A new phase of aluminium silicon carbide, $Al_4Si_2C_5$

X-ray powder diffraction data of α- and β-aluminium silicon carbide of Al_4SiC_4 was reported by Barczak [1] in 1961. Subsequently, a new unit cell dimension of α-phase different from Barczak's was proposed by Schneider [2] in 1978. He gave a new index, different from that given by Barczak on the X-ray powder diffraction profiles of the α-phase.

We have recently succeeded in synthesizing a new compound of aluminium silicon carbide, $Al_4Si_2C_5$. An attempt has been made to determine the unit cell dimensions of this new compound. The X-ray powder diffraction pattern has been successfully indexed here.

Silicon carbide (a product of Ibigawa Denko Co Ltd, β-type, particle size $< 3\,\mu m$, the purity $> 99.9\%$, oxygen content ≈ 0.2 wt %) and Al_4C_3 powder (a product of Alfa Products Co, − 100 mesh) were mixed according to the composition of $Al_4Si_2C_5$ with a ball mill made of polyethylene. Approximately 3 g of the mixture was packed into a graphite die (15 mm diameter) and heated at a rate of $50^\circ\,C\,min^{-1}$ to 1970° C in an argon atmosphere. The specimens were maintained at that temperature for a few minutes and then rapidly cooled by turning off the electric power of the heater. The time constant calculated from the recorded cooling curve was ~ 3 min. During this procedure, hot-pressing of the specimen was avoided in order to prevent the extrusion of the specimen from the die. After cooling, the recovered specimen was crushed and powdered for the X-ray investigation. The X-ray powder diffraction data showed that the specimen consisted mainly of $Al_4Si_2C_5$ together with a small amount of α-phase.

The X-ray powder diffraction data was taken by Rigaku Geigerflex using Cu*Kα* X-ray radiation with an Ni-filter and a scintillation counter detector scanning at $2\theta - 1^\circ$ per minute. The reflections were collected in the 2θ-range from 10° to 110°. The X-ray diffraction symmetry in the single crystal method [3] revealed that the space group of the crystal belongs to $R\bar{3}m$ or $R3m$. The unit cell dimension is $a_0 = 13.50$ Å, $\alpha = 13.83^\circ$ in the rhombohedral lattice and $a = 3.25$ Å, $c = 40.11$ Å in the hexagonal lattice.

Using the hexagonal cell dimension mentioned above, the powder diffraction profiles were successfully indexed in the range of 2θ from 10° to 110°. The calculated and observed planar spacings, observed 2θ, and observed intensity distribution I/I_0 are shown in Table I together with their indexes.

The new compound, $Al_4Si_2C_5$ was synthesized only when the ingredients were rapidly quenched

TABLE I X-ray powder diffraction data for $Al_4Si_2C_5$. In this table, *h k l* refer to the hexagonal unit cell

hkl	d_{calc}	d_{obs}	$2\theta_{obs}$	I/I_0
$0\,0\,3$	13.37	13.37	6.60	12
$0\,0\,9$	4.46	4.46	19.91	10
*$0\,0\cdot12$	3.34	3.35	26.57	90
$1\,0\,1$	2.81	2.81	31.86	71
$1\,0\,\bar{2}$	2.79	2.79	32.07	59
$0\,0\cdot15$	2.67	2.67	33.48	27
$1\,0\,\bar{5}$	2.66	2.66	33.71	31
$1\,0\,7$	2.53	2.53	35.49	5
$1\,0\,\bar{8}$	2.46	2.45	36.59	41
$1\,0\cdot10$	2.30	2.30	39.05	62
$1\,0\cdot\overline{11}$ $0\,0\cdot18$	2.23	2.23	40.47	100
$1\,0\cdot13$	2.08	2.08	43.47	13
$1\,0\cdot16$	1.87	1.87	48.59	25
$1\,0\cdot\overline{17}$	1.81	1.81	50.42	16
$1\,1\,0$	1.63	1.63	56.57	55
$1\,0\cdot22$	1.53	1.53	60.44	11
$1\,0\cdot\overline{23}$	1.48	1.48	62.60	19
$2\,0\,\bar{1}$ $2\,0\,2$	1.41 1.40	1.41	66.45	4
$1\,1\cdot15$ $2\,0\,5$	1.39	1.39	67.41	2
$2\,0\,8$ $1\,0\cdot\overline{26}$	1.36 1.35	1.35	69.32	11
$2\,0\cdot\overline{10}$	1.33	1.33	70.88	7
$2\,0\cdot11$ $1\,1\cdot18$	1.31	1.31	71.82	32
$2\,0\cdot\overline{13}$ $1\,0\cdot28$	1.28	1.28	74.20	4
$2\,0\cdot\overline{16}$	1.23	1.23	77.73	2
$2\,0\cdot17$	1.21	1.21	79.16	2
$1\,0\cdot\overline{32}$	1.15	1.15	84.53	1
$2\,0\cdot\overline{22}$ $0\,0\cdot36$	1.11	1.11	87.47	3
$2\,0\cdot23$	1.10	1.10	89.36	3
$2\,1\,1$ $2\,1\,\bar{2}$ $1\,0\cdot\overline{35}$	1.06	1.06	92.89	3
$2\,1\,\bar{8}$ $2\,0\cdot26$	1.04	1.04	95.43	3
$2\,1\cdot10$ $0\,0\cdot39$	1.03	1.03	96.98	4
$2\,1\cdot16$	0.98	0.98	103.68	1
$1\,0\cdot40$	0.95	0.95	109.26	4

