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CRYSTAL STRUCTURE AND PROPERTIES OF THEORETICALLY PREDICTED AlB_{12}

Jelena Zagorac[1,2*], Branko Matovic[1,2], Milan Pejic[1,3], Katarina Milutinovic[4], Dejan Zagorac[1,2]

[1] VINCA Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

[2] Centre of Excellence "CextremeLab", Centre for synthesis, processing, and characterization of materials for application in the extreme conditions, Belgrade, Serbia

[3]Faculty of Physics, University of Belgrade, Belgrade, Serbia

[4] Technicum Scientific Publishing, Stuttgart, Germany

Corresponding author: jelena@vinca.rs*

Abstract: *Aluminum borides have various industrial applications, used in fuels, explosives, abrasives, and as additives to consolidated materials based on boron carbide. The structure of AlB_{12} is similar to that of boron carbide, including almost regular icosahedrons of boron atoms. The absence of the structure data of some higher aluminum borides and the presence of a large number of reflexes in their diffraction patterns makes the identification of phase compositions very difficult and limits the possibilities of the computer modeling of the AlB_{12}. The crystal structure of AlB_{12} is usually considered as tetragonal α-AlB_{12} (space group $P4_32_12$) and orthorhombic γ-AlB_{12} (space group $P2_12_12_1$) which can be synthesized from high-temperature Al-B melts.*

In our work, we have performed ab initio optimization of the experimentally observed Yannoni's AlB_{12} using GGA-PBE functional and obtained relaxed unit cell parameters and atomic positions. Furthermore, we have predicted three different AlB_{12} structure candidates obtained as a result of the ICSD data mining. The most favorable structure according to total energy ranking was found in the UB_{12} structure type, which crystallizes in the cubic space group Fm-3m. Therefore, for the new cubic AlB_{12}, we have calculated mechanical properties on different pressures and made the comparison with available experimental data in the AlB_{12} system.

Keywords: Aluminium borides, crystal structure, *ab initio* optimization, AlB_{12}.

1. Introduction

Investigation of aluminum borides' properties and development of methods of their production has been studied since the 1950s [1]. However, up to now, not all crystalline structures of the known modifications of aluminum dodecaborides are decoded and the industrial and half-industrial technologies of their powder production remain yet to be developed (at present these materials have not found widespread use and can only be synthesized in small amounts in laboratories). [2, 3] Characteristic properties of aluminum dodecaboride (AlB_{12}) are similar to those of boron carbide (B_4C) due to the similarity of their structures: it is believed that they exhibit high hardness values and thus belong to superhard materials due to their almost regular icosahedral boron configuration [4]. Lightweight ceramics based on polycrystalline AlB_{12} exhibit high fracture toughness, thermal stability, and hardness (they easily produce scratches on silicon carbide, and even on boron carbide).[5]

Of the five phases of binary Al-B systems (AlB_2, AlB_{10}, α-AlB_{12}, β-AlB_{12}, γ-AlB_{12}), which are known for more than 50 years [6], two are shown to be stabilized by impurities (AlB_{10} and β-AlB_{12}) [7-9] and three are considered to be pure binary aluminum borides (AlB_2, α-AlB_{12}, and γ-AlB_{12}). The phases AlB_{10} and β-AlB_{12} were shown to be ternary Al-B-C systems

Aluminium dodecaboride (AlB_{12}) is the hardest boride of the aluminium-boron system. There are two very similar crystalline forms, α-AlB_{12}, and γ-AlB_{12}, and a combination of three-dimensional networks of icosahedra B_{12} and B_{20} is characteristic for both. Crystals of orthorhombic γ-AlB_{12} ($P2_12_12$; a = 16.57, b = 17.51, c = 10.14 Å) are usually obtained as intergrown crystals with tetragonal α-AlB_{12} ($P4_12_12$ or $P4_32_12$; a = 10.16, c =14.28 Å) from high-temperature Al-B

solutions.[10, 11] Efforts to prepare single crystals of boron-rich γ-AlB_{12} showed it's instability, where after pulverizing γ-AlB_{12} transforms completely to α-AlB_{12}.[10, 12]

