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X-ray investigation of the Al–B–N ternary system: isothermal section at 1500 °C: Crystal structure of the $Al_{0.185}B_6CN_{0.256}$ compound

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Abstract

The equilibrium phase diagram has been established using X-ray powder diffraction for the ternary Al–B–N system over the whole concentration region at 1500 °C. No ternary compounds have been observed. The crystal structure of the $Al_{0.185}B_6CN_{0.256}$ compound (*Cmcm* space group, $Z=8$, $a=5.685(2)$ Å, $b=8.903(3)$ Å, $c=9.122(3)$ Å, $V=461.70$ Å^3, $\rho=2.563$ g/cm^3, $\mu=0.17$ mm^{-1}, $R=0.0424$ for 407 reflections with $F_o > 4\sigma(F_o)$) was determined from single crystal X-ray diffraction (automatic diffractometer BRUKER AXS CCD, Mo Kα radiation) and electron microprobe analysis. The structure is related to the $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$ and $Al_{0.325}B_6C$ structures.

Keywords: Alloys; Crystal structure; Phase diagram; X-ray diffraction

1. Introduction

This paper is a part of our investigation of the interaction of Al and B with the elements of groups IV–V of the Periodic Table of Elements.

The ternary and quaternary boride-based compounds receive widespread attention since they often exhibit very interesting magnetic and/or superconducting properties. Aluminum nitride (AlN) is an attractive material for use as substrate and heat sink in electronic devices due to its excellent properties: high electrical resistivity, high thermal conductivity, a moderately low dielectric constant [1–3].

Phase diagrams for the binary boundary systems Al–B, Al–N and B–N have been studied sufficiently [4–11]. Crystallographic data of the elements and binary phases that occur in the Al–B–N system are listed in Table 1. In a review Neronov [12] concludes that there are no reliable data confirming the existence of the AlB_{10} and β-AlB_{12} compounds in the Al–B binary system. Will [7] reported on the crystal structure investigation of the AlB_{10} ($Al_{0.61}B_{6.50}$) compound (space group *Cmcm*, $Z=8$, $a=5.690$, $b=8.881$, $c=9.100$). There is still a controversy as to whether the structure contains carbon. Based on microprobe analysis, Perrotta et al. [13] state that the crystal contains C and the composition of the compound is $Al_{0.253}B_{6.37}C$ whereas Will [7] maintains that no carbon is present, based on chemical analyses. In Ref. [14] Will presented the result of a single crystal investigation of the ternary $AlB_{24}C_4$ or $Al_{0.325}B_6C$ compound with exactly the same lattice parameters and symmetry as was reported previously in Refs. [7,13]. The β-AlB_{12} compound appeared to be a carbon-stabilized ternary compound with the formula $Al_3B_{48}C_2$ [15].

Petzow et al. [16] earlier reported on the investigation of Al–B–N ternary system at 25 °C within the concentration range 0–50 at.% N (Fig. 1). Below we present the result of our investigation of this system at 1500 °C. Moreover, during our studies of the Al–B–C–N samples we were able to obtain several new compounds and the results of an X-ray single crystal investigation and electron microprobe analysis for one of them, $Al_{0.185}B_6CN_{0.256}$, is included in this paper.

2. Experimental procedure

The samples, each with a total weight of 1 g, were synthesized using a computer controlled (program

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Table 1
Crystallographic data of the elements and the binary phases of the Al–B–N ternary system

Compound	Structure type	Space group	Lattice parameters, Å			Ref.
			a	*b*	*c*	
Al	Cu	$Fm\bar{3}m$	4.048			[4,5]
α-B	B	$R\bar{3}m$				[4,5]
β-B	B	$R\bar{3}m$	10.925		23.814	[4,5]
β-B	B	$P4_2/nnm$	8.800		5.050	[4,5]
AlB_2	Own	$P6/mmm$	3.005		3.257	[4–6]
AlB_{10}	Own	$Cmcm$	5.690	8.881	9.100	[4,5,7]
α-AlB_{12}	Own	$P4_32_12$	10.116		14.283	[4–8]
β-AlB_{12}		Orthorhombic	12.343	12.631	10.610	[4,9]
γ-AlB_{12}	Own	$P2_12_12_1$	16.623	17.540	10.180	[5,6,10]
AlB_{31}	Own	$R\bar{3}m$	10.955		23.868	[11]
AlN	ZnS	$P6_3mc$	3.110		4.980	[4,5]
AlN		Cubic	4.104			[5]
BN	C	$P6_3/mmc$	2.5039		6.6612	[5]
BN	ZnS	$F\bar{4}3m$	3.615			[5]
BN	ZnS	$P6_3mc$	2.550		4.240	[5]

