Structure boron rich type b25c space group P-4 2 m the lattice is accentric primitive tetragonal laue symmetry 4/mm

Structure boron rich type $b_{25}c$ space group P-4 2 m the lattice is accentric primitive tetragonal laue symmetry 4/mm

M C Fajrah[1,*], B Soegijono[2], and F B Susetyo[3]

[1]Departement Of Physics, Faculty, Institut Sains Dan Teknologi Nasional,
[2]Departement Of Physics, Universitas Indonesia,
[3]Departement of Mechanical Engineering, Universitas Negeri Jakarta

[*]Email: musfirah@istn.ac.id

Abstarct. A reaction between carbon and boric acid has been carried out through a solid state reaction. The sample is heated at 400ºC. Characterization tests were carried out with X-Ray Diffraction (XRD) equipment and GSAS analysis. Based on the analysis of the results of the sample has the structure of boron rich type $B_{25}C$ initial lattice parameters a = b = 8.753 Å, c = 5, 093Å after refine chi 1.8 a = b = 8.730469Å c = 5.827706Å, with angles α = β = ϒ = 90º Space Group P -4 2 m the lattice is accentric primitive tetragonal laue symmetry 4/mm multiplicity of a general site is 8 at the atomic position (x, y, z) B_1 B_2 B_3 B_4 B_5 B_7 B_8 B_9 B_{10} B_{11} B_{12} B_{13} B_{14} B_{15} B_{25}.

1. Introduction

Boron Carbide is one of the hardest materials ever known, third rank below diamond and boron nitride. This material is the hardest material that can be produced in large quantities. It was discovered in the mid-19th century as a result of the production of borid metal, and was studied in detail in 1930 [1].Chemically boron carbide is expressed as B_4C, but in reality it has a wide composition range to form the composition of B_4C, usually through a composition $B_{13,65}C_{2,85}$, $B_{10}C$, B_8C, $B_{13}C$, $B_{25}C$ and others to reach B_4C [2]. Certain phases of composition variation may be in the mixture. Boron carbide is generally produced by reacting carbon (C) with B_2O_3 in an electric arc furnace, through a carbothermal reduction process or by a gas phase reaction [3].Based on thermodynamic instability it has been reported about some of the evolution of crystal structures and phases in micropyretics formed by boron rich, namely B_4C and B_8C [4].This research specifically studies the evolution of the $B_{25}C$ rich type boron crystal structure, using the results of the X-Ray Diffraction experiment then analyzed with the GSAS program and partly analyzed in theory based on a review of the book.

2. Experiment Methode

The Mixing process between boric acid-activated carbon using the mole ratio 7: 4 was done at 100°C. The mixing continued until the mixture dry and become grayish black powder. The grayish black powders were heated for 5 hours at 100°C, which aims to remove residual H_2O present in the sample during the mixing process. The combustion process is done in a furnace at 400ºC for 3 hours. The high crystallinity of boron carbide was obtained. The Characterization were done by means of X-ray diffractometer with radiation Cu kα with wavelength 1.54187 Å and 2θ between angle 15º-90º. The results were analyzed using the program package GSAS (General Sructure Analysis System), to

determine the crystal structure of the phases formed, also uses theory based on book reviews. Scanning electron microscopy analysis was conducted to determine the pattern of morphology that is formed[5].

3. Result and Discussion

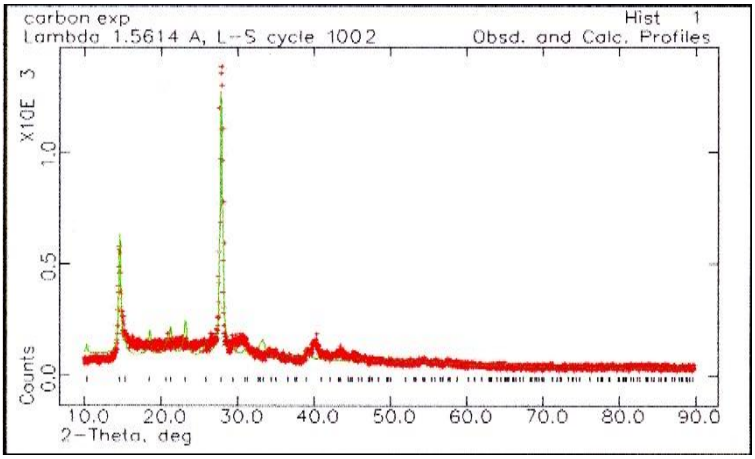

Figure 1. X Ray Difraction Pattern Boron carbide Boron Rich Type $B_{25}C$[5].

