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A SiC bicrystal junction on the (0 0 0 1) plane

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A SiC bicrystal junction in which two crystals superpose with a common (0 0 0 1) plane has been investigated by optical microscopy and X-ray precession camera techniques. The behaviour of such a junction is discussed from the viewpoint of sintering and grain boundaries in SiC using a crystallographic concept of compound tessellation. Six examples of bicrystals are considered with respect to the observed and calculated superposing rotation angles and the densities of the superpositions.

1. Introduction

The concept of compound tessellations, which has been described by Coxeter [1, 2], is useful in illustrating the aggregation behaviour of layered structures, super structures and twin crystals. Only a few SiC crystals grown in a Lely's furnace demonstrated bicrystal junction behaviour in which two crystals superimpose on the (0001) plane. This two-dimensional junction behaviour is extremely important because it involves sintering and grain boundaries [3–6] in SiC. While investigating three-dimensional behaviour, we determined a relationship between the rotation angle (θ) of the hexagonal primitive lattice net overlaying the other net and the density ($1/n$) of superpositions of two hexagonal nets caused by the rotation. In this paper we shall give actual examples of SiC bicrystals superposing with several rotation angles θ_0 and then give a comparison between observed θ_0 and calculated θ_c values. In addition, we shall discuss these bicrystal junctions in relation to compound tessellation of two-dimensional hexagonal crystallographic nets [7].

2. Observations

In a Lely's furnace [8, 9] many plate-like SiC crystals grow as a result of a reaction between silicon and carbon at 2500° C in an argon atmosphere. Among these crystals, excluding those with twinning, one can occasionally find a few specimens of bicrystals in which two plate-like crystals superpose at the (0001) plane. We have so far found six samples of bicrystals excluding twinning and we have examined their crystallographic orientation under an optical microscope and with an X-ray precession camera. The external shapes of the crystals are shown in Fig. 1a to f. It is evident from Fig. 1 that in all six bicrystals the c-axes of the two crystals composing a bicrystal are nearly parallel. The angle Ω between the c-axes of each of the six bicrystals, $c_\mathrm{I} \wedge c_\mathrm{II}$, was measured using an X-ray precession camera. The suffixes I and II refer to the Crystals I and II which constitute a bicrystal by superposing on the (0001) plane. The rotation angle θ for each bicrystal was also observed from the X-ray precession photograph of $h\,k\,0$. These X-ray photographs of $h\,k\,0$ were taken with $\mu = 25°$ with Mo-radiation of 40 kV and 25 mA. These photographs are shown in Fig. 2a to f. In Figs 1 and 2, a to f correspond to one each of the six bicrystals. The angle Ω between the c-axes, namely, $c_\mathrm{I} \wedge c_\mathrm{II}$, and the angle θ between the a-axes, namely, $a_\mathrm{I} \wedge a_\mathrm{II}$, for each of the six bicrystals are shown in Fig. 2. The angle θ is equal to the rotation angle and will be discussed later.

3. Calculations

When one hexagonal primitive lattice plane lies on another hexagonal plane in parallel, and one of the two rotates around the axis perpendicular to the lattice plane, passing the origin of the lattice, many lattice points of both planes can super-

