On the Periodicity of {001} Symmetrical Tilt Grain Boundaries

Kazutoshi Inoue^{1,*}, Mitsuhiro Saito^{1,2}, Zhongchang Wang¹,
 Motoko Kotani¹ and Yuichi Ikumura^{1,2}

¹WPI Research Center, Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

²Institute of Engineering Innovation, School of Engineering, The University of Tokyo, Tokyo 113-8656, Japan

We report an application of the O-lattice theory to systematically analyse the structures of symmetrical tilt grain boundaries with the rotation axis of {001} and demonstrate a theoretical interpretation of the experimentally observed structures of a near Σ5 grain boundary in MgO in terms of the structural-units model and the periodicity of the O-points on the boundary. We further derive generalised decomposition formulae for the symmetrical tilt grain boundaries which are closely related to the distribution of irreducible rational numbers.

[doi:10.2320/matertrans.M2014394]

(Received November 7, 2014; Accepted December 16, 2014; Published February 6, 2015)

Keywords: atomic structure, crystal structure, dislocations, symmetrical tilt grain boundary, structural unit, O-lattice

1. Introduction

Grain boundaries with a large index rarely exist in nature, and can be decomposed into the ones with a smaller index due to relaxation. Over two decades ago, both symmetrical and asymmetrical tilt grain boundaries were intensively studied^{1–16)} and a general consensus was that actual configurations of grain boundaries could be realised by arranging smaller structural units. Since then, numerous experiments and calculations on the grain boundary geometries have been conducted and the study of interfaces in crystalline materials was summarised by A. P. Sutton and R. W. Balluffi.¹⁷⁾ R. C. Pond and his collaborators provided a general theoretical framework in regard to the symmetry of space groups and point groups on the dichromatic pattern and complex of two adjacent lattices^{18,19)} that was closely related to the periodic appearance of structural units as energetically stable configurations.

Recently, observations due to high resolutional microscopy combined with theoretical calculations have been conducted^{20–23)} and M. Saito *et al.*²⁴⁾ observed the atomic-scale structures of symmetrical tilt grain boundaries with a bonding angle of 35.3° in a bicrystal of MgO. They demonstrated that the {410}-structural units of Σ17 are periodically intercalated in between the {310}-structural units of Σ5 and recognised such phenomenon as the periodic appearance of displacement-shift-complete (DSC) dislocations.

While most of the successful works relied on microscopical observations and extensive numerical calculations, we propose a novel method to analyse the structures of symmetrical tilt grain boundaries of simple cubic crystals with the rotation axis of {001} with a mathematically evident argument. Sutton *et al.* gave an algorithm to obtain the arrangement of structural units assuming that the boundary structure can be described by two favoured boundaries as a linear combination of them with coprime integral coefficients and the structure changes as continuously as possible according to the misorientation.³⁾ Our approach to describe the boundary structure is the converse of their argument. We directly derive the decomposition formula of the {001} grain

boundaries and reproduce the previously observed results by the aid of the structural-units model and conventionally-called the O-lattice theory. The ratio of the number of the structural units is precisely given as a corollary.

The O-lattice theory was introduced by W. Bollmann^{25–29)} as a way of generalisations of the coincidence-site-lattice (CSL) theory.³⁰⁾ We utilise the O-lattice as an indicator of the periodicity of the structural units and therefore, it is different from the way Bollmann proposed. In this theory, let L_0 be a 2-dimensional square lattice and L_1, L_2 be lattices which satisfy $L_i = A_i(L_0)$ ($i = 1, 2$) for a non-degenerate linear transformation A_i . Let $U(L_0)$ denote the unit cell of L_0 and $|U(L_0)|$ denote its area. In what follows, the pair of lattices (L_0, L_1) is assumed to be a configuration slightly deviated from the optimal configuration (L_0, L_2) . For the dichromatic pattern^{18,19)} of a pair of lattices (L_0, L_i) , an O-point $\mathbf{a}$ with respect to A_i can be expressed by the following basic equation which can be derived by the Frank-Bilby formula:^{31–34)}

$$(I - A_i^{-1})\mathbf{a} = \mathbf{t}_0, \quad (1)$$

where I is the identity matrix and $\mathbf{t}_0$ is an arbitrary translational vector in L_0 . From the eq. (1), $\mathbf{a}$ is recognized as the centre of the linear transformation A_i in the dichromatic pattern of (L_0, L_i) . In this sense, the O-lattice is a way of generalisation of the CSL since any of the CSL points can be the centre of a rotational transformation. One of the points the O-lattice theory has been criticised is that the choice of A_i is not unique. However, this ambiguity allows us to choose an appropriate transformation according to the problem. Let $\mathcal{O}_{A_i}(L_0, L_i)$ denote the O-lattice of (L_0, L_i) with respect to A_i . Conversely, given an O-point and the transformation A_i , the configuration of the lattices around it is recovered. From the eq. (1), one can see that $|U(L_0)|/|\det(I - A_i^{-1})|$ gives the area of the unit cell of the O-lattice and therefore that $|\det(I - A_i^{-1})|$ is a sort of the density of O-points as with Σ in the CSL theory. Generally, an O-lattice is a super-lattice of the CSL in a CSL configuration if A_i is a rotational transformation and thus the unit cell of an O-lattice is smaller than that of the CSL. The O-points can be classified in terms of the internal coordinates. Two O-points are equivalent if their internal coordinates coincide, the representatives of which are called the reduced O-points. It can be shown that

*Corresponding author, E-mail: kinoue@wpi-aimr.tohoku.ac.jp

Table 1 Examples of reduced O-points for the small Σ 's if A_i is a rotational transformation.

Σ	2θ	$\cot\theta$	g.b. plane	reduced O-points
$\Sigma 13$	22.62°	5	(510)	(0, 0), (1/2, 1/2)
$\Sigma 17$	28.07°	4	(410)	(0, 0), (1/2, 1/2), (0, 1/2), (1/2, 0)
$\Sigma 5$	36.87°	3	(310)	(0, 0), (1/2, 1/2)
$\Sigma 5$	53.13°	2	(210)	(0, 0), (1/2, 1/2), (0, 1/2), (1/2, 0)

there are two types (resp. four types) of reduced O-points for the $(m \ 1 \ 0)$ -plane where m is an odd (resp. even) integer if A_i is a rotational transformation. Table 1 shows the examples of the reduced O-points for the small Σ 's.