Aluminum borides can be synthesized using different powder metallurgy routes [13]: high current impulse arc discharge, mixing and annealing of elemental powders, grinding in a ball mill and annealing of AlB_2, grinding of elemental powders in an agate mortar (compacted and annealed afterward), plasma recondensation, radiofrequency thermal plasma method, as well as other techniques used to synthesize aluminum borides [14], such as: grinding of amorphous boron or boron oxide and metal aluminum in a ball mill, laser treatment of aluminum and boron-containing materials, crystallization from the melt of aluminum and boron-containing materials, spark plasmic sintering, thermodynamic, electroarc and other methods.

AlB_{12} is a diamond-hard semiconductor and this extreme hardness makes it a favorable component of polycrystalline cubic boron nitride (PCBN) inserts, which are mainly used in cutting and grinding to replace diamond or corundum. It was also studied in terms of the possibility to be used as the fuel [15] and explosives, as additives to consolidated materials based on boron carbide, and as abrasives [3]. Furthermore, boron treatment is a widely used practice in the industry for removing transition metals such as Ti, V, and Zr that decrease electrical conductivity. For this procedure called boron treatment, Al-B alloys containing AlB_2 and AlB_{12} are mostly used. Also, the AlB_{12}, a wide band gap semiconductor, is an interesting candidate for the detection of thermal neutrons.[16] Because of their hardness, high melting temperature, and semiconductive properties, which are useful in different applications, aluminum borides show promising applications in metallurgy, aerospace field, automotive industry [17], military industry, [18] and electrotechnics [19]. Materials based on AlB_{12} hold great potential for a wide range of applications: because of their lightweight combined with high hardness and fracture toughness, they can be used as shock wave resistant ceramics [3]; since ^{10}B isotope has large thermal neutron absorption cross-section, high-boron materials (of which AlB_{12} has one of the highest among boron compounds – about 83% by mass) is indispensable in nuclear energy application [4]; also aluminum dodecaborides can be used as a fuel, explosives or abrasives [20], impact-resistant and armor materials [18], ceramic filling in metal matrix composites and it is shown to be a promising material for radiation detection (in solid-state devices for the detection of thermal neutrons) [16].

2. Computational details

The idea of this work was to use theoretical *ab initio* methods to relax the structures of α-AlB_{12} and γ-AlB_{12} and calculate their electronic and mechanical properties since there is no enough experimental data on this topic. In order to search for experimental and theoretical structures of AlB_{12} the ICSD database [21, 22] was used. The crystal structures of α-AlB_{12} [12, 23] and γ-AlB_{12} [24, 25] were identified, wherein in both cases aluminum atoms only partially occupy their positions in the structure. This introduces complexity in theoretical models and makes calculations extremely computationally demanding.

To overcome this problem, we took the AlB_{12} model of Yannoni [26], where positions of aluminium atoms are not partially occupied. Furthermore, we have used a data mining procedure [27] and found structure types with the general formula AN_{12}. For every candidate, we have performed local optimization for the AlB_{12} composition. More details of such *ab initio* data mining explorations can be found elsewhere [28, 29]. Structure optimization was performed using GGA functional inside of the Crystal17 code [30]. After DFT optimization, the total energies have been obtained for all calculated structures, which were further analyzed.

For both boron and carbon, an all-electron basis set based on Gaussian-type orbitals was employed. In the case of boron, a [3*s*2*p*1*d*] basis set was used [31, 32] and for aluminium, a [4*s*3*p*1*d*] basis set was used, [33, 34] respectively. The calculation of elastic constants and mechanical properties is fully automated in the Crystal17 code [35, 36]. Space group determination for the investigated modifications was performed using KPLOT software [37]. VESTA code [38] was used for crystal structure visualization.

