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The preparation and characterization of a new layered yttrium nickel borocarbide

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Abstract

A new layered borocarbide with nominal composition of Y_2NiBC_2 has been prepared. The lattice constants $a_p = 3.570(1)$ Å and $c_p = 13.064(5)$ Å based on a primitive unit cell were obtained from least-squares fitting of the strong X-ray diffraction peaks. However, the actual cell dimensions were found to be $a = \sqrt{5}a_p$, $c = 2c_p$ from the electron diffraction patterns. The structure of the compound can be viewed as an intergrowth of Ni_2B_2 and quadruple YC rock salt layers. A.c. susceptibility measurements showed that the samples were non-superconducting down to 4.2 K.

Keywords: Yttrium nickel borocarbide; Preparation; Layered borocarbides; A.c. susceptibility measurements

Superconductivity with transition temperature T_c up to 23 K has recently been reported in the quaternary lanthanide–transition metal–borocarbide (Ln–M–B–C) system [1–3]. Such a T_c record is already equivalent to the highest T_c achieved in the classical intermetallic compounds. This finding opens new possibilities to search for even higher T_c in the quaternary intermetallic systems. The structures of the new superconducting and related compounds can be derived from the intergrowth of an M_2B_2 layer and rock salt LnC layers [4]. The building principle is very similar to the principle already observed in the cuprate superconductors [5]. Following a route to develop new layered cuprates [6], we aimed at the synthesis of new borocarbides with different combinations of the rock salt layer and M_2B_2 layer. If $m = 1$ in the homologous series $(M_2B_2)_m(LnC)_n$, we would obtain the structure models shown in Fig. 1 for $n = 1$, 2, 3, 4. The members with $n = 1$ and 2 correspond to the reported superconducting YNi_2B_2C ($n = 1$) and the non-superconducting compound YNiBC ($n = 2$). In the present letter, we report the preparation and characterization of a new layered borocarbide Y_2NiBC_2 which corresponds to the member with $m = 1$ and $n = 4$.

The samples of Y_2NiBC_2 were prepared in a water-cooled copper boat by induction heating. The elemental Y, Ni, B, C were weighed according to the ratios 2:1:1:2 and 3:1:1:3. The mixtures of the starting materials were first loaded into the copper boat. The samples were heated to melting under a protecting atmosphere of argon. Then they were allowed to cool to room temperature and were turned over for a second heating. In order to obtain a homogeneous sample, such a process was repeated 10 times and the whole treatment lasted about 10 h.

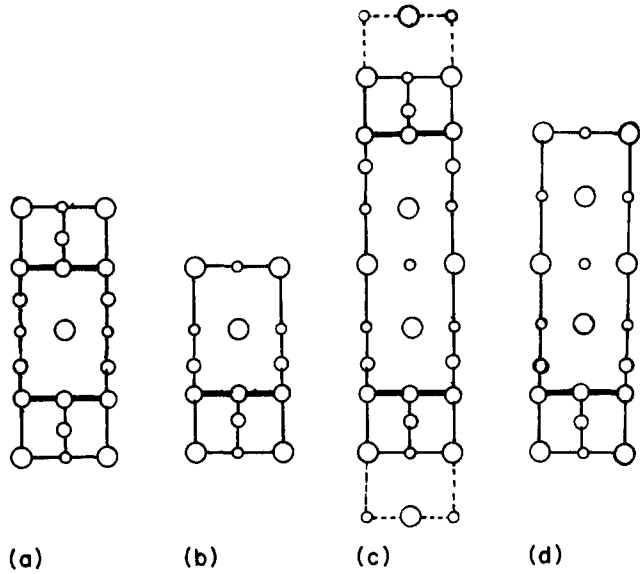

Fig. 1. The ideal structure models of the homologous series $(Ni_2B_2)_m(YC)_n$ with $m = 1$ and $n = 1$, 2, 3, 4.

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The as-prepared samples were characterized by X-ray diffraction (XRD), electron diffraction (ED) and a.c. susceptibility measurements. The XRD patterns were recorded with a Rigaku D_{MAX}-rB diffractometer with a step size of 0.02° and a scan rate of 1.8° min^{-1}. Cu Kα radiation was used and a graphite monochromater was placed in the diffraction path. Silicon powder was used as an external standard to calibrate the diffractometer. ED was performed on a Hitachi H-800 transmission electron microscope equipped with a double tilt sample holder. The a.c. susceptibilities of the samples were measured by the mutual induction bridge method.