The O-lattice defined above is called the primary O-lattice or simply the O_1 -lattice. As an alternative, we can also define a secondary O-lattice or simply an O_2 -lattice. The O_1 -lattice $\mathcal{O}_{A_i}(L_0, L_i)$ can be defined for each $i = 1, 2$. Then the transformation $A_1 A_2^{-1}$ maps L_2 to L_1 and thus the transformation $(I - A_1^{-1})^{-1}(I - A_2^{-1})$ maps $\mathcal{O}_{A_2}(L_0, L_2)$ to $\mathcal{O}_{A_1}(L_0, L_1)$. Letting $B = (I - A_1^{-1})^{-1}(I - A_2^{-1})$, the O_2 -lattice is defined to be the O_1 -lattice of two O_1 -lattices with respect to the transformation B . Namely, an O_2 -point $\mathbf{b}$ is given by²⁵⁾

$$(I - B^{-1})\mathbf{b} = \mathbf{t}_1, \quad (2)$$

where $\mathbf{t}_1$ is an arbitrary translational vector in the reference O_1 -lattice $\mathcal{O}_{A_2}(L_0, L_2)$. The basic equation of the O_2 -lattice is also given by

$$(I - A_1 A_2^{-1})\mathbf{b} = \mathbf{t}_2, \quad (3)$$

where $\mathbf{t}_2$ is an arbitrary translational vector of the DSC lattice of (L_0, L_2) . The O_2 -lattice is in general a sub-lattice of the reference O_1 -lattice. It is expected that the secondary dislocations (or the DSC dislocations) are introduced into the boundary of the Wigner-Seitz cells of the O_2 -points under the assumptions that the deviation of (L_0, L_1) from the optimal configuration (L_0, L_2) is small enough.^{28,35,36)}

2. Application of the O-Lattice Theory

We first demonstrate the application of the O-lattice theory by focusing on the symmetrical tilt CSL grain boundaries. The term *near CSL*³⁷⁾ can be defined as a configuration of a pair of two lattices which are, in a sense, close to an optimal configuration (a favoured boundary,³⁾ or a preferred state²⁸⁾). Note that the term near CSL can be used even for a CSL configuration with a high Σ . Let L_i be given by the rotation of L_0 with a rotational transformation $R(2\theta_i)$ of the angle of $2\theta_i$ ($i = 1, 2$), respectively. It is assumed that a CSL configuration with a high Σ can be approximated by two of the optimal reference configurations with low Σ 's. In this way, the periodicity of grain boundaries can be easily evaluated by the structural-units model.²⁻⁵⁾ In this paper, we consider the $(q \ p \ 0)$ -planes. As highlighted in Fig. 1, the *structural unit* of symmetrical $(q \ p \ 0)$ -grain boundary can be defined to be a kite-shaped tetragon which is made by gluing a pair of right triangles of a group of atoms at their hypotenuses whose sides in the right angles are qa and pa where a is the average atomic distance. Since a desired resolution around the

Fig. 1 (a) The (310)-structural units of the $\Sigma 5$ boundary and (b) the (410)-structural units of the $\Sigma 17$ boundary. The reference lattice L_0 , the rotated lattice L_1 and the O-lattice $\mathcal{O}(L_0, L_1)$ are presented.

boundary may not always be obtained, we take a larger cell enclosing the structural unit defined above. Figure 1 shows the atomic configurations of the (310)-structural units of the $\Sigma 5$ boundary and the (410)-structural units of the $\Sigma 17$ boundary where two lattices L_0 and L_1 are superposed. The CSL boundary is defined by the line passing through the CSL points below which there are points of L_0 and above which there are points of L_1 .

If (L_0, L_1) is of a CSL configuration, it holds that $\tan\theta_1 = p/q$ for coprime positive integers p and q . It is shown that the periodicity of the structural units in the $(q \ p \ 0)$ -plane is p . By taking $A = R(2\theta_1)$ in the eq. (1), we have

$$(I - R(2\theta_1)^{-1})^{-1} = \frac{1}{2} \begin{pmatrix} 1 & q/p \\ -q/p & 1 \end{pmatrix}. \quad (4)$$

By applying the eq. (4) to a translational vector $(0, l)$ of L_0 for an integer l to obtain the O-points on the $(q \ p \ 0)$ -plane, one can have

$$(I - R(2\theta_1)^{-1})^{-1} \begin{pmatrix} 0 \\ l \end{pmatrix} = \frac{l}{2} \begin{pmatrix} q/p \\ 1 \end{pmatrix}. \quad (5)$$

Then the point $l/2(q/p \ 1 \ 0)$ belongs to the $(q \ p \ 0)$ -plane. The CSL points are obtained by the eq. (5) if the parameter l is divisible by $2p$. If l is odd, the first component of the eq. (5) varies while the second component is maintained at $1/2$ in terms of the internal coordinates. It is concluded that the internal coordinates in the eq. (5) is periodic and the periodicity can be precisely given by $2p$. By drawing *virtual* structural units passing through O_1 -points alternately, it can be shown that the periodicity of the structural units is given by p .