Basic98) high-frequency furnace. The starting materials were taken in the form of powders of high purity aluminum, amorphous boron, graphite and aluminum nitride. Pressed mixtures of these materials with different composition were heated in boron nitride crucibles at 1500 °C for 12–14 h in argon or nitrogen atmosphere, and then rapidly cooled to room temperature (during 2–3 h). The samples containing more than 50% of nitrogen were melted in N-atmosphere. Finally, the ground powder of each sample was back pressed into standard holders for powder XRD. Diffracted X-ray intensities were collected on a Philips automated diffractometer system PW1877 (Bragg Brentano goniometer, graphite crystal monochromator, normal focus Cu tube operated at 40 kV and 50 mA). The data were recorded with a 2θ-step size of 0.02° in a 2θ-range of 20.00–100.00° and a counting time of 1 s at each step. The isotypism of the phases was proven by the agreement of the observed powder patterns with those calculated using the program LAZY PULVERIX [17]. The lattice parameters were refined by means of the LATCON [18] and Powder Cell [19] programs.

Single crystals suitable for the X-ray measurements were isolated from the alloys, glued on the top of glass fibres and mounted on the goniometer head. X-ray single crystal diffraction data were obtained using a four circle diffractometer Philips PW1100 and BRUKER AXS CCD with graphite monochromatized Mo Kα radiation (λ = 0.71073 Å). Least squares refinements of the 2θ values of different numbers of strong and well-centred reflections from the various regions of reciprocal space were used to obtain the unit-cell parameters. The data set was recorded at room temperature and the intensities were corrected for absorption, polarization and Lorentz effect.

Electron microprobe analysis of a single crystal was performed using an analyzer JOEL JXA-8600MX to determine the composition. AlN, LaB_6 and C of high purity were used as standards.

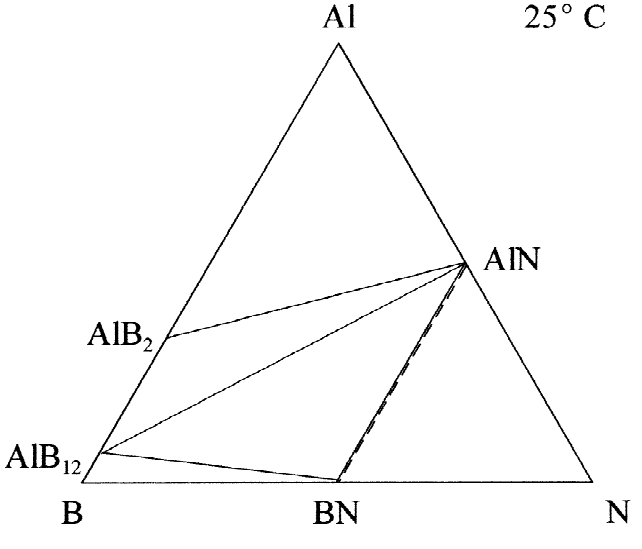

Fig. 1. Isothermal section of the Al–B–N system at 25 °C.

3. Results

3.1. Al–B–N phase diagram: binary boundary systems and isothermal section of the Al–B–N system at 1500 °C

Our investigations of the binary boundary systems at 1500 °C confirmed the existence of the AlB_{12}, AlN and BN compounds.

