substance: boron compounds with group III elements
property: properties of γ-AlB_{12}

Crystals of γ-AlB_{12} are almost always obtained as syntactically intergrown crystals with α-AlB_{12}. When such intergrown crystals are pulverized, they are entirely transformed into the α-AlB_{12} phase [99H1, 99H2]. Single phase crystals of the γ-AlB_{12} structure type are obtainable by cooling an Al-B solution containing a small quantity of Mg [99H2]. Those crystals are not transformed to α-AlB_{12} by pulverization.

preparation [77S, 77H, 60K], crystalline structure [77K, 77H, 60K, 75S, 77M1, 77M2]

Space group: $P2_12_12_1$ [87H].

Structure of γ-AlB_{12} in Fig. 1 [83H, 87H].

Crystal chemistry of α-AlB_{12} and γ -AlB_{12} [99H3].

Preparation of α-AlB_{12} and γ -AlB_{12} [99H4].

lattice parameters
(in Å)

a	16.57	*T* = 300 K	single crystal, X-ray diffraction	85H,
b	17.51			87H,
c	10.14			94W
V	2942 $Å^3$			
a	16.66(10)	*T* = 300 K	single crystal, X-ray diffraction	87K
b	17.69(10)			
c	10.195(35)			

lattice parameters of Si-doped γ-AlB_{12} ($Al_{1.0}Si_{0.7}B_{15.6}$)

a	16.629	*T* = 300 K	X-ray diffraction	87G
b	17.551			
c	10.220			

occupancies of metal sites
(in %)

Al(1)	96.14	*T* = 300 K	X-ray diffraction	87H,
Al(2)	95.34			83H
Al(3)	94.64			
Al(4)	52.34			
Al(5)	74.74			
Al(6)	76.44			87H,
Al(7)	51.14			83H
Al(8)	44.44			
Al(9)	18.84			
Al(10)	19.04			
Al(11)	6.84			

B_{20}-(C_2) and B_{20}-(C_3) units in the γ-AlB_{12} structure in Fig. 2 [83H].

energy gap of Si-doped γ-AlB_{12} ($Al_{1.0}Si_{0.7}B_{15.6}$)
(in eV)

E_g	0.36	T = 300 K	deep level	88W
	0.56		deep level	
	0.69		deep level	
	0.78		deep level	
	0.91		deep level	
	1.00		indirect allowed or non-direct	
	1.71		indirect allowed or non-direct	

Absorption edge of Si-doped γ-AlB_{12} ($Al_{1.0}Si_{0.7}B_{15.6}$) in Fig. 3 [87G, 98W].

IR active phonon wavenumbers
(ν/c in cm^{-1})

ν/c	1110	T = 300 K	obtained from the original data of	94W
	1054		the spectrum in Fig. 4	
	1013			
	968			
	939			
	876			
	792			
	775			
	757			
	731			
	694			
	680			
	640			
	593			
	564			
	503			
	483			
	453			
	411			
	373			
	327			
	298			
	269			
	225			
	190			

Phonon absorption spectrum in Fig. 4 [94W].

activation energies

E_A	0.22 eV	T = 100...375 K	electrical conductivity	91P

electrical conductivity

σ	$2.5 \cdot 10^{-4}\ \Omega^{-1}cm^{-1}$	T = 293 K		91P

microhardness
(in GPa)

H_K	22.8(8)	load 1.96 N	91P
H_V	27.3(12)	load 1.96 N	87K
H	25.56	(+ Cr) hardness type not specified	88B
	24.45	(+ W) hardness type not specified	

microstrength

σ	1.6 GPa	(+ Cr)	88B
	1.46 GPa	(+ W)	

microbrittleness

γ	9.6	(+ Cr)	88B
	19.5	(+ W)	