In order to validate the above method, we consider the $(22 \ 7 \ 0)$ -structure as a model case which corresponds to the misorientation of the angle of 35.300° ($\tan(35.300^\circ/2) \simeq 7/22$) and is a near (310) $\Sigma 5$ -structure of the angle of 36.869° ($\tan(36.869^\circ/2) \simeq 1/3$). Figure 2 shows the dichromatic pattern of the $(22 \ 7 \ 0)$ -structure with the unit cells of L_0 . It can be seen that O-points in the virtual structural unit shifts periodically in $U(L_0)$. In the fourth structural unit from the left, one finds an O-point at the edge of $U(L_0)$ whose internal

Fig. 2 The (22 7 0)-structure with virtual structural units. The reference lattice L_0 , the rotated lattice L_2 of the angle of 35.30° and the O_1 -lattice $O(L_0, L_2)$ are presented, indicating that O_1 -point is shifted in the unit cell of L_0 . After the relaxation, the virtual structural units are transformed to (possibly deformed) six (310)-units and one (410)-unit.

coordinates are $(0, 1/2)$ with respect to the coordinate system of L_0 . Since the theoretical grain boundary is on the (22 7 0)-plane the above argument suggests that the periodicity of the structural units is 7. The deviation of the angle 35.300° identifies this CSL configuration as $\Sigma 533$ which is in between 36.869° ($\Sigma 5$) and 28.072° ($\Sigma 17$). Therefore this grain boundary can be described by the combination of the (310) and the (410)-planes. The internal coordinates of the eq. (5) becomes $(0, 1/2)$ if $l = 7 + 14k$ for each integer k which appears not in the $\Sigma 5$ but in the $\Sigma 17$ configuration (Table 1). The decomposition is thus given by the linear combination with integral coefficients of the reference boundaries.³⁾ Namely, it holds that $(22\ 7\ 0) = 6(3\ 1\ 0) + 1(4\ 1\ 0)$, which is viewed as a decomposition of a reciprocal vector. Once two reference structures are determined appropriately, one can obtain the integral coefficients uniquely for a specific grain boundary. Figure 3 shows an ABF-STEM image of the MgO grain boundary with a bonding angle of 35.3° and a corresponding schematic plot of the structural units, indicating that the periodicity of the structural units is 7 though it can be varied in the presence of impurities.²⁴⁾

For each $m = 2, 3, 4, 5, \dots$, let p/q be a rational number for coprime positive integers p and q with $1/m < p/q < 1/(m-1)$. Since the $(m\ 1\ 0)$ and the $(m-1\ 1\ 0)$ -planes can be the reference structures for the $(q\ p\ 0)$ -plane, the first decomposition rule is summarised as follows:

$$(q\ p\ 0) = n_1(m\ 1\ 0) + n_2(m-1\ 1\ 0), \quad (6)$$

where $n_1 = q - (m-1)p$ and $n_2 = -q + mp$ are positive integers. Similar equations were discussed by A. A. Levi *et al.*¹⁵⁾ and by Sutton *et al.*³⁸⁾ to describe the arrangement of the structural units. Note that $n_1 + n_2 = p$ defines the periodicity of the structural units. It holds that $n_1 > n_2$ if the $(q\ p\ 0)$ -plane is close to the $(m\ 1\ 0)$ -plane i.e. $1/m < p/q < 2/(2m-1)$ and $n_1 < n_2$ holds otherwise where $2/(2m-1)$ is the harmonic average of $1/m$ and $1/(m-1)$. The eq. (6) not only agrees with the microscopical observation by Saito *et al.*²⁴⁾ but successfully generalise the results of theoretical calculations by G. J. Wang *et al.*,^{8,9)} relatively recent results by S. P. Chen *et al.*,¹⁴⁾ and most of the experimental results by N. D. Browning *et al.*¹⁶⁾ It should be remarked that our argument goes in the opposite direction of Sutton's.³⁾ Although we only focus on the near $(3\ 1\ 0)\ \Sigma 5$ grain boundaries in this paper, the formula can be valid in more general cases which will be discussed further. Readers can refer to the decomposition table of the $(qp0)$ -planes

Fig. 3 An ABF-STEM image of the grain boundary in MgO with a bonding angle of 35.3° ²⁴⁾ and the schematic plot of structural units.

around $\Sigma 5$ ($2\theta = 36.869^\circ$) with $p < 10$ presented in Table 2 and more detailed cases for larger p 's in the appendix.

We may assume that the periodicity p is smaller than 10 since *nature might not prefer a long periodicity*. Then it can be shown that the numerators of the irreducible rational numbers in between $1/m$ and $1/(m-1)$ which are smaller than 10 form a mirror-symmetric sequence $\{p_l\}_{l=1}^{29}$:

$$\begin{aligned} &1, \underline{9}, 8, 7, 6, 5, \underline{9}, 4, \underline{7}, 3, \underline{8}, 5, 7, \underline{9}, 2, \\ &\underline{9}, 7, 5, \underline{8}, 3, \underline{7}, 4, \underline{9}, 5, 6, 7, 8, \underline{9}, 1. \end{aligned} \quad (7)$$

For instance, irreducible rational numbers in between $1/4$ and $1/3$ whose numerators are less than 10 can be given by $1/4, 9/35, 8/31, 7/27, 6/23, 5/19, 9/34, 4/15, 7/26, 3/11, 8/29, 5/18, 7/25, 9/32, 2/7, 9/31, 7/24, 5/17, 8/27, 3/10, 7/23, 4/13, 9/29, 5/16, 6/19, 7/22, 8/25, 9/28, 1/3$. Therefore, if $p_1 = 1$ and $p_{29} = 1$ correspond to the (410)-plane with 28.072° and the (310)-plane with 36.869° , respectively, $p_{26} = 7$ corresponds to the (22 7 0)-plane with $2\theta = 35.300^\circ$. It is observed that $p_l = p_{l-1} + p_{l+1}$ holds for $l = 2, 7, 9, 11, 14, 16, 19, 21, 23, 28$ (underlined) corresponding to the decomposition of a periodicity p_l to p_{l-1} and p_{l+1} which can be also shown by the periodicity of the O-points. Let q_l be the denominator that corresponds to p_l . We can now propose the second decomposition rule as follows. If it satisfies that $p_l = p_{l-1} + p_{l+1}$, the eq. (6) can be modified to

$$\begin{aligned} (q_l\ p_l\ 0) &= [n_{l-1}^{(1)}(m\ 1\ 0) + n_{l-1}^{(2)}(m-1\ 1\ 0)] \\ &+ [n_{l+1}^{(1)}(m\ 1\ 0) + n_{l+1}^{(2)}(m-1\ 1\ 0)], \end{aligned} \quad (8)$$

