A derivation of coincidence relations utilizing quaternion and matrix based on the hexagonal lattice for material engineers

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Received 30 May 2018

Revised 17 December 2018

Accepted 22 January 2019

Published 10 April 2019

Grain-oriented silicon steel is mainly used as the core material of transformers, and it is manufactured by applying secondary recrystallization. The driving force of this process is the grain boundary energy, based on the nature of the grain boundary, which is determined by coincidence site lattice (CSL) relations. CSL relations are determined by the arrangement of lattice points in three-dimensional space and have already been shown mathematically by using advanced mathematics. However, their derivation processes are abstract, making them difficult for material engineers to understand. Therefore, in this study, a derivation of CSL relations is attempted in order to enable material engineers to easily understand the derivation. This study contributes to industrial mathematics by helping material engineers understand the essence of the mathematical method in order to use it appropriately. Specifically, a derivation method for coincidence relations is proposed using the hexagonal lattice (in the case of an axial ratio of $\sqrt{8/3}$) as an example that avoids the need for advanced mathematics. This method involves applying the scale rotation of a quaternion, and it is thus named the quaternion-matrix method. The matrix specifying the ΣN coincidence relation of a certain lattice system is expressed by a similarity transformation using the matrix comprising its primitive translation vectors and is given as the following transformation matrix: $\mathbf{H}_i = \mathbf{E}_i^{-1} \mathbf{E}_R \mathbf{E}_i$. Based on the rational number property of the transformation matrix elements, the following formula is derived: $N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2$, $N_i \in \mathbb{N}^+$, $N : \Sigma$ value. Here, $(N_0 N_1 N_2 N_3)$ is specified by the integrality (lattice point) and irreducibility (unit cell) among the elements of $\mathbf{H}_i$, and the quaternion for the CSL formation is

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thus derived. Finally, based on the polar form of this quaternion, the coincidence relation can be derived.

Keywords: Coincidence site lattice; quaternion; hexagonal lattice.

1. Introduction

Grain-oriented (GO) silicon steel is mainly used as the core material of transformers, and it is the only product in the steel industry that is manufactured by applying secondary recrystallization. The most successful texture control has been achieved on an industrial scale, and as a result, only specific oriented grains ($\{110\}\langle 001 \rangle$) cover all products. The driving force of secondary recrystallization is the grain boundary energy, based on the nature of the grain boundary,¹ which is determined by coincidence site lattice (CSL) relations. CSL relations are determined by the arrangement of lattice points between two lattices in three-dimensional space. CSL relations are derived mathematically using advanced mathematics.^{2–10} However, their derivation processes are abstract, making them difficult for material engineers to understand their derivation.

The purpose of this study is to attempt a derivation of coincidence relations that material engineers can easily understand. This study contributes to industrial mathematics by enabling material engineers to understand the essence of the mathematical method in order to use it appropriately. Therefore, this paper is presented by using only crystallography, elementary linear algebra, and algebraic number theory. In addition, the simple cubic lattice is highly symmetrical, making the expressions of certain matrices with different meanings identical and the meanings of the equation ambiguous. As an example, we propose a derivation of the hexagonal crystal using a method called the quaternion-matrix method.

Meanwhile, the definition of the CSL is “Two interpenetrating point lattices contain under certain conditions a common sublattice”. Moreover, it is the finest common sublattice of the crystal lattices formed with a three-dimensional lattice $\mathbf{L}$ (simple cubic, face-centered cubic, body-centered cubic, hexagonal, or whatever) and a three-dimensional lattice $\mathbf{RL}$ which is obtained by rotational transformation of $\mathbf{L}$. In addition, the CSL is classified with the “ Σ value” which is the reciprocal number of the fraction of lattice point in common.

The coincidence relation to be derived in this paper indicates the rotational axis and angle in three-dimensional space, and a right-handed coordinate system is applied. The report by Warrington¹⁰ on the hexagonal lattice can be used as a reference.

This paper is divided into two sections. Section 2 consists of the preliminaries, especially for non-specialists in mathematics and Sec. 3 consists of the main results for the hexagonal lattice.

2. Preliminaries

2.1. Definition of CSL

CSL is defined as follows, according to Grimmer *et al.*³:

“Two interpenetrating point lattices contain under certain conditions a common sublattice, i.e., a coincidence-site lattice The CSL is the finest common sublattice of the crystal lattices 1 and 2.”

2.2. Expanded lattice

The “expanded lattice” is expressed by using the primitive translation vectors (PTVs) of the CSL to specify the coincidence relation.

In the orthogonal (standard) coordinate system (base $\mathbf{E}_s$: ${}^t[100]$, ${}^t[010]$, ${}^t[001]$, t : transpose), the PTV indicating one unit cell (i) is expressed as $\mathbf{E}_i$, while the lattice rotated with an orthogonal matrix $\mathbf{R}$ is $\mathbf{RE}_i$. Let us consider the (expanded) lattices that are obtained by multiplying the PTVs of each of $\mathbf{E}_i$ and $\mathbf{RE}_i$ by $N \in \mathbb{N}^+$, as $N\mathbf{E}_i$ and $N\mathbf{RE}_i$, respectively. Then, the set of the ΣN -CSL points contains both the $N\mathbf{E}_i$ and the $N\mathbf{RE}_i$.

The ΣN -CSL relation can be expressed using this $N\mathbf{RE}_i$ (Theorem).

Here, $N\mathbf{E}_i$ is termed as the expanded-standard lattice (ESL), and $N\mathbf{RE}_i$ as the expanded-rotated lattice (ERL).