The sample of $Al_{33.3}B_{66.7}$ composition ('AlB_2') was found to contain two phases, Al and AlB_{12}. The X-ray diffraction data were collected for a single crystal isolated from the surface of this sample in the range $3 \leq \theta \leq 27°$ using a Philips PW1100 diffractometer. The cell parame-

ters were obtained from 33 well-centered reflections ($4.7 \leq \theta \leq 19.7°$). The symmetry was found to be tetragonal: $a = 10.182(2)$ Å, $c = 14.301(2)$ Å. A total of 1864 reflections were observed and collected and 1407 were considered ($I > 2\sigma(I)$). The space group extinctions led to the possible space groups $P4_12_12$ or $P4_32_12$. The obtained result correlates well with the data presented in Refs. [8,20] for the structure of the α-AlB_{12} compound. No evidence for the existence of the AlB_{10}, β- and γ-AlB_{12} and AlB_2 compounds was found. The solubility of the third component in the observed binary compounds was found to be negligible.

The equilibrium phase diagram of the Al–B–N system at 1500 °C was derived using X-ray powder diffractograms of 21 samples. The results of the X-ray phase analyses for several selected samples are presented in Table 2. The isothermal section of the Al–B–N system at 1500 °C is shown in Fig. 2. No ternary compounds were observed.

A critically evaluated isothermal section of part of the

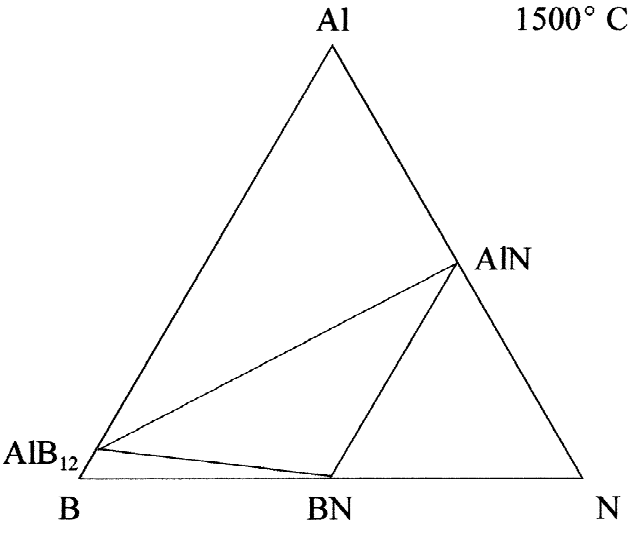

Fig. 2. Isothermal section of the Al–B–N system at 1500 °C.

Table 2
Results of the X-ray phase analyses for the selected samples of the Al–B–N system

N	Nominal composition (in at.%)	Phase analyses	Space group	Structure type	Lattice parameters, Å	
					a	*c*
1	$Al_{80}B_{10}N_{10}$	Al	$Fm\bar{3}m$	Cu	4.0419	
		AlN	$P6_3mc$	ZnS	3.1215	4.9770
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
2	$Al_{63}B_{20}N_{17}$	Al	$Fm\bar{3}m$	Cu	4.0418	
		AlN	$P6_3mc$	ZnS	3.1179	4.9915
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
3	$Al_{52}B_{38}N_{10}$	Al	$Fm\bar{3}m$	Cu	4.0413	
		AlN	$P6_3mc$	ZnS	3.1127	4.9781
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
4	$Al_{65}B_8N_{27}$	Al	$Fm\bar{3}m$	Cu	4.0299	
		AlN	$P6_3mc$	ZnS	3.1196	4.9795
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
5	$Al_{40}B_{43}N_{17}$	Al	$Fm\bar{3}m$	Cu	4.0424	
		AlN	$P6_3mc$	ZnS	3.1109	4.9747
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
6	$Al_{30}B_{10}N_{60}$	AlN	$P6_3mc$	ZnS	3.1120	4.9725
		BN (traces)	$F\bar{4}3m$	ZnS		
7	$Al_{30}B_{30}N_{40}$	AlN	$P6_3mc$	ZnS	3.1190	4.9756
		BN	$F\bar{4}3m$	ZnS	3.6181	
		AlB_{12} (traces)	$P4_32_12$	α-AlB_{12}		
8	$Al_{35}B_{50}N_{15}$	Al	$Fm\bar{3}m$	Cu	4.0428	
		AlB_{12}	$P4_32_12$	α-AlB_{12}		
		AlN	$P6_3mc$	ZnS		
9	$Al_{35}B_{60}N_5$	Al	$Fm\bar{3}m$	Cu	4.0462	
		AlB_{12}	$P4_32_12$	α-AlB_{12}	10.179	14.2937
		AlN (traces)	$P6_3mc$	ZnS		
10	$Al_{25}B_{65}N_{10}$	AlN	$P6_3mc$	ZnS	3.1120	4.9725
		AlB_{12}	$P4_32_12$	α-AlB_{12}	10.179	14.2928
		Al (traces)	$Fm\bar{3}m$	Cu		
11	$Al_{20}B_{70}N_{10}$	AlN	$P6_3mc$	ZnS	3.1120	4.9725
		AlB_{12}	$P4_32_12$	α-AlB_{12}	10.1798	14.2778
12	$Al_{10}B_{80}N_{10}$	AlB_{12}	$P4_32_12$	α-AlB_{12}	10.1860	14.2875
		AlN	$P6_3mc$	ZnS	3.1190	4.9754
		BN (traces)	$F\bar{4}3m$	ZnS		
13	$Al_{10}B_{90}$	AlB_{12}	$P4_32_12$	α-AlB_{12}	10.1824	14.2918
14	$Al_{33.3}B_{66.7}$	AlB_{12}	$P4_32_12$	α-AlB_{12}	10.1915	14.2839
		Al	$Fm\bar{3}m$	Cu	4.0423	

