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Dirhodium Triyttrium Disilicide, $Y_3Rh_2Si_2$

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Abstract. $M_r = 528{\cdot}7$, *Pbcm*, $a = 5{\cdot}5661\ (5)$, $b = 7{\cdot}7171\ (5)$, $c = 13{\cdot}043\ (1)$ Å, $V = 560{\cdot}26$ Å^3, $Z = 4$, $D_x = 6{\cdot}26$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 376{\cdot}1$ cm^{-1}, $F(000) = 940$, room temperature, final $R = 0{\cdot}045$ for 678 unique reflections. The structure is made of Y and Si trigonal prisms centred by Si and Rh atoms and can be derived from a hexagonal close-packed model using the concept of unit-cell twinning. The stacking of these units is the same as in binary alloys with Fe_3C- or Mn_5C_2-type structures.

Introduction. Structures of R_3M binary alloys of Fe_3C, Mn_5C_2 and CrB type have been studied (*e.g.* Moreau, Le Roy & Paccard, 1982). These structures can be derived from a hexagonal close-packed model through twinning of unit cells (Andersson & Hyde, 1974). Here, the study is extended to the three-component alloy $Rh_2Y_3Si_2$.

Experimental. Alloys made from commercially available elements of high purity (Y:99·9%, Rh:99·99%, Si:99·999%). Samples prepared by conventional arc-melting techniques. Small crystals of $Y_3Rh_2Si_2$ suitable for X-ray analysis isolated by mechanical fragmentation from crushed melt. Weissenberg photographs showed crystals to have space group *Pbcm* or $Pbc2_1$. Single crystal $40 \times 60 \times 80$ μm, intensities measured with graphite-monochromated Mo $K\alpha$ radiation, CAD-4 Enraf–Nonius diffractometer, $\theta/2\theta$ scan mode; accurate cell dimensions by least-squares analysis of 25 θ values; three standard reflections monitored at intervals of 3600s, intensity variation during data collection <1%. Intensities of 1275 independent reflections, to limit of $\theta = 35°$, measured and corrected for background, Lorentz and polarization factors with *START* (Frenz, 1983). $0 \le h \le 8$, $0 \le k \le 12$, $0 \le l \le 20$. Structure solved by direct methods with *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Positions of Y, Rh and Si atoms revealed in corresponding E map for space group *Pbcm*. Full-matrix least-squares refinement of 36 positional and anisotropic thermal parameters converged after a few cycles using F values of 678 reflections* with $I > 3\sigma(I)$. $R = R_w = 0{\cdot}045$, Dunitz & Seiler (1973) weighting scheme where $w = \exp(36\sin\theta/\lambda)$ for each reflection. Zero Δ/σ in final least-squares cycle; peak height in final difference map $< |5{\cdot}0|$ e Å^{-3}. All calculations performed on PDP 11/23 computer using *SDP* (Frenz, 1983). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Atomic positions and equivalent isotropic temperature factors are listed in Table 1, interatomic distances are in Table 2.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39420 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atomic positions for* $Y_3Rh_2Si_2$ *with e.s.d.'s in parentheses*

B_{eq} is defined as $\frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B(Å^2)
Y(1)	0·1377 (2)	0·6057 (1)	0·10313 (6)	0·785 (8)
Y(2)	0·3713 (3)	0·2472 (2)	¼	0·76 (1)
Rh	0·6361 (1)	0·46771 (9)	0·09020 (5)	0·756 (5)
Si(1)	0·8584 (8)	0·3976 (6)	¼	0·77 (4)
Si(2)	0·3836 (7)	¼	0	0·75 (4)

Table 2. *Interatomic distances in* $Y_3Rh_2Si_2$ *up to* 4·0 Å

All e.s.d.'s are less than 0·001 Å.