Note. Strictly, all matrices of PTV should be expressed as $\mathbf{E}_i\mathbf{E}_s$ with $\mathbf{E}_s$, because all calculations

are performed in the orthogonal coordinate system. However, as $\mathbf{E}_s$ does not cause any change in the calculation, $\mathbf{E}_s$ is omitted in this paper.

Note. Matrix $\mathbf{E}_s$ is given as follows:

$$\mathbf{E}_s := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

2.3. Theorem

Here, the theorem on ΣN -CSL points is presented. This theorem has already been shown by many mathematicians using advanced mathematics.⁷

Theorem. The set of ΣN -CSL points contains both of the $N\mathbf{E}_i$ and the $N\mathbf{RE}_i$. That is, $N\mathbf{E}_i$ and $N\mathbf{RE}_i$ are expressed as the linear combination of PTVs for the CSL with integer coefficients, which have no common factor among nine elements.

Proof. The PTVs of the original lattice ($\mathbf{A}$) under consideration are expressed as $\mathbf{E}_i$, which consists of three column vectors in the orthogonal coordinate system, and the PTVs of the CSL as $\mathbf{C}$.

Based on the definition of CSL,

- (a) CSL can be expressed as the linear combinations of the integer coefficients of each of $\mathbf{E}_i$ and $\mathbf{RE}_i$, which have no common factor among nine elements.
- (b) $N\mathbf{E}_i$ and $N\mathbf{RE}_i$ can be expressed as the linear combination of the integer coefficients of $\mathbf{E}_i$ and $\mathbf{RE}_i$, respectively.

Based on (a), the CSL points are also lattice points for the original lattice, and therefore, $\mathbf{C}$ is expressed as the linear combination of integer coefficients ($\mathbf{K}$) for $\mathbf{E}_i$, which have no common factor among nine elements:

$$\mathbf{C} = \mathbf{E}_i \mathbf{K}. \quad (1)$$

Similarly, for another lattice $\mathbf{B}$, the linear combination of integer coefficients is expressed by $\mathbf{L}$:

$$\mathbf{C} = \mathbf{RE}_i \mathbf{L}. \quad (2)$$

Here, $\mathbf{K}$ and $\mathbf{L}$ are 3×3 matrices of integer elements, which are normal as their volume is not zero.

Based on (b),

$$\begin{aligned} \text{ESL: } \mathbf{A} &:= N\mathbf{E}_i, \text{ therefore, } N^{-1}\mathbf{A} = \mathbf{E}_i \text{ and} \\ \text{ERL: } \mathbf{B} &:= N\mathbf{RE}_i, \text{ therefore, } \mathbf{R}^{-1}N^{-1}\mathbf{B} = \mathbf{E}_i. \end{aligned} \quad (3)$$

As (1) and (2) are commutative with N ,

$$\begin{aligned} \mathbf{C} &= \mathbf{E}_i \mathbf{K}, \text{ therefore,} \\ N\mathbf{CK}^{-1} &= \mathbf{CNK}^{-1} = \mathbf{A}, \text{ similarly} \\ N\mathbf{CL}^{-1} &= \mathbf{CNL}^{-1} = \mathbf{B}. \end{aligned} \quad (4)$$

Therefore, the expanded lattices of (4), $\text{ESL}(N\mathbf{E}_i)$ and $\text{ERL}(N\mathbf{RE}_i)$, are formed by the linear combination of $\mathbf{C}$ (the PTVs of CSL) as the coefficients $N\mathbf{K}^{-1}$ and $N\mathbf{L}^{-1}$, respectively.

Furthermore, inverse matrices for $\mathbf{K}$ and $\mathbf{L}$ are $1/\det[\mathbf{K}] = 1/\det[\mathbf{L}] = 1/N$ times the cofactor matrix for each. Since all elements of $\mathbf{K}$ and $\mathbf{L}$ are integers, the cofactors are also all integers, and the elements of $N\mathbf{K}^{-1}$ and $N\mathbf{L}^{-1}$, which were multiplied by $1/N$ and N , are all integers. That is, both expanded lattices $\mathbf{A}$ and $\mathbf{B}$ are formed by the linear combination of the integer coefficients of PTVs of CSL.

This theorem might be a corollary of Theorem 1 in Ref. 2. However, its proof might be difficult to understand for material engineers owing to the application of group theory. $\square$

2.4. Quaternion

Quaternions are considered to be an extension of complex numbers, and are widely used for expressing three-dimensional rotation; however, they are uncommon in the field of material engineering. In this study, quaternions are applied for the expression of three-dimensional rotation of lattice points.

Using the base $\{1, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$, which satisfies $\mathbf{i}\mathbf{i} = \mathbf{j}\mathbf{j} = \mathbf{k}\mathbf{k} = -1$, $\mathbf{i}\mathbf{j} = -\mathbf{j}\mathbf{i} = \mathbf{k}$, $\mathbf{j}\mathbf{k} = -\mathbf{k}\mathbf{j} = \mathbf{i}$, $\mathbf{k}\mathbf{i} = -\mathbf{i}\mathbf{k} = \mathbf{j}$, $\mathbf{i}\mathbf{j}\mathbf{k} = -1$, a quaternion is expressed as $\mathbf{q} := a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k} = |\mathbf{q}|(\cos\theta + \mathbf{u}\sin\theta)$, $|\mathbf{u}| = 1 = |\mathbf{q}|(\cos\theta + h/R\sin\theta\mathbf{i} + k/R\sin\theta\mathbf{j} + l/R\sin\theta\mathbf{k})$, $R^2 := h^2 + k^2 + l^2$, $|\mathbf{q}|^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2$, $a_i \in \mathbb{R}$.

