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Combination Rule of Σ Values at Triple Junctions in Cubic Polycrystals

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Abstract

In cubic polycrystals, combinations of coincidence orientation relationships at a triple junction of grains A, B and C can be obtained by using the equation

$$\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}/d^2,$$

where d is a common divisor of Σ_{AB} and Σ_{BC}. This paper describes the derivation of this equation and shows several models of polycrystals composed of specially selected coincidence boundaries using the above equation.

1. Introduction

The orientation relationship between two overlapping cubic crystal lattices forming a coincidence-site lattice (CSL) is expressed by a special rotation matrix R (CSL matrix) (Warrington & Bufalini, 1971; Grimmer, Bollmann & Warrington, 1974),

$$R = (1/\Sigma)\tilde{R}, \qquad (1)$$

where every element of $\tilde{R}$ $[(\tilde{R})_{ij,1\leq i,j\leq 3}]$ is integral and $(\tilde{R})_{ij,1\leq i,j\leq 3}$ and Σ have no common factors. Σ is an odd integer and defined as 'the ratio of the total number of lattice sites of one crystal to the number of coinciding lattice sites' (Warrington & Bufalini, 1971). Since coincidence boundaries are known to exhibit important properties in energy, fracture strength, corrosion resistivity, diffusion coefficients, electrical conductivity *etc.*, it is of great interest to design such a polycrystalline material as composed of specially selected grains with coincidence orientation relationships. Since crystal grains in a polycrystal are bound to triple junctions, it is necessary to investigate the rule that governs the orientation relationships of the grains around the triple junctions. For this purpose of grain boundary design, a formula to describe the CSL orientation relationships among the grains at triple junctions has been proposed (Miyazawa, Ishida & Mori, 1983; Takahashi, Miyazawa, Mori & Ishida, 1986). The purpose of this paper is to describe the formula in detail and to give several models of grain-boundary design in cubic polycrystals.

2. Combinations of Σ values at a triple junction

Consider a triple junction O formed by grains A, B and C with the same cubic unit cell. $X_j(P)$ is a coordinate vector of a point P expressed by orthogonal coordinates fixed to the crystallographic axis system of grain j. The rotation matrix R_{ij} denoting the orientation relationship between grains i and j is defined by $X_j(P) = R_{ij}^{-1}X_i(P)$. From these definitions, the following equations are obtained if three orthogonal coordinates bound to the grains A, B and C have the same origin at the triple junction O:

$$X_B(P) = R_{AB}^{-1}X_A(P), \qquad (2)$$

$$X_C(P) = R_{BC}^{-1}X_B(P), \qquad (3)$$

$$X_A(P) = R_{CA}^{-1}X_C(P). \qquad (4)$$

From (2), (3) and (4),

$$X_A(P) = R_{CA}^{-1}R_{BC}^{-1}R_{AB}^{-1}X_A(P), \qquad (5)$$

then,

$$R_{AB}R_{BC}R_{CA} = E. \qquad (6)$$

E is the unit matrix. It can be seen in (6) that, if two of the three rotation matrices express CSL orientation relationships, the third matrix also expresses a CSL orientation relationship.

The matrices at the triple junction are written as follows from (1) when grain boundaries AB, BC and CA are the coincidence boundaries:

$$R_{AB} = (1/\Sigma_{AB})\tilde{R}_{AB}, \quad R_{BC} = (1/\Sigma_{BC})\tilde{R}_{BC}, \quad R_{CA} = (1/\Sigma_{CA})\tilde{R}_{CA}. \qquad (7)$$

From (6) and (7),

$$(1/\Sigma_{CA})\tilde{R}_{CA} = (1/\Sigma_{BC})^t\tilde{R}_{BC}(1/\Sigma_{AB})^t\tilde{R}_{AB} = (1/\Sigma_{AB}\Sigma_{BC})^t\tilde{R}_{BC}\,{}^t\tilde{R}_{AB}, \qquad (8)$$

where t means transpose.

Since every element of the product ${}^t\tilde{R}_{BC}\,{}^t\tilde{R}_{AB}$ is integral, there must be an integer l such that

$$\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}/l. \qquad (9)$$

Similarly,

$$\Sigma_{AB} = \Sigma_{BC}\Sigma_{CA}/m \tag{10}$$

and

$$\Sigma_{BC} = \Sigma_{CA}\Sigma_{AB}/n \tag{11}$$

for some integers m and n. From (9), (10) and (11),

$$\Sigma^2_{AB} = ln, \tag{12}$$

$$\Sigma^2_{BC} = lm, \tag{13}$$

$$\Sigma^2_{CA} = mn. \tag{14}$$

If Σ_{AB} and Σ_{BC} are relatively prime, Σ^2_{AB} and Σ^2_{BC} are also relatively prime, therefore l must be equal to 1. Hence, $\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}$. The following result is obtained.

Proposition 1

If Σ_{AB} and Σ_{BC} are the Σ values of coincidence boundaries AB and BC at a triple junction of A, B and C grains and are relatively prime, then, at the boundary CA,

$$\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}. \tag{15}$$

Equation (15) appeared in Doni & Bleris (1988) but it is a special case of the general expression (51).

Consider the case that R_{AB} and R_{BC} are the CSL matrices with π rotation axes. The π rotation matrix around the rotation axis $[HKL]$ (matrix with $[HKL]$ rotation axis of 180°) can be expressed as

$$R = \frac{1}{M}\begin{bmatrix} 2H^2 - M & 2HK & 2HL \\ 2HK & 2K^2 - M & 2KL \\ 2HL & 2KL & 2L^2 - M \end{bmatrix}, \tag{16}$$

where integers H, K and L do not have a common divisor except 1 and

$$M \equiv H^2 + K^2 + L^2. \tag{17}$$

The matrix R is defined as

$$R = R'/M. \tag{18}$$

If M is an odd number, M and all elements of R' do not have a common divisor except 1 and the matrix R is called 'irreducible'. This is proved as follows. Let us use the notation $\alpha|\beta$, which expresses that β is divisible by α. Suppose d is a prime common divisor of M and $R'_{ij,1\leq i,j\leq 3}$, *i.e.* $d|M$ and $d|R'_{ij,1\leq i,j\leq 3}$, which leads to $d|2H^2 - M$, $d|2K^2 - M$ and $d|2L^2 - M$. If M is odd, $d \neq 2$. Then, since d/M and $d \neq 2$, $d|H^2$, *i.e.* $d|H$. Similarly, $d|K$ and $d|L$. d must be equal to 1 because H, K and L were assumed to be relatively prime. Therefore, (16) is irreducible when M is odd, and $\Sigma = M$ from (1)

When M is even, two of H, K and L must be odd and one of them must be even, *i.e.* (H, K, L) must be of type (odd, odd, even), (odd, even, odd) or (even, odd, odd). Then, $M/2$ is found to be odd. When M is even, (16) can be written as

$$R = [1/(M/2)] \times \begin{bmatrix} H^2 - (M/2) & HK & HL \\ HK & K^2 - (M/2) & KL \\ HL & KL & L^2 - (M/2) \end{bmatrix}, \tag{19}$$

where $\Sigma = M/2$ in this case.

At a triple junction, if R_{AB} and R_{CA} are the π rotation matrices such that

$$R_{AB} = \frac{1}{M_1}\begin{bmatrix} 2H_1^2 - M_1 & 2H_1K_1 & 2H_1L_1 \\ 2H_1K_1 & 2K_1^2 - M_1 & 2K_1L_1 \\ 2H_1L_1 & 2K_1L_1 & 2L_1^2 - M_1 \end{bmatrix}$$
$$\equiv (1/M_1)\tilde{R}_{AB}, \tag{20}$$

$$R_{BC} = \frac{1}{M_2}\begin{bmatrix} 2H_2^2 - M_2 & 2H_2K_2 & 2H_2L_2 \\ 2H_2K_2 & 2K_2^2 - M_2 & 2K_2L_2 \\ 2H_2L_2 & 2K_2L_2 & 2L_2^2 - M_2 \end{bmatrix}$$
$$\equiv (1/M_2)\tilde{R}_{BC}, \tag{21}$$

then, from (6), the following equation is derived:

$$\begin{aligned} R^{-1}_{CA} &= R_{AB}R_{BC} \\ &= (1/M_1M_2) \\ &\times \begin{bmatrix} M_1M_2 - 2(K_3^2 + L_3^2) & 2WL_3 + 2H_3K_3 & -2WK_3 + 2H_3L_3 \\ -2WL_3 + 2H_3K_3 & M_1M_2 - 2(H_3^2 + L_3^2) & 2WH_3 + 2K_3L_3 \\ 2WK_3 + 2H_3L_3 & -2WH_3 + 2K_3L_3 & M_1M_2 - 2(H_3^2 + K_3^2) \end{bmatrix}, \end{aligned} \tag{22}$$

where

$$(H_3, K_3, L_3) \equiv (H_1, K_1, L_1) \times (H_2, K_2, L_2) \tag{23}$$

and

$$W = (H_1, K_1, L_1) \cdot (H_2, K_2, L_2). \tag{24}$$

Let the matrix $\tilde{R}_{CA}$ be defined such that

$$R^{-1}_{CA} = (1/M_1M_2)\tilde{R}_{CA}. \tag{25}$$

Suppose that an odd integer d is a prime common divisor of M_1 and M_2 and that d divides all elements of $\tilde{R}_{CA}$ $[= (\tilde{R}_{CA})_{ij,1\leq ij\leq 3}]$. Then,

$$d|M_1M_2 - 2(K_3^2 + L_3^2), \tag{26}$$

$$d|M_1M_2 - 2(H_3^2 + L_3^2), \tag{27}$$

$$d|M_1M_2 - 2(H_3^2 + K_3^2). \tag{28}$$

Therefore, $d|K_3^2 + L_3^2$, $d|H_3^2 + L_3^2$ and $d|H_3^2 + K_3^2$, leading to $d|2H_3^2$, $d|2K_3^2$, $d|2L_3^2$. Since d is odd, $d|H_3^2$, $d|K_3^2$, $d|L_3^2$ and, since d is prime,

$$d|H_3, \quad d|K_3, \quad d|L_3. \tag{29}$$

From the condition of normalization,

$$\{M_1M_2 - 2(K_3^2 + L_3^2)\}^2 + (-2WL_3 + 2H_3K_3)^2 + (2WK_3 + 2H_3L_3)^2 = (M_1M_2)^2,$$

then

$$(K_3^2 + L_3^2)W^2 = (K_3^2 + L_3^2)(M_1M_2 - H_3^2 - K_3^2 - L_3^2). \tag{30}$$

Case 1: $K_3^2 + L_3^2 \neq 0$

In this case,

$$W^2 = M_1M_2 - H_3^2 - K_3^2 - L_3^2, \tag{31}$$

therefore $d|W^2$ from (29) and then $d|W$ because d is prime. Since d is a common divisor of H_3, K_3, L_3 and W, d^2 is a common divisor of $(\tilde{R}_{CA})_{ij, 1\leq i,j\leq 3}$ and M_1M_2. If $M_1', M_2', H_3', K_3', L_3'$ and W' are defined as $M_1 = M_1'd$, $M_2 = M_2'd$, $H_3 = H_3'd$, $K_3 = K_3'd$, $L_3 = L_3'd$ and $W = W'd$, (22) becomes

$$R_{CA}^{-1} = (1/M_1'M_2') \times \begin{bmatrix} M_1'M_2' - 2(K_3'^2 + L_3'^2) & 2W'L_3' + 2H_3'K_3' & -2W'K_3' + 2H_3'L_3' \\ -2W'L_3' + 2H_3'K_3' & M_1'M_2' - 2(H_3'^2 + L_3'^2) & 2W'H_3' + 2K_3'L_3' \\ 2W'K_3' + 2H_3'L_3' & -2W'H_3' + 2K_3'L_3' & M_1'M_2' - 2(H_3'^2 + K_3'^2) \end{bmatrix}. \tag{32}$$

Since (32) has the same matrix form as (22), each element in parentheses in (32) is shown to be divided by d'^2 again if d' is an odd prime common divisor of M_1' and M_2' and if d' divides every element in parentheses in (32).

Case 2: $K_3^2 + L_3^2 = 0$

This time, $K_3 = L_3 = 0$, hence

$$K_3 = L_1H_2 - H_1L_2 = 0 \tag{33}$$

and

$$L_3 = H_1K_2 - K_1H_2 = 0. \tag{34}$$

If $H_1 \neq 0$, then $H_3 = K_1L_2 - L_1K_2 = K_1(L_1H_2/H_1) - L_1(K_1H_2/H_1) = 0$. This leads to

$$R_{CA}^{-1} = E = (1/M_1M_2)\tilde{R}_{CA} \tag{35}$$

and hence $R_{AB} = R_{BC}^{-1}$ and $\Sigma_{AB} = \Sigma_{BC}$. It is obvious that every element of $\tilde{R}_{CA}$ can be divided by d^2 if d is defined as an odd common divisor of M_1 and M_2.

If $H_1 = 0$, then $L_1H_2 = 0$ and $K_1H_2 = 0$ from (33) and (34). If $H_2 \neq 0$, then $K_1 = L_1 = 0$. Because the rotation axis $[H_1K_1L_1]$ is not defined as the zero vector, H_2 must be zero. The rotation matrices R_{AB} and R_{CA} with the rotation axes $[0K_1L_1]$ and $[0K_2L_2]$ are written as

$$R_{AB} = [1/(K_1^2 + L_1^2)] \times \begin{bmatrix} -(K_1^2 + L_1^2) & 0 & 0 \\ 0 & K_1^2 - L_1^2 & 2K_1L_1 \\ 0 & 2K_1L_1 & -(K_1^2 - L_1^2) \end{bmatrix}, \tag{36}$$

$$R_{BC} = \frac{1}{K_2^2 + L_2^2} \begin{bmatrix} -(K_2^2 + L_2^2) & 0 & 0 \\ 0 & K_2^2 - L_2^2 & 2K_2L_2 \\ 0 & 2K_2L_2 & -(K_2^2 - L_2^2) \end{bmatrix}. \tag{37}$$

R_{CA}^{-1} is written as

$$R_{CA}^{-1} = [1/(K_1^2 + L_1^2)(K_2^2 + L_2^2)] \times \begin{bmatrix} (K_1^2 + L_1^2)(K_2^2 + L_2^2) & 0 & 0 \\ 0 & (K_1K_2 + L_1L_2)^2 - (K_1L_2 - L_1K_2)^2 & 2(K_1K_2 + L_1L_2)(K_1L_2 - L_1K_2) \\ 0 & -2(K_1K_2 + L_1L_2)(K_1L_2 - L_1K_2) & (K_1K_2 + L_1L_2)^2 - (K_1L_2 - L_1K_2)^2 \end{bmatrix} \tag{38}$$

$$= \frac{1}{x^2 + y^2} \begin{bmatrix} x^2 + y^2 & 0 & 0 \\ 0 & x^2 - y^2 & 2xy \\ 0 & -2xy & x^2 - y^2 \end{bmatrix} \tag{39}$$

$$\equiv \tilde{R}_{CA}/M_1M_2, \tag{40}$$

where

$$M_1 \equiv K_1^2 + L_1^2 \tag{41}$$

and

$$M_2 \equiv K_2^2 + L_2^2. \tag{42}$$

In (39), x and y are defined such that

$$x = K_1K_2 + L_1L_2, \tag{43}$$

$$y = K_1L_2 - L_1L_2. \tag{44}$$

Let us assume here that d is an odd prime number common to M_1 and M_2. If d divides every element of $\tilde{R}_{CA}$, it can be shown that d^2 also divides every element of $\tilde{R}_{CA}$. This is proved as follows. From the assumption $d|2xy$, then $d|x$ or $d|y$, since d is an odd prime number.

(i) If $d|x$, then $d|y^2$, from the assumption that d divides every element of $\tilde{R}_{CA}$. Since d is prime, $d|y$. Therefore, it is found the d^2 divides every element of $\tilde{R}_{CA}$.

(ii) If $d|y$, d^2 is also proved to divide every element of $\tilde{R}_{CA}$.

From (i) and (ii), for an odd prime number d common to M_1 and M_2, every element of $\tilde{R}_{CA}$ can be divided by d^2 if d divides every element of $\tilde{R}_{CA}$.

If M_1', M_2', x' and y' are defined as

$$M_1 = M_1'd, \quad M_2 = M_2'd, \quad x = x'd \quad \text{and} \quad y = y'd,$$

(39) becomes

$$R_{CA}^{-1} = \frac{1}{x'^2 + y'^2} \begin{bmatrix} x'^2 + y'^2 & 0 & 0 \\ 0 & x'^2 - y'^2 & 2x'y' \\ 0 & -2x'y' & x'^2 - y'^2 \end{bmatrix}. \tag{45}$$

Since (45) has the same matrix form as (39), every element in square brackets in (45) can be divided by d'^2 again if d' is an odd prime common divisor of M_1' and M_2' and if d' divides every element in square brackets in (45).