The as-prepared samples were aggregates of fibrous thin platelets. X-ray powder diffractions of the samples from the two starting compositions resulted in similar patterns (Fig. 2). The XRD pattern of the sample annealed at 900 °C for 150 h also did not exhibit any significant differences. Thus, it indicates that Y_2NiBC_2 is the equilibrium composition and the compound is at least stable between the annealing and melting temperature. The main peaks in the XRD patterns can be indexed by a primitive tetragonal cell. Cell parameters $a=3.570(1)$ Å and $c=13.064(5)$ Å, which agree with the hypothetical structure model (Fig. 1(d)), were obtained by least-squares fitting of the strong peaks (Table 1). As aforementioned, the structure can be viewed as built up by alternate stacking of a single Ni_2B_2 layer and four layers of the YC rock salt unit. The strong intensities of 001 diffraction may reveal a 001 preferred orientation. A minor phase of YNiBC was found to coexist with the main phase. The remaining peaks might be due to matrix or superstructure diffractions.

The ED pattern of the 001 zone is shown in Fig. 3. From the figure we found that the pattern can only be indexed with a parameter $a=7.98$ Å. The larger cell of the basal plane is thus related to the primitive subcell (from XRD) by the equation $a=\sqrt{5}a_p$ (Fig. 3(b)). Furthermore, the diffractions extinct in the substructure such as 130 and 420 exhibited intensities comparable with those of 310 and 240. The intensities of the latter two diffractions should be the strongest

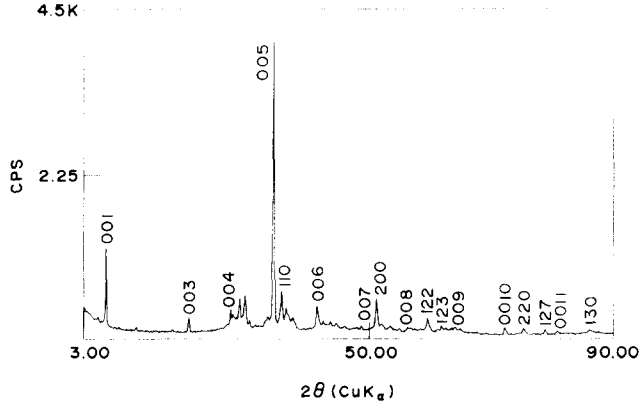

Fig. 2. The XRD pattern of a Y_2NiBC_2 sample.

Table 1
The X-ray diffraction pattern of Y_2NiBC_2 (indexed with a primitive tetragonal cell, $a=3.56965(4)$ Å, $c=13.064(5)$ Å)

h k l	d_{obs} (Å)	d_{calc} (Å)	I_{obs}
0 0 1	13.03	13.06	31
0 0 3	4.354	4.355	7
0 0 4	3.266	3.266	10
0 0 5	2.614	2.613	100
1 1 0	2.518 [a]	2.524	17
0 0 6	2.178	2.177	11
0 0 7	1.867	1.866	5
2 0 0	1.784	1.785	14
0 0 8	1.634	1.633	4
1 2 2	1.551	1.551	7
1 2 3	1.499	1.499	5
0 0 9	1.453	1.452	4
1 2 4	1.4347	1.4342	4
0 0 10	1.3060	1.3064	4
2 2 0	1.2621	1.2621	4
1 2 7	1.2133	1.2131	3
0 0 11	1.1875	1.1877	3
1 3 0	1.1286	1.1288	3

[a] Not included in the fitting.