Since

$$(1) \quad \theta: \cos\theta = a_0/\sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2}, \quad \sin\theta = \sqrt{a_1^2 + a_2^2 + a_3^2}/\sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2}, \quad 0 \leq \theta \leq \pi.$$

In addition, θ is the argument, $\arg(\mathbf{q})$.

- (2) $\mathbf{q}^* = a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k}$ is the conjugate quaternion for $\mathbf{q} = a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$, and they satisfy

$$\begin{aligned} (\mathbf{q}_1 \mathbf{q}_2)^* &= \mathbf{q}_2^* \mathbf{q}_1^* \quad \text{and} \\ \mathbf{q} \mathbf{q}^* &= a_0^2 + a_1^2 + a_2^2 + a_3^2 = \mathbf{q}^* \mathbf{q}. \end{aligned} \quad (5)$$

It is possible to “rotate and expand” vectors using the quaternion, which is known as “scale rotation”, as described in Lemma B.1.

2.5. Expansion and rotation of $\mathbf{E}_s$

Using Lemma B.1, “quaternion a_i expression” ($\mathbf{E}_R$: rotational angle; $\theta = 2 \arg(\mathbf{q})$, expansion rate; $(a_0^2 + a_1^2 + a_2^2 + a_3^2)$ for a rotation and expansion of the base ($\mathbf{E}_s$: ${}^t[100]$, ${}^t[010]$, ${}^t[001]$, t : transpose) of the standard (orthogonal) coordinate system is derived.)

$$\mathbf{E}_R = \begin{pmatrix} a_0^2 + a_1^2 - a_2^2 - a_3^2 & 2(a_1 a_2 - a_0 a_3) & 2(a_1 a_3 + a_0 a_2) \\ 2(a_2 a_1 + a_0 a_3) & a_0^2 - a_1^2 + a_2^2 - a_3^2 & 2(a_2 a_3 - a_0 a_1) \\ 2(a_3 a_1 - a_0 a_2) & 2(a_3 a_2 + a_0 a_1) & a_0^2 - a_1^2 - a_2^2 + a_3^2 \end{pmatrix}. \quad (6)$$

Therefore, the operation for expansion and rotation of one PTV of the lattice (i) is $\mathbf{E}_R \mathbf{E}_i = N \mathbf{R} \mathbf{E}_i$ and, based on Theorem, this can be expressed by means of the linear combination of irreducible integer coefficients for $\mathbf{E}_i$ through $\mathbf{C}$. Its coefficient matrix is expressed as $\mathbf{H}_i$.

$$\begin{aligned} \text{ERL: } \mathbf{E}_R \mathbf{E}_i &= N \mathbf{R} \mathbf{E}_i \\ &:= \mathbf{E}_i \mathbf{H}_i, \text{ then } \mathbf{E}_i^{-1} \mathbf{E}_R \mathbf{E}_i = \mathbf{H}_i. \end{aligned} \quad (7)$$

Therefore, $\mathbf{H}_i = \mathbf{E}_i^{-1} \mathbf{E}_R \mathbf{E}_i$ is a similarity transformation of (6) and the coefficient matrix of integer elements for which there is no common factor. Here, $\det[\mathbf{E}_R \mathbf{E}_i] = \det[N \mathbf{R} \mathbf{E}_i] = N^3 \det[\mathbf{E}_i]$. The volume of ERL is smaller than N^3 if there is a common factor, indicating that the Σ value is not N .

Based on the integrality and irreducibility of the elements for this $\mathbf{H}_i$, the restriction of quaternion coefficient a_i is derived, and the CSL relation is derived in the following section.

$$\begin{aligned} \mathbf{H}_h &= \mathbf{E}_h^{-1} \mathbf{E}_R \mathbf{E}_h = [H_{ij}] \\ &= \begin{pmatrix} a_0^2 + a_1^2 - a_2^2 - a_3^2 + 2\sqrt{3}/3(a_1 a_2 + a_0 a_3) & -a_1^2 + a_2^2 + 2\sqrt{3}/3(a_1 a_2 - 2a_0 a_3) & 4\sqrt{6}/3(a_1 a_3 + a_0 a_2) + 4\sqrt{2}/3(a_2 a_3 - a_0 a_1) \\ 4\sqrt{3}/3(a_1 a_2 + a_0 a_3) & a_0^2 - a_1^2 + a_2^2 - a_3^2 - 2\sqrt{3}/3(a_1 a_2 + a_0 a_3) & 8\sqrt{2}/3(a_2 a_3 - a_0 a_1) \\ \sqrt{6}/2(a_1 a_3 - a_0 a_2) & -\sqrt{6}/4(a_1 a_3 - a_0 a_2) + 3\sqrt{2}/4(a_2 a_3 + a_0 a_1) & a_0^2 - a_1^2 - a_2^2 + a_3^2 \end{pmatrix}. \end{aligned} \quad (9)$$

The conditions of CSL relation (i.e., the necessary and sufficient conditions to be rational) can be derived by the lattice (integrality) and the unit cell (irreducibility: existence of common divisors for matrix elements), which are verified to restrict these conditions for elements in (9) hereafter.

3.2. Formula based on rationality of $\mathbf{H}_h$ matrix elements

The conditions for the elements of (9) to be rational are expressed by applying the concept of “extension of field”. First, the rationality of elements is examined, followed by an investigation of integrality (based on lattice points). Mathematically, the set of rational numbers forms the field, but one of the integers does not.

That is, $\mathbf{q}^t[100]\mathbf{q}^*$, $\mathbf{q}^t[010]\mathbf{q}^*$, and $\mathbf{q}^t[001]\mathbf{q}^*$ are derived by using $\mathbf{q} = a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$.