A summary of the above discussions gives the following result.

Proposition 2

For two CSL matrices with π rotation axes, $R_{AB} = (1/M_1)\tilde{R}_{AB}$ and $R_{BC} = (1/M_2)\tilde{R}_{BC}$, if d is an odd common divisor of M_1 and M_2 and if d divides every element of the product $\tilde{R}_{AB}\tilde{R}_{BC}$, then every element of $\tilde{R}_{AB}\tilde{R}_{BC}$ can be divided by d^2.

Suppose $d_1^\alpha d_2^\beta \ldots d_n^\gamma$ to be the odd greatest common divisor of M_1 and M_2, where $d_1, d_2, \ldots$ and d_n ($d_i \neq d_j$ for $i \neq j$) are odd prime numbers and the integers $\alpha, \beta, \ldots, \gamma \geq 1$. M_1 and M_2 are denoted as $M_1 = (d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_1'$ and $M_2 = (d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_2'$, where M_1' and M_2' have no common divisor except 1 or 2. Then, (25) is written as

$$R_{CA}^{-1} = \tilde{R}_{CA}/(d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_1'(d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_2' \quad \text{for } \alpha, \beta, \gamma, \ldots \geq 1. \tag{46}$$

If the integers $d_{1'}, d_{2'}, \ldots$ and $d_{n'}$ ($d_{i'} \neq d_{j'}$ for $i' \neq j'$) are assumed to be some of the prime numbers $d_1, d_2, \ldots$ and d_n, the product $d_{1'}d_{2'} \ldots d_{n'}$ is a common divisor of M_1 and M_2. If the product $d_{1'}d_{2'} \ldots d_{n'}$ divides $(\tilde{R}_{CA})_{ij,1\leq i,j\leq 3}$, it is shown from the above discussion that $(d_{1'}d_{2'} \ldots d_{n'})^2$ can also divide $(\tilde{R}_{CA})_{ij,1\leq i,j\leq 3}$. If the quotient $(\tilde{R}_{CA})_{ij,1\leq i,j\leq 3}/(d_{1'}d_{2'} \ldots d_{n'})^2$ is denoted as $(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}$, the following equation is obtained:

$$\frac{(\tilde{R}_{CA})_{ij,1\leq i,j\leq 3}/(d_{1'}d_{2'} \ldots d_{n'})^2}{(d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_1'(d_1^\alpha d_2^\beta \ldots d_n^\gamma)M_2'/(d_{1'}d_{2'} \ldots d_{n'})^2} = \frac{(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}}{(d_1^{\alpha'} d_2^{\beta'} \ldots d_n^{\gamma'})M_1'(d_1^{\alpha'} d_2^{\beta'} \ldots d_n^{\gamma'})M_2'} \equiv (\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}/M_1''M_2'' \tag{47}$$

for integers $\alpha', \beta', \gamma', \ldots \geq 0$.

Further, if $(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}$ can be divided by the odd common divisor $d_{1''}d_{2''} \ldots d_{n''}$ ($d_{i''} \neq d_{j''}$ for $i'' \neq j''$) of M_1'' and M_2'', and the quotient $(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}/(d_{1''}d_{2''} \ldots d_{n''})^2$ is denoted as $(\tilde{R}''_{CA})_{ij,1\leq i,j\leq 3}$, then

$$\frac{(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}/(d_{1''}d_{2''} \ldots d_{n''})^2}{(d_1^{\alpha'} d_2^{\beta'} \ldots d_n^{\gamma'})M_1'(d_1^{\alpha'} d_2^{\beta'} \ldots d_n^{\gamma'})M_2'/(d_{1''}d_{2''} \ldots d_{n''})^2} = \frac{(\tilde{R}''_{CA})_{ij,1\leq i,j\leq 3}}{(d_1^{\alpha''} d_2^{\beta''} \ldots d_n^{\gamma''})M_1'(d_1^{\alpha''} d_2^{\beta''} \ldots d_n^{\gamma''})M_2'} \equiv (\tilde{R}''_{CA})_{ij,1\leq i,j\leq 3}/M_1'''M_2''' \tag{48}$$

for integers $\alpha'', \beta'', \gamma'', \ldots \geq 0$. The above process is repeated until $(\tilde{R}^{''\ldots'}_{CA})_{ij,1\leq i,j\leq 3}$ cannot be divided by the common factor of $M_1^{''\ldots'}$ and $M_2^{''\ldots'}$. Therefore, Σ_{CA} is found to have the form of the following equation when M_1 and M_2 are odd:

$$\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}/d^2, \tag{49}$$

where d is a common divisor of Σ_{AB} and Σ_{BC}.

The process to obtain (49) is applicable also when even factors are contained in M_1 and M_2 because the elements of matrix $(\tilde{R}'_{CA})_{ij,1\leq i,j\leq 3}$ are divisible by the even factors after the successive divisions by odd factors. In this case, the following equation holds for $\alpha, \beta = 0, 1$:

$$\Sigma_{CA} = (M_1/2^\alpha)(M_2/2^\beta)/d^2 = \Sigma_{AB}\Sigma_{BC}/d^2. \tag{50}$$

Table 1 shows the numerically calculated axis and angle pairs of the CSL matrices that satisfy $R_1R_2R_3 = E$. $\Sigma 3([1\,1\,1], 180.00)$ means the $\Sigma 3$ CSL matrix whose rotation axis and angle are [1 1 1] and 180.0°, respectively. Equation (49) has been deduced using two coincidence matrices with the π rotation axes, whereas Table 1 shows that (49) holds also when R_{AB} and R_{BC} do not have the π rotation axis. From the numerical calculations, (49) is conjectured to be valid in general for the CSL matrices that do not have π rotation axes and is called 'the combination rule of Σ values at a triple junction' here.

The above discussions may be summarized as follows.

Proposition 3

At the triple junction of Σ_{AB}, Σ_{BC} and Σ_{CA} coincidence boundaries, the following equation is obtained for a common divisor d of Σ_{AB} and Σ_{BC}:

$$\Sigma_{CA} = \Sigma_{AB}\Sigma_{BC}/d^2. \tag{51}$$

Similarly, for a common divisor d' of Σ_{BC} and Σ_{CA} and for a common divisor d'' of Σ_{CA} and Σ_{AB}, the following equations hold at the triple junction:

$$\Sigma_{AB} = \Sigma_{BC}\Sigma_{CA}/d'^2 \tag{52}$$

$$\Sigma_{BC} = \Sigma_{AB}\Sigma_{CA}/d''^2. \tag{53}$$

From (51), (52) and (53), the following equation is obtained:

$$(\Sigma_{AB}\Sigma_{BC}\Sigma_{CA})^{1/2} = dd'd''. \tag{54}$$

Proposition 4

$(\Sigma_{AB}\Sigma_{BC}\Sigma_{CA})^{1/2}$ is an odd integer at the triple junction of coincidence boundaries with Σ_{AB}, Σ_{BC} and Σ_{CA}.

Values of $(\Sigma_{AB}\Sigma_{BC}\Sigma_{CA})^{1/2}$ are shown in Table 1. The value $(\Sigma_{AB}\Sigma_{BC}\Sigma_{CA})^{1/2}$ is conjectured to be the unit-cell volume of the lattice that is formed from the