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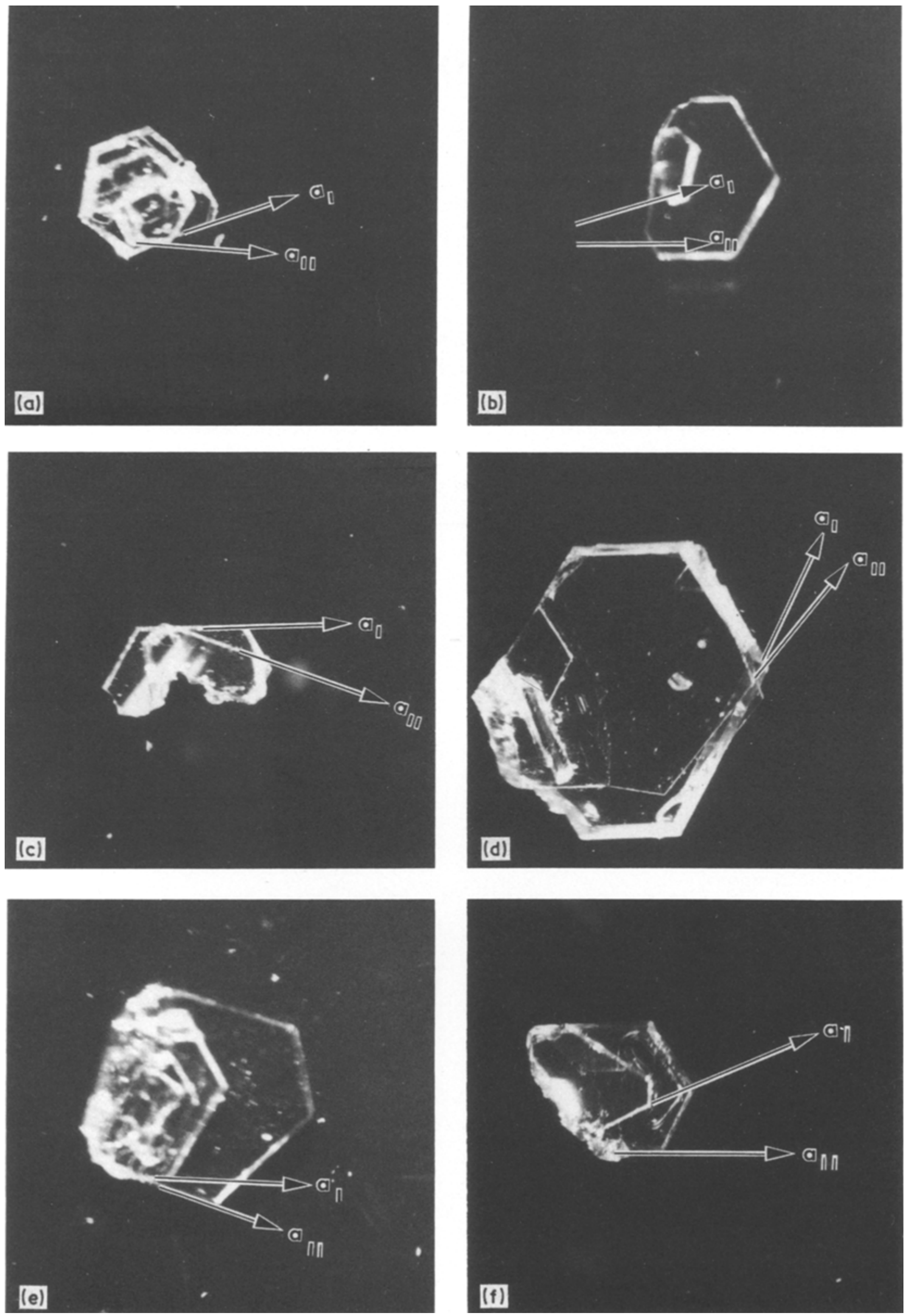

Figure 1 The external shapes of six bicrystals of SiC. The crystallographic orientations of superimposition of their a-axes are shown by a_{I} and a_{II}.