The a_i ($i = 0-3$) expression for $\mathbf{E}_R$ ($:=$ the operation of expansion and rotation of $\mathbf{E}_s = (a_0^2 + a_1^2 + a_2^2 + a_3^2)\mathbf{R}\mathbf{E}_s$, strictly) is as follows:

3. Hexagonal Lattice Case

3.1. $\mathbf{H}_h$ matrix elements using quaternion

The PTV for the hexagonal lattice (axial ratio $c/a = \sqrt{8/3}$): $\mathbf{E}_h$ (the suffix i is replaced by h indicating hexagonal) and its dual vectors, $\mathbf{E}_h^{-1}$, are expressed in the standard coordinate system as follows¹⁰:

$$\begin{aligned} \mathbf{E}_h &= \begin{pmatrix} 1 & -1/2 & 0 \\ 0 & \sqrt{3}/2 & 0 \\ 0 & 0 & 2\sqrt{6}/3 \end{pmatrix}, \\ \mathbf{E}_h^{-1} &= \begin{pmatrix} 1 & \sqrt{3}/3 & 0 \\ 0 & 2\sqrt{3}/3 & 0 \\ 0 & 0 & \sqrt{6}/4 \end{pmatrix}. \end{aligned} \quad (8)$$

Therefore, based on (6)–(8), we have

Based on Lemma B.5, $a_i = N_i \sqrt{m_i}$ ($N_i \in \mathbb{Z}^\times$, m_i : square-free integer). Each element of $\mathbf{H}_h$ can be expressed in this form. In addition, the rationality conditions are restricted. Lemmas B.8 and B.9 are also applied hereafter.

Each element of H_{ij} is replaced by N_i in Table 1, and examined as follows:

- H_{11} : We consider extension field $\mathbb{Q}(\sqrt{3})$, so that it is rational.

Since the square members are rational (integers), the remaining part must satisfy

$$\begin{aligned} 2\sqrt{3}/3(a_1 a_2 + a_0 a_3) &\in \mathbb{Q}, \\ \text{i.e., } \{N_1 N_2 \sqrt{m_1 m_2} + N_0 N_3 \sqrt{m_0 m_3}\} \sqrt{3} &\in \mathbb{Q}. \end{aligned}$$

Table 1. H_{ij} , the elements of $\mathbf{H}_h$ with a_i replaced by N_i .

$N = a_0^2 + a_1^2 + a_2^2 + a_3^2 = (N_0)^2 + 2(N_1)^2 + 6(N_2)^2 + 3(N_3)^2$, $a_0 = N_0$, $a_1 = \sqrt{2}N_1$, $a_2 = \sqrt{6}N_2$, $a_3 = \sqrt{3}N_3$	
$H_{11} : a_0^2 + a_1^2 - a_2^2 - a_3^2 + 2\sqrt{3}/3(a_1a_2 + a_0a_3)$	$-6N_2^2 + 4N_1N_2 + 2N_0N_3 + 2N_1^2 - 3N_3^2 + N_0^2$: integer, parity judgment: $-3N_3^2 + N_0^2$
$H_{12} : -a_1^2 + a_2^2 + 2\sqrt{3}/3(a_1a_2 - 2a_0a_3)$	$2(2N_1N_2 - 2N_0N_3 - N_1^2 + 3N_2^2)$: even
$H_{13} : 4\sqrt{6}/3(a_1a_3 + a_0a_2) + 4\sqrt{2}/3(a_2a_3 - a_0a_1)$	$8(N_1N_3 + N_0N_2 + N_2N_3) - 8/3N_0N_1$
$H_{21} : 4\sqrt{3}/3(a_1a_2 + a_0a_3)$	$4(2N_1N_2 + N_0N_3)$: even
$H_{22} : a_0^2 - a_1^2 + a_2^2 - a_3^2 - 2\sqrt{3}/3(a_1a_2 + a_0a_3)$	$6N_2^2 - 4N_1N_2 - 2N_0N_3 - 2N_1^2 - 3N_3^2 + N_0^2$: integer, parity judgment: $-3N_3^2 + N_0^2$
$H_{23} : 8\sqrt{2}/3(a_2a_3 - a_0a_1)$	$16N_2N_3 - 16/3N_0N_1$
$H_{31} : \sqrt{6}/2(a_1a_3 - a_0a_2)$	$3(N_1N_3 - N_0N_2)$: integer
$H_{32} : -\sqrt{6}/4(a_1a_3 - a_0a_2) + 3\sqrt{2}/4(a_2a_3 + a_0a_1)$	$3(-N_1N_3 + N_0N_2 + 3N_2N_3 + N_0N_1)/2$
$H_{33} : a_0^2 - a_1^2 - a_2^2 + a_3^2$	$-6N_2^2 - 2N_1^2 + 3N_3^2 + N_0^2$: integer, parity judgment: $+3N_3^2 + N_0^2$

Therefore, $m_1m_2 = 3 \cdot p_{12}^2$, $m_0m_3 = 3 \cdot p_{03}^2$, p_{ij} , q_{ij} , r_{ij} , $s_{ij} \in \mathbb{Z}$ (m_i is square-free, but $m_i m_j$ may not be). Similarly,

- H_{12} : $m_1m_2 = 3 \cdot p_{12}^2$, $m_0m_3 = 3 \cdot p_{03}^2$
- H_{13} : $m_1m_3 = 6 \cdot q_{13}^2$, $m_0m_2 = 6 \cdot q_{02}^2$, $m_2m_3 = 2 \cdot r_{23}^2$, $m_0m_1 = 2 \cdot r_{01}^2$, since base $\sqrt{6}$ and $\sqrt{2}$ are linearly independent.
- H_{21} : m_1m_2 , $m_0m_3 = 3 \cdot p_{ij}^2$
- H_{22} : m_1m_2 , $m_0m_3 = 3 \cdot p_{ij}^2$
- H_{23} : $m_2m_3 = 2 \cdot r_{23}^2$, $m_0m_1 = 2 \cdot r_{01}^2$
- H_{31} : m_1m_3 , $m_0m_2 = 6 \cdot q_{ij}^2$
- H_{32} : m_1m_3 , $m_0m_2 = 6 \cdot q_{ij}^2$, $m_2m_3 = m_0m_1 = 2 \cdot r_{ij}^2$
- H_{33} : $m_i m_i = \mathbb{Q} \cdot s_{ij}^2 = 1 \cdot s_{ij}^2$.

