($\overline{B}$) for the five h.c.p. elements studied in this work are given in Table 1. It can be seen from the values that for these elements $B_c \approx B_a$ within limits of the errors. The c/a values are also given in Table 1; they are also close to 1.63. The near-equality of B_c and B_a and the closeness of the c/a ratio to 1.63 are in comformity with the observation referred to in §1 that the two Debye–Waller factors in h.c.p. elements differ significantly only in those cases where the c/a ratio differs significantly from 1.63.

Table 1
Debye–Waller factors and Debye temperatures of some h.c.p. elements.

Parameter Reference†	c/a [*a*]	B_c (Å^2) [*b*]	B_a (Å^2) [*b*]	$\overline{B}$ (Å^2) [*b*]	θ_M (K) [*b*]	θ_D (K) [*c*]	E_f (eV) [*b*]
α-Ti	1.59	0.48 (6)	0.54 (1)	0.52 (3)	391 (22)	420	1.28
Zr	1.59	0.51 (4)	0.52 (1)	0.52 (2)	267 (20)	291	1.37
Ru	1.58	0.15 (1)	0.14 (2)	0.14 (2)	495 (24)	494	3.64
Tm	1.58	0.84 (1)	0.82 (1)	0.83 (1)	155 (10)	167	1.01
Hf	1.58	0.41 (1)	0.41 (2)	0.41 (2)	217 (20)	248	1.72

† Source references: [*a*] Wyckoff (1960); [*b*] present work; [*c*] Gschneidner (1964) for Tm and Singh & Varshni (1982) for the rest.

The values of θ_M are given in Table 1. The values of 391 (22) K and 495 (24) K obtained in this work for the Debye temperatures of Ti and Ru are higher than the values of 270 (30) K and 350 K reported by Spreadborough & Christian (1959) and Brill & Chopra (1962), respectively, from the temperature variation of X-ray intensities. Values of the Debye temperature (θ_D) obtained from specific heat data are also quoted in Table 1. The θ_M values agree fairly well with the θ_D values although it may be mentioned that exact agreement is not expected.

Glyde (1967) and Tewary (1971) have semi-empirically derived the following relation between the X-ray Debye temperature (θ_M) and energy of formation (E_f) of vacancies:

$$E_f = A(k_B/h)^2 M\theta_M^2 a^2,$$

where A is a constant, a is the interatomic distance and the other quantities have already been defined. Glyde (1967) showed that for h.c.p. elements the value of A is 1.17×10^{-2}. Using the values of θ_M obtained in this work, values of E_f have been estimated; these are included in Table 1. Gopi Krishna *et al.* (1986) obtained values in the range 1–1.5 eV for several h.c.p. metals. The E_f values for the metals studied here are of this order with the exception of Ru, which has a much larger E_f value.

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