Table 3
Parameters for the single crystal X-ray data collections

Compound	$Al_{0.185}B_6CN_{0.256}$
Space group [10]	*Cmcm* (N.63)
Lattice parameters	
a, Å	5.685(2)
b, Å	8.903(3)
c, Å	9.122(3)
Formula per unit cell	8
Cell volume, $Å^3$	461.70(27)
Calculated density, g cm^{-3}	2.459
Linear absorption coefficient, mm^{-1}	0.17
Number of measured reflections	2970
Maximum scattering angle, deg	73.62
hkl range	$-9 \le h \le 9,\ -14 \le k \le 14,\ -10 \le l \le 9$
Number of unique reflections	488 ($R_{int} = 0.0215$)
Number of reflections with $F_o > 4\sigma(F_o)$	407
Number of refined parameters	60
R, wR_2	0.0424, 0.1174
Goodness of fit	1.080
Highest/lowest residual electron density (e $Å^{-3}$)	0.89/−0.25

Al–B–N system at 25 °C, for the concentration range 0–50 at.% N, is given in Ref. [16] (Fig. 1). The difference between these and our results consists of the existence of the AlB_2 compound at 25 °C. Our results agree well with the data on the binary phase diagram of the Al–B system presented in Ref. [21].

3.2. Single crystal investigation of the $Al_{0.185}B_6CN_{0.256}$ compound

The lattice parameters ($a = 5.685(2)$ Å, $b = 8.903(3)$ Å, $c = 9.122(3)$ Å) and the possible space group *Cmcm* [22] for the blue coloured single crystal indicated isotypism or similarity in the crystal structures with the $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$ and $Al_{0.325}B_6C$ compounds [7,13,14]. The structure was solved in space group *Cmcm* by means of direct methods using SHELXS-86 [23] and refined by a full-matrix least squares program using atomic scattering factors provided by the program package SHELXL-93 [24] and SHELXL-97 [25]. The absorption correction was performed with the assistance of program SADABS [26]. The weighting schemes included a term, which accounted for the counting statistics and the parameter correcting for isotropic secondary extinction was optimized. The final residuals are presented in Table 3. The atomic coordinates, which correspond to their standardized form according to STIDY [27], equivalent and anisotropic thermal parameters and interatomic distances are shown in Tables 4–6, respectively. The projection of the $Al_{0.185}B_6CN_{0.256}$ unit cell on the *YZ* plane is shown in Fig. 3.

3.3. Electron microprobe analysis

The results of electron microprobe analysis of several locations on the single crystal are presented in Table 7 and conform well with the results from our X-ray structural investigation.

