substance: boron compounds, general properties
property: structure group of the REB_{50} type borides

Structure: orthorhombic

Space group: Pbam [97H, 97T]

Crystal structure in Figs. 1–4 [97H], see also, for $TbB_{41}Si_{1.2}$ [99M1].

Preparation by the borothermal reduction of RE oxides [97T, 99M2]

Since REB_{50} decomposes above 1800 °C, it is not possible to grow single crystals from the melt. However, with the addition of Si isostructural single crystal with the composition $YB_{41}Si_{1.2}$ [97T, 99H] and $TbB_{41}Si_{1.2}$ [99M1] could be grown by the floating zone method

Representatives of the YB_{50} type borides

Chemical formula	
YB_{50}	94T
TbB_{50}	99M4
DyB_{50}	99M4
HoB_{50}	99M4
ErB_{50}	99M4
$YB_{41}Si_{1.2}$	97H
$YB_{44}Si_{1.0}$	97T
$TbB_{41}Si_{1.2}$	99M2

Rare earth elements from Tb to Lu form the same structure [94T].

Investigations on the electronic properties have not yet become available.

The outstanding properties of this structure group are the magnetic ones. Till now, they have been the only icosahedral boron-rich solids, that exhibit antiferromagnetic-like transitions [99M1, 99M2]. For TbB_{50} and $TbB_{41}Si_{1.2}$ see [99M3].

Magnetic field dependence of the magnetization of DyB_{50}, TbB_{50}, ErB_{50}, HoB_{50}, $TbB_{41}Si_{1.2}$, in Fig. 5 [99M1].

Magnetic susceptiblity of $TbB_{41}Si_{1.2}$ in Fig. 6 [99M1].

Specific heat of $TbB_{41}Si_{1.2}$ in Fig. 7 [99M1]

References:

94T Tanaka, T., Okada, S., Ishizawa, Y.: J. Alloys Compounds 205 (1994) 281.

97H Higashi, I., Tanaka, T., Kobayashi, K., Ishizawa, Y., Takami, M.: J. Solid State Chem. 133 (1997) 11 (Proc. 12th Int. Symp. Boron, Borides and Rel. Compounds, Baden, Austria, 1996).

97T Tanaka, T., Okada, S., Ishizawa, Y.: J. Solid State Chem. 133 (1997) 55 (Proc. 12th Int. Symp. Boron, Borides and Rel. Compounds, Baden, Austria, 1996).

99H Higashi, I., Ishii, T., Kobayashi, K., Tanaka, T.: J. Solid State Chem. (2000) (Proc. 13th Int. Symp. Boron, Borides and Rel. Compounds, Dinard, France, Sept. 1999).

99M1 Mori, T., Tanaka, T.: J. Solid State Chem. (2000) (Proc. 13th Int. Symp. Boron, Borides and Rel. Compounds, Dinard, France, Sept. 1999).

99M2 Mori, T., Tanaka, T.: J. Phys. Soc. Jpn. 68 (1999) 2033.

99M3 Mori, T., Tanaka, T.: J. Alloys Compounds 288 (1999) 32.

99M4 Mori, T., Tanaka, T.: J. Phys. Soc. Jpn. (1999) (submitted).

Fig. 1.

$YB_{41}Si_{1.2}$. Icosahedral B_{12} arrangement as seen along the *c* axis (only the icosahedra within the range *z* = 0.17...0.42 are drawn) [97H].

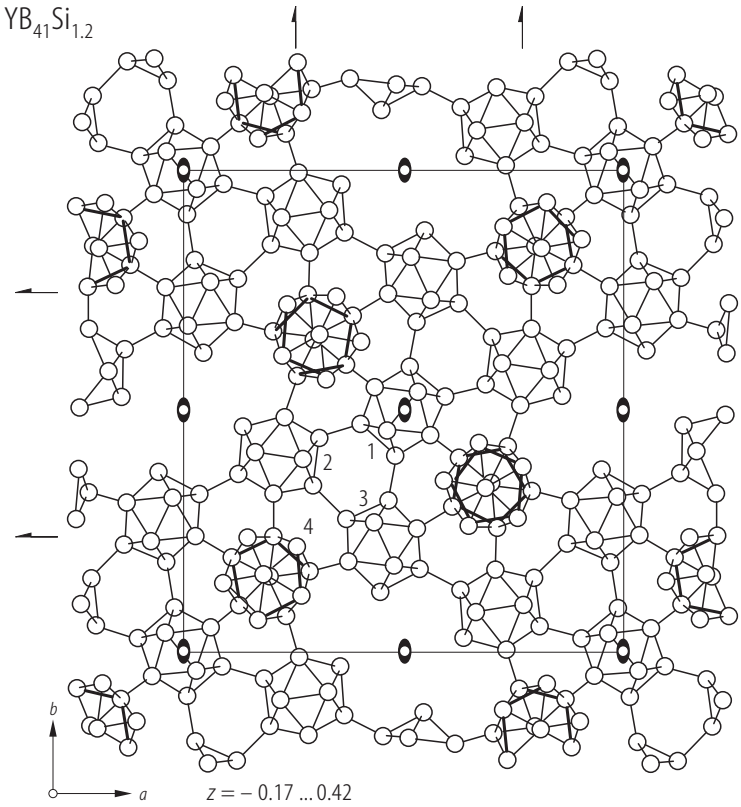

Fig. 2

$YB_{41}Si_{1.2}$.Arrangement of B_{12} icosahedra and $B_{12}Si_3$ units as seen along the *c* axis. Polyhedra within the range *z* = 0.30...0.92 are drawn [97H].