Table 1. *Axis–angle pairs of the CSL matrices that satisfy* $R_1R_2R_3 = E$

No.	R_1	R_2	R_3	$(\Sigma_1\Sigma_2\Sigma_3)^{1/2}$
1	Σ3([1 1 1], 180.00)	Σ9([−1 2 2], 180.00)	Σ3([0 −1 1], 109.47)	9
2	Σ3([1 1 1], 180.00)	Σ5([2 1 0], 180.00)	Σ15([−1 2−1], 78.46)	15
3	Σ3([1 1 1], 180.00)	Σ7([3 2 1], 180.00)	Σ21b([−1 2−1], 44.42)	21
4	Σ3([1 1 1], 180.00)	Σ7([0 1 −2], 73.40)	Σ21a([0 −5 −4], 162.25)	21
5	Σ3([1 1 1], 180.00)	Σ9([2 2 1], 180.00)	Σ27a([−1 1 0], 31.59)	27
6	Σ3([1 1 1], 180.00)	Σ9([0 1 −2], 96.38)	Σ27b([1 −4 −3], 157.81)	27
7	Σ3([1 1 1], 180.00)	Σ11([3 1 1], 180.00)	Σ33c([0 1 −1], 58.99)	33
8	Σ3([1 1 1], 180.00)	Σ33a([1 4 4], 180.00)	Σ11([0 −1 1], 50.48)	33
9	Σ3([1 1 1], 180.00)	Σ11([−1 0 3], 144.90)	Σ33b([4 −3 2], 139.25)	33
10	Σ3([1 1 1], 180.00)	Σ13a([3 2 0],180.00)	Σ39b([−2 3 −1],73.62)	39
11	Σ3([1 1 1], 180.00)	Σ13b([4 3 1], 180.00)	Σ39b([−2 3 −1], 50.13)	39
12	Σ3([1 1 1], 180.00)	Σ13b([0 1 −3], 76.66)	Σ39a([0 −7 −5], 153.82)	39
13	Σ3([1 1 1], 180.00)	Σ15([5 2 1], 180.00)	Σ45c([−1 4 −3], 65.03)	45
14	Σ3([1 1 1], 180.00)	Σ15([0 1 −2], 48.19)	Σ45a([−2 −7 −6], 167.90)	45
15	Σ3([1 1 1], 180.00)	Σ15([−1 0 5], 137.17)	Σ45b([7 −4 3], 130.12)	45
16	Σ5([2 1 0], 180.00)	Σ25a([3 4 0], 180.00)	Σ5([0 0 1], 53.13)	25
17	Σ5([2 1 0], 180.00)	Σ5([3 −1 1], 95.74)	Σ25b([7 1 −5], 120.00)	25
18	Σ5([2 1 0], 180.00)	Σ7([3 2 1], 180.00)	Σ35a([1 −2 1], 34.05)	35
19	Σ5([2 1 0], 180.00)	Σ7([0 1 −2], 73.40)	Σ35b([4 7 2], 166,27)	35
20	Σ5([2 1 0], 180.00)	Σ9([2 2 1], 180.00)	Σ45c([1 −2 2], 53.13)	45
21	Σ5([2 1 0], 180.00)	Σ9([3 1 1], 67.11)	Σ45b([1 3 −1], 117.10)	45
22	Σ5([2 1 0], 180.00)	Σ9([−5 1 −1], 120.00)	Σ45a([−5 −5 −7], 95.74)	45
23	Σ7([3 2 1], 180.00)	Σ49c([2 6 3], 180.00)	Σ7([0 −1 2], 73.40)	49
24	Σ7([3 2 1], 180.00)	Σ7([3 3 −1], 110.93)	Σ49b([2 6 3], 90.00)	49
25	Σ7([3 2 1], 180.00)	Σ49a([8 3 5], 180.00)	Σ7([1 −1 −1], 38.21)	49
26	Σ9([2 2 1], 180.00)	Σ9([−5 1−1], 120.00)	Σ9([−1 −1 −5], 120.00)	27
27	Σ9([2 2 1], 180.00)	Σ15([5 2 1], 180.00)	Σ15([0 1 −2], 48.19)	45
28	Σ9([2 2 1], 180.00)	Σ21b([3 7 −5], 167.47)	Σ21a([−5 5 3], 113.88)	63
29	Σ9([2 2 1], 180.00)	Σ27b([−3 −4 2], 94.25)	Σ27a([−6 −1 −1], 114.04)	81
30	Σ9([2 2 1], 180.00)	Σ27b([3 5 −4], 148.41)	Σ27b([−3 5 2], 114.04)	81
31	Σ9([2 2 1], 180.00)	Σ33a([1−7 −9], 170.01)	Σ33b([3 −7 5], 104.93)	99
32	Σ9([2 2 1], 180.00)	Σ33b([−1 −5 −6], 151.50)	Σ33b([1 −5 2], 84.78)	99
33	Σ9([2 2 1], 180.00)	Σ39a([−2 7 5], 180.00)	Σ39b([1 −4 6], 111.04)	117
34	Σ9([2 2 1], 180.00)	Σ45c([−3 −4 −1], 65.03)	Σ45b([−6 −5 −2], 116.39)	135
35	Σ9([2 2 1], 180.00)	Σ45b([−3 −11 7], 171.45)	Σ45a([−9 5 5], 117.10)	135
36	Σ15([5 2 1], 180.00)	Σ15([−4 2 1], 113.58)	Σ25b([−5 1 −7], 120.00)	75
37	Σ15([5 2 1], 180.00)	Σ25a([0 7 1], 180.00)	Σ15([−1 −1 7], 134.43)	75
38	Σ15([5 2 1], 180.00)	Σ21b([3 7 −5], 167.47)	Σ35a([−2 5 5], 122.88)	105
39	Σ15([5 2 1], 180.00)	Σ35a([5 −3 1], 180.00)	Σ21a([1 0 −5], 103.77)	105
40	Σ15([5 2 1], 180.00)	Σ21a([−1 −9 −1], 167.47)	Σ35b([−2 −1 7], 122.88)	105
41	Σ15([5 2 1], 180.00)	Σ45a([5 −8 1], 180.00)	Σ27a([1 0 −5], 157.81)	135
42	Σ15([5 2 1], 180.00)	Σ27a([5 −3 5], 95.31)	Σ45c([8 −1 −3], 130.12)	135
43	Σ15([5 2 1], 180.00)	Σ27a([7 −3 −5], 122.48)	Σ45b([3 7 −4], 130.12)	135
44	Σ15([5 2 1], 180.00)	Σ45b([5 4 2], 180.00)	Σ27b([0 −1 2], 35.43)	135
45	Σ15([5 2 1], 180.00)	Σ27b([3 5 −4], 148.41)	Σ45c([−1 9 7], 117.10)	135
46	Σ15([5 2 1], 180.00)	Σ27b([−3 7 7], 168.96)	Σ45a([2 −6 7], 167.90)	135
47	Σ21b([4 2 1], 180.00)	Σ21b([−1 −5 −7], 141.79)	Σ49c([−1 −11 5], 120.00)	147
48	Σ21b([4 2 1], 180.00)	Σ49b([9 1 4], 180.00)	Σ21b([1 −1 −2], 44.42)	147
49	Σ21b([4 2 1], 180.00)	Σ49a([−8 3 5], 180.00)	Σ21b([−1 4 −4], 124.85)	147
50	Σ21b([4 2 1], 180.00)	Σ21a([4 −5 0], 162.25)	Σ49c([3 2 −9], 156.69)	147
51	Σ21b([4 2 1], 180.00	Σ21a([5 5 −3], 113.88)	Σ49b([3 9 5], 99.99)	147
52	Σ21a([5 4 1], 180.00)	Σ49a([8 5 3], 180.00)	Σ21a([1 −1 −1], 21.79)	147
53	Σ25a([4 3 0], 180.00)	Σ25b([4 3 0], 90.00)	Σ25b([4 3 0], 90.00)	125
54	Σ25b([4 3 5], 180.00)	Σ25b([4 3 0], 90.00)	Σ25b([1 7 5], 120.00)	125
55	Σ25a([4 3 0], 180.00)	Σ35a([7 −1 3], 80.96)	Σ35b([9 3 −5], 130.01)	175
56	Σ25b([5 4 3], 180.00)	Σ35a([5 3 1], 180.00)	Σ35a([−1 2 −1], 34.05)	175
57	Σ25b([4 3 0], 90.00)	Σ35a([−1 −7−9], 150.63)	Σ35b([2 −1 7], 122.88)	175
58	Σ25b([5 4 3], 180.00)	Σ35b([4 1 2], 66.42)	Σ35b([4 3 1], 119.06)	175
59	Σ25a([4 3 0], 180.00)	Σ45c([−1 8 3], 130.12)	Σ45c([5 0 7], 130.12)	225
60	Σ25a([4 3 0], 180.00)	Σ45b([−11 3 −1], 117.1)	Σ45a([−5 −5 −9], 117.10)	225
61	Σ25b([5 4 3], 180.00)	Σ45c([1 −4 −8], 143.13)	Σ45b([1 −11 3], 117.10)	225
62	Σ25b([4 3 0], 90.00)	Σ45c([8 1 −4], 143.13)	Σ45a([4 3 −4], 145.31)	225
63	Σ25b([5 4 3], 180.00)	Σ45b([2 −5 5], 101.54)	Σ45a([13 1 −3], 171.45)	225
64	Σ25b([5 4 3], 180.00)	Σ45b([−6 5 5], 155.66)	Σ45b([3 −7 11], 171.45)	225
65	Σ25b([4 3 0], 90.00)	Σ45a([4 3 −2], 106.79)	Σ45a([6 7 −2], 167.90)	225
66	Σ25b([4 3 0], 90.00)	Σ45a([−3 4 4], 145.31)	Σ45b([−1 −2 −9], 155.65)	225
67	Σ35a([5 3 1], 180.00)	Σ49c([3 6 2], 180.00)	Σ35a([0 −1 3], 64.62)	245
68	Σ35a([5 3 1], 180.00)	Σ35a([5 4 −2], 106.60)	Σ49b([3 6 2], 90.00)	245
69	Σ35a([5 3 1], 180.00)	Σ35b([4 1 2], 66.42)	Σ49a([8 3 0], 119.33)	245
70	Σ35a([5 3 1], 180.00)	Σ35b([−7 2 −1], 122.88)	Σ49b([−3 −2 −7], 105.39)	245
71	Σ35a([5 3 1], 180.00)	Σ35b([−3 3 1], 43.23)	Σ49c([−11 −5−7], 171.81)	245
72	Σ35b([6 5 3], 180.00)	Σ49c([6 −2 3], 180.00)	Σ35b([1 0 −2], 106.60)	245
73	Σ35b([6 5 3], 180.00)	Σ35b([3 5 9], 130.00)	Σ49b([6 −2 3], 90.00)	245
74	Σ49c([6 3 2], 180.00)	Σ49c([−11 5 1], 120.00)	Σ49c([−5 1 −11], 120.00)	343
75	Σ49c([6 3 2], 180.00)	Σ49a([−3 −13 −3], 155.25)	Σ49b([−5 −3 9], 99.99)	343
76	Σ49c([6 3 2], 180.00)	Σ49b([9 5 −3], 99.99)	Σ49b([5 9 3], 99.99)	343