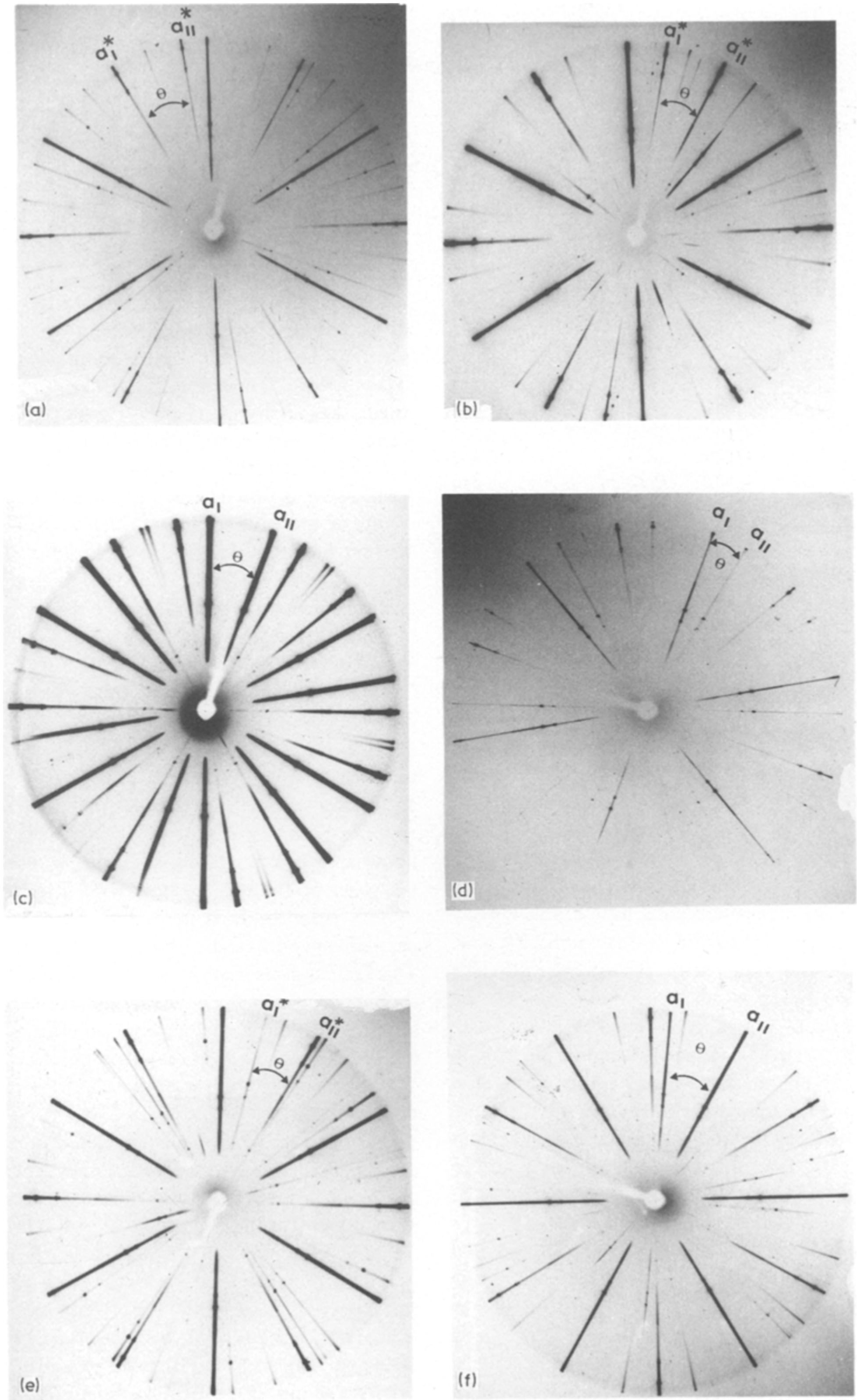

Figure 2 The precession photographs of the six bicrystals. Their orientations are shown by a_{I}^* and a_{II}^* or a_{I} and a_{II}.

TABLE I The calculated rotation angle θ_c ranging from $n = 7$ to 397

(u, v)	$\theta_c(°)$	$1/n$	(u, v)	$\theta_c(°)$	$1/n$
3, 1	21.79	1/7	15, 1	6.84	1/211
4, 1	27.80	1/13	16, 3	20.32	1/217
5, 2	13.17	1/19	17, 8	3.89	1/217
6, 1	17.90	1/31	17, 6	19.27	1/223
7, 3	9.43	1/37	17, 5	26.75	1/229
7, 1	15.18	1/43	16, 1	6.40	1/241
8, 3	16.43	1/49	17, 3	19.03	1/247
9, 4	7.34	1/61	18, 7	14.62	1/247
9, 2	24.43	1/67	17, 2	12.36	1/259
9, 1	11.64	1/73	18, 5	28.78	1/259
10, 3	26.01	1/79	19, 9	3.48	1/271
10, 1	10.42	1/91	19, 7	17.28	1/277
11, 5	6.01	1/91	19, 6	24.02	1/283
11, 3	29.41	1/97	19, 4	23.04	1/301
10, 2	19.65	1/103	20, 9	6.61	1/301
12, 5	10.99	1/109	18, 1	5.67	1/307
13, 6	5.09	1/127	19, 3	16.89	1/313
12, 1	8.61	1/133	21, 10	3.15	1/331
13, 4	25.04	1/133	21, 8	15.65	1/337
13, 3	25.46	1/139	19, 1	5.36	1/343
14, 5	18.73	1/151	20, 3	15.99	1/349
13, 1	7.93	1/157	21, 5	26.35	1/361
14, 3	23.48	1/163	22, 9	11.99	1/367
15, 7	4.41	1/169	21, 4	20.67	1/373
15, 4	29.84	1/181	22, 7	23.71	1/379
16, 7	8.26	1/193	23, 11	2.88	1/397
15, 2	14.11	1/199			