3. Results and discussion

3.1. *Ab initio* data mining analysis

Local optimization of existing AlB_{12} structures was performed only for the model of Yannoni [26] since this is the unique structure where positions of aluminum atoms are not partially occupied. Results of local optimization including space group, unit cell parameters, and total energy are given in Table 1. Besides Yannoni's model of AlB_{12}, we have found three different structure type candidates using the *ab initio* data mining investigation of the ICSD crystal structure database.[21, 22, 27, 39, 40] Starting from these three models we have optimized AlB_{12} composition with UB_{12}[41], $Al_{12}W$ [42], and $Mn_{12}Th$ [43] structure types. The results for these three phases are also given in Table 1.

Optimized unit cell parameters of the Yannoni's model show good agreement with the experimental values (Table 1). The unit cell parameter a = 10.18 Å is almost the same as the experimental parameter a = 10.17 Å. The difference occurs for the value of the unit cell parameter c, where the theoretical value c = 15.67 Å, is increased in comparison with the experimental c = 14.28 Å. If we follow the coordination of the boron atoms in Figure 1a and after analyzing distances using KPLOT software, one can observe that each boron atom is mostly coordinated with 11 or 12 boron atoms, but there is no regular icosahedral network as in α-AlB_{12} and γ-AlB_{12} compounds. Among the predicted structures obtained using the data mining procedure, the best in total energy ranking is the cubic AlB_{12}-UB_{12} structure type. It appears in the *Fm*-3*m* space group (no. 225), and the unit cell parameters are shown in Table 1, while the predicted structure is shown in Figure 1b. The structure shows the network of regular icosahedra whose presence usually is also characteristic for α-AlB_{12} and γ-AlB_{12} compounds. This structure arrangement is probably the reason why this structure type is ranked as the best in total energy.

Interestingly, there is another predicted AlB_{12} structure with cubic symmetry appearing in space group *Im*-3*m*. It has been calculated in the $Al_{12}W$ structure type and the optimized unit cell parameters are given in Table 1. It has a different arrangement of boron atoms if compared with the UB_{12} structure type. Each of the boron atoms is in the center of 8-fold coordinated polyhedra (Figure 1c). Nevertheless, the $Al_{12}W$ structure type in AlB_{12} is high in energy, supporting the fact that this sort of packing of boron atoms is not favorable for AlB_{12} composition. Finally, the structure type that is highest in the calculated total energy is obtained in the $Mn_{12}Th$ modification of AlB_{12}. Figure 1d shows the characteristic planar arrangement of the boron atoms in this structure type. Similar to the previous case, lacking icosahedral boron arrangement causes a bad ranking in total energy for the AlB_{12} system.

Furthermore, we have calculated curves showing the dependence of Energy vs. Volume and they are shown in Figure 2. The structure type that has the best energy ranking is the UB_{12}. Yannoni's model is presented only with a single point since calculating energy-volume dependence was computationally expensive. Since there is no experimental evidence for the existence of AlB_{12} with the UB_{12} structure type, but keeping in mind that Yannoni's model is experimentally observed, it would be reasonable to expect the existence of UB_{12} structure type in the AlB_{12} system, especially since it has better total energy ranking than Yannoni'model.

Table 1. Space group, unit cell parameters (Å), atomic positions, and total energy values in Hartrees (E_h) for four optimized AlB_{12} modifications obtained using GGA functional.