Summing the above,

$$m_1m_2 = m_0m_3 = 3 \cdot p_{ij}^2,$$

$$m_1m_3 = m_0m_2 = 6 \cdot q_{ij}^2, \quad m_2m_3 = m_0m_1 = 2 \cdot r_{ij}^2,$$

$$m_i m_i = 1 \cdot s_{ii}^2 \in \mathbb{Q}, \quad p_{ij}, q_{ij}, r_{ij}, s_{ij} \in \mathbb{Z}.$$

These equations indicate that $\sqrt{m_1m_2}$ and $\sqrt{m_0m_3}$ contend the irrational adjoint element $\sqrt{3}$, $\sqrt{m_1m_3}$ and $\sqrt{m_0m_2}$ contend $\sqrt{6}$, and $\sqrt{m_2m_3}$ and $\sqrt{m_0m_1}$ contend $\sqrt{2}$. Additionally, $\sqrt{m_i m_i} = m_i$ is not an irrational number.

That is, a_i , which contends $\sqrt{2}$, $\sqrt{3}$, and $\sqrt{6}$ as adjoint elements, causes every H_{ij} to be rational.

Furthermore, as m_i is a square-free integer and the square roots of p^2 , q^2 , r^2 , and s^2 are integers, in the extension field: $\mathbb{Q}(\sqrt{2}, \sqrt{3})$,

$$\begin{aligned} m_1m_2 &= m_0m_3 = 3, \\ m_1m_3 &= m_0m_2 = 6, \quad \text{and} \\ m_2m_3 &= m_0m_1 = 2 \end{aligned} \quad (10)$$

are concluded.

In addition, based on Lemmas B.2, B.12 and B.13, $a_0 = N_0$, $a_1 = \sqrt{2}N_1$, $a_2 = \sqrt{6}N_2$, $a_3 = \sqrt{3}N_3$,

$$\begin{aligned} N &= a_0^2 + a_1^2 + a_2^2 + a_3^2 \\ &= N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2, \\ N_i &\in \mathbb{N}^+, \quad i = 0-3. \end{aligned} \quad (11)$$

In the case that $N \leq 50$, all the combinations of $\{(N_0, N_1, N_2, N_3), N_i \in \mathbb{N}^+\}$ are listed in Table 2. They were calculated by substituting numbers from 0 to $\lfloor \sqrt{N} \rfloor$, $\lfloor \sqrt{N/2} \rfloor$, $\lfloor \sqrt{N/6} \rfloor$, and $\lfloor \sqrt{N/3} \rfloor$ for each N_i based on (11).

Note. Here, the brackets $[]$ indicate Gauss' symbol.

This is the necessary and sufficient condition for all elements of $\mathbf{H}_h$ to be rational numbers, as well as the necessary condition for them to be integers.

Similarly, this method can be applied for three cubic lattices, and the Σ -value N satisfies the formula $N = a_0^2 + a_1^2 + a_2^2 + a_3^2 = N_0^2 + N_1^2 + N_2^2 + N_3^2$: ($N_i \in \mathbb{N}^+$), and are odd numbers.⁴

3.3. Integrality and irreducibility

Integrality refers to $\mathbf{H}_h$ being a CSL point (necessary condition), and irreducibility means the condition for it to be an ERL (unit cell of expanded-rotated lattice), for which $\det[\mathbf{H}_h] = N^3$ (sufficient condition). Consequently, the necessary and sufficient conditions for a quaternion for CSL formation are derived, and are specifically calculated below by applying Lemma B.10.

3.3.1. Examination of integrality

Because elements other than H_{13} , H_{23} , and H_{32} are integers, these three elements are examined. Using the fact that the remainder by “3” and “2” is 0.

Table 2. All cases of CSL for hexagonal lattice.

