Crystal structure of erbium vanadium tantal boride, $\text{Er}(\text{V}_{0.77}\text{Ta}_{0.23})\text{VB}_6$

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Abstract

$\text{B}_6\text{ErTa}_{0.23}\text{V}_{1.77}$, orthorhombic, *Pbam* (No. 55), $a = 11.280(2)$ Å, $b = 8.940(2)$ Å, $c = 3.390(1)$ Å, $V = 341.9$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.034$, $wR_{\text{obs}}(F) = 0.034$, $T = 293$ K.

Source of material

The title compound was obtained as by-product during systematic investigation in ternary Er–V–B system. A pellet pressed from erbium filings (99.9 %), vanadium powder (99.5 %), and crystalline boron (99.99 %) in ratio of 2:1:6 was wrapped in tantalum foil, sealed in quartz ampoule and sintered at 1270 K. Needle-shaped crystal were formed on contact surfaces of the pellet and tantalum foil. The presence of tantalum in the crystal was suspected during the structure refinement and was confirmed by EDAX. A detected atomic ratio between vanadium and sum of erbium with tantalum of 1.27(2) : 1 agrees with values of 1.44(1) : 1 obtained from crystal structure refinement.

Experimental details

The lattice parameters of $\text{Er}(\text{V}_{0.77}\text{Ta}_{0.23})\text{VB}_6$ were determined from least-square procedure of 1978 reflections measured during the data collection.

Discussion

The crystal structure of $\text{Er}(\text{V}_{0.77}\text{Ta}_{0.23})\text{VB}_6$ adopts Y_2ReB_6 type [1]. The boron atoms form two-dimensional planar nets of condensed five-, six-, and seven-membered rings. All prismatically coordinated centers between two slabs are filled by metals, according to the atomic radii, the largest Er and the smallest V atoms occupy the centers of heptagonal and pentagonal prisms, respectively. The hexagonal prisms contain statistically distributed Ta (intermediate size) and V atoms. Coordination polyhedra around Er, (Ta,V), and V atoms have 23, 20, and 17 vertices, respectively. Each boron atom is trigonal prismatically coordinated by metal atoms. The environment is completed by three additional boron neighbors, which are situated in the same plane as the central atom. The B–B bond lengths vary between 1.74(2) Å and 1.85(2) Å and agree very well with average distance of 1.776 Å in α -rhombohedral boron [2]. The shortest contacts between another pairs of atoms are $d(\text{Er}—\text{Ta},\text{V}) = 3.391(2)$ Å, $d(\text{Er}—\text{V}) = 3.046(3)$ Å, $d(\text{Er}—\text{B}) = 2.631(1)$ Å, $d(\text{Ta},\text{V}—\text{V}) = 2.764(3)$ Å, $d(\text{Ta},\text{V}—\text{B}) = 2.426(1)$ Å, and $d(\text{V}—\text{B}) = 2.254(9)$ Å. Ternary compounds with Y_2ReB_6 structure type are observed in numerous rare-earth transition metal boron systems: RE_2MB_6 (RE = Y, Gd–Tm; M = Ru, Re, Os), RE_2MB_6 (RE = Yb, Lu; M = Ru, Os), Lu_2FeB_6 , Yb_2AlB_6 , U_2MB_6 (M = Mo, W, Re, Os) [3]; Sc_2ReB_6 [4]; RE_2MoB_6 (RE = Er, Tm, Yb, Lu) [4,5]; $\text{Lu}_{1.34}\text{V}_{1.66}\text{B}_6$ [6]; Lu_2WB_6 [7]. Nevertheless, a formation of isotopic phases was not detected during systematic investigation of ternary Er–V–B [8] and Ta–V–B [9] systems. $\text{Er}(\text{V}_{0.77}\text{Ta}_{0.23})\text{VB}_6$ is the first quasi-ternary representative of Y_2ReB_6 type and the third example of described structure, where transition metal atoms have hexagonal-prismatic environment. Recently reported borides Zr_2CrB_6 and ZrCr_2B_6 contain in the centers of hexagonal prisms Cr and statistically distributed Cr and Zr atoms, respectively [10].

Table 1. Data collection and handling.

Crystal:	metallic needle, size $0.02 \times 0.03 \times 0.08$ mm
Wavelength:	Mo K_{α} radiation (0.7107 Å)
μ :	377.5 cm^{-1}
Diffractionmeter, scan mode:	Rigaku Mercury CCD, φ/ω
$2\theta_{\text{max}}$:	64.06°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2542, 565
Criterion for F_{obs} , $N(hkl)_{\text{gt}}$:	$F_{\text{obs}} > 4 \sigma(F_{\text{obs}})$, 545
$N(\text{param})_{\text{refined}}$:	38
Programs:	WinCSD [11], ATOMS [12]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U _{iso}
B(1)	4g	0.237(1)	0.202(1)	0	0.005(2)
B(2)	4g	0.213(1)	0.518(2)	0	0.004(2)
B(3)	4g	0.081(1)	0.241(2)	0	0.005(2)
B(4)	4g	0.067(1)	0.447(2)	0	0.005(2)
B(5)	4g	0.320(1)	0.371(2)	0	0.006(2)
B(6)	4g	0.024(1)	0.907(2)	0	0.007(2)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Er	4h	0.91475(5)	0.32152(6)	1/2	0.0040(3)	0.0021(2)	0.0037(3)	−0.0005(2)	0	0
V/Ta(1) ^a	4h	0.37194(1)	0.55391(1)	1/2	0.0050(5)	0.0041(5)	0.0047(5)	−0.0012(4)	0	0
V(2)	4h	0.1840(2)	0.3555(2)	1/2	0.0052(8)	0.0030(8)	0.0044(8)	0.0022(7)	0	0

a: V/Ta(1) = 0.768(3)V + 0.232Ta

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