Y(1)–Rh	2·875	Y(2)–Si(1)	2·949
–Si(1)	2·944	–Si(1)	2·985
–Si(1)	2·957	–2Rh	3·000
–Rh	2·875	–2Rh	3·068
–Rh	2·993	–Si(1)	3·082
–Rh	3·069	–2Si(2)	3·262
–Si(2)	3·186	–2Y(1)	3·512
–2Si(2)	3·386	–2Y(1)	3·590
–Y(1)	3·492	–2Y(1)	3·607
–Y(1)	3·500		
–Y(2)	3·512	Rh–Si(2)	2·478
–Y(2)	3·590	–Si(1)	2·483
–Y(2)	3·607	–Si(2)	2·486
–Y(1)	3·831	–Rh	2·842
		–Y(1)	2·875
Si(1)–2Rh	2·483	–Y(1)	2·976
–2Y(1)	2·944	–Y(1)	2·993
–Y(2)	2·949	–Y(2)	3·000
–2Y(1)	2·957	–Y(2)	3·068
–Y(2)	2·985	–Y(1)	3·069
–Y(2)	3·082		
		Si(2)–2Rh	2·478
		–2Rh	2·486
		–2Y(1)	3·186
		–2Y(2)	3·262
		–2Y(1)	3·349
		–2Y(1)	3·386

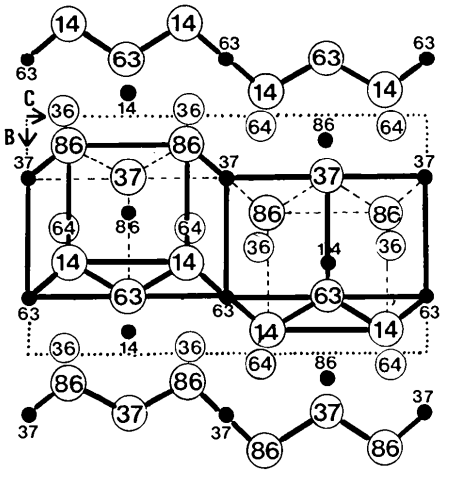

Fig. 1. Projection along the a axis for $Y_3Rh_2Si_2$. Numbers correspond to x parameters multiplied by 100. Drawing of trigonal prisms becomes significant if 100 is added to inscribed values of 100 x for upper atoms and if 100 is subtracted for lower atoms. Large circles are Y atoms, small circles Rh atoms and filled circles Si atoms.

Discussion. The structure of $Y_3Rh_2Si_2$ is shown in Fig. 1 in projection along the a axis. All Y atoms participate in the formation of trigonal prisms centred by Si atoms. On each side of the central Y prism, there is a prism made of one common face of four Y atoms and one edge of two Si atoms. These two adjacent prisms are centred by one Rh atom. The $Y_3Rh_2Si_2$ structure involves units of three adjacent trigonal prisms centred by Si and Rh atoms. The linkage of these units along the b direction and the stacking along the a direction are identical to those found in binary alloys crystallizing with the Fe_3C or Mn_5C_2 type structures (Parthé & Moreau, 1977). Also indicated on Fig. 1 are zig-zag chains of atoms along the c axis. It has been shown that these chains can be geometrically derived from a hexagonal close-packed structure (Andersson & Hyde, 1974). Twinning along particular planes leads to the formation of trigonal prismatic holes on the twin planes. Structures of YPd_2Si (Moreau, Le Roy & Paccard, 1982) of Fe_3C type and R_5Ir_2 (R = rare earth) of Mn_5C_2 (Le Roy, Paccard & Moreau, 1980) and CrB type (Parthé, 1976) have been interpreted using this concept of unit-cell twinning. In $Y_3Rh_2Si_2$ the hexagonal close-packed structure is made of Y and Si atoms and the prismatic holes are occupied by Rh and Si atoms. In YPd_2Si the hexagonal close-packed structure was made of Y and Pd atoms and the prismatic holes were occupied by Si atoms only. The radii of metallic atoms given by Teatum, Gschneider & Waber (1960) are 1·319 for Si, 1·345 for Rh and 1·376 Å for Pd, so that it is not surprising to find both Rh and Si atoms either in prismatic holes or in the chains.

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