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Crystal structure of erbium palladium phosphor (3:20:6), $Er_3Pd_{20}P_6$

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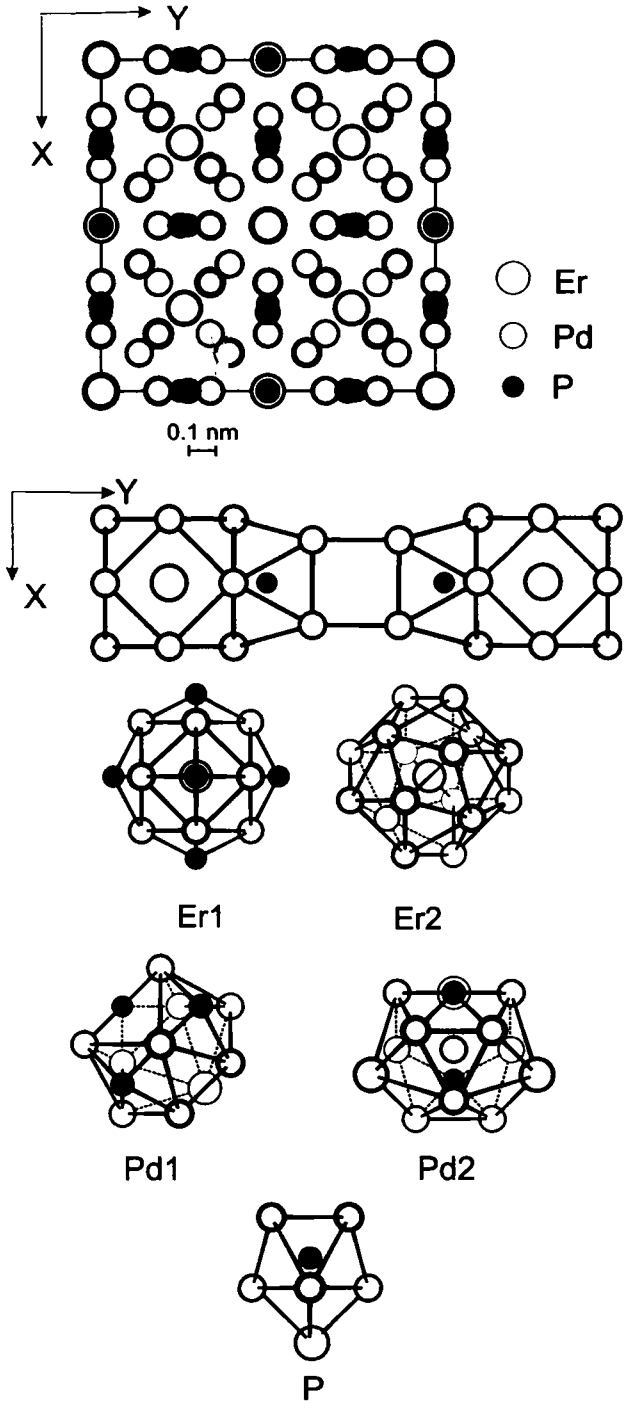

Abstract

$Er_3P_{20}Pd_6$, cubic, $Fm\bar{3}m$ (no. 225), a = 12.111(1) Å, V = 1776.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.030, $wR_{ref}(F)$ = 0.032, T = 293 K.

Source of material

Erbium, red phosphorus, and palladium were of 99.99 wt.-% purity. A mixture of the starting components with nominal composition $Er_3Pd_{20}P_6$ was pressed into a small pellet (1 g) and melted in an arc furnace under a Ti/Zr-gettered argon atmosphere at normal pressure. The alloy was heat-treated at 1070 K for 20 d in evacuated fused silica ampules, followed by quenching in cold water. After the sample was crushed, bar-like air-stable single crystals with metallic luster were extracted and were for the structure determination. Energy-dispersive analysis of several crystals in a scanning electron microscope confirmed the presence of erbium, palladium, and phosphorus as the only components in atomic percentages of Er:Pd:P = 11:68:21 (with estimated standard deviations of 2 %).

Discussion

$Er_3Pd_{20}P_6$ adopts the $Cr_{23}C_6$-type structure (Pearson symbol cF116) [1], which is built up of fragments of columns of cuboctahedra (figure, top), two tetragonal antiprisms, and cubes (figure, middle). The Er atoms substitute for the transition metals in sites 4*a* and 8*c*. The P atoms have tetragonal antiprismatic coordination (figure, bottom). The shortest interatomic distance found (d(Pd1—P) = 235.6(2) pm) is by < 5 % smaller than the sum of atomic radii. Because of the low rare-earth content, the Er atoms remain isolated, and interatomic distances to them are larger than the sum of atomic radii. The greatest contraction (9.4 %) occurs for the Er2—Pd2 distance of 281.95(5) pm, indicating that the bonding between Er and Pd atoms is probably stronger than that between Pd and P, or Er and P. $Er_3Pd_{20}P_6$ is paramagnetic and its susceptibility follows the Curie-Weiss law.

Table 1. Data collection and handling.

Crystal:	black, bar-like, size 0.05 × 0.05 × 0.15 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	342.2 cm^{-1}
Diffractometer, scan mode:	Nonius KappaCCD, ω
$2\theta_{max}$:	79.5°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	327, 327
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 302
$N(param)_{refined}$:	14
Programs:	WinCSD [2], ORTEP-3 [3]

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Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Er(1)	4*a*	0	0	0	0.0074(2)	U_{11}	U_{11}	0	0	0
Er(2)	8*c*	¼	¼	¼	0.0094(2)	U_{11}	U_{11}	0	0	0
Pd(1)	48*h*	0.17278(4)	0	x	0.00676(1)	0.0175(3)	U_{11}	0	−0.0001(2)	0
Pd(2)	32*f*	0.11559(4)	x	x	0.00759(1)	U_{11}	U_{11}	−0.00073(1)	U_{12}	U_{12}
P(1)	24*e*	0.2379(3)	0	½	0.009(1)	0.0065(7)	U_{22}	0	0	0

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