coincidence points of three crystal grains. This will be discussed elsewhere.

Candidate Σ values at a triple junction are easily obtained by putting $\Sigma_1 = pq$, $\Sigma_2 = qr$ and $\Sigma_3 = rp$ for odd integers p, q and r.

3. Application of the combination rule to two-dimensional polycrystals

Using (51), two-dimensional polycrystals with various combinations of coincidence boundaries can be designed. But, in this paper, design of coincidence boundaries with a finite number of Σ values is considered. To construct grain boundaries of a two-dimensional polycrystal using a finite number of $\Sigma (\neq 1)$ values is identical to assigning a finite number of CSL matrices to the grains so that no adjacent grains have the same matrix. According to Foulds (1992), based on the four-colour theorem by Appel & Haken (1976), 'Any map on a plane surface can be colored with at most four colors so that no two adjacent regions have the same color'. If the four colors are substituted by the four CSL matrices E, R_1, R_2 and R_3, every crystal grain can have one of the CSL matrices so that no two adjacent grains have the same CSL matrix.

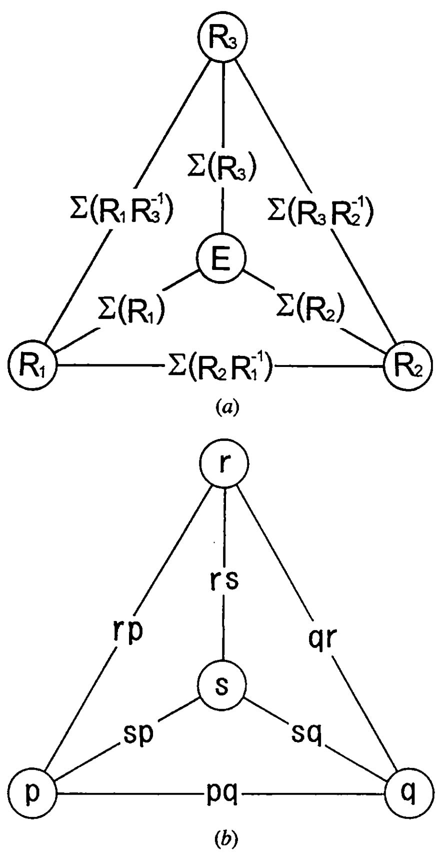

Fig. 1. (a) Relationships among the CSL matrices E, R_1, R_2 and R_3. (b) A diagram to search the candidate Σ values in (a) using odd integers p, q, r and s.

Relationships among E, R_1, R_2 and R_3 are schematically shown in Fig. 1(a) with the Σ values derived from the orientation difference between two matrices. Fig. 1(a) shows that all grain boundaries in a two-dimensional polycrystal can be constructed from at most six different Σ values. Fig. 1(a) contains four triangles, ER_1R_2, ER_2R_3, ER_1R_3 and $R_1R_2R_3$. When three matrices of each triangle's vertices are assumed to be the coincidence matrices of grains forming a triple junction, the Σ values on the triangle edges must satisfy the combination rule. A diagram to find the candidate Σ values is therefore proposed in Fig. 1(b) for odd integer p, q, r and s.

In reality, it is possible to construct grain boundaries from a more limited number of Σ values. For example, if the matrices are selected as

$$R_1 = \frac{1}{3}\begin{bmatrix} \bar{1} & 2 & 2 \\ 2 & \bar{1} & 2 \\ 2 & 2 & \bar{1} \end{bmatrix}, \quad R_2 = \frac{1}{3}\begin{bmatrix} \bar{1} & 2 & \bar{2} \\ 2 & \bar{1} & \bar{2} \\ \bar{2} & \bar{2} & \bar{1} \end{bmatrix},$$

$$R_3 = \frac{1}{3}\begin{bmatrix} \bar{1} & \bar{2} & 2 \\ \bar{2} & \bar{1} & \bar{2} \\ 2 & \bar{2} & \bar{1} \end{bmatrix},$$

Σ values other than 3 and 9 do not appear because

$$R_2R_1^{-1} = \frac{1}{9}\begin{bmatrix} 1 & \bar{8} & 4 \\ 8 & \bar{1} & 4 \\ \bar{4} & \bar{4} & \bar{7} \end{bmatrix}, \quad R_3R_2^{-1} = \frac{1}{9}\begin{bmatrix} \bar{7} & \bar{4} & 4 \\ 4 & 1 & 8 \\ \bar{4} & 8 & 1 \end{bmatrix},$$

$$R_1R_3^{-1} = \frac{1}{9}\begin{bmatrix} 1 & \bar{4} & \bar{8} \\ 4 & \bar{7} & 4 \\ \bar{8} & \bar{4} & 1 \end{bmatrix}.$$

If these matrices are assigned to the grains, the grain boundaries are made up of only $\Sigma3$ and $\Sigma9$ boundaries as shown in Fig. 2, where the combination rule is seen to hold at every triple junction.

Using the following CSL matrices,

$$R_1 = \frac{1}{9}\begin{bmatrix} \bar{1} & 8 & 4 \\ 8 & \bar{1} & 4 \\ 4 & 4 & \bar{7} \end{bmatrix}, \quad R_2 = \frac{1}{9}\begin{bmatrix} \bar{7} & 4 & 4 \\ \bar{4} & \bar{1} & \bar{8} \\ 4 & \bar{8} & \bar{1} \end{bmatrix},$$

$$R_3 = \frac{1}{9}\begin{bmatrix} \bar{1} & \bar{4} & \bar{8} \\ \bar{4} & \bar{7} & 4 \\ \bar{8} & 4 & \bar{1} \end{bmatrix},$$

it is possible to make a polycrystal model that contains only $\Sigma9$ boundaries since the following relationships are obtained in this case:

$$R_2R_1^{-1} = \frac{1}{9}\begin{bmatrix} \bar{1} & \bar{4} & \bar{8} \\ \bar{4} & \bar{7} & 4 \\ \bar{8} & 4 & \bar{1} \end{bmatrix}, \quad R_3R_2^{-1} = \frac{1}{9}\begin{bmatrix} \bar{1} & 8 & 4 \\ 8 & \bar{1} & 4 \\ 4 & 4 & \bar{7} \end{bmatrix},$$

$$R_1R_3^{-1} = \frac{1}{9}\begin{bmatrix} \bar{7} & \bar{4} & 4 \\ \bar{4} & \bar{1} & \bar{8} \\ 4 & \bar{8} & \bar{1} \end{bmatrix}.$$

Table 2 shows such combinations of CSL matrices that are closed about one, two or three kinds of Σ values.