Space group and modification	Cell parameters (Å) and fractional coordinates	The energy on PBE level (Hartrees, E_h)
	PBE	
AlB_{12}-UB_{12} type *Fm*-3*m* (225)	*a* = 7.39 Al (0 0 0) B (0.3304 0.3304 1/2)	-540.0656
AlB_{12}-Yannoni $P4_12_12$ (92)	*a* = 10.18, *c* = 15.67 Al (0.0696 0.1814 0.1976) B(0.9609 0.0620 0.1170) Al (0.9290 0.7478 0.0183) B (0.8544 0.0930 0.1981) B (0.3043 0.1836 0.1761) B (0.7823 0.8362 0.1138) B (0.4875 0.8582 0.2874) B (0.4894 0.8872 0.0291) B (0.3606 0.8842 0.1030) B (0.6818 0.1945 0.0420) B (0.0770 0.9592 0.9887) B (0.9042 0.9241 0.1667) B (0.4134 0.0544 0.1419) B (0.5234 0.9462 0.1893) B (0.3129 0.0376 0.2358) B (0.6961 0.0032 0.1832) B (0.0189 0.8544 0.2394) B (0.6241 0.9100 0.0997) B (0.2237 0.8868 0.1778) B (0.8070 0.1235 0.9841) B (0.1964 0.9401 0.0652) B (0.7230 0.1683 0.1461) B (0.2160 0.0976 0.0071) B (0.5821 0.0869 0.1084) B (0.1991 0.2425 0.0906) B (0.0794 0.9632 0.1559) Exp. *a* = 10.17(1); *c* = 14.28(1) [26]	-539.9941
AlB_{12}-$Al_{12}W$ type *Im*-3*m* (229)	*a* = 5.74 Al (0 0 0) B (0.2196 0.2196 1/2)	-539.8059
AlB_{12}-$Mn_{12}Th$ type *I*4/*mmm* (139)	*a* = 8.80, *c* = 3.17 Al (0 0 0) B (1/4 1/4 3/4) B (0.7436 0 0) B (1/2 0.2615 0)	-539.7554