4. Discussion

4.1. Atomic coordination and chemical bonds

The Al atoms located between icosahedra of B are surrounded by 10 and 9 neighbors and occupy up to 16.3%

Table 4
Atomic coordinates, occupancy factors (*G*) and equivalent thermal parameters for the $Al_{0.185}B_6CN_{0.256}$ compound

Atom	Wyckoff notation	*x*	*y*	*z*	*G*%	*U* (eq.)
Al1	4*c*	0	0.70906(28)	0.25	16.3(1)	0.00757(86)
Al2	16*h*	0.17223(86)	0.03847(45)	0.05140(74)	5.1(1)	0.01234(149)
C	8*f*	0	0.15342(9)	0.56090(16)	100	0.00773(29)
N	4*a*	0	0	0	51.3(1)	0.00251(53)
B1	8*f*	0	0.45300(11)	0.08590(17)	100	0.00726(30)
B2	8*f*	0	0.24897(11)	0.08960(16)	100	0.00795(30)
B3	8*g*	0.33829(16)	0.01634(11)	0.25	100	0.00772(30)
B4	8*g*	0.15948(17)	0.18043(11)	0.25	100	0.00796(30)
B5	16*h*	0.25424(12)	0.34800(7)	0.15187(12)	100	0.00806(27)

Table 5
Anisotropic thermal parameters for atoms in the $Al_{0.185}B_6CN_{0.256}$ compound

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al1	0.00777(107)	0.00673(221)	0.00820(0)	0.00000	0.00000	0.00000
Al2	0.02032(216)	0.00772(189)	0.00899(421)	0.00446(138)	0.00133(179)	0.00665(135)
C	0.00595(36)	0.01111(43)	0.00612(82)	0.00272(28)	0.00000	0.00000
N	0.00264(64)	0.00294(72)	0.00195(153)	−0.00027(60)	0.00000	0.00000
B1	0.00765(39)	0.00914(41)	0.00499(87)	0.00048(33)	0.00000	0.00000
B2	0.00806(37)	0.00960(45)	0.00618(85)	−0.00167(35)	0.00000	0.00000
B3	0.00815(38)	0.00905(41)	0.00596(89)	0.00000	0.00000	0.00131(26)
B4	0.01080(41)	0.00789(40)	0.00518(90)	0.00000	0.00000	0.00039(27)
B5	0.00822(31)	0.01032(39)	0.00564(74)	−0.00077(21)	0.00049(25)	−0.00101(17)

and 5.1% of the atomic sites. One of these atoms competes statistically with nitrogen. The shortest Al–B and Al–C distances are somewhat shorter than the sum of the radii of Al, B and C. Similar features of the interatomic distances were observed in Refs. [7,13,14].

The structure of the $Al_{0.185}B_6CN_{0.256}$ compound clearly reveals the distorted hexagonal close packing of B icosahedra. The distances between B atoms which form these icosahedra are 1.79–1.84 Å. The B_{12} icosahedra are interconnected via direct bonds ($d_{B-B}=1.78$ Å) (Fig. 4a) and –C– bridges to form a 3D-framework ($d_{B-C}=1.62$ Å). Analogous interatomic distances for these type of bonds are presented in Refs. [13,14,28] for the $Al_{0.253}B_{6.37}C$, $Al_{0.325}B_6C$ and B_4C compounds. The carbon atom is connected with two boron atoms and two of such groups form a hexagon. These hexangular layers are linked via a nitrogen atom (Fig. 4b) to form linear chains –C–N–C–. The interatomic distance C–N = 1.47 Å is in very good agreement with the sum of the covalent radii of the atoms ($R_C=0.77$ Å, $R_N=0.7$ Å). The same values of distances were observed for the $Al_{0.253}B_{6.37}C$ [13] compound, however for the C–B–C chains.

Table 6
Selected interatomic distances (*d*, Å) and coordination numbers of atoms (CN) for the $Al_{0.185}B_6CN_{0.256}$ compound