4. Application of the combination rule to three-dimensional polycrystals

In three-dimensional polycrystals, quadruple junctions where four crystal grains meet appear. Fig. 3 shows a model of quadruple junction O formed by the gains 1, 2, 3 and 4 with a shape of a truncated octahedron. Six grain boundaries denoted as $OP_1P_2P_3$ (GB1), $OP_1P_4P_5P_6P_7$ (GB2), $OP_1P_{18}P_{17}P_{16}P_{12}$ (GB3), $OP_3P_8P_9P_{10}P_7$ (GB4), $OP_3P_{15}P_{14}P_{13}P_{12}$ (GB5) and $OP_7P_{11}P_{12}$ (GB6) meet at point O and are assumed to be coincidence boundaries with Σ values of Σ_{GB1}, Σ_{GB2}, Σ_{GB3}, Σ_{GB4}, Σ_{GB5} and Σ_{GB6}, respectively. The coincidence boundaries form four sets of Σ values, $\Sigma_{GB1} - \Sigma_{GB2} - \Sigma_{GB3}$, $\Sigma_{GB2} - \Sigma_{GB4} - \Sigma_{GB6}$, $\Sigma_{GB3} - \Sigma_{GB5} - \Sigma_{GB6}$ and $\Sigma_{GB1} - \Sigma_{GB4} - \Sigma_{GB5}$, around the triple lines OP_1, OP_7, OP_{12} and OP_3, respectively, and their relationships are schematically shown in Fig. 4. The Σ values of each set must satisfy the combination rule but are confined to the values that are determined by the crystal orientation relationships around the quadruple junction. Since the orientation relationships of grains at quadruple junction are described by the same diagram as Fig. 1(a), the CSL matrices of Table 2 are also applicable to the case of a quadruple junction.

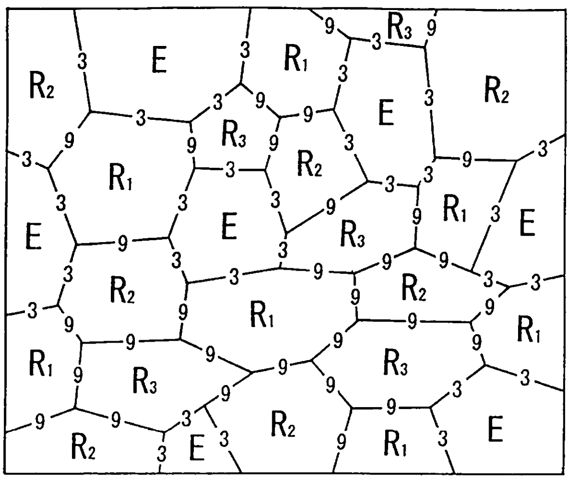

Fig. 2. A two-dimensional polycrystal model composed of only $\Sigma 3$ and $\Sigma 9$ boundaries. Matrices E, R_1, R_2 and R_3 represent orientation of grains.

Fig. 5 shows a cubic unit cell composed of eight b.c.c. sub unit cells. Four CSL matrices E, R_1, R_2 and R_3 are put to each lattice point so that the same matrix does not come to the nearest neighbors by three-dimensional translations of the unit cell. The figure demonstrates that whole grain boundaries in a polycrystalline aggregate become the coincidence boundaries with specially selected Σ values if crystal grains have the shape of a truncated octahedron. For example, three-dimensional polycrystal with only $\Sigma 3$ and $\Sigma 9$ boundaries, or $\Sigma 9$ boundaries or $\Sigma 3$, $\Sigma 5$ and $\Sigma 15$ boundaries, or $\Sigma 25$ boundaries can be con-

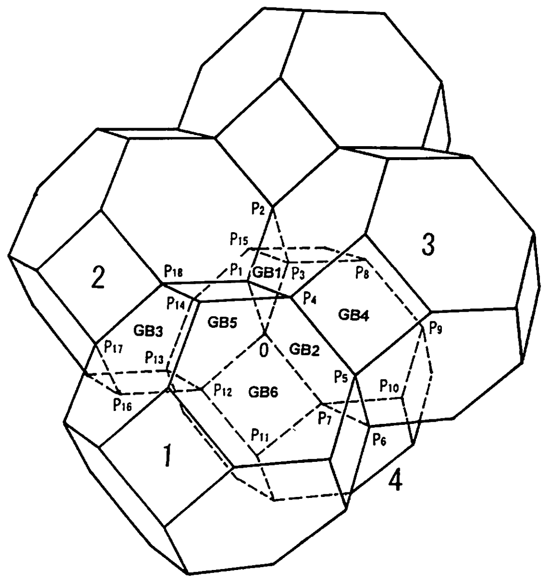

Fig. 3. A model of quadruple junction O formed by the truncated octahehdrons 1, 2, 3 and 4.

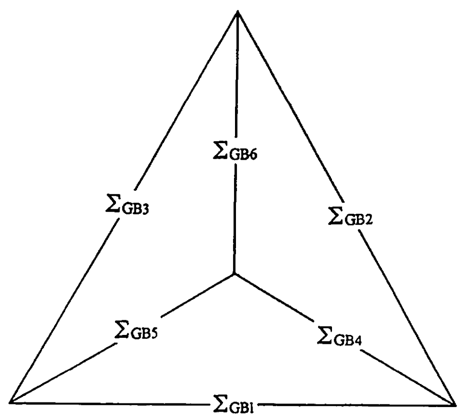

Fig. 4. A diagram showing the relationships among the six coincidence boundaries meeting at the quadruple junction O of Fig. 3.

Table 2. *Combinations of the CSL matrices (axis–angle pairs) closed for* Σ *values* ≤ 49