* This reflection is affected by the presence of graphite as an impurity.

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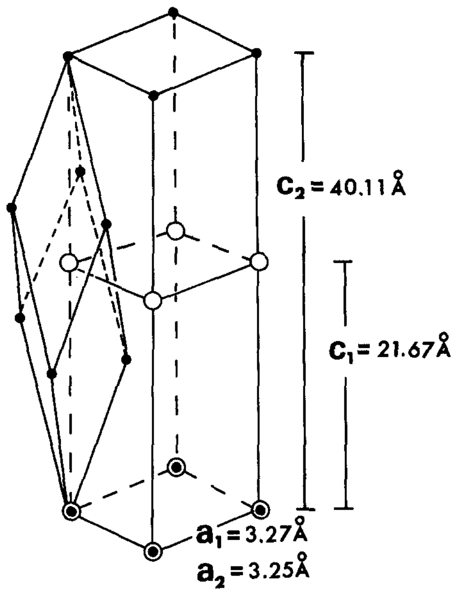

Figure 1 A crystal axial relation between α-Al_4SiC_4 and $Al_4Si_2C_5$ of aluminium silicon carbide. The lattice points of Al_4SiC_4 are shown with white circles and those of $Al_4Si_2C_5$ with black dots. The hexagonal lattice points of the latter corresponding rhombohedral are also given. Suffixes 1 and 2 indicate the lattice of α-Al_4SiC_4 and $Al_4Si_2C_5$, respectively.

from 1970° C to room temperature. If the compound $Al_4Si_2C_5$ is cooled slowly from 1970° C to 1900° C, the $Al_4Si_2C_5$ phase does not appear at all, but α-Al_4SiC_4 phase and silicon carbide are formed. Therefore, this new compound may be considered to be a stable phase at temperatures above 1900° C. Other experimental results showed that at temperatures below 1900° C, α-Al_4SiC_4 is more stable than the $Al_4Si_2C_5$.

The X-ray diffraction profiles of $Al_4Si_2C_5$ are quite different from those of α- and β-aluminium silicon carbide reported by Barczak [1] and Schneider [2]. The axial relation of the crystal lattices between Al_4SiC_4 and $Al_4Si_2C_5$ is shown in Fig. 1. The *a*-axis dimension in the hexagonal lattice of $Al_4Si_2C_5$ is very similar to that of α-Al_4SiC_4 and the *c*-axis dimension of the former is nearly twice as long as the latter.

The intensity distribution of X-ray diffraction and the unit cell dimension of $Al_4Si_2C_5$ are very similar to those of aluminium carbonitride, $Al_6C_3N_2$ reported by Jefferey and Wu [4]. Therefore, the crystal structure of the former may be similar to that of the latter. It can be postulated that the layer structure of $Al_4Si_2C_5$ is formed by substituting the two SiC layers for two AlN layers in the $Al_6C_3N_2$ structure.

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The preparation and properties of single crystal copper phosphide

Copper–phosphorus alloys are used in the metal industry instead of pure phosphorus for deoxidizing brass and bronze alloys and in the preparation of phosphor bronze. As a result there have been several studies of the copper–phosphorus phase diagram [1–3]. All of the diagrams indicate the presence of a compound with the formula Cu_3P, tricopper phosphide or, more commonly, copper phosphide. The crystal structure and some of the properties have been investigated [4, 5]. This compound has analogues in copper arsenide (Cu_3As) and copper antimonide (Cu_3Sb) and the former has been shown to have semiconducting

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