where $n_l^{(i)} = n_{l-1}^{(i)} + n_{l+1}^{(i)}$ ($i = 1, 2$) satisfying that $n_L^{(1)} = q_L - (m-1)p_L$ and $n_L^{(2)} = -q_L + mp_L$ ($L = l-1, l, l+1$). For instance, the $(32\ 9\ 0)$ -structure corresponding to the misorientation angle of 31.417° decomposes into $5(4\ 1\ 0) + 4(3\ 1\ 0)$ according to the eq. (6). On the other hand, since $9/32$ is in between $7/25$ and $2/7$, the $(32\ 9\ 0)$ -structure can be composed of the $(25\ 7\ 0)$ and the $(7\ 2\ 0)$ -structures, each of which decomposes into $4(4\ 1\ 0) + 3(3\ 1\ 0)$ and $(4\ 1\ 0) + (3\ 1\ 0)$, respectively, corresponding to the decomposition of the periodicity 9 into 7 and 2. It can be easily seen in Table 2. Note that the $(m\ 1\ 0)$ -plane can be decomposed into smaller indices when m is greater than 4.

Table 2 The decomposition table for the $(qp0)$ -plane around $\Sigma 5$ ($2\theta = 36.869^\circ$) with $p < 10$ is presented. The reference configurations are denoted by $A = (4\ 1\ 0)$, $B = (3\ 1\ 0)$ and $C = (2\ 1\ 0)$ which are represented in boldstyle. The second rule of decomposition in the eq. (8) is observed.

$2\theta[^\circ]$	$\tan\theta$	Σ	g.b. plane	decomposition
28.072	1/4	17	(4 1 0)	A
28.841	9/35	653	(35 9 0)	8A + 1B
28.940	8/31	1025	(31 8 0)	7A + 1B
29.068	7/27	389	(27 7 0)	6A + 1B
29.241	6/23	565	(23 6 0)	5A + 1B
29.487	5/19	193	(19 5 0)	4A + 1B
29.652	9/34	1237	(34 9 0)	7A + 2B
29.862	4/15	241	(15 4 0)	3A + 1B
30.136	7/26	725	(26 7 0)	5A + 2B
30.510	3/11	65	(11 3 0)	2A + 1B
30.844	8/29	905	(29 8 0)	5A + 3B
31.048	5/18	349	(18 5 0)	3A + 2B
31.284	7/25	337	(25 7 0)	4A + 3B
31.417	9/32	1105	(32 9 0)	5A + 4B
31.890	2/7	53	(7 2 0)	1A + 1B
32.378	9/31	521	(31 9 0)	4A + 5B
32.520	7/24	625	(24 7 0)	3A + 4B
32.779	5/17	157	(17 5 0)	2A + 3B
33.008	8/27	793	(27 8 0)	3A + 5B
33.398	3/10	109	(10 3 0)	1A + 2B
33.855	7/23	289	(23 7 0)	2A + 5B
34.205	4/13	185	(13 4 0)	1A + 3B
34.482	9/29	461	(29 9 0)	2A + 7B
34.708	5/16	281	(16 5 0)	1A + 4B
35.051	6/19	397	(19 6 0)	1A + 5B
35.300	7/22	533	(22 7 0)	1A + 6B
35.489	8/25	689	(25 8 0)	1A + 7B
35.637	9/28	865	(28 9 0)	1A + 8B
36.869	1/3	5	(3 1 0)	B

Continued on next column.

Continued.

$2\theta[^\circ]$	$\tan\theta$	Σ	g.b. plane	decomposition
36.869	1/3	5	(3 1 0)	B
38.186	9/26	757	(26 9 0)	8B + 1C
38.358	8/23	593	(23 8 0)	7B + 1C
38.580	7/20	449	(20 7 0)	6B + 1C
38.880	6/17	325	(17 6 0)	5B + 1C
39.307	5/14	221	(14 5 0)	4B + 1C
39.597	9/25	353	(25 9 0)	7B + 2C
39.966	4/11	137	(11 4 0)	3B + 1C
40.449	7/19	205	(19 7 0)	5B + 2C
41.112	3/8	73	(8 3 0)	2B + 1C
41.708	8/21	505	(21 8 0)	5B + 3C
42.075	5/13	97	(13 5 0)	3B + 2C
42.501	7/18	373	(18 7 0)	4B + 3C
42.741	9/23	305	(23 9 0)	5B + 4C
43.602	2/5	29	(5 2 0)	1B + 1C
44.498	9/22	565	(22 9 0)	4B + 5C
44.760	7/17	169	(17 7 0)	3B + 4C
45.239	5/12	169	(12 5 0)	2B + 3C
45.667	8/19	425	(19 8 0)	3B + 5C
46.397	3/7	29	(7 3 0)	1B + 2C
47.258	7/16	305	(16 7 0)	2B + 5C
47.924	4/9	97	(9 4 0)	1B + 3C
48.455	9/20	481	(20 9 0)	2B + 7C
48.887	5/11	73	(11 5 0)	1B + 4C
49.550	6/13	205	(13 6 0)	1B + 5C
50.033	7/15	137	(15 7 0)	1B + 6C
50.402	8/17	353	(17 8 0)	1B + 7C
50.692	9/19	221	(19 9 0)	1B + 8C
53.130	1/2	5	(2 1 0)	C

The findings by Saito *et al.*²⁴⁾ can be interpreted from a viewpoint of the O_2 -lattice. Figure 4 shows the dichromatic pattern of the $(22\ 7\ 0)$ -structure with the virtual structural units in which the line passing through the CSL points indicates the $(22\ 7\ 0)$ -boundary connecting two CSL O_2 -points and the diagonal lines are the boundary of the Wigner-Seitz cells of O_2 -points. Given $\cot\theta_2$ is an odd integer, $A_1 = R(2\theta_1)$ and $A_2 = R(2\theta_2)$ in the eqs. (1) and (3), the area of the unit cells of the O_1 -lattice of (L_0, L_2) and the O_2 -lattice of (L_0, L_1, L_2) can be given by $V_{O_1} = 1/4 \sin^2 \theta_2$, $V_{O_2} = \sin^2 \theta_1 / 2 \sin^2 \Delta\theta$, respectively, where $\Delta\theta = \theta_2 - \theta_1$. Since their unit cells are square, the ratio of the length of the side l_{O_1} and l_{O_2} can be given by

$$\frac{l_{O_2}}{l_{O_1}} = \frac{\sqrt{2}}{|\cot\theta_1 - \cot\theta_2|}. \quad (9)$$

