Refinement of the crystal structure of ytterbium nickel tetraboride, $YbNiB_4$

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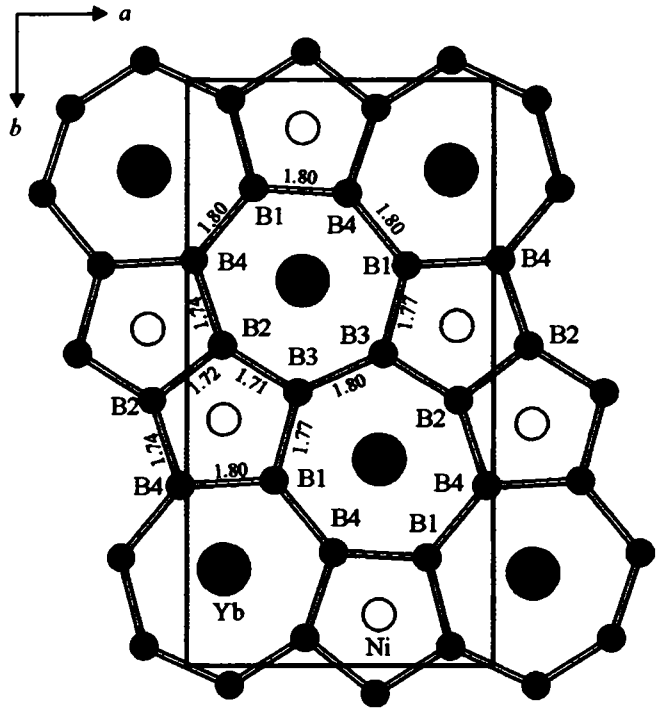

Abstract

B_4NiYb, orthorhombic, *Pbam* (no. 55), $a = 5.8645(2)$ Å, $b = 11.3680(5)$ Å, $c = 3.3850(2)$ Å, $V = 225.7$ Å^3, $Z = 4$, $R_{gt}(F) = 0.025$, $wR_{ref}(F) = 0.026$, $T = 295$ K.

Source of material

A mixture of ytterbium filings (99.95 %), nickel powder (99.98 %) and crystalline boron (99.98 %) with nominal composition $YbNiB_4$ was compacted into a pellet and sealed into Ta tube. The primary reaction was performed at 800 °C during three days. The homogenization annealing was carried out at 1100 °C for four days. Single crystals were separated from the annealed sample by mechanical fragmentation.

Experimental details

Lattice parameters were refined from 51 reflections obtained from X-ray powder diffraction data using Cu $K\alpha_1$ radiation and LaB_6 ($a = 4.15692(1)$ Å) as internal standard.

Discussion

Based on powder X-ray diffraction patterns the crystal structure of $YbNiB_4$ was previously assigned to the $YCrB_4$ structure type ($a = 5.888$ Å, $b = 11.54$ Å, $c = 3.412$ Å) [1]. The structure of the $YCrB_4$ type is the most widespread among the ternary borides. However, only for few representatives of this structure type atomic coordinates have been determined [2,3].

The crystal structure of $YbNiB_4$ contains planar boron nets perpendicular to [001], composed of five- and seven-membered rings. The metal atoms are located between the boron nets. Ytterbium atoms are situated between the seven-membered rings, and the nickel atoms between the five-membered rings. The distances between boron atoms in the net range from 1.71(1) Å (B2—B3) to 1.80(1) Å (B1—B4) and are close to the sum of the covalent radii of the boron atom (r(B) = 0.88 Å [4]). The minimal distances Yb—B2 (2.553(6) Å) and Yb—Ni (2.9720(9) Å) are less than a sum of atomic radii of Yb, Ni and B atoms, respectively (r(Yb) = 1.94 Å, r(Ni) = 1.246 Å [4]). The minimal distances Ni—Ni (2.551(1) Å) and Ni—B (2.197(5) Å) are slightly larger than the sum of atomic radii of the components. The volume of the unit cell increases in the sequence of isomorphic compounds $YbFeB_4$ ($V = 221.4$ Å^3) [5], $YbCoB_4$ ($V = 223.2$ Å^3 [6]) and $YbNiB_4$ ($V = 225.7$ Å^3).

Table 1. Data collection and handling.

Crystal:	gray needle, size 0.050 × 0.030 × 0.020 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	511.3 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7 & Mercury CCD, ω/φ
$2\theta_{max}$:	62°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1780, 1780
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 4\,\sigma(I_{obs})$, 375
$N(param)_{refined}$:	26
Programs:	SHELXL-97 [7], ATOMS [8], CSD [9]

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

Atom	Site	x	y	z	U_{iso}
B(1)	4g	0.785(1)	0.1841(7)	½	0.003(1)
B(2)	4g	0.386(1)	0.0475(7)	½	0.006(1)
B(3)	4g	0.861(2)	0.0332(7)	½	0.008(1)
B(4)	4g	0.479(1)	0.1929(7)	½	0.004(1)

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Table 3. 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	4*h*	0.12738(5)	0.15020(2)	0	0.0035(2)	0.0018(2)	0.00485(2)	0.00003(1)	0	0
Ni	4*h*	0.63401(2)	0.08839(8)	0	0.0045(4)	0.0029(4)	0.0050(3)	0.0006(4)	0	0

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