Atom	*d*, Å	CN	Atom	*d*, Å	CN
Al1–2B3	1.9466(25)		B2–C	1.6150(20)	
–2B4	1.9526(12)	10	–2B5	1.7858(11)	
–4B5	2.0696(17)		–B1	1.8168(16)	8
–2C	2.1153(20)		–2B4	1.8262(14)	
			–2Al2	2.1430(43)	
Al2–2C	1.7480(52)				
–B5	1.9724(45)		B3–B4	1.7798(15)	
–B1	2.0372(47)		–2B5	1.8233(12)	
–B3	2.0523(64)	9	–B3	1.8386(19)	9
–B2	2.1430(43)		–2B1	1.8450(14)	
–B5	2.1528(62)		–Al1	1.9466(25)	
–B1	2.2465(56)		–2Al2	2.0523(64)	
–Al2	2.2767(109)				
			B4–B3	1.7798(15)	
C–N	1.4746(11)		–2B5	1.8213(12)	
–B2	1.6150(20)		–2B2	1.8262(14)	9
–2B5	1.6251(12)	10	–B4	1.8133(21)	
–2Al2	1.7480(52)		–Al1	1.9526(12)	
–2Al	1.9710(47)		–2Al2	2.2101(62)	
–2Al1	2.1153(20)				
			B5–C	1.6251(12)	
N–2C	1.4746(11)	2	–B2	1.7858(11)	
			–B5	1.7903(23)	
B1–B1	1.7766(29)		–B4	1.8213(12)	
–B2	1.8168(16)		–B1	1.8235(11)	9
–2B5	1.8235(11)		–B3	1.8233(12)	
–2B3	1.8450(14)	10	–Al2	1.9724(45)	
–2Al2	2.0372(47)		–Al1	2.0696(17)	
–2Al2	2.2465(56)		–Al2	2.1528(62)	

4.2. Relationship of the $Al_{0.185}B_6CN_{0.256}$, $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$ and $Al_{0.325}B_6C$ structures

The lattice parameters, space group and atomic distributions in the $Al_{0.185}B_6CN_{0.256}$ structure show similarity with $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$ and $Al_{0.325}B_6C$. All these structures contain groups of B atoms that form B_{12} icosahedra interconnected analogously as those in the B_4C

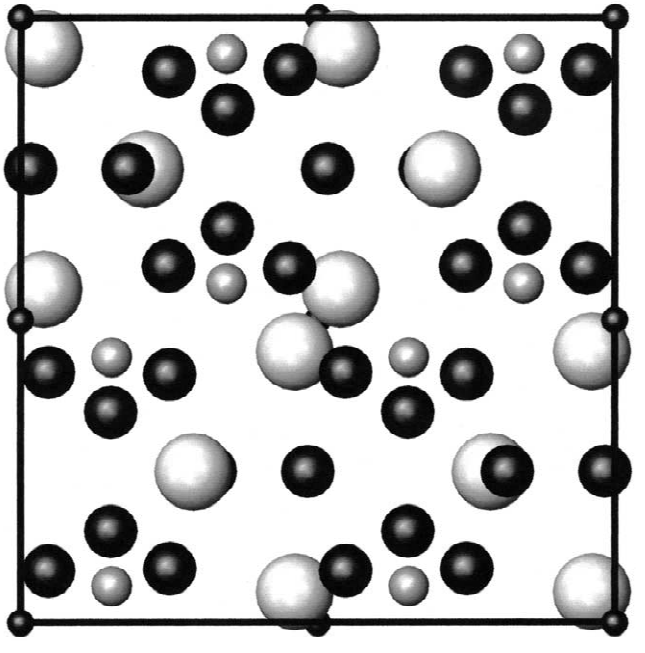

Fig. 3. Projection of the $Al_{0.185}B_6CN_{0.256}$ structure onto the *YZ* plane (white large circles mean Al atoms, black middle size circles are used for boron atoms, grey small circles for carbon atoms and black small ones for nitrogen atoms).

Table 7
Results of the microprobe analyses of the $Al_{0.185}B_6CN_{0.256}$ single crystal

Atom	1	2	3	4	5	6	7	8	9	10
Al, at.%	3.5194	3.6371	3.6018	3.5438	3.6550	3.5265	3.5285	3.6106	3.5421	3.4216
B, at.%	77.8184	78.4648	77.7795	77.8094	77.6309	77.9937	77.1156	78.8483	77.2260	77.6254
N, at.%	5.5646	4.5558	5.5577	6.1209	6.1604	5.6484	6.6392	4.4618	6.7235	5.1707
C, at.%	13.0976	13.3422	13.0609	12.5358	12.5537	12.8314	12.7167	13.0794	12.5083	13.7823
Total, at.%	100.00	100.00	100.00	100.00	100.0	100.00	100.00	100.00	100.00	100.00

