substance: boron compounds, general properties
property: further structure groups

Structure group of YB_{25}

Structure: monoclinic [97T, 99M]

Space group: I112, I11m, or I112/m

Isostructural compounds with lanthanoides from Gd to Ho are possible as well.

Because of the very similar lattice parameters of YB_{25} and $YAlB_{14}$ it is assumed that the structure is very similar to that of the orthorhombic $MgAlB_{14}$ type borides [97T, 99M].

Information on the electronic properties is still missing

Structure group of BeB_3 87L, 75M

Information on the electronic properties is still missing.

Structure group of orthorhombic SiB_6 87L, 86V

Information on the electronic properties is missing.

Structure group of the YB_{66} type borides

Many of the lanthanide metals form boron-rich compounds of the composition MB_{66}. The compounds NdB_{66}, SmB_{66}, GdB_{66}, TbB_{66}, DyB_{66}, HoB_{66}, ErB_{66}, TmB_{66}, YbB_{66}, LuB_{66} are known at now. [72S1, 72S2, 72S3, 76K, 76S, 77N, 77S2, 75B, 81S].

The boron framework is composed of $(B_{12})_{13}$ giant icosahedra consisting of a central and 12 surrounding B_{12} icosahedra and B_{80} clusters. The $(B_{12})_{13}$ units are located in one orientation at the face-centered cubic lattice points. They also occur at the centers of the cell and of the cell edges with orientation rotated by 90°. In total they contribute with eight $(B_{12})_{13}$ units = 1248 boron atoms to the unit cell (Fig. 1). The B_{80} clusters consist of 80 boron sites belonging to four crystallographic positions of the space group Fm3c: (3×192j, 64g)/8. In this cluster, all the sites are only partially occupied with occupancies ranging between 28 and 71 % leading to about 42 boron atoms per B_{80} cluster in agreement with previous structure description [69R]. The B_{80} cluster is centered at the 8(a) position (1/4, 1/4, 1/4), and thus there are eight of such clusters (336 B atoms) per unit cell. Accordingly, the total number of B atoms is 1584 per unit cell. The Y sites are enclosing the B_{80} clusters in an octahedral arrangement, each, hence there are eight octahedral Y arrangements per unit cell. They are connected to their neighboring six octahedra through their apical Y sites (Fig. 1). The actual composition is determined by the occupancy of the Y sites, for example 0.5, 0.5324 and 0.575(5) for YB_{66}, YB_{62} and YB_{56} respectively. In the case of simultaneously occupied neighbored Y sites (for occupancies > 0.5 inevitable) the repulsive force between the ionized Y atoms increases the Y-Y distance [97H].

Representatives of the YB_{66} type borides

Chemical formula (idealized)	Structural formula	
YB_{66}	$Y_3 \cdot (B_{12})_{13} \cdot B_{42}$	97H
YB_{62}	$Y_{3.2} \cdot (B_{12})_{13} \cdot B_{42}$	77I
YB_{56}	$Y_{3.5} \cdot (B_{12})_{13} \cdot B_{42}$	97H
GdB_{66}		94G
DyB_{66}		86G

So far as electronic properties of representatives of the YB_{66} type borides have become known, they indicate semiconducting behavior.

Thermal properties

Temperature dependence of the thermal conductivity of some representatives of the YB_{66} structure group: $YB_{66\pm x}$ ($YB_{61.7}$ [92R, 94M]; YB_{66} [71S, 94M], YB_{66} [87C, 89C, 94M; YB_{66} [77S2, 94M]); $GdB_{66\pm x}$ (GdB_{66} [86G]; $GdB_{62.5}$ [94M]) in Fig. 2.

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Fig. 1.

YB_{66} structure group. Structure containing $(B_{12})_{13}$ giant icosahedra, B_{80} clusters (80 B sites, about 42 of which are statistically occupied) and Y-Y pairs [97H].

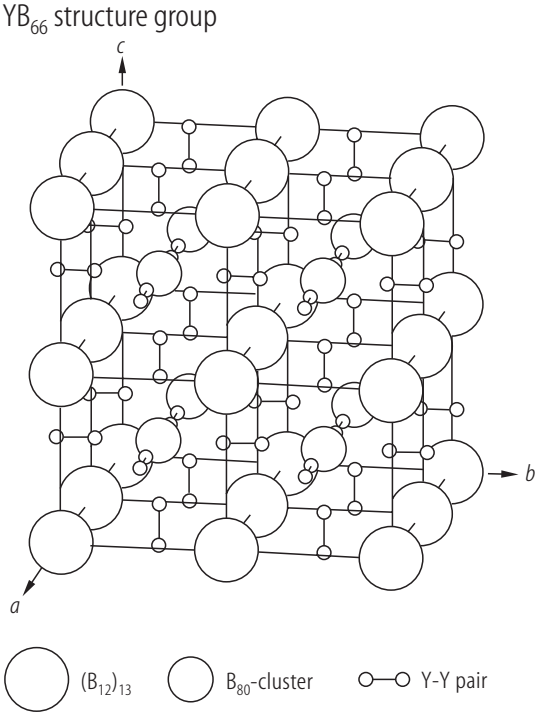

Fig. 2.

YB_{66} structure group. Temperature dependence of thermal conductivity. Open symbols: $YB_{66\pm X}$ (squares, $YB_{61.7}$ [92R, 94M]; triangles, YB_{66} [71S, 94M], circles, YB_{66} [87C, 89C, 94M], diamonds, YB_{66} [77S1, 94M]); closed symbols: $GdB_{66\pm X}$ (circles, GdB_{66} [86G], triangles down, $GdB_{62.5}$ [94M]).