impose on each other depending on the rotation. The number of superpositions caused by this rotation should vary discontinuously according to the rotation angle θ. In addition, the origin and the superpositions produce a new super hexagonal net [7]. The super hexagonal lattice thus created is n times larger than the primitive one. (n is an integer and the multiplicity of the super cell.) The number of superpositions in the unit area, i.e. the density of superpositions, is reflected in the value of $1/n$ and can be indirectly regarded as an indicator of the binding force between the two crystals overlapping on the (0001) plane of the bicrystal. As $1/n$ becomes larger, the binding force becomes stronger. For instance, when two crystals join in a bicrystal with $\theta \equiv 0°$ (mod 60°), the primitive lattice points of both crystals coincide perfectly with each other and the value of $1/n$ reaches a maximum. Therefore, the bicrystal with $\theta \equiv 0$ combines most strongly.

Here, the relationship between the rotation angle θ and the density of superpositions of a hexagonal net have been examined using a simple example. Let us suppose that two identical hexagonal primitive lattice planes superpose exactly parallel with each other and each of them has an infinite number of lattice points in the $h\,k\,0$ net. When either of the two planes rotates around an axis perpendicular to the lattice plane, passing the origin, the density of superpositions of both lattice planes will vary according to the rotations. From this, we calculated the variations of these superpositions as a function of the rotation angle. The results of the calculation are given in Table I with $1/n$ ranging from 1/7 to 1/397 together with the (u, v) co-ordinate and θ_c. The nearest superpositions from the origin can be represented by (u, v). This notation distinguishes a hexagonal super lattice from the primitive hexagonal lattice. θ_c values thus calculated were then compared with θ_0 which appeared in real SiC bicrystals as shown in Figs 1 and 2. The observed θ_0 agreed closely but not perfectly with the calculated θ_c. This slight disagreement may be caused by errors in the measurement of θ_0 and the inclination of Ω between overlapping hexagonal planes. θ_c and θ_0 are given in Table II together with Ω values. It is evident from Table II that all of the observed θ_0 can correspond to some of the calculated θ_c values. This fact suggests that the junction of SiC bicrystals should occur only when the rotation angle θ accords with a specific angle which creates a super lattice by the superposition lattice points.

TABLE II A comparison between observed θ_0 and calculated θ_c values. The compound tessellation of each of the six bicrystals are represented by Schläfli's symbol

θ_c	θ_0	Ω	Schläfli's symbol
21.79°	22.1°	6°	{3, 6} [7{3, 6}] with $(u, v) = (3, 1)$
17.90°	18.0°	3°	{3, 6} [31{3, 6}] with $(u, v) = (6, 1)$
19.65°	19.7°	0°	{3, 6} [103{3,6}] with $(u,v) = (11,2)$
10.99°	11.1°	0°	{3, 6} [109{3,6}] with $(u,v) = (12,5)$
17.28°	17.0°	7°	{3, 6} [277{3,6}] with $(u,v) = (19,7)$
23.71°	23.7°	0°	{3, 6} [379{3,6}] with $(u,v) = (22,7)$

4. Discussion

The concept of compound tessellations has been applied to twinning, superstructure and aggregation of layered structures. This concept should also be useful in illustrating the bicrystal behaviour of SiC. A compound tessellation can be created [7] by a suitable rotation and translation of one vertex with co-ordinate (u, v) of the original regular tessellation. For instance, starting with a vertex (u, v) of {3, 6} regular tessellation, the rotation about the origin through multiples of 60° produce six new vertices: (u, v), $(u-v, u)$, $(-v, u-v)$, $(-u, -v)$, $(v-u, -u)$ and $(v, v-u)$.