fracture toughness

K_c	1.8(2) MN $m^{-3/2}$		91P, 87K

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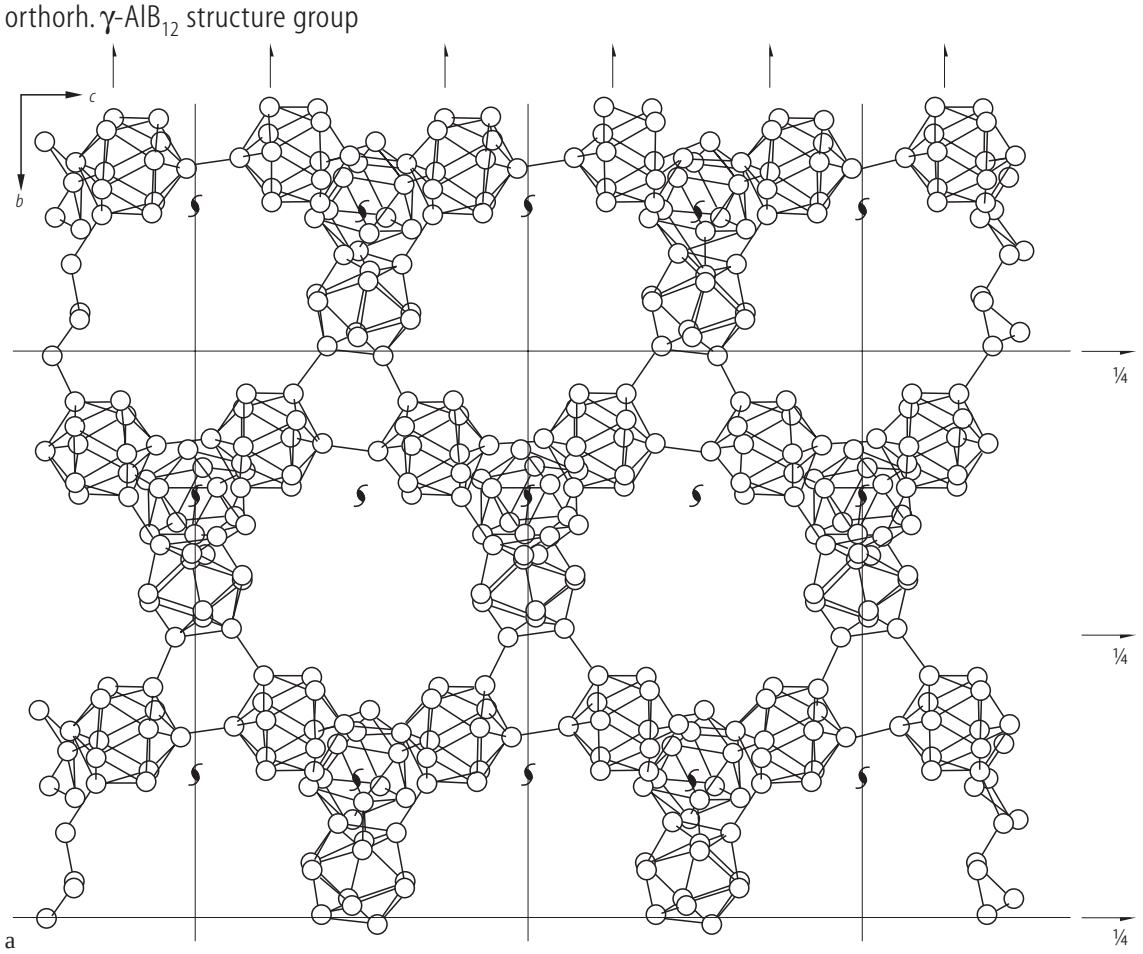
Fig. 1.

Orthorhombic γ-AlB_{12} structure group. Structure in a view parallel to [100]; **(a)** B_{12} icosahedral arrangement, **(b)** features of the linkages between a $B_{20}(C_2)$ unit and B_{12} icosahedra, **(c)** arrangement of the $B_{48}(T_d)$ subunit showing B_{144} (T_d) and truncated tetrahedral holes (the circles represent B_{12} icosahedra) [83H]. For stereoscopic views of the $B_{20}(C_2)$ and $B_{20}(C_3)$ units and of the coordination of the metal sites to the boron framework see [83H].