By taking $\cot\theta_1 = 22/7$ ($2\theta_1 = 35.30^\circ$) and $\cot\theta_2 = 3$ ($2\theta_2 = 36.87^\circ$), the value of the eq. (9) is given by $7\sqrt{2}$. The length of the diagonal line of the unit O_2 -cell is therefore estimated to be $14\ l_{O_1}$, indicating that there are 15 O_1 -points that are arrayed regularly on the CSL boundary in Fig. 4. The theory of the O_2 -lattice suggests that a DSC dislocation can

Fig. 4 The dichromatic pattern of the $(22\ 7\ 0)$ -structure with virtual structural units. The reference lattice L_0 , the rotated lattice L_1 of angle of 35.30° , the O_1 -lattice $O(L_0, L_1)$ and the O_2 -lattice are presented. The diagonal lines crossing perpendicularly shows the boundary of the Wigner-Seitz cells of O_2 -points. In the fourth structural unit from the left, a DSC dislocation can be introduced.

be introduced at the intersection of the CSL boundary and the boundary of the Wigner-Seitz cells of the O₂-lattice. It occurs at the middle of the array of 15 O₁-points where the internal coordinates of it are (0, 1/2). One of the atoms around the point should be shifted by the DSC Burgers vector close to [3 1 0]/10 of the $\Sigma 5$ configuration through relaxation in order to localise the misfit.

3. Conclusion

We have applied the O-lattice theory to analyse the structures of symmetrical tilt grain boundaries of cubic crystals with the rotation axis {001} and successfully derived a decomposition formula for symmetrical tilt near $\Sigma 5$ grain boundaries. We provide a convincing theoretical interpretation for the observed structures of a near $\Sigma 5$ grain boundary in MgO both from the structural-units model and the theory of the secondary O-lattice. The established theoretical formulae help to elucidate the fundamental structural relationship in a grain boundary and provide an approach for understanding structures of random grain boundaries.

Acknowledgements

The authors are grateful to Prof. Hideo Yoshinaga and Prof. Wenzheng Zhang for valuable discussions. This work is supported in part by Nippon Steel & Sumitomo Metal Corporation, the Elements Strategy Initiative for Structural Materials (ESISM) by the MEXT of Japan, the JSPS Grant-in-Aid for Scientific Research on Innovative Areas “Nano Informatics” (Grant No. 251006005), the Grant-in-Aid for Young Scientists (A) (grant no. 24686069), NSFC (grant no. 11332013) and, JSPS and CAS under the Japan-China Scientific Cooperation Program.

REFERENCES

- G. H. Bishop and B. Chalmers: *Scr. Metall.* **2** (1968) 133–139.
- A. P. Sutton and V. Vitek: *Acta Metall.* **14** (1980) 129–132.
- A. P. Sutton and V. Vitek: *Philos. Trans. R. Soc. Lond. A* **309** (1983) 1–36.
- A. P. Sutton and V. Vitek: *Philos. Trans. R. Soc. Lond. A* **309** (1983) 37–54.
- A. P. Sutton and V. Vitek: *Philos. Trans. R. Soc. Lond. A* **309** (1983) 55–68.
- R. C. Pond, D. A. Smith and V. Vitek: *Acta Metall.* **27** (1979) 235–241.
- R. W. Balluffi and P. D. Bristowe: *Surf. Sci.* **144** (1984) 28–43.
- G.-J. Wang, A. P. Sutton and V. Vitek: *Acta Metall.* **32** (1984) 1093–1104.
- G.-J. Wang and V. Vitek: *Acta Metall.* **34** (1986) 951–960.
- R. C. Pond: *Proc. R. Soc. A* **357** (1977) 471–483.
- R. C. Pond and V. Vitek: *Proc. R. Soc. A* **357** (1977) 453–470.
- V. Vitek, D. A. Smith and R. C. Pond: *Philos. Mag.* **41** (1980) 649–663.
- M. Kohyama: *Phys. Stat. Sol. (b)* **141** (1987) 71–83.
- S. P. Chen, D. J. Srolovitz and A. F. Voter: *J. Mat. Res.* **4** (1989) 62–77.
- A. A. Levi, D. A. Smith and J. T. Wetzell: *J. Appl. Phys.* **69** (1991) 2048–2056.
- N. D. Browning, S. J. Pennycook, M. F. Chisholm, M. M. McGibbon and A. J. McGibbon: *Interface Sci.* **2** (1995) 397–423.
- A. P. Sutton and R. W. Balluffi: *Interfaces in Crystalline Materials*, (Clarendon Press, Oxford, 1995).
- R. C. Pond and W. Bollmann: *Philos. Trans. R. Soc. Lond. A* **292** (1979) 449–472.
- R. C. Pond and D. S. Vlachavas: *Proc. R. Soc. A* **386** (1983) 95–143.
- C. Schmidt, M. W. Finnis, F. Ernst and V. Vitek: *Philos. Mag. A* **77** (1998) 1161–1184.
- N. Shibata, F. Oba, T. Yamamoto and Y. Ikuhara: *Philos. Mag.* **84** (2004) 2381–2415.
- M. Imaeda, T. Mizoguchi, Y. Sato, H.-S. Lee, S. D. Findlay, N. Shibata, T. Yamamoto and Y. Ikuhara: *Phys. Rev. B* **78** (2008) 245320.
- H. Hojo, T. Mizoguchi, H. Ohta, S. D. Findlay, N. Shibata, T. Yamamoto and Y. Ikuhara: *Nano Lett.* **10** (2010) 4668–4672.
- M. Saito, Z. Wang, S. Tsukimoto and Y. Ikuhara: *J. Mater. Sci.* **48** (2013) 5470–5474.
- W. Bollmann: *Crystal Defects and Crystalline Interfaces*, (Springer-Verlag, Berlin, 1970).
- W. Bollmann: *Surf. Sci.* **31** (1972) 1–11.
- R. C. Pond and D. A. Smith: *Int. Met. Rev.* **June** (1976) 61–74.
- W. Bollmann: *Crystal Lattices, Interfaces, Matrices*, published by the author, Geneva, (1982).
- C. Solenthaler and W. Bollmann: *Mater. Sci. Eng.* **81** (1986) 35–49.
- S. Ranganathan: *Acta Cryst.* **21** (1966) 197–199.
- F. C. Frank: *Symposium on the Plastic Deformation of Crystalline Solids*, (1950) pp. 150–154.
- B. A. Bilby: *Report on the Conference on Defects in Crystalline Solids*, (1955) pp. 124–133.
- J. W. Christian: *The Theory of Transformations in Metals and Alloys*, 3rd ed., (Pergamon, Oxford, 2002).
- J. P. Hirth, R. C. Pond, R. G. Hoagland, X.-Y. Liu and J. Wang: *Prog. Mat. Sci.* **58** (2013) 749–823.
- Z.-Z. Shi, F.-Z. Dai, M. Zhang, X.-F. Gu and W.-Z. Zhang: *Metall. Mat. Trans. A* **44** (2013) 2478–2486.
- W.-Z. Zhang: *Metall. Mat. Trans. A* **44** (2013) 4513–4531.
- G. A. Bruggeman, G. H. Bishop and W. H. Hartt: *The Nature and Behavior of Grain Boundaries*, (Plenum Press, New York, 1972) pp. 83–122.
- A. P. Sutton: *Prog. Mat. Sci.* **36** (1992) 167–202.

