Crystal structure of ytterbium copper stannide, $Yb_4Cu_2Sn_5$

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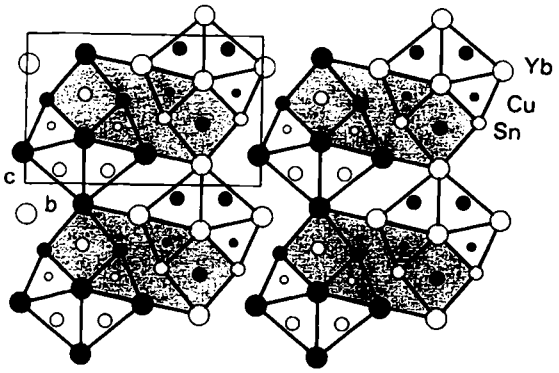

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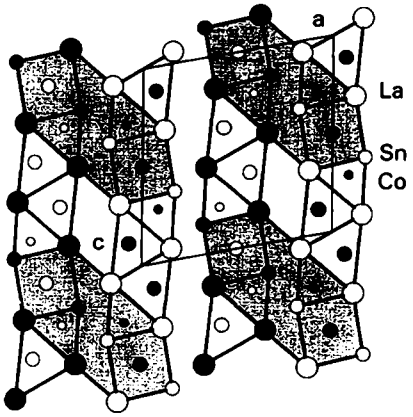

$La_4Co_2Sn_5$

Abstract

$Cu_2Sn_5Yb_4$, orthorhombic, *Pmmn* (No. 59), $a = 4.413(1)$ Å, $b = 13.887(2)$ Å, $c = 8.830(1)$ Å, $V = 541.1$ Å^3, $Z = 2$, $R_{gt}(F) = 0.032$, $wR_{all}(F^2) = 0.065$, $T = 293$ K.

Source of material

The title compound has been synthesized by induction melting of stoichiometric amounts of the elements in small tantalum crucibles sealed by arc welding under argon. The metals used had a nominal purity of 99.9 mass % for ytterbium and 99.999 mass % for tin and copper. The sample was annealed in the same induction furnace at 923 K for 45 minutes and then slowly cooled. Metallographic analysis (optical and electronic) and electron-probe microanalysis were carried out on the sample.

Experimental details

The atomic coordinates have been standardized using the program STRUCTURE TIDY [1].

Discussion

$Yb_4Cu_2Sn_5$ (Pearson code *oP*22), crystallizing in a new structure type, corresponds to the τ_{10} phase, identified during the study of the isothermal section at 673 K of the Yb-Cu-Sn system [2]. In the figure it is compared with the monoclinic $La_4Co_2Sn_5$ structure (*I*2/*m*, $a = 11.074$ Å, $b = 4.607$ Å, $c = 11.373$ Å, $\beta = 100.87°$) [3]. They both are built up by two layers (open and full circles) alternating along the short axis, *a* for the Yb compound and *b* for the La compound. The stippled motif is identical. The remaining part is formed by the same three trigonal prisms, two of them around Sn and one around a Cu (or Co) atom, but differently oriented in the two structures. This particular relationship causes all coordination polyhedra of the non-rare-earth atoms be equal, namely Cu(Yb) = Co(La); Sn(1)(Yb) = Sn(1)(La); Sn(2)(Yb) = Sn(3)(La); Sn(3)(Yb) = Sn(2)(La). In this last polyhedron some vertices are occupied by the same atoms, but in a different sequence. The shortest distances in $Yb_4Cu_2Sn_5$ are Cu—Sn(1) 2.634(2) Å, Sn(1)—Sn(1) 2.877(2) Å, Yb(3)—Cu 3.044(1) Å and Yb(3)—Sn(2) 3.188(1) Å. The topology of the copper-centered trigonal prisms is similar to that found around part of the palladium atoms in the YPdSi structure, having the same space group [4].

Table 1. Data collection and handling.

Crystal:	metallic grey, prism, size 0.04 × 0.08 × 0.11 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	492.71 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω/θ
$2\theta_{max}$:	59.86°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1824, 914
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 738
$N(param)_{refined}$:	38
Programs:	STRUCTURE TIDY [1], SIR92 [5], SHELXL-97 [6],

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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}
Yb(1)	4*e*	1/4	0.01007(4)	0.79630(7)	0.0139(3)	0.0130(3)	0.0090(3)	0	0	-0.0025(2)
Yb(2)	2*b*	1/4	3/4	0.1356(1)	0.0132(4)	0.0184(4)	0.0077(4)	0	0	0
Yb(3)	2*b*	1/4	3/4	0.6990(1)	0.0108(4)	0.0091(3)	0.0064(4)	0	0	0
Cu	4*e*	1/4	0.1078(1)	0.3810(2)	0.0140(8)	0.0165(8)	0.0073(7)	0	0	0.0020(7)
Sn(1)	4*e*	1/4	0.14642(7)	0.0890(1)	0.0147(5)	0.0102(4)	0.0052(4)	0	0	-0.0002(3)
Sn(2)	4*e*	1/4	0.58695(7)	0.4447(1)	0.0115(4)	0.0127(4)	0.0064(4)	0	0	-0.0019(4)
Sn(3)	2*a*	1/4	1/4	0.5933(2)	0.0129(7)	0.0135(6)	0.0065(6)	0	0	0

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