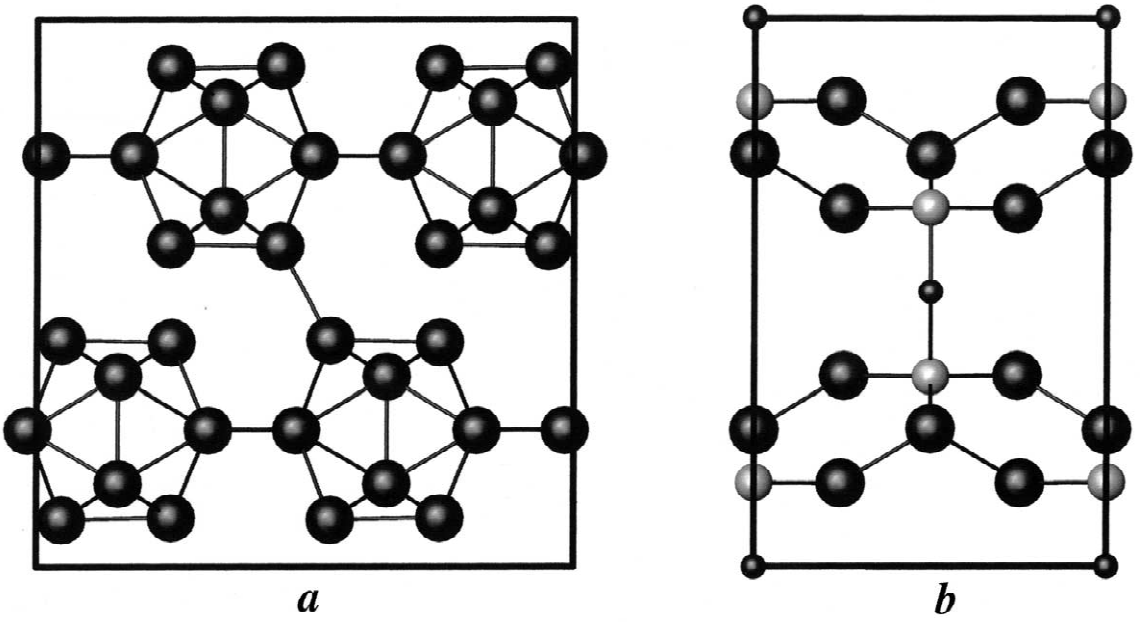

Fig. 4. Arrangement of the B_{12} icosahedra (a) and interconnection between hexagonal layers (b) in the $Al_{0.185}B_6CN_{0.256}$ structure.

and $B_{25}C$ structures. The occupation of the Wyckoff positions by the atoms in the $Al_{0.185}B_6CN_{0.256}$, $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$ and $Al_{0.325}B_6C$ structures are presented in Table 8. In $Al_{0.61}B_{6.50}$, and $Al_{0.253}B_{6.37}C$, the Al atom occupies one of the 8*f* positions which is unoccupied in the $Al_{0.185}B_6CN_{0.256}$ and $Al_{0.325}B_6C$ structures. The 4*a* position is filled by Al in $Al_{0.61}B_{6.50}$ and $Al_{0.325}B_6C$, by B in $Al_{0.253}B_{6.37}C$ and by nitrogen in $Al_{0.185}B_6CN_{0.256}$.

Table 8
Occupancy of the atomic positions in the $Al_{0.61}B_{6.50}$, $Al_{0.253}B_{6.37}C$, $Al_{0.325}B_6C$ and $Al_{0.185}B_6CN_{0.256}$ compounds

Wyckoff position	$Al_{0.61}B_{6.50}$		$Al_{0.253}B_{6.37}C$		$Al_{0.325}B_6C$		$Al_{0.185}B_6CN_{0.256}$	
	Atom	*G*%	Atom	*G*%	Atom	*G*%	Atom	*G*%
16*h*	B	100	B	100	B	100	B	100
16*h*	Al	6.4	Al	7.2	Al	5.6	Al	5.1
8*g*	B	100	B	100	B	100	B	100
8*g*	B	100	B	100	B	100	B	100
8*f*	$Al_{0.31}B_{0.69}$	72.9	C	100	C	100	C	100
8*f*	B	100	B	100	B	100	B	100
8*f*	Al	3	Al	1.5	–	–	–	–
8*f*	B	100	B	100	B	100	B	100
4*c*	Al	18.8	Al	18.8	Al	16.6	Al	16.3
4*a*	Al	26.5	B	73.5	Al	26.6	N	51.1