Appendix

Table A.1 The decomposition table for the (q p 0)-plane around $\Sigma 5$ ($2\theta = 36.869^\circ$) with $p < 20$ is presented. The reference configurations are denoted by A = (4 1 0), B = (3 1 0) and C = (2 1 0) which are represented in boldstyle.

$2\theta[^\circ]$	$\tan \theta$	Σ	g.b. plane	decomposition
28.072	1/4	17	(4 1 0)	A
28.431	19/75	2993	(75 19 0)	18A + 1B
28.451	18/71	5365	(71 18 0)	17A + 1B
28.474	17/67	2389	(67 17 0)	16A + 1B
28.500	16/63	4225	(63 16 0)	15A + 1B
28.529	15/59	1853	(59 15 0)	14A + 1B
28.562	14/55	3221	(55 14 0)	13A + 1B
28.600	13/51	1385	(51 13 0)	12A + 1B
28.645	12/47	2353	(47 12 0)	11A + 1B
28.698	11/43	985	(43 11 0)	10A + 1B
28.762	10/39	1621	(39 10 0)	9A + 1B
28.800	19/74	5837	(74 19 0)	17A + 2B
28.841	9/35	653	(35 9 0)	8A + 1B
28.888	17/66	4645	(66 17 0)	15A + 2B
28.940	8/31	1025	(31 8 0)	7A + 1B
29.000	15/58	3589	(58 15 0)	13A + 2B
29.068	7/27	389	(27 7 0)	6A + 1B
29.148	13/50	2669	(50 13 0)	11A + 2B
29.177	19/73	2845	(73 19 0)	16A + 3B
29.241	6/23	565	(23 6 0)	5A + 1B
29.313	17/65	2257	(65 17 0)	14A + 3B
29.352	11/42	1885	(42 11 0)	9A + 2B
29.394	16/61	3977	(61 16 0)	13A + 3B
29.487	5/19	193	(19 5 0)	4A + 1B

Continued on next page.

