Refinement of the crystal structure of neodymium palladium phosphide, NdPdP

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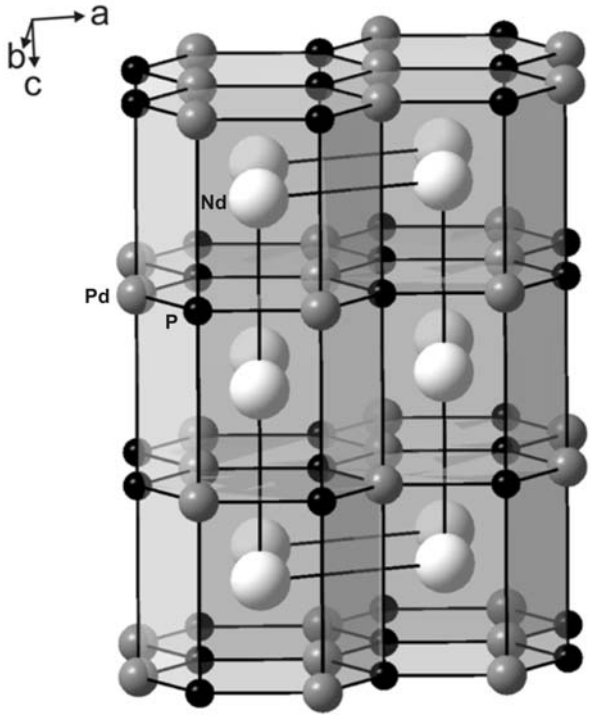

Abstract

NdPPd, hexagonal, $P6_3/mmc$ (no. 194), $a = 4.206(1)$ Å, $c = 7.653(2)$ Å, $V = 117.2$ Å^3, $Z = 2$, $R_{gt}(F) = 0.033$, $wR_{ref}(F^2) = 0.081$, $T = 293$ K.

Source of material

Polycrystalline samples of composition NdPdP were prepared from the elements: red phosphorus as powder, neodymium and palladium as ingots, all supplied with minimum purity of 99.9 %. Powder and freshly filed chips of the constituents in the nominal ratio of Nd : Pd : P = 1 : 1 : 1 were mixed and pressed into pellets. A small excess of phosphorus (2 at.%) was added to compensate for possible evaporation losses during the arc melting process. Prior to arc-melting, the pellets (about 1 g each) were pre-reacted in evacuated silica tubes by gradual heating them to 1070 K, holding at this temperature for 3 days and then slowly cooling to room temperature. Then the buttons were arc melted, again heated just above the melting point in a high-frequency furnace (TIG-10/300, Hüttinger) under purified argon atmosphere for 1 hour at 1640 K and slowly cooled down to room temperature. After the sample was crushed, air-stable single crystals with prismatic shape and metallic luster were separated from the crushed sample and used for structure determination. The composition of samples was checked using energy-dispersive X-ray spectroscopy (TESCAN 5130MM scanning electron microscope with Oxford Si-detector). The presence of only neodymium, palladium and phosphorus in an atomic ratio of Nd : Pd : P = 32.3 : 34.6 : 33.1 was revealed (standard deviation estimated to be about 1.5 at.%).

Discussion

The ternary phosphide NdPdP [1] belongs to the ZrBeSi type structure, the ternary ordered variant of the binary AlB_2 type [2]. The coloring of the hexagonal net by Be and Si atoms and the alternating stacking of such nets changes the space group from $P6/mmm$ to $P6_3/mmc$. Phosphorus and palladium atoms center the trigonal prisms formed by neodymium atoms. The nearest neighbours of Nd atoms are six Pd and six P atoms which form the hexagonal prism $[Pd_6P_6]$. The interatomic distances in the NdPdP structure are in the good agreement with the sum of atomic radii of the components.

Table 1. Data collection and handling.

Crystal:	metallic prism, size 0.006 × 0.048 × 0.061 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	157.72 cm^{-1}
Diffractometer, scan mode:	STOE IPDS 1, φ
$2\theta_{max}$:	56.14°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2128, 139
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 119
$N(param)_{refined}$:	8
Programs:	SHELXL-97 [3], DIAMOND [4]

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}
Nd(1)	2*a*	0	0	½	0.0053(3)	U_{11}	0.0064(4)	½U_{11}	0	0
Pd(2)	2*c*	⅓	⅓	¾	0.0052(4)	U_{11}	0.0108(5)	½U_{11}	0	0
P(3)	2*d*	⅔	⅔	¾	0.005(1)	U_{11}	0.014(2)	½U_{11}	0	0

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