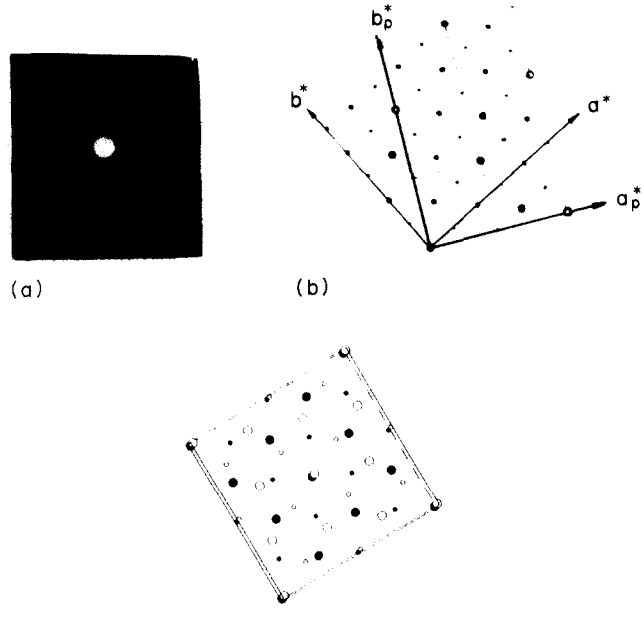

Fig. 3. (a) The (001) zone ED pattern of Y_2NiBC_2 sample and its indexing (b) with the supercell ($a=\sqrt{5}a_p$) and (c) with the primitive cell (a_p). The atom positions projected down to the basal plane (the larger circles are Y, smaller circles are Ni atoms and the open (full) circles represent atoms in the upper (lower) subcell).

since they are related to 110 and 200 when indexed with the primitive subcell. This is an indication that for the 001 zone pattern new 100, 010, 110 mirror planes are introduced in the supercell and the mirror planes in the subcell are destroyed. Such a phenomenon can be tentatively explained by using the structure

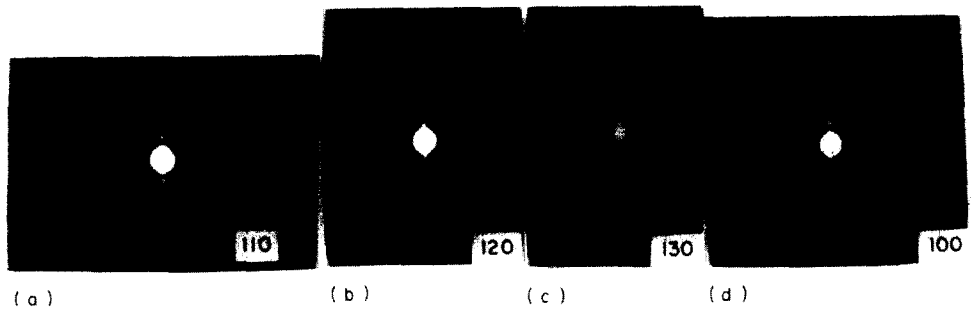

Fig. 4. The ED patterns of a Y_2NiBC_2 sample rotated around the c^* direction: (a) −18.4°; (b) 0°; (c) +8.1°; (d) +26.6°.

model shown in Fig. 3(c). The unit cell in the model is composed of two parts alternately stacking along c direction. Each part is the same as the substructure and relate to the other by a rotation of 26.6° around the c axis. The rotation not only leads to the appearance of the equivalent spots of 130–310 and 240–420, but also leads to the appearance of $hk0$ $(h+k=2n)$ diffractions in the 001 zone ED pattern.

Fig. 4 shows the ED patterns of ($hk0$) zones obtained by tilting the sample around the c^* direction. The patterns generally agree with that of the 001 zone diffraction. Fig. 4(d) (100 zone) reveals that an enlarged cell with $a=\sqrt{5}a_p$ and $c=2c_p$ must be chosen. However, the superstructure spots in Figs. 4(b) and 4(c) which lead to a quadruple structure ($c=4c_p$) along the c axis were not completely understood. They may be due to double diffraction or complex ordering in the c direction. The streaks along the c^* direction in all the patterns can be assigned to the stacking default of the YC and Ni_2B_2 layers.

The a.c. susceptibilities of the samples did not reveal any evidence for superconductivity down to 4.2 K. The non-superconducting nature of this compound and structurally related compound YNiBC might provide the clue that the close contact of Ni_2B_2 layers in YNi_2B_2C is a prerequisite for the appearance of superconductivity.

In conclusion, we have obtained a new layered borocarbide which is built up from Ni_2B_2 and quadruple layers of rock salt YC layers. Although it possesses a structural resemblance to the superconducting YNi_2B_2C compound, it did not exhibit any evidence of superconductivity.

Acknowledgments

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