N	*All combinations of (N_0, N_1, N_2, N_3)				M**
	N_0	N_1	N_2	N_3	
1	1	0	0	0	○
2	0	1	0	0	
3	1	1	0	0	
3	0	0	0	1	
4	2	0	0	0	
4	1	0	0	1	
5	0	1	0	1	
6	2	1	0	0	
6	1	1	0	1	
6	0	0	1	0	
7	2	0	0	1	○
7	1	0	1	0	
8	0	2	0	0	
8	0	1	1	0	
9	3	0	0	0	
9	1	2	0	0	
9	2	1	0	1	
9	1	1	1	0	
9	0	0	1	1	
10	2	0	1	0	○
10	1	0	1	1	○
11	3	1	0	0	
11	0	2	0	1	○
11	0	1	1	1	○
12	2	2	0	0	
12	3	0	0	1	
12	1	2	0	1	
12	0	0	0	2	
12	2	1	1	0	
12	1	1	1	1	
13	1	0	0	2	○
13	2	0	1	1	
14	3	1	0	1	○
14	0	1	0	2	○
14	0	2	1	0	
15	2	2	0	1	
15	1	1	0	2	
15	3	0	1	0	
15	1	2	1	0	
15	2	1	1	1	
16	4	0	0	0	
16	2	0	0	2	
17	3	2	0	0	○
17	3	1	1	0	○
17	0	2	1	1	
18	4	1	0	0	
18	0	3	0	0	
18	2	1	0	2	
18	2	2	1	0	
18	3	0	1	1	○
18	1	2	1	1	
18	0	0	1	2	○
19	1	3	0	0	
19	4	0	0	1	○
19	1	0	1	2	
20	3	2	0	1	
20	0	2	0	2	
20	3	1	1	1	
20	0	1	1	2	
21	4	1	0	1	
21	0	3	0	1	
21	3	0	0	2	
21	1	2	0	2	
21	2	2	1	1	
21	1	1	1	2	
22	2	3	0	0	○
22	1	3	0	1	○
22	4	0	1	0	
22	2	0	1	2	
23	3	1	0	2	
23	3	2	1	0	
24	4	2	0	0	
24	2	2	0	2	
24	4	1	1	0	
24	0	3	1	0	
24	2	1	1	2	
24	0	0	2	0	
25	5	0	0	0	
25	2	3	0	1	
25	1	3	1	0	○
25	4	0	1	1	
25	1	0	2	0	○
26	3	2	1	1	○
26	0	2	1	2	○
26	0	1	2	0	

N	*All combinations of (N_0, N_1, N_2, N_3)				M**
	N_0	N_1	N_2	N_3	
27	5	1	0	0	
27	3	3	0	0	
27	4	2	0	1	
27	0	0	0	3	
27	4	1	1	1	
27	0	3	1	1	○
27	3	0	1	2	
27	1	2	1	2	
27	1	1	2	0	
27	0	0	2	1	○
28	5	0	0	1	
28	4	0	0	2	
28	1	0	0	3	
28	2	3	1	0	
28	1	3	1	1	
28	2	0	2	0	
28	1	0	2	1	
29	3	2	0	2	○
29	0	1	0	3	
29	3	1	1	2	○
29	0	1	2	1	
30	5	1	0	1	
30	3	3	0	1	
30	4	1	0	2	
30	0	3	0	2	
30	1	1	0	3	
30	4	2	1	0	
30	2	2	1	2	
30	2	1	2	0	
30	1	1	2	1	
31	1	3	0	2	
31	2	0	0	3	○
31	5	0	1	0	
31	2	3	1	1	○
31	2	0	2	1	○
32	0	4	0	0	
32	0	2	2	0	
33	5	2	0	0	
33	1	4	0	0	
33	2	1	0	3	
33	5	1	1	0	
33	3	3	1	0	
33	4	2	1	1	
33	0	0	1	3	
33	3	0	2	0	
33	1	2	2	0	
33	2	1	2	1	
34	4	3	0	0	
34	2	3	0	2	
34	5	0	1	1	○
34	4	0	1	2	○
34	1	0	1	3	○
35	0	4	0	1	○
35	0	2	0	3	○
35	3	2	1	2	
35	0	1	1	3	○
35	3	1	2	0	
35	0	2	2	1	○
36	6	0	0	0	
36	2	4	0	0	
36	5	2	0	1	
36	1	4	0	1	
36	4	2	0	2	
36	3	0	0	3	
36	1	2	0	3	
36	5	1	1	1	
36	3	3	1	1	
36	4	1	1	2	
36	0	3	1	2	
36	1	1	1	3	
36	2	2	2	0	
36	3	0	2	1	
36	1	2	2	1	
36	0	0	2	2	
37	4	3	0	1	
37	5	0	0	2	○
37	1	3	1	2	○
37	2	0	1	3	
37	1	0	2	2	○
38	6	1	0	0	○
38	3	1	0	3	○
38	0	4	1	0	
38	3	1	2	1	○
38	0	1	2	2	○

N	*All combinations of (N_0, N_1, N_2, N_3)				M**
	N_0	N_1	N_2	N_3	
39	6	0	0	1	
39	2	4	0	1	
39	5	1	0	2	
39	3	3	0	2	
39	2	2	0	3	
39	5	2	1	0	
39	1	4	1	0	
39	2	1	1	3	
39	2	2	2	1	
39	1	1	2	2	
40	4	3	1	0	
40	2	3	1	2	
40	4	0	2	0	
40	2	0	2	2	
41	3	4	0	0	○
41	6	1	0	1	
41	0	4	1	1	
41	0	2	1	3	
41	3	2	2	0	○
42	6	0	1	0	
42	2	4	1	0	
42	5	2	1	1	
42	1	4	1	1	
42	4	2	1	2	
42	3	0	1	3	
42	1	2	1	3	
42	4	1	2	0	
42	0	3	2	0	
42	2	1	2	2	
43	5	3	0	0	
43	4	0	0	3	○
43	4	3	1	1	○
43	5	0	1	2	
43	1	3	2	0	
43	4	0	2	1	○
44	6	2	0	0	
44	3	4	0	1	
44	0	4	0	2	
44	3	2	0	3	
44	6	1	1	0	
44	3	1	1	3	
44	3	2	2	1	
44	0	2	2	2	
45	5	2	0	2	
45	1	4	0	2	
45	4	1	0	3	
45	0	3	0	3	
45	6	0	1	1	
45	2	4	1	1	
45	5	1	1	2	
45	3	3	1	2	○
45	2	2	1	3	
45	4	1	2	1	
45	0	3	2	1	
45	3	0	2	2	○
45	1	2	2	2	
46	5	3	0	1	○
46	4	3	0	2	○
46	1	3	0	3	○
46	2	3	2	0	○
46	1	3	2	1	○
47	6	2	0	1	○
47	3	4	1	0	
47	6	1	1	1	○
47	3	1	2	2	
48	4	4	0	0	
48	6	0	0	2	
48	2	4	0	2	
48	0	0	0	4	
48	4	2	2	0	
48	2	2	2	2	
49	7	0	0	0	
49	2	3	0	3	
49	1	0	0	4	○
49	5	3	1	0	○
49	4	0	1	3	
49	5	0	2	0	○
49	2	3	2	1	
50	0	5	0	0	
50	6	1	0	2	
50	0	1	0	4	
50	6	2	1	0	○
50	3	4	1	1	○
50	0	4	1	2	○
50	3	2	1	3	○