The results of X-Ray Diffraction were analyzed using GSAS, the initial crystal structure data identified was phase $B_{25}C$ space group P -4 2 m, lattice parameters a = b = 8.753Å c = 5.093Å angles α = β = γ = 90 tetragonal crystal system. After refine until the residue $\chi 2$ = 1.8 phase B25C space group P -4 2 m the lattice parameter becomes a = b = 8.730469Å c = 5.827706Å angles α = β = γ = 90 tetragonal crystal system

This final result is still in the $B_{25}C$ type boron rich phase, thus the above evidence supports the formation of the boron carbide system from elementary boron. That the lattice parameter results are very compatible with the tetragonal crystal system, Same as the Isometric system, the Tetragonal crystal system has 3 crystal axes, each perpendicular to each other. Axes a and b have the same length units. While the c axis is different, it can be longer or shorter but generally longer [6]. In actual conditions, Tetragonal has an axial ratio a = b ≠ c, which means that the length of the a axis is the same as the b axis but not the c axis and has a crystallographic angle α = β = γ = 90° [7]. This means, in this system, all the crystallographic angles (α, β and γ) are perpendicular to each other (90˚) as shown in Figure 2.6 below.

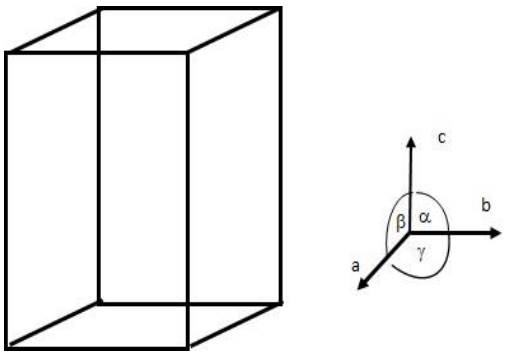

Figure 2. Boron Rich Type $B_{25}C$ Crystal Lattice Simple Tetragonal-P[7].

Tetragonal system -P crystal lattice a = b ≠ c, α = β = γ = 90˚ when connected to the P-4 2 m space group, the P symbol indicates that the system is primitive where the atoms are only located in each corner shows that this is a simple tetragonal.

In the crystal system it is determined by the presence of a single -4 axis in the crystal, which means it produces a group of -4 (S_4) points which have the order h = 4 [8]. That this symmetry operation can be

added and is always in the crystal system, means that it has a mirror reflection and 2-fold rotation placed in a very strategic orientation [9] [8]. For example, if we add a 2-fold rotation about the direction perpendicular to the 4-fold axis, say along a [10] [8], consider other symmetry operations if something is produced. Note that the so-called direction 4 or -4 in the P -4 2 m space group is a 4-fold direction where this direction becomes so important, because this is the main axis or direction unique to tetragonal crystals [11] [8].

It is conventional to place the symbol "4" first, in international notation the first "2" after the "4" refers to the 2-fold rotation about a and to an equivalent 2-fold rotation about b as a consequence of the 4-fold rotation. While the second "2 "refers to diagonal the 2-fold rotation. As before this illustrates a direction perpendicular to the main axis 2 fold [12] [8] This symmetry operation can be seen by referring to the point group 422 (D_4) [13] [8]. That a symmetry operation to groups of points 4 and -4, for example, reflections even though the mirror plane is placed normally on a 4-fold axis produces a centrosymmetric point 4 / m (C_{4h}) group [14] [8].

Another related thing is that it can make reflections through a 4-fold axis on fields a and c [15] [8]. With the argument that this means another mirror area diagonally between axes a and b, giving a 4mm point group, and can add a mirror plane on the 2-fold axis perpendicular to c [16] [8].

The result is another centrosymmetric point group 4 / m 2 / m or 4 / mm, and finally we can add to the axis point group 2 times perpendicular to c along a. Whereas the mirror plane is diagonal along from the -ab plane in the point group -42m (D_{2d}) [17].

Space Group P -4 2 m the lattice is acentric primitive tetragonal laue symmetry 4 / mm, has eight operations of this position equivalent positions are, as table 1.

Table 1. Position of P-4 2 m equivalent atoms which have eight operations on Boron Rich Type $B_{25}C$.

No	Posisi Atom			No	Posisi Atom		
(1)	x	y	Z	(2)	y	-x	-z
(3)	-x	-y	-z	(4)	-z	x	-z
(5)	-x	y	-z	(6)	y	x	Z
(7)	x	-y	-z	(8)	-y	-x	Z

That eight equal positions are generated by the space group P -4 2 m by placing the -4 (S_{34}) symmetry operating axis parallel to c and in the cell unit [18] [8], as shown in Figure 3.

