The Crystal Structure of Pd_2Al

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In the course of phase analysis and crystal structure studies on the palladium-aluminium system a phase with the composition Pd_2Al has been studied.

The alloy was prepared by arc-melting palladium and aluminium in a ratio 2:1 in an argon atmosphere. Crystals of Pd_2Al were obtained from the crushed melt. The single crystal and Guinier powder photographs showed the structure to be orthorhombic with the following unit cell dimensions:

$a = 5.40_7$Å, $b = 4.06_1$Å, $c = 7.76_9$Å.

The single crystal data were registered in a Weissenberg camera using CuK radiation. The crystal (less than 0.02 mm in all dimensions) was rotated around the b-axis. The multiple film technique was used and the intensities were estimated visually. The symmetry, the unit cell dimensions and the appearance of the Patterson projection along [010] suggested that the phase is of the C 23 type. The signs of most the structure factors were calculated starting from approximate values of the x and z parameters taken from isostructural Rh_2Ge [1]. The parameters were then refined from successive $\varrho_o(xz)$ and $\varrho_c(xz)$ syntheses. No serious influence from absorption could be detected and $\log I_o/I_c$ decreased linearly with $\sin^2\Theta/\lambda^2$. The temperature factor B was found to be 1.50 Å^2. The final R-value was 7.1 % for the $h0l$ reflexions.

The following structure was thus derived:

Unit cell content: 4 Pd_2Al
Space-group: *Pnma*, No. 62
Pd_1 in 4(c): $x = 0.833$, $y = \frac{1}{4}$, $z = 0.065$.
Pd_2 in 4(c): $x = 0.957$, $y = \frac{1}{4}$, $z = 0.713$.
Al in 4(c): $x = 0.303$, $y = \frac{1}{4}$, $z = 0.101$.

Table 1. Interatomic distances in Pd_2Al.

Atom	Neighbour	C.N.	Distance in Å
Pd_1	Pd_1	2	2.90
	Pd_2	1	2.82
		2	2.90
		2	2.81
		1	2.97
	Al	1	2.88
		1	2.56
		2	2.52
		1	2.60
Pd_2	Pd_1	1	2.82
		2	2.90
		2	2.81
		1	2.97
	Pd_2	2	2.76
	Al	2	2.86
		2	2.56
		1	2.58
Al	Pd_1	1	2.88
		1	2.56
		2	2.52
		1	2.60
	Pd_2	2	2.86
		2	2.56
		1	2.58

The interatomic distances are given in Table 1.

Further studies on phases of this system are in progress and good single crystals have been found in arc-melted samples of the compositions PdAl and $PdAl_4$.

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