<i>Continued.</i>					<i>Continued.</i>				
$2\theta[^\circ]$	$\tan \theta$	Σ	g.b. plane	decomposition	$2\theta[^\circ]$	$\tan \theta$	Σ	g.b. plane	decomposition
29.565	19/72	5545	(72 19 0)	15A + 4B	33.398	3/10	109	(10 3 0)	1A + 2B
29.593	14/53	3005	(53 14 0)	11A + 3B	33.565	19/63	2165	(63 19 0)	6A + 13B
29.652	9/34	1237	(34 9 0)	7A + 2B	33.596	16/53	3065	(53 16 0)	5A + 11B
29.717	13/49	1285	(49 13 0)	10A + 3B	33.642	13/43	1009	(43 13 0)	4A + 9B
29.751	17/64	4385	(64 17 0)	13A + 4B	33.716	10/33	1189	(33 10 0)	3A + 7B
29.862	4/15	241	(15 4 0)	3A + 1B	33.773	17/56	3425	(56 17 0)	5A + 12B
29.963	19/71	2701	(71 19 0)	14A + 5B	33.855	7/23	289	(23 7 0)	2A + 5B
29.990	15/56	3361	(56 15 0)	11A + 4B	33.932	18/59	3805	(59 18 0)	5A + 13B
30.036	11/41	901	(41 11 0)	8A + 3B	33.981	11/36	1417	(36 11 0)	3A + 8B
30.075	18/67	4813	(67 18 0)	13A + 5B	34.041	15/49	1313	(49 15 0)	4A + 11B
30.136	7/26	725	(26 7 0)	5A + 2B	34.075	19/62	4205	(62 19 0)	5A + 14B
30.202	17/63	2129	(63 17 0)	12A + 5B	34.205	4/13	185	(13 4 0)	1A + 3B
30.248	10/37	1469	(37 10 0)	7A + 3B	34.351	17/55	1657	(55 17 0)	4A + 13B
30.308	13/48	2473	(48 13 0)	9A + 4B	34.397	13/42	1933	(42 13 0)	3A + 10B
30.345	16/59	3737	(59 16 0)	11A + 5B	34.482	9/29	461	(29 9 0)	2A + 7B
30.371	19/70	5261	(70 19 0)	13A + 6B	34.562	14/45	2221	(45 14 0)	3A + 11B
30.510	3/11	65	(11 3 0)	2A + 1B	34.601	19/61	2041	(61 19 0)	4A + 15B
30.666	17/62	4133	(62 17 0)	11A + 6B	34.708	5/16	281	(16 5 0)	1A + 4B
30.700	14/51	2797	(51 14 0)	9A + 5B	34.835	16/51	2857	(51 16 0)	3A + 13B
30.752	11/40	1721	(40 11 0)	7A + 4B	34.894	11/35	673	(35 11 0)	2A + 9B
30.791	19/69	2561	(69 19 0)	12A + 7B	34.949	17/54	3205	(54 17 0)	3A + 14B
30.844	8/29	905	(29 8 0)	5A + 3B	35.051	6/19	397	(19 6 0)	1A + 5B
30.922	13/47	1189	(47 13 0)	8A + 5B	35.142	19/60	3961	(60 19 0)	3A + 16B
30.957	18/65	4549	(65 18 0)	11A + 7B	35.184	13/41	925	(41 13 0)	2A + 11B
31.048	5/18	349	(18 5 0)	3A + 2B	35.300	7/22	533	(22 7 0)	1A + 6B
31.145	17/61	2005	(61 17 0)	10A + 7B	35.400	15/47	1217	(47 15 0)	2A + 13B
31.185	12/43	1993	(43 12 0)	7A + 5B	35.489	8/25	689	(25 8 0)	1A + 7B
31.221	19/68	4985	(68 19 0)	11A + 8B	35.567	17/53	1549	(53 17 0)	2A + 15B
31.284	7/25	337	(25 7 0)	4A + 3B	35.637	9/28	865	(28 9 0)	1A + 8B
31.359	16/57	3505	(57 16 0)	9A + 7B	35.700	19/59	1921	(59 19 0)	2A + 17B
31.417	9/32	1105	(32 9 0)	5A + 4B	35.757	10/31	1061	(31 10 0)	1A + 9B
31.502	11/39	821	(39 11 0)	6A + 5B	35.855	11/34	1277	(34 11 0)	1A + 10B
31.561	13/46	2285	(46 13 0)	7A + 6B	35.938	12/37	1513	(37 12 0)	1A + 11B
31.605	15/53	1517	(53 15 0)	8A + 7B	36.008	13/40	1769	(40 13 0)	1A + 12B
31.638	17/60	3889	(60 17 0)	9A + 8B	36.068	14/43	2045	(43 14 0)	1A + 13B
31.664	19/67	2425	(67 19 0)	10A + 9B	36.120	15/46	2341	(46 15 0)	1A + 14B
31.890	2/7	53	(7 2 0)	1A + 1B	36.166	16/49	2657	(49 16 0)	1A + 15B
32.119	19/66	4717	(66 19 0)	9A + 10B	36.207	17/52	2993	(52 17 0)	1A + 16B
32.147	17/59	1885	(59 17 0)	8A + 9B	36.243	18/55	3349	(55 18 0)	1A + 17B
32.181	15/52	2929	(52 15 0)	7A + 8B	36.276	19/58	3725	(58 19 0)	1A + 18B
32.226	13/45	1097	(45 13 0)	6A + 7B	36.869	1/3	5	(3 1 0)	B
32.288	11/38	1565	(38 11 0)	5A + 6B	37.482	19/56	3497	(56 19 0)	18B + 1C
32.378	9/31	521	(31 9 0)	4A + 5B	37.517	18/53	3133	(53 18 0)	17B + 1C
32.440	16/55	3281	(55 16 0)	7A + 9B	37.556	17/50	2789	(50 17 0)	16B + 1C
32.520	7/24	625	(24 7 0)	3A + 4B	37.599	16/47	2465	(47 16 0)	15B + 1C
32.588	19/65	2293	(65 19 0)	8A + 11B	37.649	15/44	2161	(44 15 0)	14B + 1C
32.627	12/41	1825	(41 12 0)	5A + 7B	37.706	14/41	1877	(41 14 0)	13B + 1C
32.672	17/58	3653	(58 17 0)	7A + 10B	37.772	13/38	1613	(38 13 0)	12B + 1C
32.779	5/17	157	(17 5 0)	2A + 3B	37.849	12/35	1369	(35 12 0)	11B + 1C
32.880	18/61	4045	(61 18 0)	7A + 11B	37.940	11/32	1145	(32 11 0)	10B + 1C
32.920	13/44	2105	(44 13 0)	5A + 8B	38.051	10/29	941	(29 10 0)	9B + 1C
33.008	8/27	793	(27 8 0)	3A + 5B	38.115	19/55	1693	(55 19 0)	17B + 2C
33.069	19/64	4457	(64 19 0)	7A + 12B	38.186	9/26	757	(26 9 0)	8B + 1C
33.114	11/37	745	(37 11 0)	4A + 7B	38.267	17/49	1345	(49 17 0)	15B + 2C
33.174	14/47	2405	(47 14 0)	5A + 9B	38.358	8/23	593	(23 8 0)	7B + 1C
33.213	17/57	1769	(57 17 0)	6A + 11B	38.461	15/43	1037	(43 15 0)	13B + 2C

*Continued on next column.**Continued on next page.*

Continued.

