Experimental

Crystal data

$KY_{0.95}Er_{0.05}F_4$
M_r = 209.4
Trigonal
$P3_1$
a = 14.075 (2) Å
b = 14.075 (2) Å
c = 10.115 (2) Å
V = 1735.2 Å^3
Z = 18
D_x = 3.607 Mg m^{-3}
Ag $K\alpha$ radiation
λ = 0.5608 Å
Cell parameters from 25 reflections
θ = 10–17°
μ = 8.953 mm^{-1}
T = 293 K
Sphere
0.14 mm (radius)
Pink

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: spherical
T_{min} = 0.165, T_{max} = 0.190
21625 measured reflections
6834 independent reflections
4503 observed reflections [$I \geq 3\sigma^2(I)$]
R_{int} = 0.04
θ_{max} = 30°
$h = -25 \rightarrow 25$
$k = -25 \rightarrow 25$
$l = -18 \rightarrow 18$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F
Final R = 0.032
wR = 0.035
S = 3.494
2667 reflections
325 parameters
w = 1
$(\Delta/\sigma)_{max}$ = 0.10
$\Delta\rho_{max}$ = 1.613 e Å^{-3}
$\Delta\rho_{min}$ = −1.487 e Å^{-3}
Extinction correction: Stout & Jensen (1968)
Extinction coefficient: 2.56882×10^{-7}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Lists of structure factors, anisotropic thermal parameters and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55258 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU1003]

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Structure of $LaPd_2In$

B. Xue, H. Schwer and F. Hulliger

Laboratorium für Festkörperphysik, ETH Hönggerberg, CH-8093 Zürich, Switzerland

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Abstract

Lanthanum dipalladium indide, $LaPd_2In$, was found to crystallize with a hexgonal $GdPt_2Sn$-type structure, an ordered version of the TiAs structure. Pd—In bond lengths are similar to those reported for Pt—In in isotypic YPt_2In [Dwight (1987). *Mater. Res. Bull.* **22**, 201–204]; although La is larger than Y, the La—Pd and Pd—Pd distances are slightly shorter than the corresponding Pt—Y and Pt—Pt bond lengths.

Comment

The structure determination of $LaPd_2In$ was carried out as part of an investigation of LnT_2X compounds (Ln = rare earth, T = transition element, X = B element).

The sample was synthesized by arc melting the constituent elements under purified argon in a water-cooled copper hearth. Traces of a second phase were detectable on the Cu $K\alpha$ Guinier powder photograph. All crystals found in the crushed ingot were intergrown or twinned. The diffraction data were taken using the best crystal which showed only slight twinning. The result is summarized in Table 1 and visualized in Fig. 1. The relevant interatomic distances are listed in Table 2.

The strongest bonds are found between the In and Pd atoms. The shortest bond length (In—Pd) is 2.777 Å, equivalent to an 8.3% contraction with respect to the element radii (Dwight, 1987). The bond lengths and angles are comparable with those of YPt_2In [shortest bond length

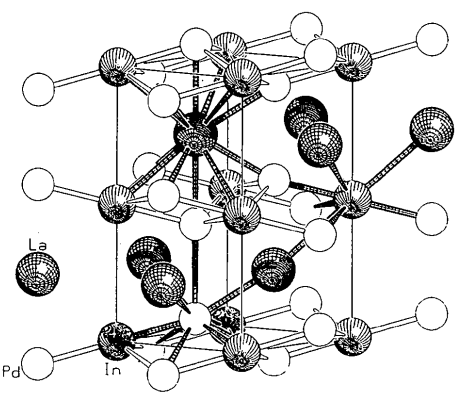

Fig. 1. *SCHAKAL88* plot of the unit cell of $LaPd_2In$. The coordinations of the La, In and Pd atoms are emphasized by thick bondsticks.

(Pt—In) 2.746 Å, corresponding to a largest contraction of 10%]. With 5*d* La and 4*d* Pd replacing 4*d* Y and 5*d* Pt respectively, the size of the unit cell increases slightly. Similar La—La, In—In and La—In distances are found in related La—In compounds such as La_2In (Palenzona, 1968) and La_3In (McMasters & Gschneidner, 1974).

A disordered distribution was considered because of the nearly equal scattering powers of In and Pd, but the corresponding refinement yielded larger *R* values. Equal distances between the 2(*a*) (In) and 4(*f*) (Pd) sites would be expected within a disordered Pd—In layer; this is contrary to the observed bond lengths.

Experimental

Crystal data

$LaPd_2In$
M_r = 466.53
Hexagonal
$P6_3/mmc$
a = 4.6445 (7) Å
c = 9.354 (2) Å
V = 174.75 (5) Å^3
Z = 2
D_x = 8.866 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 20 reflections
θ = 8.30–30.85°
μ = 28.327 mm^{-1}
T = 295 K
Lath
0.19 × 0.09 × 0.04 mm
Pink
Arc melting

Data collection

Siemens *P3/PC* diffractometer
$\theta/2\theta$ scans
Absorption correction: Gaussian (*SHELX*76; Sheldrick, 1976)
T_{min} = 0.3837, T_{max} = 0.0925
2503 measured reflections
2506 independent reflections
1909 observed reflections [$I>2\sigma(I)$]
R_{int} = 0.0622
θ_{max} = 32.54°
$h = -7 \rightarrow 7$
$k = -7 \rightarrow 7$
$l = -14 \rightarrow 14$
2 standard reflections monitored every 48 reflections
intensity variation: 1.4%

Refinement

Refinement on F^2
Final R = 0.0369
wR = 0.0974
S = 1.572
148 reflections
9 parameters
Calculated weights $w = 1/[\sigma^2(F_o^2)+(0.0306P)^2+6.3988P]$, $P = (F_o^2+2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.000
$\Delta\rho_{max}$ = 1.551 e Å^{-3}
$\Delta\rho_{min}$ = −2.266 e Å^{-3}
Extinction correction: *SHELXL*92 (Sheldrick, 1992)
Extinction coefficient: 0.0302 (38)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Data collection: *P3/PC* diffractometer software (Siemens, 1989). Cell refinement: *P3/PC* diffractometer software. Data reduction: *XDISK* (Siemens, 1991). Program(s) used to solve structure: *SHELXL*92. Program(s) used to refine structure: *SHELXL*92. Molecular graphics: *SCHAKAL*88 (Keller, 1988). Software used to prepare material for publication: *SHELXL*92.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

		x	y	z	U_{eq}
Pd	4(*f*)	$\frac{1}{3}$	$\frac{2}{3}$	0.5773 (2)	0.0118 (5)
La	2(*c*)	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.0102 (6)
In	2(*a*)	0	0	0	0.0126 (6)

Table 2. *Interatomic distances* (Å)

La—2Pd	3.062 (2)	Pd—3In	2.777 (1)
6Pd	3.130 (2)	3Pd	3.047 (1)
6In	3.558 (1)	1La	3.062 (2)
In—6Pd	2.777 (1)	3La	3.130 (1)
6La	3.558 (1)	1Pd	3.231 (1)

Refinement was by full-matrix least-squares methods on F^2 (for all reflections except those flagged for possible systematic errors) using *SHELXL*92. As this program performs a refinement on F^2 rather than F, it yields larger R values. A parallel refinement on F using *SHELX*76 and taking atomic scattering factors from Cromer & Mann (1968) gave similar positional parameters but better R values (R = 0.0355, wR = 0.0269). The observation threshold $I>2\sigma(I)$ was used only to calculate values for R(obs.) *etc.* which are given here for comparison with refinements on F.

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