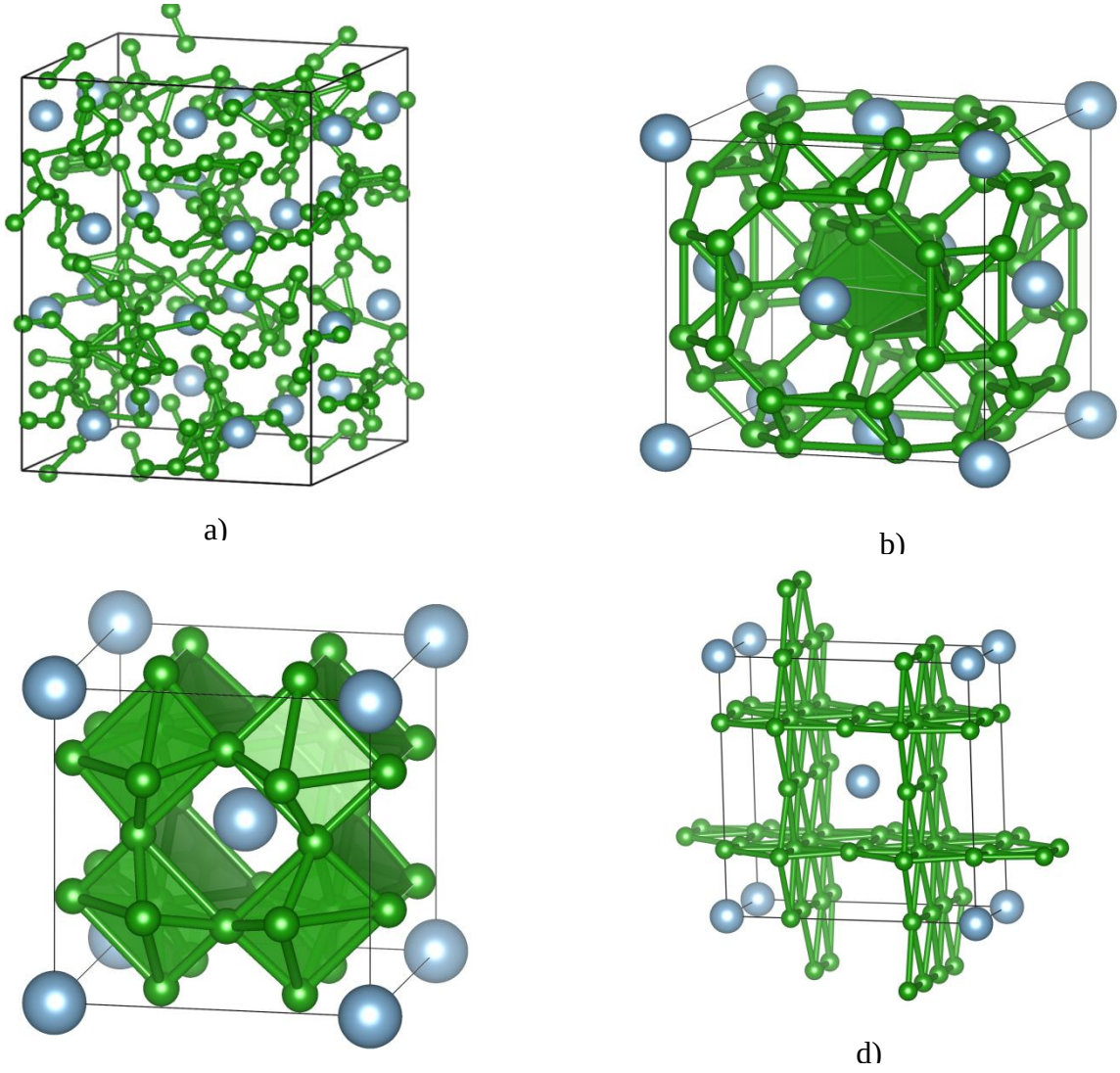

Figure 1. Crystal structures of the: a) AlB_{12}-Yannoni model; which is experimentally observed; and b) UB_{12} type; c) $Al_{12}W$ type and d) $Mn_{12}Th$ type in AlB_{12} system, which is theoretically predicted in this study.

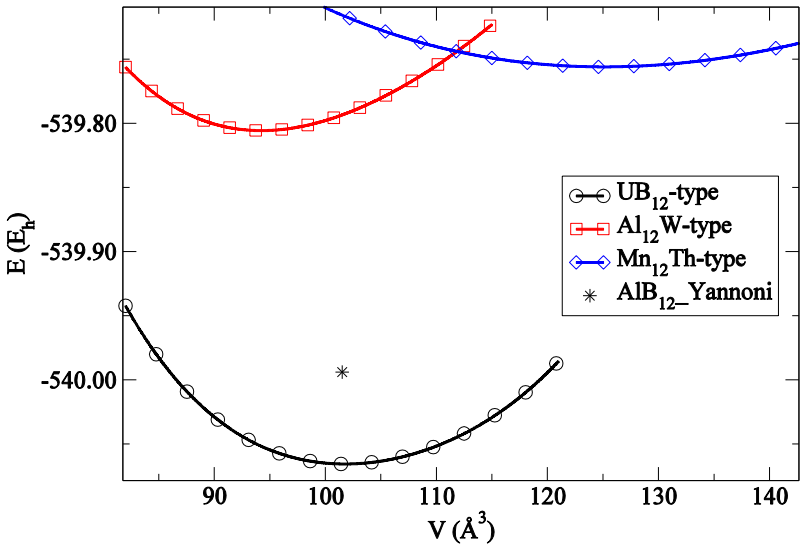

Figure 2. Energy-volume curves calculated using PBE functional for four different structure arrangements in the AlB_{12} system.

