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THE YNi_4B COMPOUND IN YTTRIUM-NICKEL-BORON SYSTEM

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A new-type compound, YNi_4B, has been prepared by an arc-melting technique. The unit cell is hexagonal with $a=4.977\pm0.004$Å and $c=6.942\pm0.005$Å, probable space group P6/mmm, and contains two formula units. The structure consists of two units of YNi_5 structure ($CaCu_5$-type), the nickel positions partly substituted for by boron atoms.

It is reported that there exist the ternary phases[1-5] such as $RCrB_4$, RCo_2B_2, RCo_3B_2, $RCo_{12}B_6$ and RCo_4B_4 in rare earth-transition metal-boron system. In examining the phase equilibrium of Y-Ni-B system, a new ternary compound with a hexagonal unit cell was found to have a composition of 16.7 at% Y, 66.7 Ni, and 16.7 B. The stoichiometric composition of YNi_4B is proposed. This is the first compound in Y-Ni-B system.

The sample weighing about 10g was prepared by arc-melting the mixture of Y, Ni and B in a purified argon atmosphere. The purities of Y, Ni and B used were 99.9 wt% 99.99 and 99.9 respectively. The sample was ground in an agate mortar and then examined by chemical analysis and X-ray diffraction.

The X-ray diffraction patterns were taken by a Debye-Scherrer camera and a diffractometer using Fe radiation ($FeK\alpha_1=1.9360$Å, $FeK\alpha_2=1.9399$Å, and $FeK\bar{\alpha}=1.9373$Å). The X-ray diffraction intensities were measured by a diffractometer with an NaI(Tl) scintillation counter and a pulse height analyser.

The YNi_4B pattern was indexed on the basis of hexagonal unit cell. As seen in Table 1, the agreement is fairly good between the observed and the calculated d-spacings. The lattice parameters are $a=4.977\pm0.004$Å, $c=6.942\pm0.005$Å and $c/a=1.395$. The unit cell content is 2 YNi_4B. The experimental and the theoretical density are 7.38 g/cm^3 and 7.46 g/cm^3 respectively.

No systematic extinction is not observed (Table 1). Space group P6/mmm is considered for YNi_4B because the diffraction pattern is similar to that of YNi_5 or YCo_3B_2. The relative intensities were computed, assuming that 2Y, 8Ni and 2B in the YNi_4B structure occupy the atomic sites as shown in Table 2 respectively. The reliability factor, $R=\Sigma|I_{ob}-I_{cal}|/\Sigma I_{ob}$, is 0.148. From the value of R-factor, the assumption concerning the atomic position of Y and Ni is considered to be valid. In the metal-rich borides, B atom is generally situated at the center of the trigonal prism formed by six metal atoms[6]. It is therefore reasonable to consider that B atoms in the YNi_4B structure occupy 2(d) sites with the simple geometrical arguments.

The structure of YNi_4B consists of two layers of YNi_5 structure ($CaCu_5$-type) in

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which the nickel positions are partly substituted for by boron atoms. Projection of the YNi_4B structure on the (001) plane is shown in Fig 1.

Ternary borides of the same structure are also observed for (La, Ce, Pr, Sm, Gd, Tb, Dy, Ho, Er, and Yb)-Ni-B system. The typical patterns are shown in Fig 2. Crystal structure and magnetic properties of these compounds will be described in a later report.

Table 1. X-ray Diffraction Data for YNi_4B

hkl	$d_{ob.}$	$d_{cal.}$	$I_{ob.}$	$I_{cal.}$
100	—	4.310	0	0.7
002	—	3.471	0	0.3
102	2.701	2.703	57.9	70.8
110	2.482	2.489	17.0	22.6
111	2.344	2.343	10.3	16.9
003	2.316	2.314	15.1	18.4
200	2.155	2.155	87.8	80.7
201	2.057	2.058	9.3	12.2
103	2.093	2.093	10.3	10.4
112	2.023	2.023	103.2	103.1
202	1.829	1.831	19.9	19.7
004	1.734	1.736	19.8	19.5
104	—	1.610	0	0.8
203	1.577	1.577	5.6	5.4
212	1.475	1.474	20.7	19.8
300	1.438	1.437	6.9	6.6
114	1.422	1.424	14.3	11.6
005	1.389	1.388	2.1	1.5
204	1.351	1.352	19.8	15.1
213	1.328	1.332	32.2	5.3
302		1.328		26.9
220	1.244	1.244	26.0	30.6
115	1.213	1.212	7.9	7.9
214	1.189	1.188	2.3	1.1
205	1.167	1.167	21.0	21.4
006	1.156	1.157	2.3	2.0
312	1.130	1.130	19.4	14.0
304	1.107	1.107	12.4	9.5
223	1.097	1.096	12.4	20.1
400	1.078	1.078	25.7	17.2
401	1.064	1.065	6.1	3.2
313		1.062		2.7
116	1.049	1.049	24.9	18.5
402	1.029	1.029	5.2	6.4
224	1.012	1.011	58.6	57.8

B (the temperature factor)=0.80
R (the reliability factor)=0.148

Table 2. Parameters of the atom positions for YNi_4B

	Hexagonal, Z=2, P6/mmm	
2Y :	1(a),1(b)	$(0,0,0;0,0,\frac{1}{2})$
2Ni :	2(c)	$(\frac{1}{3},\frac{2}{3},0;\frac{2}{3},\frac{1}{3},0)$
6Ni :	6(i)	$(\frac{1}{2},0,z;0,\frac{1}{2},z;\frac{1}{2},\frac{1}{2},z;$ $\frac{1}{2},0,\bar{z};0,\frac{1}{2},\bar{z};\frac{1}{2},\frac{1}{2},\bar{z})$ z=0.29
2B :	2(d)	$(\frac{1}{3},\frac{2}{3},\frac{1}{2};\frac{2}{3},\frac{1}{3},\frac{1}{2})$

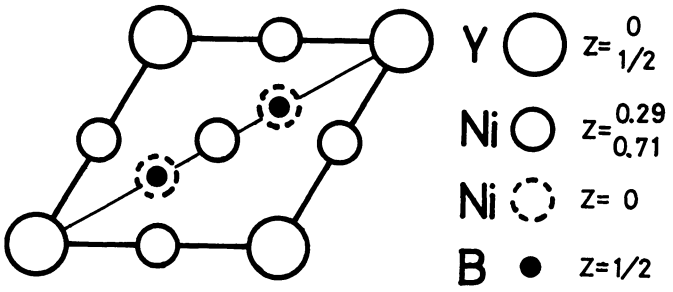

Fig 1. The projection of YNi_4B structure on (001) plane.

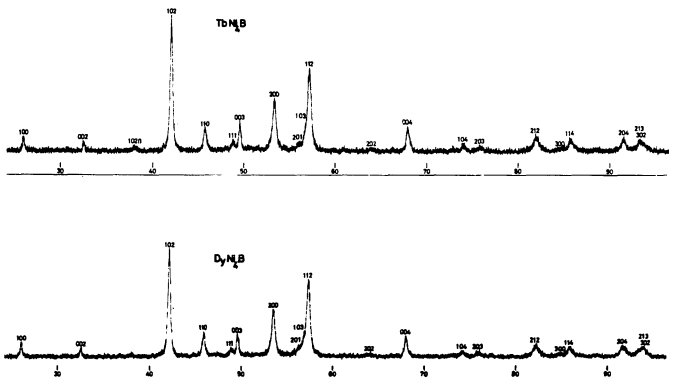

Fig 2. The X-ray diffraction patterns for $TbNi_4B$ and $DyNi_4B$.

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