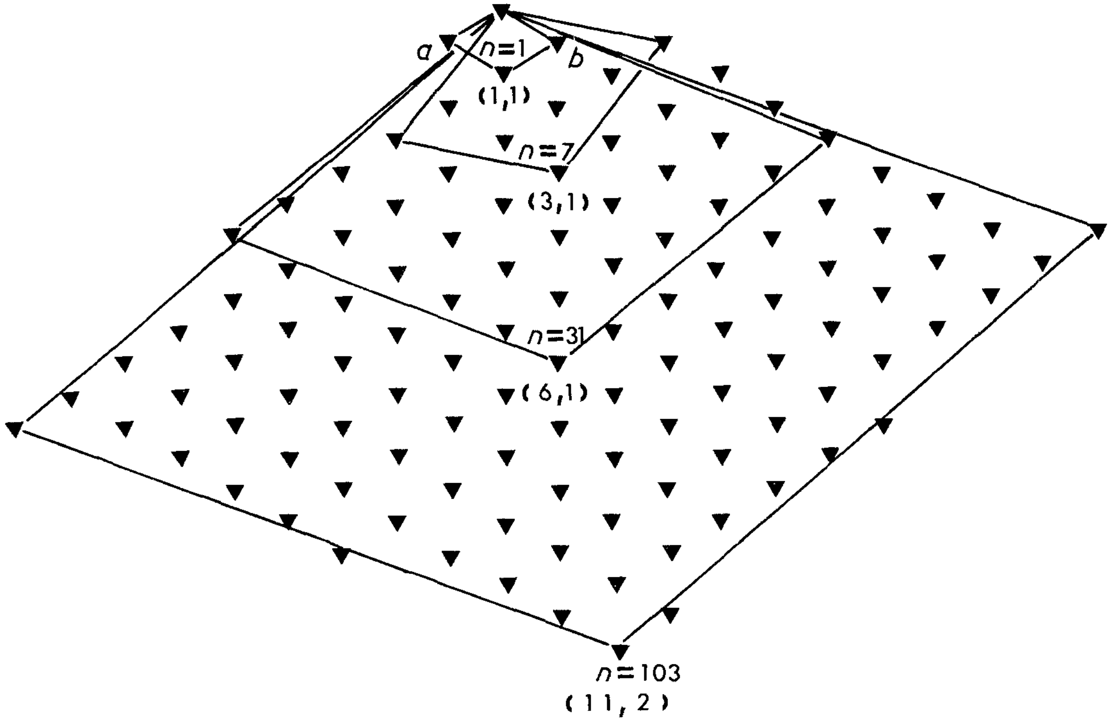

Figure 3 Three examples of bicrystals are illustrated by the compound tessellations. The vertices co-ordinating (u, v) and the multiplicity of the super cell, n, are given. The smallest hexagonal mesh represents the primitive hexagonal lattice with $(u, v) = (1, 1)$ and $n = 1$.