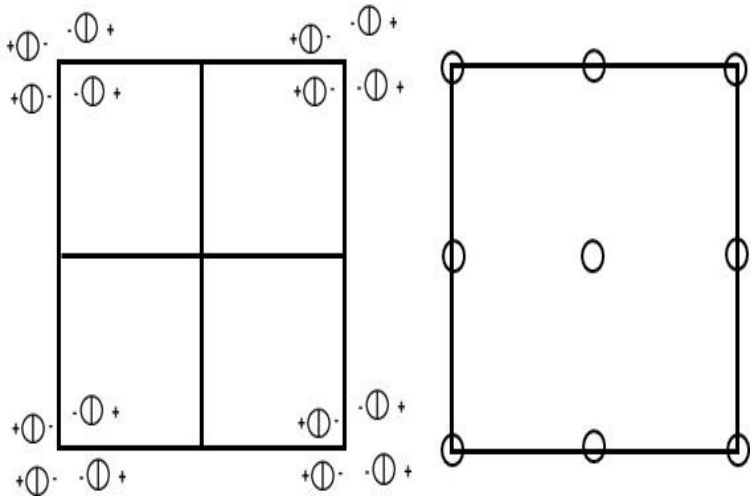

Figure 3. Boron rich type $B_{25}C$ symmetry operation -4 parallel to the c axis [8].

This results in atomic position points as described in table 2.

Table 2. Boron rich type B25C operation symmetry -4 produces an atomic position[8].

No	Posisi Atom		
1	x	y	Z
2	-y	x	-z
3	-x	-y	z
4	y	-x	z

Figure 3 illustrates the axis of the screw which is placed perpendicular to the axis as is the case with 2 fold axes in the point group -4 2 m (D_{2d}) and this intersects the -4 axis along the line at the atomic position x ¼ 0 and this results in a four position equivalent with atomic positions [19] [8], in table 3.

Table 3. Atomic positions resulting from symmetry operations of -4 2 m Boron Rich Type $B_{25}C$ [8].

No	Posisi Atom		
1	½+y	½+x	Z
2	½-x	½+y	-z
3	½-y	½-x	z
4	½+y	½-y	-z

The last four points relate to the first four by the mirror plane parallel to c at position 45° to the screw axis (such as the mirror plane 45° to the 2-fold axis in the -4 2 m point group) [20] [8]. Regarding boron carbide type boron rich type $B_{25}C$, the relationship with the position of the atoms produced both on the B atom and the C atom with symmetry can be explained in table 4.

Table 4. Relationship of atomic positions B and C with symmetry operations on Boron Rich $B_{25}C$ Type.

No	Type u23 pn	Atom	Multi	Symmetry	frac	X	Y	Z
1	B	B1	1	-4 2 m	1.0000	0.0000	0.0000	0.0000
2	B	B2	1	-4 2 m	-8.2826	0.5000	0.5000	0.5000
3	B	B3	4	2	1.0000	0.4345	0.0000	0.0000
4	B	B4	4	2	9.8552	0.9273	0.5000	0.5000
5	B	B5	4	2	-2.6148	0.0000	0.5000	0.8390
6	B	B6	4	2	-1.6728	0.0000	0.5000	0.3930
7	B	B7	4	M	5.4981	0.1241	0,1141	0,3803
8	B	B8	4	M	2.9517	0,6183	0.6113	0.1207
9	B	B9	4	M	-5,4952	0.2473	0.2473	0,5849
10	B	B10	4	M	7.8129	0.7443	0.7443	0.9150
11	B	B11	8	1	-3.1999	0.3260	0.0889	0.3995
12	B	B12	8	1	-2.9072	0.8260	0.5892	0.1019
13	B	B13	8	1	5.8670	0.2268	0.0809	0.8780
14	B	B14	8	1	8.0336	0.7252	0.5802	0.4135
15	C	C15	1	-4 2 m	6.1598	0.0000	0.0000	0.5000
16	C	C16	1	-4 2 m	1.0000	0.5000	0.5000	0.5000

If the X-Ray Diffraction results have been analyzed to produce Boron carbide boron Rich Type $B_{25}C$ Space Group P -4 2 m the lattice is accentric primitive tetragonal laue symmetry 4 / mm multiplicity of a general site is 8 at the atomic position (x, y, z) B_1 B_2 B_3 B_4 B_5 B_7 B_8 B_9 B_{10} B_{11} B_{12} B_{13} B_{14} B_{15} B_{25},

the morphological results can be explained based on the results of the Scanning Electron Microscopy (SEM) magnification.