$2\theta[^\circ]$	$\tan \theta$	Σ	g.b. plane	decomposition
38.580	7/20	449	(20 7 0)	6B + 1C
38.717	13/37	769	(37 13 0)	11B + 2C
38.769	19/54	3277	(54 19 0)	16B + 3C
38.880	6/17	325	(17 6 0)	5B + 1C
39.004	17/48	2593	(48 17 0)	14B + 3C
39.073	11/31	541	(31 11 0)	9B + 2C
39.146	16/45	2281	(45 16 0)	13B + 3C
39.307	5/14	221	(14 5 0)	4B + 1C
39.444	19/53	1585	(53 19 0)	15B + 4C
39.493	14/39	1717	(39 14 0)	11B + 3C
39.597	9/25	353	(25 9 0)	7B + 2C
39.710	13/36	1465	(36 13 0)	10B + 3C
39.770	17/47	1249	(47 17 0)	13B + 4C
39.966	4/11	137	(11 4 0)	3B + 1C
40.143	19/52	3065	(52 19 0)	14B + 5C
40.190	15/41	953	(41 15 0)	11B + 4C
40.272	11/30	1021	(30 11 0)	8B + 3C
40.341	18/49	2725	(49 18 0)	13B + 5C
40.449	7/19	205	(19 7 0)	5B + 2C
40.565	17/46	2405	(46 17 0)	12B + 5C
40.646	10/27	829	(27 10 0)	7B + 3C
40.752	13/35	697	(35 13 0)	9B + 4C
40.819	16/43	2105	(43 16 0)	11B + 5C
40.865	19/51	1481	(51 19 0)	13B + 6C
41.112	3/8	73	(8 3 0)	2B + 1C
41.390	17/45	1157	(45 17 0)	11B + 6C
41.451	14/37	1565	(37 14 0)	9B + 5C
41.544	11/29	481	(29 11 0)	7B + 4C
41.613	19/50	2861	(50 19 0)	12B + 7C
41.708	8/21	505	(21 8 0)	5B + 3C
41.849	13/34	1325	(34 13 0)	8B + 5C
41.911	18/47	2533	(47 18 0)	11B + 7C
42.075	5/13	97	(13 5 0)	3B + 2C
42.249	17/44	2225	(44 17 0)	10B + 7C
42.322	12/31	1105	(31 12 0)	7B + 5C
42.388	19/49	1381	(49 19 0)	11B + 8C
42.501	7/18	373	(18 7 0)	4B + 3C
42.635	16/41	1937	(41 16 0)	9B + 7C
42.741	9/23	305	(23 9 0)	5B + 4C
42.895	11/28	905	(28 11 0)	6B + 5C
43.002	13/33	629	(33 13 0)	7B + 6C
43.081	15/38	1669	(38 15 0)	8B + 7C
43.142	17/43	1069	(43 17 0)	9B + 8C
43.190	19/48	2665	(48 19 0)	10B + 9C
43.602	2/5	29	(5 2 0)	1B + 1C
44.022	19/47	1285	(47 19 0)	9B + 10C
44.072	17/42	2053	(42 17 0)	8B + 9C
44.135	15/37	797	(37 15 0)	7B + 8C
44.218	13/32	1193	(32 13 0)	6B + 7C
44.332	11/27	425	(27 11 0)	5B + 6C
44.498	9/22	565	(22 9 0)	4B + 5C
44.612	16/39	1777	(39 16 0)	7B + 9C
44.760	7/17	169	(17 7 0)	3B + 4C
44.885	19/46	2477	(46 19 0)	8B + 11C
44.958	12/29	985	(29 12 0)	5B + 7C
45.041	17/41	985	(41 17 0)	7B + 10C

*Continued on next column.**Continued.*

$2\theta[^\circ]$	$\tan \theta$	Σ	g.b. plane	decomposition
45.239	5/12	169	(12 5 0)	2B + 3C
45.428	18/43	2173	(43 18 0)	7B + 11C
45.501	13/31	565	(31 13 0)	5B + 8C
45.667	8/19	425	(19 8 0)	3B + 5C
45.781	19/45	1193	(45 19 0)	7B + 12C
45.864	11/26	797	(26 11 0)	4B + 7C
45.977	14/33	1285	(33 14 0)	5B + 9C
46.050	17/40	1889	(40 17 0)	6B + 11C
46.397	3/7	29	(7 3 0)	1B + 2C
46.711	19/44	2297	(44 19 0)	6B + 13C
46.770	16/37	1625	(37 16 0)	5B + 11C
46.857	13/30	1069	(30 13 0)	4B + 9C
46.997	10/23	629	(23 10 0)	3B + 7C
47.104	17/39	905	(39 17 0)	5B + 12C
47.258	7/16	305	(16 7 0)	2B + 5C
47.405	18/41	2005	(41 18 0)	5B + 13C
47.498	11/25	373	(25 11 0)	3B + 8C
47.611	15/34	1381	(34 15 0)	4B + 11C
47.677	19/43	1105	(43 19 0)	5B + 14C
47.924	4/9	97	(9 4 0)	1B + 3C
48.204	17/38	1733	(38 17 0)	4B + 13C
48.291	13/29	505	(29 13 0)	3B + 10C
48.455	9/20	481	(20 9 0)	2B + 7C
48.609	14/31	1157	(31 14 0)	3B + 11C
48.682	19/42	2125	(42 19 0)	4B + 15C
48.887	5/11	73	(11 5 0)	1B + 4C
49.134	16/35	1481	(35 16 0)	3B + 13C
49.247	11/24	697	(24 11 0)	2B + 9C
49.353	17/37	829	(37 17 0)	3B + 14C
49.550	6/13	205	(13 6 0)	1B + 5C
49.727	19/41	1021	(41 19 0)	3B + 16C
49.809	13/28	953	(28 13 0)	2B + 11C
50.033	7/15	137	(15 7 0)	1B + 6C
50.229	15/32	1249	(32 15 0)	2B + 13C
50.402	8/17	353	(17 8 0)	1B + 7C
50.555	17/36	1585	(36 17 0)	2B + 15C
50.692	9/19	221	(19 9 0)	1B + 8C
50.815	19/40	1961	(40 19 0)	2B + 17C
50.926	10/21	541	(21 10 0)	1B + 9C
51.119	11/23	325	(23 11 0)	1B + 10C
51.282	12/25	769	(25 12 0)	1B + 11C
51.419	13/27	449	(27 13 0)	1B + 12C
51.538	14/29	1037	(29 14 0)	1B + 13C
51.641	15/31	593	(31 15 0)	1B + 14C
51.732	16/33	1345	(33 16 0)	1B + 15C
51.813	17/35	757	(35 17 0)	1B + 16C
51.884	18/37	1693	(37 18 0)	1B + 17C
51.948	19/39	941	(39 19 0)	1B + 18C
53.130	1/2	5	(2 1 0)	C