A Ternary Rare Earth Boride with a $ThCr_2Si_2$-type Structure

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In the study of the phase diagram in the yttrium-cobalt-boron system, a ternary compound with a tetragonal unit cell was found to have a composition of 19.8%Y, 40.5%Co, and 39.7%B (by atomic). The stoichiometric composition of YCo_2B_2 is proposed. This is the first compound found in the Y–Co–B system.

The samples were prepared by arc-melting from stoichiometric amounts of Y, Co, and B under purified argon. The purities of the Y, Co, and B used were 99.9%, 99.99%, and 99.9% (by weight) respectively. For homogenizing, the samples were wrapped with tantalum foil, sealed in quartz capsules under a vacuum, and annealed for 150 hr at 800°C. After these heat treatments, the samples were ground in an agate mortar under an inert atmosphere to prevent oxidation and then examined by chemical and X-ray analyses.

TABLE 1. X-RAY POWDER DATA FOR YCo_2B_2
($a=3.561\pm0.003$Å, $c=9.358\pm0.005$Å)

hkl	$d_{obs.}$(Å)	$d_{calc.}$(Å)	$I_{obs.}$	$I_{calc.}$
002	4.678	4.679	5.9	5.4
101	3.319	3.328	48.5	49.2
110	n.obs.	2.518	n.obs.	0.4
103	2.344	2.346	67.6	27.9
004		2.340		30.4
112	2.215	2.217	100.0	110.0
200	1.781	1.781	25.1	30.5
202	n.obs.	1.664	n.obs.	0.1
105	1.656	1.657	10.0	9.7
211	1.570	1.570	10.3	10.7
006	n.obs.	1.560	n.obs.	0.1
213	1.418	1.418	31.1	12.2
204		1.417		23.3
116	1.326	1.326	26.4	23.2
220	1.258	1.259	9.0	12.2
107	1.251	1.252	3.7	3.3
222	n.obs.	1.216	n.obs.	0.3
215	1.213	1.213	7.9	9.9
301	1.177	1.178	4.5	3.2
206	n.obs.	1.173	n.obs.	0.3
008	1.169	1.170	6.0	6.1
310	n.obs.	1.126	n.obs.	0.1
303	1.109	1.109	21.3	5.5
224		1.109		20.4
312	1.094	1.095	16.6	24.1
118	n.obs.	1.061	n.obs.	0.2
217	1.025	1.024	10.0	10.3
305	1.002	1.002	11.3	10.1
321	0.982	0.982	18.5	20.6
226	n.obs.	0.980	n.obs.	1.9
208	0.978	0.978	71.4	94.4

n. obs.=not observed.

The X-ray patterns were taken using Fe radiation with a Debye-Scherrer camera and a diffractometer equipped with an X-ray monochromator. The observed intensities were measured with a Geiger-Müller counter.

The YCo_2B_2 pattern was indexed as tetragonal. As is shown in Table 1, there is a good agreement between the observed and calculated interplanar spacings. The tetragonal unit cell of the YCo_2B_2 structure has the dimensions of $a=3.561\pm0.003$ Å, $c=9.358\pm0.005$ Å, and $c/a=2.628$, and it contains two YCo_2B_2 formula units. Pycnometric-density measurements were also carried out. The experimental and theoretical densities are 6.30 g/cm³ and 6.39 g/cm³ respectively.

The relative intensities were computed assuming that YCo_2B_2 crystallizes isostructurally to the $ThCr_2Si_2$ type,[1-4] which is an ordered ternary version of the $BaAl_4$ type, the two nonequivalent sites of the Al atoms being occupied by different kinds of atoms. The reliability factor, $R=\sum|I_{ob}-I_{cal}|/\sum I_{ob}$, is 0.16. This good agreement between the observed and calculated intensities (Table 1) shows that this is the most probable structure. The space group is number 139, $I4/mmm(D_{4h}^{17})$. The atom locations and the projection of the YCo_2B_2 structure on (010) are shown in Table 2 and in Fig. 1 respectively.

TABLE 2. THE PARAMETER OF ATOM POSITION FOR YCo_2B_2

Tetragonal, $Z=2$, $I4/mmm$ (D_{4h}^{17})			
Equivalent positions (0,0,0; $^1/_2$, $^1/_2$, $^1/_2$)+			
2Y	2(a)	(0,0,0)	
4Co	4(d)	(0,$^1/_2$,2z;$^1/_2$,0,2z)	$z=0.125$
4B	4(e)	(0,0,z; 0,0,$\bar{z}$)	$z=0.378$

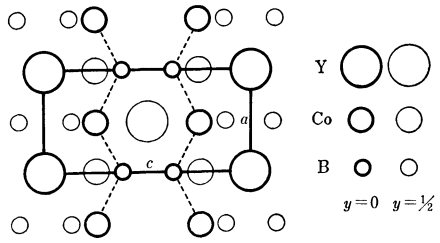

Fig. 1. The projection of YCo_2B_2 structure on (010).

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