No.	R_1	R_2	R_3	$R_2R_1^{-1}$	$R_3R_2^{-1}$	$R_1R_3^{-1}$
1	Σ3([1 1 1], 180.00)	Σ3([−1 1 1], 180.00)	Σ3([1 −1 1], 180.00)	Σ9([0 −1 1], 141.06)	Σ9([−1 −1 0], 141.06)	Σ9([−1 0 1], 141.06)
2	Σ3([1 1 1], 180.00)	Σ5([0 2 1], 180.00)	Σ15([5 −1 2], 180.00)	Σ15([−1 −1 2], 78.46)	Σ3([−1 −1 2], 180.00)	Σ5([−1 −1 2], 101.54)
3	Σ3([1 1 1], 180.00)	Σ7([3 2 1], 180.00)	Σ21b([−2 1 4], 180.00)	Σ21b([−1 2 −1], 44.42)	Σ3([1 −2 1]), 180.00)	Σ7([−1 2 −1], 135.59)
4	Σ3([1 1 1], 180.00)	Σ7([−3 2 1], 180.00)	Σ21a([−1 −4 5], 180.00)	Σ21a([−1 −4 5], 180.00)	Σ3([1 1 1], 180.00)	Σ7([−3 2 1], 180.00)
5	Σ3([1 1 1], 180.00)	Σ9([2 2 1], 180.00)	Σ9([1 −2 2], 180.00)	Σ27a([−1 1 0], 31.59)	Σ9([−2 1 2], 180.00)	Σ27b([−4 1 3], 157.81)
6	Σ3([1 1 1], 180.00)	Σ9([−2 2 1], 180.00)	Σ9([−1 −2 2], 180.00)	Σ27b([−1 −3 4], 157.81)	Σ9([2 1 2], 180.00)	Σ27b([4 −3 −1], 157.81)
7	Σ3([1 1 1], 180.00)	Σ11([3 1 1], 180.00)	Σ33a([1 4 4], 180.00)	Σ33c([0 1 −1], 58.99)	Σ3([0 −1 −1], 109.47)	Σ11([0 1 −1], 50.48)
8	Σ3([1 1 1], 180.00)	Σ13a([3 2 0], 180.00)	Σ39b([−2 3 −1], 50.13)	Σ39b([−2 3 −1], 73.62)	Σ3([−2 −1 1], 180.00)	Σ13b([4 3 1], 180.00)
9	Σ5([1 0 0], 36.87)	Σ7([3 −2 1], 180.00)	Σ35a([−5 1 3], 180.00)	Σ35a([9 −7 1], 150.63)	Σ5([1 2 1], 101.54)	Σ7([−3 0 2], 149.00)
10	Σ5([2 1 0], 180.00)	Σ9([1 −2 2], 180.00)	Σ45b([−2 4 5], 180.00)	Σ45b([−2 4 5], 180.00)	Σ5([2 1 0], 180.00)	Σ9([1 −2 2], 180.00)
11	Σ9([2 2 1], 180.00)	Σ9([1 −2 2], 180.00)	Σ9([−2 1 2], 180.00)	Σ9([−2 1 2], 180.00)	Σ9([2 2 1], 180.00)	Σ9([1 −2 2], 180.00)
12	Σ9([2 2 1], 180.00)	Σ27a([5 −1 1], 180.00)	Σ27b([1 7 2], 180.00)	Σ27b([1 1 −4], 109.47)	Σ9([−1 −1 4], 180.00)	Σ27a([1 1 −4], 70.53)
13	Σ9([2 2 1], 180.00)	Σ27a([5 −1 1], 180.00)	Σ27b([−1 2 7], 180.00)	Σ27b([1 1 −4], 109.47)	Σ9([−1 −4 1], 180.00)	Σ27b([−4 5 −2], 131.81)
14	Σ9([2 2 1], 180.00)	Σ27b([1 7 2], 180.00)	Σ27b([−1 2 7], 180.00)	Σ27a([−1 −1 4], 70.53)	Σ9([5 −1 1], 120.00)	Σ27b([−4 5 −2], 131.81)
15	Σ9([2 2 1], 180.00)	Σ45b([2 5 4], 180.00)	Σ45a([8 5 1], 180.00)	Σ45c([1 −2 2], 53.13)	Σ9([−1 2 −2], 90.00)	Σ45b([1 −2 2], 36.87)
16	Σ9([2 2 1], 180.00)	Σ45c([−7 5 4], 180.00)	Σ45a([1 −5 8], 180.00)	Σ45a([1 −5 8], 180.00)	Σ9([2 2 1], 180.00)	Σ45c([−7 5 4], 180.00)
17	Σ9([2 2 1], 180.00)	Σ45c([4 7 5], 180.00)	Σ45b([−2 4 5], 180.00)	Σ45b([1 −2 2], 36.87)	Σ9([1 −2 2], 90.00)	Σ45a([−1 2 −2], 126.87)
18	Σ15([5 2 1], 180.00)	Σ21a([5 −1 4], 180.00)	Σ35a([−5 1 3], 180.00)	Σ35b([3 −5 −5], 80.96)	Σ15([1 5 0], 137.17)	Σ21b([1 −4 3], 103.77)
19	Σ15([5 2 1], 180.00)	Σ21b([2 −1 4], 180.00)	Σ35a([5 1 3], 180.00)	Σ35a([1 −2 −1], 122.88)	Σ15([−1 2 1], 78.46)	Σ21b([−1 2 1], 44.42)
20	Σ15([5 2 1], 180.00)	Σ21b([−1 2 4], 180.00)	Σ35a([5 −3 1], 180.00)	Σ35b([2 −7 4], 166.27)	Σ15([−2 −3 1], 150.07)	Σ21a([−1 0 5], 103.77)
21	Σ15([5 2 1], 180.00)	Σ21b([1 4 2], 180.00)	Σ35b([5 6 3], 180.00)	Σ35b([0 −1 2], 106.60)	Σ15([0 1 −2], 48.19)	Σ21b([0 1 −2], 58.41)
22	Σ15([5 2 1], 180.00)	Σ21b([2 −4 1], 180.00)	Σ35b([5 −3 6], 180.00)	Σ35a([2 −1 −8], 166.27)	Σ15([−3 −1 2], 86.18)	Σ21a([−3 5 5], 113.88)
23	Σ25a([4 3 0], 180.00)	Σ25b([4 3 0], 90.00)	Σ25b([−4 −3 0], 90.00)	Σ25b([−4 −3 0], 90.00)	Σ25a([4 3 0], 180.00)	Σ25b([−4 −3 0], 90.00)
24	Σ25a([4 3 0], 180.00)	Σ25b([4 3 0], 90.00)	Σ25b([−3 4 0], 90.00)	Σ25b([−4 −3 0], 90.00)	Σ25b([−7 1 5], 120.00)	Σ25b([−4 −3 5], 180.00)
25	Σ49a([8 5 3], 180.00)	Σ49b([−9 4 1], 180.00)	Σ49b([−1 9 4], 180.00)	Σ49c([1 5 −11], 120.00)	Σ49c([1 5 −11], 120.00)	Σ49c([1 5 −11], 120.00)
26	Σ49b([9 4 1], 180.00)	Σ49b([1 9 4], 180.00)	Σ49b([4 1 9], 180.00)	Σ49c([1 −5 11], 120.00)	Σ49c([11 1 −5], 120.00)	Σ49c([−5 11 1], 120.00)
27	Σ49c([6 3 2], 180.00)	Σ49a([8 −3 5], 180.00)	Σ49b([−1 −4 9], 180.00)	Σ49b([3 −2 −6], 90.00)	Σ49c([−1 −11 −5], 120.00)	Σ49a([−5 8 3], 180.00)
28	Σ49c([6 3 2], 180.00)	Σ49a([8 −3 5], 180.00)	Σ49b([−4 −9 1], 180.00)	Σ49b([3 −2 −6], 90.00)	Σ49c([−3 2 6], 180.00)	Σ49b([3 −2 −6], 90.00)
29	Σ49c([6 3 2], 180.00)	Σ49b([−1 −4 9], 180.00)	Σ49b([−4 −9 1], 180.00)	Σ49a([−5 8 3], 180.00)	Σ49c([11 −5 −1], 120.00)	Σ49b([3 −2 −6], 90.00)
30	Σ49c([6 3 2], 180.00)	Σ49c([2 −6 3], 180.00)	Σ49a([8 −3 5], 180.00)	Σ49c([−3 2 6], 180.00)	Σ49b([−3 2 6], 90.00)	Σ49b([−3 2 6], 90.00)
31	Σ49c([6 3 2], 180.00)	Σ49c([2 −6 3], 180.00)	Σ49b([−1 −4 9], 180.00)	Σ49c([−3 2 6], 180.00)	Σ49b([6 3 2], 90.00)	Σ49a([−5 8 3], 180.00)
32	Σ49c([6 3 2], 180.00)	Σ49c([2 −6 3], 180.00)	Σ49b([−4 −9 1], 180.00)	Σ49c([−3 2 6], 180.00)	Σ49b([3 −2 −6], 90.00)	Σ49b([3 −2 −6], 90.00)
33	Σ49c([6 3 2], 180.00)	Σ49c([2 −6 3], 180.00)	Σ49c([−3 2 6], 180.00)	Σ49c([−3 2 6], 180.00)	Σ49c([6 3 2], 180.00)	Σ49c([2 −6 3], 180.00)

structed. Fig. 6 shows a model of polycrystal that contains only $\Sigma 3$ and $\Sigma 9$ boundaries.

As previously discussed, four CSL matrices are sufficient in constructing a two-dimensional polycrystal with only the coincidence boundaries whose Σ values are not equal to 1. But when columnar crystal grains are formed on a single-crystalline substrate with the same lattice constant as the columnar grains, at least one more CSL matrix is necessary so that the grain–substrate interfaces and the grain boundaries can be made of the coincidence boundaries ($\Sigma \neq 1$) only. Fig. 7(*a*) gives a diagram to find those matrices, and contains 13 triangles: $E_1R_1R_2$, $E_1R_1R_3$, $E_1R_2R_3$, $R_1R_2R_3$, $E_2R_1R_3$, $E_2R_1R_4$, $E_2R_3R_4$, $R_1R_3R_4$, $E_3R_1R_2$, $E_3R_1R_4$, $E_3R_2R_4$, $R_1R_2R_4$ and $R_2R_3R_4$. Each triangle corresponds to a set of coincidence boundaries at a

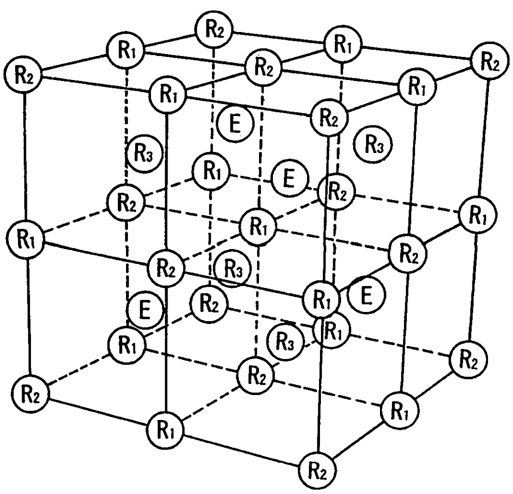

Fig. 5. CSL matrices E, R_1, R_2 and R_3 assigned to the lattice points of a cubic unit cell composed of eight b.c.c. sub unit cells.