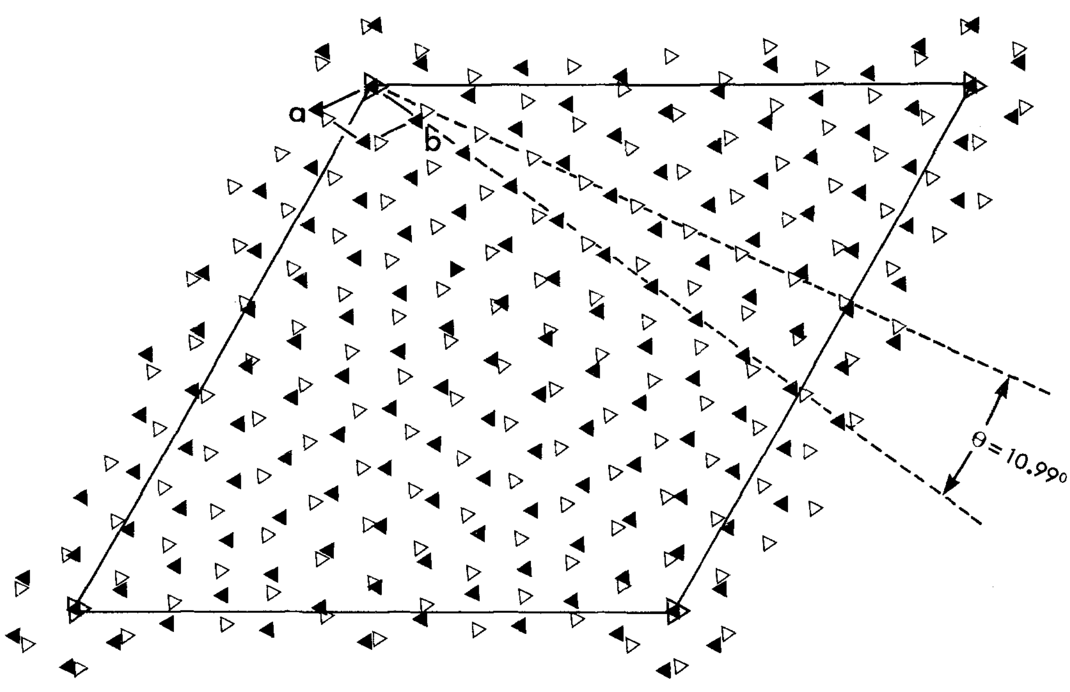

Figure 4 The compound tessellation of $\{3, 6\}$ $[109\{3, 6\}]$, with $(u, v) = (12, 5)$. Open triangle and filled triangle represent Crystal I and Crystal II, respectively, which are composed of a bicrystal superimposing on the (0001) plane. The perfect coincident superpositions between Crystals I and II can be seen in the co-ordinate of $(u, v) = (12, 5)$. The rotation angle θ is 10.99°.

The origin and these six points compose a new $\{3, 6\}$ tessellation bearing edge $(u^2 - uv + v^2)^{1/2}$. In addition, a suitable translation produces a distribution of all the vertices of the original $\{3, 6\}$ among $n = u^2 - uv + v^2$. Thus, induced compound tessellation can be represented by

$$\{3, 6\}\ [n\{3, 6\}], \qquad \text{with } n = u^2 - uv + v^2,$$

where n is the multiplicity of the super cell mentioned earlier.

Using this concept of compound tessellation $\{3, 6\}\ [n\{3, 6\}]$, we tried to explain the behaviour of bicrystal junctions occurring in real SiC plate-like crystals. Among the six different bicrystals observed so far, a few examples are illustrated by the compound tessellation in Fig. 3. The smallest hexagonal mesh represents the primitive hexagonal lattice and the larger ones represent the super lattice created by the superposition of two primitive lattice planes on each other.

Previous research concerning bicrystals of SiC explained the behaviour of the rotation angle $10° 54'$ using a concept of pseudo-compound tessellation [10] rather than regular compound tessellation. Sueno *et al.* [10] suggested that the junction with $\theta \fallingdotseq 11°$ was caused by the lattice points nearly in common rather than by perfectly coincident superpositions between two hexagonal layers overlaying each other. The previous work was explained in this way in the range $n < 40$. By expanding the super lattice to $n = 397$, however, we found that perfectly coincident superpositions occurred when $\theta_c = 10° 59'$ and $n = 109$, as given in Table I. These superpositions produce a hexagonal super lattice and can be explained by the concept of compound tessellation of $\{3, 6\}\ [109\{3, 6\}]$, $(u, v) = (12, 5)$, as shown in Fig. 4. The concept of compound tessellation can be applied to explain their aggregation behaviour not only for the case of $\theta \fallingdotseq 11°$ but also for all other cases of SiC bicrystals observed so far. All of the six examples reported here are explained by this concept using Schläfli's symbol in Table II. As seen in Table II, the multiplicity of $n = 379$ was observed in real bicrystals. From this fact, we conclude that the bicrystals of SiC should overlay exactly with superpositions of coinciding lattice points rather than join at pseudo superpositions of lattice points within the range of at least $n = 397$. In other words, almost all bicrystals up to $n = 397$ must accompany coinciding superpositions even though the density of superpositions is considerably lower. The concept of pseudo superpositions may be valid for the discussion of the higher order of SiC bicrystals, i.e. $n > 400$.

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