Notes: *All combinations of (N_0, N_1, N_2, N_3) in case that N is under 50.

$$N = (N_0)^2 + 2(N_1)^2 + 6(N_2)^2 + 3(N_3)^2.$$

**M(O): All combinations with $N \leq 50$, $N \in \mathbf{N}$ ($N_i \geq 0$): $N_i \in \mathbf{N}^+$ satisfying the above formula under the conditions of Integrality and Irreducibility.

H_{13} and H_{23} contain $8/3N_0N_1$ and $16/3N_0N_1$, respectively. As 3 is a prime number, it is acceptable as long as either N_0 or N_1 is a multiple of 3: $N_0 \equiv 0$ or $N_1 \equiv 0 \pmod{3}$, i.e., $N_0N_1 \equiv 0 \pmod{3}$.

H_{32} : if $(-N_1N_3 + N_0N_2 + 3N_2N_3 + N_0N_1) \equiv 0 \pmod{2}$, H_{32} is an integer.

Therefore, if $(-N_1 + N_2)N_3 + (+N_1 + N_2)N_0 \equiv -2N_2N_3 \equiv 0 \pmod{2}$, H_{32} is an integer.

If the parity for combination (N_1, N_2) matches, $(-N_1 + N_2)$ and $(N_1 + N_2)$ are even for any N_0 and N_3 . Similarly, $(+N_0 - N_3)N_1 + (+N_0 + N_3)N_2 \equiv -2N_2N_3 \equiv 0 \pmod{2}$, if the parity for combination (N_0, N_3) matches, $(-N_0 + N_3)$ and $(N_0 + N_3)$ are even for any N_1 and N_2 . Therefore, if the parity for either combination (N_1, N_2) or (N_0, N_3) matches, H_{32} is an integer. In conclusion, the condition for integrality of H_{32} is that

$$\{N_0N_1 \equiv 0 \pmod{3}\} \text{ and } \{\text{parity matching of } (N_1, N_2) \text{ or } (N_0, N_3)\}. \quad (12)$$

3.3.2. Examination of irreducibility

Irreducibility by 2:

H_{11} , H_{22} , and H_{33} : if $(N_0^2 \pm 3N_3^2) \equiv 0 \pmod{2}$, they are even. It means that $N_0^2 \equiv 3N_3^2 \pmod{2}$.

Therefore, their irreducibility by 2 matches the parity between N_0 and N_3 .

H_{31} : if $3(N_1N_3 - N_0N_2) \equiv 0 \pmod{2}$, then $(N_1N_3 - N_0N_2) \equiv 0 \pmod{2} \because (2, 3) = 1$.

$\therefore$ If the parity of N_0 and N_3 matches, H_{31} is even in the same manner as H_{11} , H_{22} , and H_{33} , (A)

i.e., $(N_1N_3 - N_0N_2) = 2nN_1 - 2mN_2 = 2(nN_1 - mN_2)$: for any N_1 and N_2 , n and $m \in \mathbb{Z}$.

$\therefore$ If the parity of N_0 and N_3 does not match, H_{31} is odd.

i.e., $2nN_1 + N_1 - 2mN_2 - N_2 = 2(nN_1 - mN_2) + N_1 - N_2$. Therefore, for $H_{31} \equiv 0 \pmod{2}$, the parity of N_1 and N_2 matches.

H_{12} and H_{21} are even.

H_{13} and H_{23} are even if they are integers.

H_{32} : if $(-N_1N_3 + N_0N_2 + 3N_2N_3 + N_0N_1) \equiv 0 \pmod{4}$, H_{32} is even.

$\therefore (N_0 - N_3)(N_1 + N_2) \equiv -4N_2N_3 \pmod{4}$, if H_{32} is even.

This equation means that

$$(N_0 - N_3) \equiv 0 \quad \text{and} \quad (N_1 + N_2) \equiv 0 \pmod{2} \quad (B1)$$

or

$$(N_0 - N_3) \equiv 0 \pmod{4} \quad (B2)$$

or

$$(N_1 + N_2) \equiv 0 \pmod{4}. \quad (B3)$$

In conclusion, the condition for “**reducibility by 2**” is

$$(A) \text{ and } \{(B1) \text{ or } (B2) \text{ or } (B3)\}. \quad (13)$$

Therefore, the condition of **irreducibility by 2** is one in which (13) is omitted from (12).

Irreducibility by 3:

Based on H_{11} , H_{22} , $N_0 \equiv 0 \pmod{3}$. Based on H_{23} , $N_2N_3 \equiv 0 \pmod{3} \because (3, 16) = 1$

Based on H_{11} , $N_1 \equiv 0 \pmod{3}$

Therefore, the cases of $\{(N_0 \equiv 0) \cap (N_1 \equiv 0) \cap (N_2N_3 \equiv 0) \pmod{3}\}$ for **irreducibility by 3** are omitted.