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References

[1] T.B. Barrett, A.V. Virkar, K.L. More, R.B. Dinwiddie, R.A. Cutler, J. Am. Ceram. Soc. 80 (1997) 1421.
[2] L.M. Sherard, Ceram. Bull. 69 (1990) 1801.
[3] K. Watari, H.J. Hwang, M. Toriyama, S. Kanzaki, J. Am. Ceram. Soc. 79 (1996) 1979.
[4] T.V. Massalski, P.R. Subramanian, H. Okamoto, L. Kacprzak, in: 2nd Edition, Binary Alloy Phase Diagrams, ASM International, Materials Park, OH, 1990.
[5] P. Villars, L.D. Calvert (Eds.), Pearson's Handbook of Crystallographic Data of Intermetallic Phases, ASM International, Materials Park, OH, 1985.
[6] P. Villars, A. Prince, H. Okamoto, Handbook of Ternary Alloy Phase Diagrams, ASM International, Materials Park, OH, USA, 1995.
[7] G. Will, Acta Cryst. 23 (1967) 1071.
[8] I. Higashi, T. Sakurai, T. Atoda, J. Solid State Chem. 20 (1977) 67.
[9] I.A. Kohn, D.W. Eckart, Anal. Chem. 32 (1960) 296.
[10] I. Higashi, J. Solid State Chem. 47 (1983) 333.
[11] I. Higashi, H. Iwamasaki, T. Ito, T. Lundstrom, S. Okada, L.-E. Tergenins, J. Solid State Chem. 82 (1989) 230.
[12] V.A. Neronov, Poroshk. Metall. 10 (1989) 58.
[13] A.J. Perrotta, W.D. Townes, J.A. Potenza, Acta Cryst. B25 (1969) 1223.
[14] G. Will, Acta Cryst. 25 (1969) 1219.
[15] V.I. Matkovic, R.F. Giese, J. Economy, Z. Kristallogr. 122 (1965) 108.
[16] G. Petzow, G. Effenberg, in: Ternary Alloys, Vol. 3, VCH Verlagsgeselschaft, Weinheim, Germany, 1990, p. 192.
[17] K. Yvon, W. Jeitschko, E. Parthé, J. Appl. Crystallogr. 10 (1977) 73.
[18] D. Schwarzenbach, Program LATCON, UNI Lausanne, Switzerland, 1975.
[19] G. Nolze, W. Kraus, Powder Cell for Windows, Version 2.2, Federal Institute for Materials Research and Testing, Berlin, Germany, 1999.
[20] J.S. Kasper, M. Vlasse, R. Naslain, J. Solid State Chem. 28 (1977) 281.
[21] H. Dushanek, P. Rogl, J. Phase Eq. 15 (1994) 543.
[22] T. Hahn (Ed.), Space-Group Symmetry, International Tables for Crystallography, Vol. A, D. Reidel, Dordrecht, 1983.
[23] G.M. Sheldrick, SHELXS-86, Program for Crystal Structure Determination, University of Göttingen, Germany, 1986.
[24] G.M. Sheldrick, SHELXS-93, Program for Crystal Structure Refinement, University of Göttingen, Germany, 1993.
[25] G.M. Sheldrick, SHELXS-97, Program for Crystal Structure Refinement, University of Göttingen, Germany, 1997.
[26] SMART, SAINT, and SADABS Packages, Version 5.1, Bruker AXS, Madison, WI, 1997–1999.
[27] E. Parthé, L. Gelato, B. Chabot, M. Penzo, K. Cenzual, R. Gladyshevskii, TYPIX. Standardized data and crystal chemical characterization of inorganic structure types, in: 8th Edition, Gmelin Handbook of Inorganic and Organometallic Chemistry, Vol. 1, Springer-Verlag, Berlin, 1993.
[28] G. Will, A. Kirfel, A. Gupta, E. Amberger, J. Less-Common Metals 67 (1979) 19.