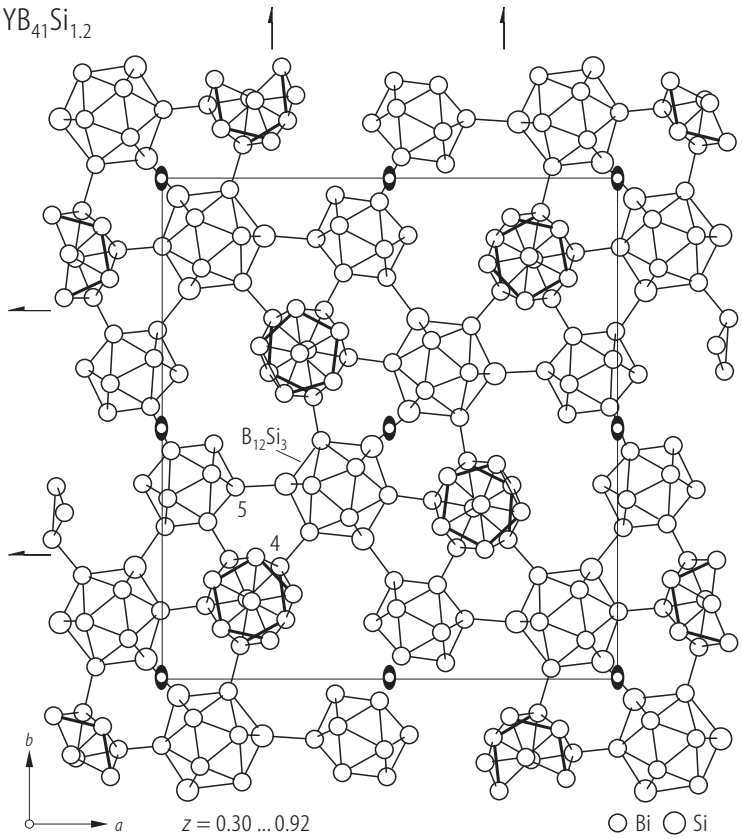

Fig. 3.

$YB_{41}Si_{1.2}$. $B_{12}Si_3$ unit as seen along the *b* axis. Large circles, Si sites; smaller circles, B sites [97H].

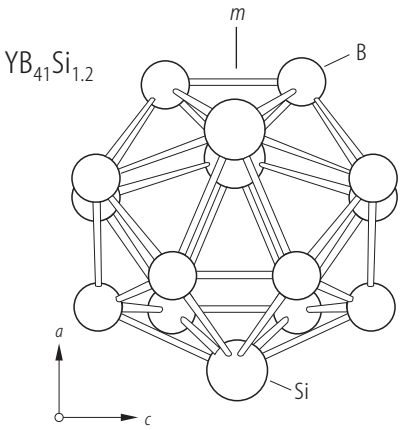

Fig. 4.

$YB_{41}Si_{1.2}$. Unusual linkage between two icosahedra effected through two apical atoms of each icosahedron [97H].

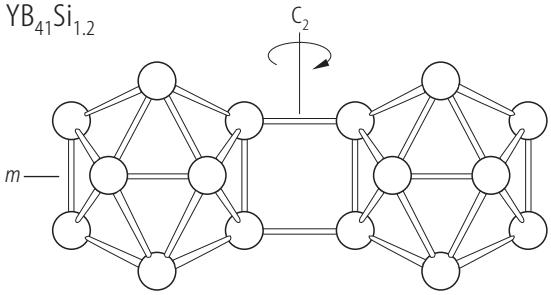

Fig. 5.

YB_{50} – type structure. Magnetization at 2K vs. magnetic field. **(a)** DyB_{50}, TbB_{50}; **(b)** ErB_{50}, HoB_{50}; **(c)** $TbB_{41}Si_{1.2}$. The critical magnetic fields H_c are indicated by arrows (H_c , field, where the derivative of the magnetization is maximum) [99M1]. p_{RE}: magnetic moment per rare earth atom.