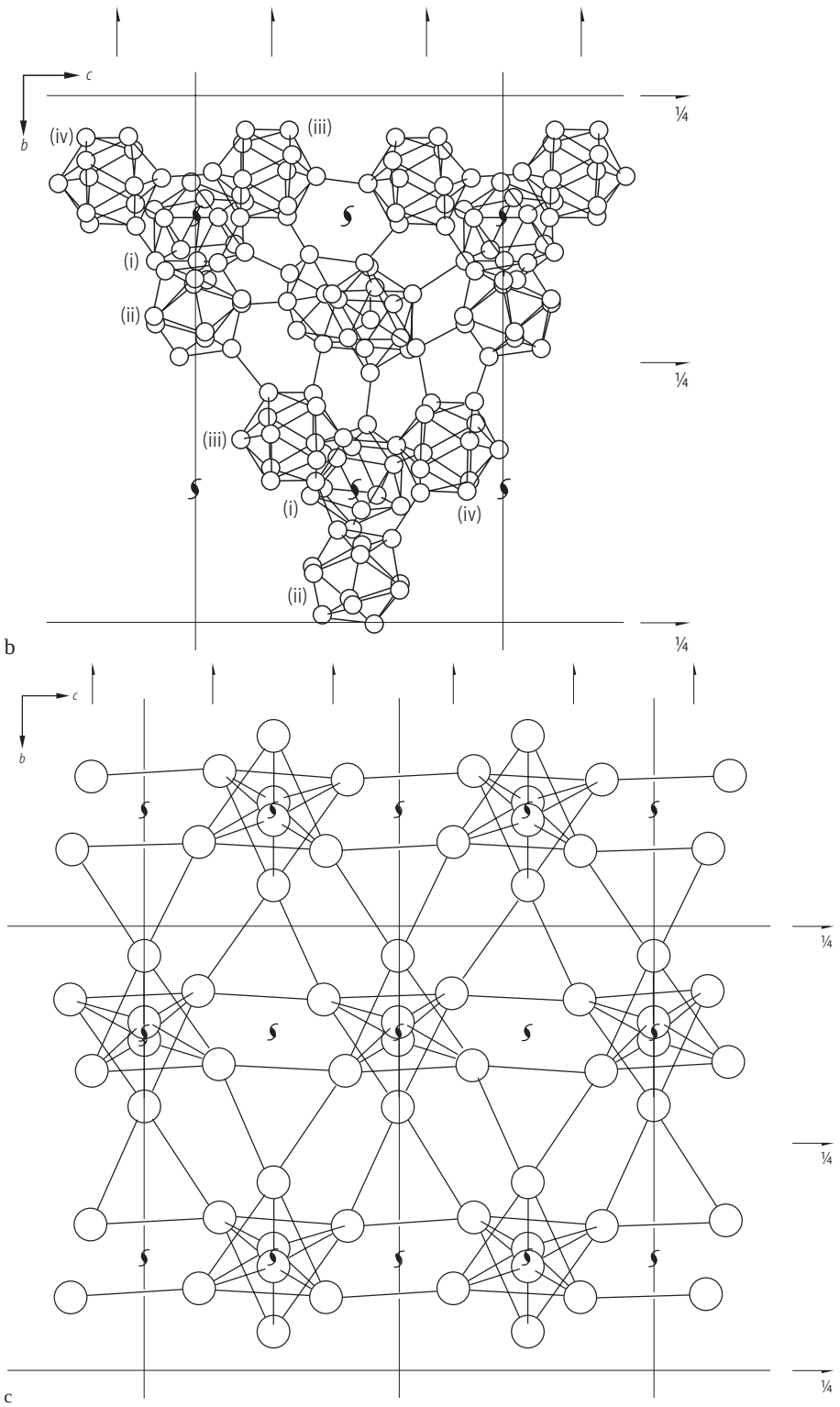

c
b
(iv)
(iii)
(i)
(ii)
(iii)
(i)
(iv)
(ii)
¼
¼
¼
b
c
b
¼
¼
¼
c

Fig. 2.

γ-AlB_{12}. Stereoscopic views of **(a)** B_{20} (C_2) and **(b)** B_{20} (C_3) units of the structure [83H].

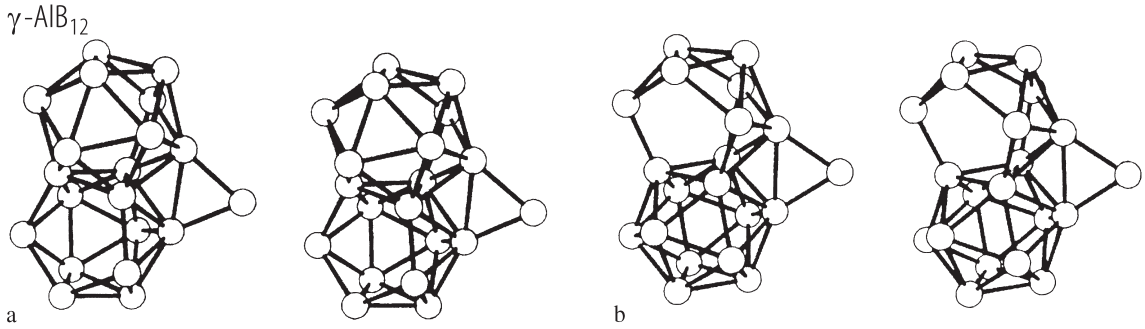


Fig. 3.

γ-AlB_{12} :Si. Absorption edge; absorption coefficient α vs. photon energy [98W] (at higher photon energies results of two different samples).

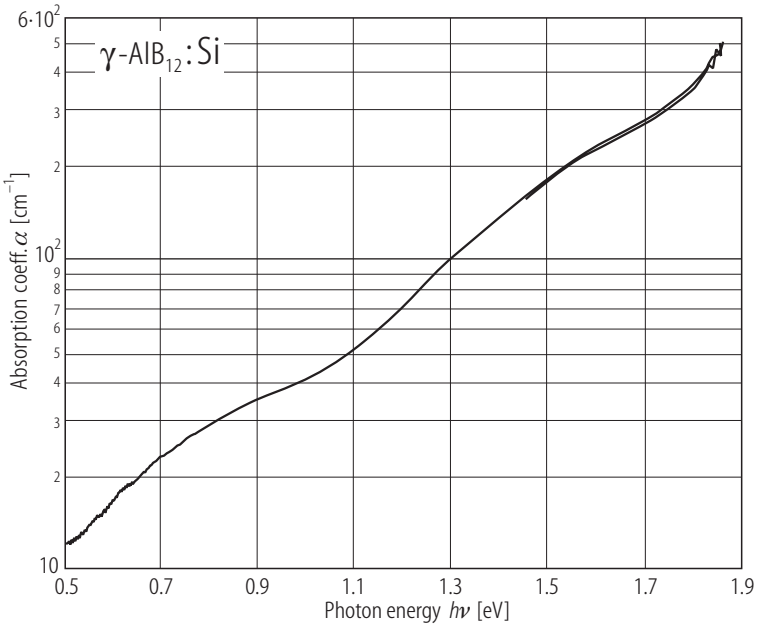


Fig. 4.

γ-AlB_{12}. IR phonon absorption spectrum. Absorption index vs. wavenumber [94W].