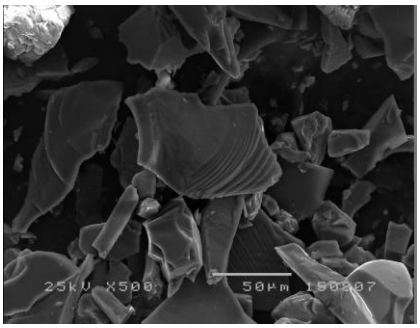

Figure 4. Morphology Boron Carbide Boron Rich $B_{25}C$.

4. Conclusion

Boron carbide boron Rich type $B_{25}C$ space group P -4 2 m, lattice parameter a = b = 8.753Å c = 5.093Å angles $\alpha = \beta = \gamma = 90$ tetragonal crystal system. After rifine until the residue $\chi 2 = 1.8$ phase $B_{25}C$ space group P -4 2 m the lattice parameter becomes a = b = 8.730469Å c = 5.827706Å angles $\alpha = \beta = \gamma = 90$ tetragonal crystal system. Boron Rich Type B25C Crystal Lattice Simple Tetragonal-P, Space Group P -4 2 m the lattice is acentric primitive tetragonal laue symmetry 4/mm, have eight symmetry operation. Boron Rich Type $B_{25}C$ symmetry operation -4 parallel with c axes. Relationship of atomic positions B and C with Symmetry Operations on Boron Rich Type B25C, the lattice is accentric primitive tetragonal laue symmetry 4 / mm multiplicity of a general site is 8 at the atomic position (x, y, z B_1 B_2 B_3 B_4 B_5 B_7 B_8 B_9 B_{10} B_{11} B_{12} B_{13} B_{14} B_{15} B_{25}.

References

[1] Kalandadze G I, Shalamberidze S O and Peikrishvili A B 2000 *J. Solid State Chem.* **154** 194-8
[2] Alizaded A, Nassaj E T and Sani N E H 2003 *J. Eur. Ceram. Soc.* **24** 3227-34
[3] Mondal S and Bathia A K 2004 *J. Eur. Ceram. Soc* **25** 287-291
[4] Mohanty R M, Balasubramanian K and Seshada S K 2011 *Advances In Ceramics, ISBN:978 953-307-504-4, InTech*, 128-138
[5] Fajrah M C and Soegijono B 2014 *Adv. Mater. Res.* **896** 609-12
[6] Rizqigeos 2013 sistim kristal tetragonal *Blok Geologi* **April 13**
[7] Slideshare.net 2014 Mineralogi dan kristalografi sistim tetragonal, *USTJ Jayapura*
[8] Burns G and Glazer A M 1990 *Space groups for solid satate scientists* (Academic Press, INC) 64-116
[9] Barlow W 1894 *On the geometric properties of homogeneous rigid structures and their aplication to crystals*, Z. Krist 23 1 (in German) (in Gerald Burns A. M Glazer)
[10] Buerger M J 1956, 1963 *Elementary crystallography an introduction to the fundamental geometric features of crystals* (New York Willey (in Gerald Burns A. M Glazer))
[11] Buerger M J 1971 *Introduction to crystal geometry* (New York McGraw-Hill (in Gerald Burns A. M Glazer)
[12] Burckhardt J J 1966 *The motion groups of crystallography* Birkhauser, Basel (in German) (in Gerald Burns A. M Glazer)
[13] Burckhard J J 1967 *His Exact Sci.* **4** 235 (in German) (in Gerald Burns A. M Glazer)
[14] Burns G 1985 *Solid state physics* (New York: Academic Press (in Gerald Burns A. M Glazer))
[15] Fedorov E S 1967 *Vseross. Min. Obshch, Zap.*(11) 28, 1 (in Russian). A Full Translation by D.

and K. Harker is Given in *The American Crystallographic Association Monograph* No.**7** (in Gerald Burns A. M Glazer).

[16] Hilton H 1963 *Mathematical crystallography and the theory of groups of moment* (New York Clarendon, Oxford; Reprinted by Dover) (in Gerald Burns A. M Glazer)

[17] Schoenflies A 1891 *Theory of crystal structure* (Teubner, Leipzig, German) (in Gerald Burns A. M Glazer)

[18] Sohncke L 1879 Development of a theory of crystal structure (Teubner, Leipzig, German) (in Gerald Burns A. M Glazer)

[19] Terpstra P 1955 Introduction to the space groups (Walters Groningen) (in Gerald Burns A. M Glazer)

[20] Wyckoff R W G 1930 *The analytical expression of the results of the theory of space groups* (Washington: Carnegie Inst., (in Gerald Burns A. M Glazer))