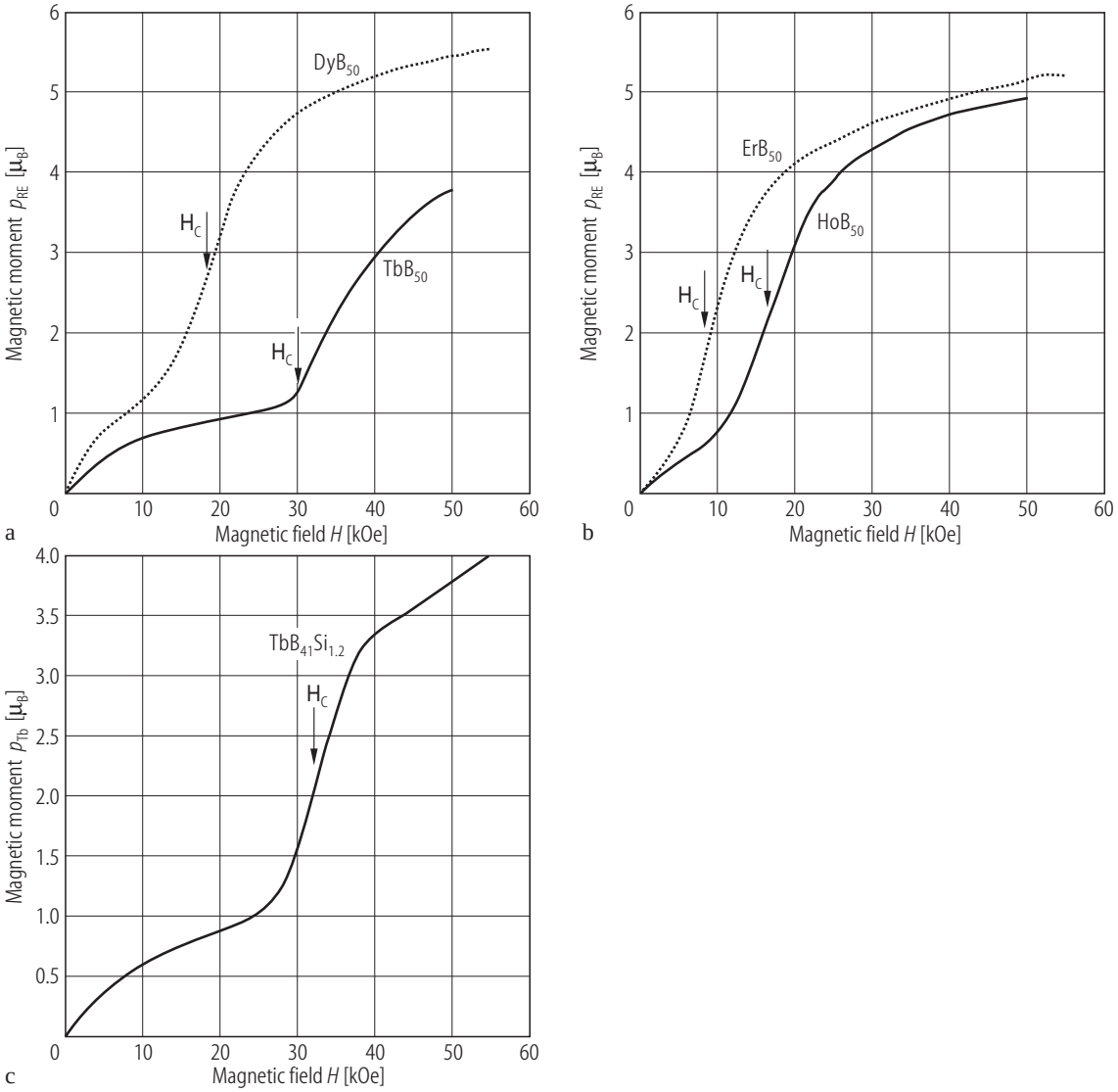

Fig. 6.

YB_{50} – type structure ($TbB_{41}Si_{1.2}$). Magnetic susceptibility vs. T. T_N ~ 18 K (peak temperature, temperature of an antiferromagnetic-like transition) [99M1].

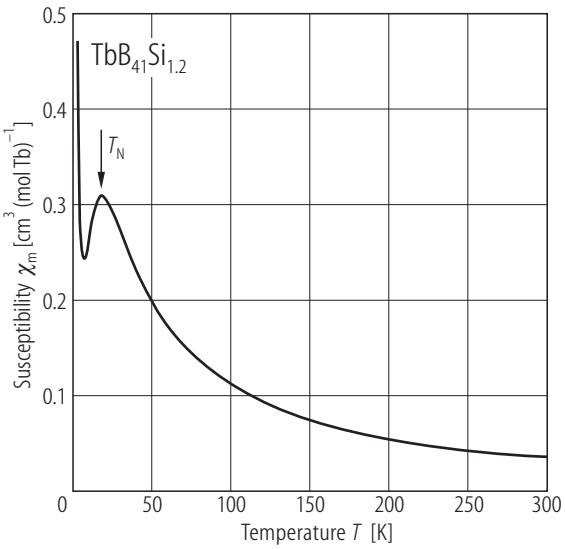

Fig. 7.

YB_{50} – type structure ($TbB_{41}Si_{1.2}$). Heat capacity C/T vs. T^2. Circles, experimental results; solid line, calculated according to $C = \gamma T + c_2 T^2$ with c_2 = 109 mJ/(mol K^3) [99M1].