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Crystal structure of neodymium palladium antimonide, $NdPd_{0.85}Sb_2$

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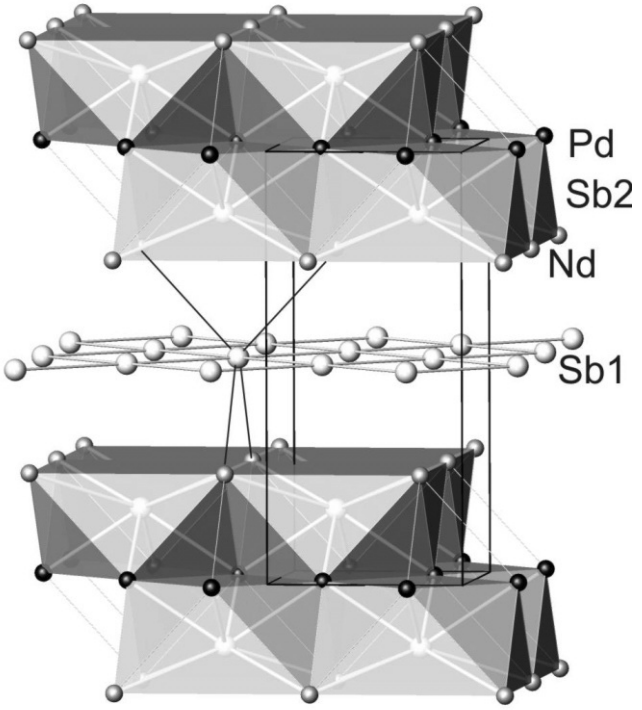

Abstract

$NdPd_{0.85}Sb_2$, tetragonal, *P*4/*nmm* (no. 129), $a = 4.4098(3)$ Å, $c = 9.6907(9)$ Å, $V = 188.4$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0369$, $wR_{ref}(F) = 0.0383$, $T = 295$ K.

Table 1. Data collection and handling.

Crystal:	metallic, prism-like, size 0.0223×0.0259×0.0712 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	311.6 cm^{-1}
Diffractometer, scan mode:	Mercury70 CCD, 2×2 bin
$2\theta_{max}$:	144.4°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	821, 821
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 4\ \sigma(I_{obs})$, 204
$N(param)_{refined}$:	7
Programs:	WINCSD [5]

Source of material

A polycrystalline sample with the nominal composition $NdPdSb_2$ was prepared from Nd (99,99 %), Pd (99,99 %) and Sb (99,99 %) ingots. The components were mixed in a ratio of Nd:Pd:Sb = 1:1:2 with an excess of 2 at.% of Sb, because of the relatively high vapor pressure of Sb and pressed into a pellet. Then the sample was repeatedly melted in an arc-furnace under purified argon atmosphere to achieve homogeneity. Afterwards it was heated in a fused quarz glass tube under vacuum at 600 ºC for 750 h, quenched with cold water. The air-stable sample was crushed and single crystals with a prismatic form and a metallic luster were selected for a single crystal structure determination.

Experimental details

The composition of the sample was checked using energy-dispersive *X*-ray spectroscopy (TESCAN 5130MM scanning electron microscope with Oxford Si-detector) and resulted in a ratio of Nd:Pd:Sb = 25.4:21.5:53.1 (standard deviation estimated to be about 1.5 at.%). No impurities were detected.

Discussion

The structure of the ternary antimonide $NdPd_{0.85}Sb_2$ [1, 2] belongs to the $HfCuSi_2$ type structure which is closely related to the structure type of $BaAl_4$ [3]. In the structure of $NdPd_{0.85}Sb_2$ the two crystallographically different Sb atoms and the Nd atoms fully occupy the positions 2*a* and 2*c*, respectively, whereas the position 2*b* is only 85 % occupied by Pd atoms. The structure of $NdPd_{0.85}Sb_2$ can be described in terms of double layers of corner sharing $[Sb(2)Pd_{4/4}Nd_{4/4}]$ square antiprisms separated by flat nets of Sb1 atoms. Within these nets the Sb1 atoms are square planar coordinated by 4 Sb1 with distances of 311 pm indicating Sb–Sb bonding interactions. In contrast the Sb2 atoms exhibit Sb–Sb distances larger than 400 pm and can therefore be considered as discrete. The Pd–Sb and Nd–Sb distances in the structure of $NdPd_{0.85}Sb_2$ are in good agreement with the sum of the adjacent atomic radii (r_{Nd} = 0,1814 nm, r_{Pd} = 0,1376 nm, r_{Sb} = 0,141 nm [4]).

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

Atom	Site	Occ.	*x*	*y*	*z*	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Nd	2*c*		¼	¼	0.7544(3)	0.65(5)	0.65(5)	0.68(8)	0	0	0
Pd	2*a*	0.85(1)	¾	¼	0	0.64(9)	0.64(9)	0.84(11)	0	0	0
Sb1	2*b*		¾	¼	½	0.50(7)	0.50(7)	1.13(9)	0	0	0
Sb2	2*c*		¼	¼	0.1507(4)	0.96(7)	0.96(7)	1.40(11)	0	0	0

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