3.2. Mechanical properties of a cubic AlB_{12} at extreme pressure conditions

Since our investigation proved cubic AlB_{12} with the UB_{12} structure type as a potential candidate for experimental synthesis, our next step was to calculate its mechanical properties, especially hardness up to 50 GPa. In the sequence of our investigation, we have calculated elastic constants C_{ij} for AlB_{12} with the UB_{12} structure type, and second-order elastic constants are given in Table 2. For the polycrystalline materials, the mechanical properties are usually described by various elastic moduli, such as bulk modulus *B*, shear modulus *K*, and Young's modulus *E*, which are the measure of the compressibility, rigidity, and stiffness. In further work, obtained elastic constants from Table 2 were used to calculate elastic moduli: *B*, *K*, *E*, and *v* for investigated AlB_{12} with the UB_{12} structure type for the pressure range 0-50 GPa.

Table 2. Calculated bulk modulus *B* (GPa), shear modulus *K* (GPa), Young's modulus *E* (GPa), Poisson's ratio *v*, hardness V_H (GPa), and elastic constants AlB_{12} (UB_{12}-type).

AlB_{12} (UB_{12}-type)	C_{11}	C_{12}	C_{44}	***B***	***K***	***E***	***v***	V_H
0	254	177.1	167.2	202.7	93.6	243.3	0.3	9.50
5	273.6	193.9	177.3	220.5	98.4	257.1	0.3	9.47
10	292.7	210.3	185.2	237.8	102.5	268.8	0.3	9.37
15	313.7	228.9	195.3	257.2	107.1	282	0.3	9.30
20	331.3	246.4	204.8	274.7	110.4	292	0.3	9.12
25	349.3	263.4	213.8	292.1	113.9	302.5	0.3	9.01
30	366	280.5	222	309	116.6	310.7	0.3	8.83
35	383.1	296.9	229.9	325.6	119.6	319.8	0.3	8.72
40	399.2	313.6	237.4	342.2	121.9	326.8	0.3	8.53
45	415.3	330.2	244.2	358.6	124	333.5	0.3	8.35
50	430.4	346.1	251	374.2	125.8	339.5	0.3	8.17

Hardness V_H is related to the elastic and plastic properties of materials, and can be calculated from bulk modulus (B) and shear modulus (K) according to equation (1) from Ref. [44]:

$$V_H = 0.92(K/B)^{1.137}K^{0.708} \quad (1)$$

Values for the hardness of AlB_{12} (UB_{12}-type) in the pressure range 0-50 GPa are given in Table 2. According to [2] materials sintered from α-AlB_{12} powders have hardness ≈ 24 GPa. With the increased pressure hardness values are decreasing from 9.50 GPa at 0 GPa pressure down to 8.17 GPa at 50 GPa pressure. Our calculations show that the hardness of AlB_{12} is drastically decreased if the UB_{12} structure type is adopted, which can have an enormous effect on future technological applications. We can conclude that the crystal structure and the boron coordination have the greatest influence on mechanical properties. Furthermore, Poisson's ration v provides information about the ductility/brittleness of the materials. If the value of v is smaller than 0.26, the material will have brittle behavior. Otherwise, as in the case with UB_{12} structure type, the AlB_{12} appears to be ductile (v=0.30). Interestingly, the value of the Poisson's ration v doesn't depend on pressure, and ductility is preserved for the whole investigated pressure range.

4. Conclusion

We have investigated the AlB_{12} system and performed structure prediction using *ab initio* data mining investigation. We have found three new structure candidates as the result of the data mining of the ICSD database (UB_{12}, $Al_{12}W$, and $Mn_{12}Th$). Besides them, we have optimized experimentally observed Yannoni's model of the AlB_{12} compound. Among these four candidates, the best ranking in total energy has been observed for the UB_{12} structure type with the cubic *Fm*-3*m* space group.
We have investigated structural properties for four structure candidates and additionally mechanical properties for the AlB_{12} with UB_{12} structure type, and the effect of extreme conditions of high pressure up to 50 GPa. According to Poisson's ratio AlB_{12} with UB_{12} exhibits ductile character, while the hardness decreases with the pressure increase. In this context, we conclude that the crystal structure and the boron coordination have the greatest influence on mechanical properties, as well on future scientific and technological applications of AlB_{12}.

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