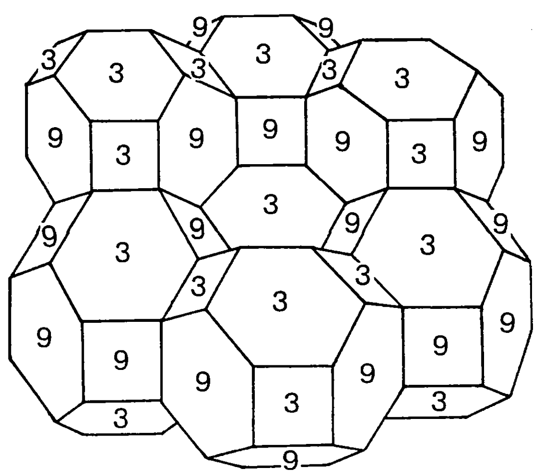

Fig. 6. A polycrystal model formed by truncated octahedrons, where grain boundaries are composed of only $\Sigma 3$ and $\Sigma 9$ boundaries.

Table 3. *Examples of the CSL matrices (axis–angle pairs) closed for Σ values $\leq$ 49*

	R_1	R_2	R_3	R_4	$R_1^{-1}R_2$	$R_1^{-1}R_3$	$R_1^{-1}R_4$	$R_2^{-1}R_3$	$R_2^{-1}R_4$	$R_3^{-1}R_4$
No. 1	Σ3 [1 1 1] 180.00	Σ9 [−2 −2 1] 180.00	Σ9 [2 −1 2] 180.00	Σ9 [−1 2 2] 180.00	Σ3 [1 −1 0] 109.47	Σ3 [−1 0 1] 109.47	Σ3 [0 1 −1] 109.47	Σ9 [−1 2 2] 180.00	Σ9 [2 −1 2] 180.00	Σ9 [−2 −2 1] 180.00
No. 2	Σ3 [−1 −1 −1] 60.00	Σ5 [−2 1 0] 180.00	Σ15 [2 −1 5] 180.00	Σ45a [−1 8 5] 180.00	Σ15 [−7 1 3] 165.17	Σ5 [−2 1 −2] 143.13	Σ15 [1 −3 −4] 137.17	Σ3 [1 2 0] 131.81	Σ9 [−1 −2 3] 123.75	Σ3 [3 1 −1] 146.44
No. 3	Σ3 [1 1 1] 180.00	Σ7 [3 2 1] 180.00	Σ7 [−3 2 1] 180.00	Σ7 [3 −2 1] 180.00	Σ21b [1 −2 1] 44.42	Σ21a [−1 −4 5] 180.00	Σ21b [−3 −2 5] 144.05	Σ49c [0 −1 2] 146.80	Σ49c [−1 0 3] 129.25	Σ49c [2 3 0] 62.01
No. 4	Σ3 [1 1 1] 180.00	Σ15 [−5 −2 1] 180.00	Σ15 [2 −1 5] 180.00	Σ15 [−1 5 2] 180.00	Σ5 [1 −2 1] 101.54	Σ5 [−2 1 1] 101.54	Σ5 [1 1 −2] 101.54	Σ25b [−1 3 1] 168.52	Σ25b [−1 1 −3] 168.52	Σ25b [3 1 −1] 168.52
No. 5	Σ15 [5 2 1] 180.00	Σ15 [−2 1 5] 180.00	Σ15 [1 −5 2] 180.00	Σ15 [2 5 1] 180.00	Σ25b [1 −3 1] 168.52	Σ25b [1 −1 −3] 168.52	Σ25a [1 1 −7] 91.15	Σ25b [−3 −1 −1] 168.52	Σ25b [2 −1 1] 156.93	Σ25b [−5 −1 5] 91.15

triple junction and each three Σ values on the triangle edges must satisfy the combination rule. Fig. 7(*b*) shows an example of candidate Σ values for Fig. 7(*a*). It is expected that the whole grain boundaries can be composed of only $\Sigma 3$, $\Sigma 7$, $\Sigma 21$ and $\Sigma 49$ coincidence boundaries. Several combinations of the CSL matrices that are closed for special Σ values are numerically obtained as shown in Table 3. Figs. 8(*a*) and (*b*) show the grain-boundary models to demonstrate the consideration. The CSL matrices E and R_1–R_4 of group No. 3 in Table 3 are assigned to the grains in Fig. 8(*a*) so that the same matrices do not adjoin each other and the calculated Σ values are given to the grain boundaries as shown in Fig. 8(*b*). The combination rule is seen to hold at every triple junction of the grain boundaries and grain–substrate interfaces.

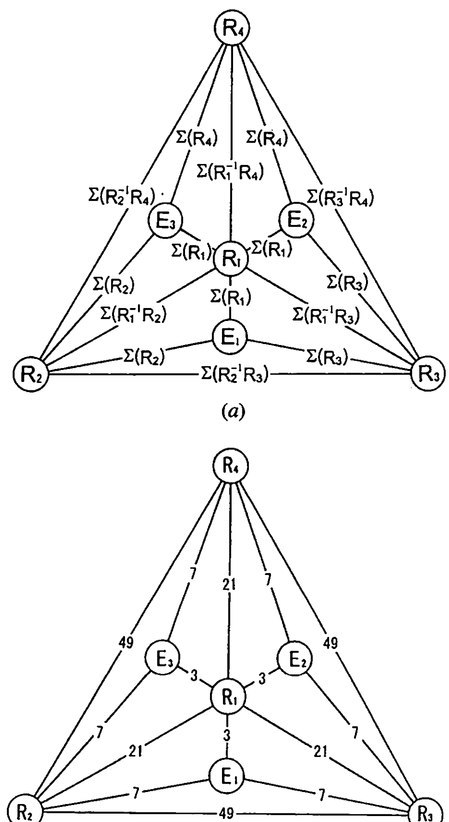

Fig. 7. (*a*) A diagram showing the relationships among five CSL matrices, E $(= E_1 = E_2 = E_3)$, R_1, R_2, R_3 and R_4. Σ values derived from the orientation difference between two CSL matrices are shown on the triangle edges. (*b*) Examples of the combinations of Σ values that satisfy (*a*).

5. Conclusions

Grain boundaries in cubic polycrystals have been discussed for the special cases that the orientation

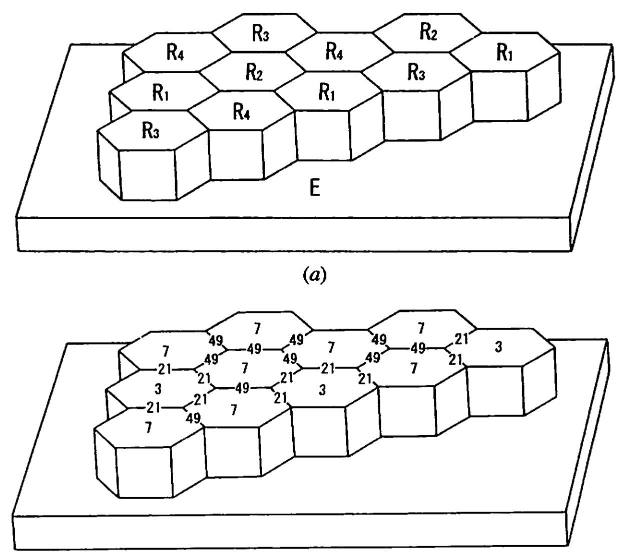

Fig. 8. (*a*) A model of columnar grains with coincidence boundaries grown on a single-crystalline substrate. CSL matrices E, R_1, R_2 and R_3 are assigned to the grains so that the same matrix may not adjoin. (*b*) Assigned Σ values according to Table 3 and (*a*). Numbers on the top surface of columnar grains indicate Σ values of grain–substrate interfaces.

relationships among the grains at triple junctions are described by the CSL matrices. Three coincidence boundaries can meet at a triple junction bound by a combination rule about the Σ values. The combination rule can be used to find candidate Σ values of coincidence boundaries at triple junctions and also at quadruple junctions. Examples of the CSL matrices that satisfy the combination rule have been tabulated and models of grain boundaries with selected Σ values have been demonstrated. The grain boundaries in the actual polycrystals are not always described by the ideal CSL orientation relationships but the combination rule is expected to be useful in the design of polycrystals with important coincidence boundaries.

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