When three zeros exist:

- In case of $a_0 = 0$, rotational angle $\theta = 2\pi$ and rotational axis: $\langle 100 \rangle$.
- When $a_0 \neq 0$, rotational angle $\theta = 0$ and the rotational axis is arbitrary. That is, this is not rotation.

Note. With Miller index in crystallography, the equivalent directions of crystal are shown as $\langle hkl \rangle$ and the specific direction is shown as $[hkl]$.¹⁰

Irreducibility by other positive integers:

Irreducibility for 4 ($= 2^2$) is included in the case for 2. Irreducibility for 6 ($= 2 \cdot 3$) is included in the cases for 2 and 3. For 5 and 7, irreducibility is evaluated by actually calculating each element to see if all can be divided by them, and these cases are a future work. Irreducibility for 8 ($= 2^3$) is included in the case for 2. For larger prime numbers, evaluation is performed by actual calculation. However, in case of $N \leq 50$, the maximum N_i is 8 since $8^2 = 64$.

The results of the above calculation are listed in Table 2 by applying the above-mentioned conditions. In this table, there are different combinations with the same ΣN and they are summarized in Table 3. It is necessary to verify whether these vary as CSL, or depend on the coordinate system (base), i.e., basis transformation (see Appendix C).

For example, in case of $N = 35$, the combinations are (0401), (0221), (0203), and (0113). These can be divided into two classes: (0401), (0221) and (0203),

Table 3. Combinations of (N_0, N_1, N_2, N_3) containing symmetry of the hexagonal lattice (equivalent quaternions to the left).

N	N_0	N_1	N_2	N_3	N	N_0	N_1	N_2	N_3
1	1	0	0	0					
7	2	0	0	1					
10	1	0	1	1	10	2	0	1	0
11	0	2	0	1	11	0	1	1	1
13	1	0	0	2					
14	0	1	0	2	14	3	1	0	1
17	3	2	0	0	17	3	1	1	0
18	0	0	1	2					
18	3	0	1	1					
19	4	0	0	1					
22	1	3	0	1	22	2	3	0	0
25	1	3	1	0	25	1	0	2	0
26	0	2	1	2	26	3	2	1	1
27	0	3	1	1	27	0	0	2	1
29	3	2	0	2	29	3	1	1	2
31	2	0	0	3					
31	2	3	1	1	31	2	0	2	1
34	5	0	1	1	34	1	0	1	3
35	0	4	0	1	35	0	2	2	1
35	0	2	0	3	35	0	1	1	3
37	1	3	1	2	37	1	0	2	2
37	5	0	0	2					
38	0	1	2	2	38	3	1	2	1
38	3	1	0	3	38	6	1	0	0
41	3	4	0	0	41	3	2	2	0
43	4	0	0	3					
43	4	3	1	1	43	4	0	2	1
45	3	3	1	2	45	3	0	2	2
46	1	3	0	3	46	5	3	0	1
46	1	3	2	1	46	2	3	2	0
47	6	2	0	1	47	6	1	1	1
49	1	0	0	4					
49	5	3	1	0	49	5	0	2	0
50	0	4	1	2	50	3	4	1	1
50	3	2	1	3	50	6	2	1	0

(0113). In the same class, they are transformed mutually by a basis transformation (Lemma B.11). However, between different classes, it cannot be transformed mutually by any basis transformation.

3.4. Calculation example

The $\Sigma 7$ case is calculated as an example, as follows.

For $\Sigma 7$, $N_0 = 2$, $N_1 = 0$, $N_2 = 0$, $N_3 = 1$: $a_0^2 = 4$, $a_1^2 = 0$, $a_2^2 = 0$, $a_3^2 = 3$, based on Table 2. Therefore, quaternion $\mathbf{q} = 2 + \sqrt{3}\mathbf{k}$ for the $\Sigma 7$ formation. Since there are plural CSL expressions (pairs of rotational angle and axis), a representative expression is derived. That is, the relation with the minimum angle is derived by basis transformation, considering the hexagonal lattice symmetry.

By means of symmetry calculation ${}^*\mathbf{R}_i\mathbf{q}\mathbf{R}_j$ of $12 \times 12 = 144$ by applying $\mathbf{q} = 2 + \sqrt{3}\mathbf{k}$ ($\mathbf{R}_i$ and $\mathbf{R}_j$ according to Lemma B.11, the minimum rotational angle 21.79° is derived by

$$\mathbf{R}_1^*\mathbf{q}\mathbf{R}_6, \quad \mathbf{R}_2^*\mathbf{q}\mathbf{R}_1, \quad \mathbf{R}_3^*\mathbf{q}\mathbf{R}_2, \quad \mathbf{R}_5^*\mathbf{q}\mathbf{R}_4, \quad \mathbf{R}_6^*\mathbf{q}\mathbf{R}_5, \\ \mathbf{B}^*\mathbf{q}\boldsymbol{\beta}, \quad \mathbf{C}^*\mathbf{q}\boldsymbol{\alpha}, \quad \boldsymbol{\alpha}^*\mathbf{q}\mathbf{B}, \quad \boldsymbol{\beta}^*\mathbf{q}\mathbf{A}, \quad \text{and} \quad \boldsymbol{\gamma}^*\mathbf{q}\mathbf{C}.$$

Here, $a_i \geq 0$ ($i = 1, 2, 3$: all rotational axis indices are considered non-negative) is satisfied by $\mathbf{R}_1^*\mathbf{q}\mathbf{R}_6$, $\mathbf{R}_2^*\mathbf{q}\mathbf{R}_1$, $\mathbf{R}_3^*\mathbf{q}\mathbf{R}_2$, $\mathbf{R}_5^*\mathbf{q}\mathbf{R}_4$, and $\mathbf{R}_6^*\mathbf{q}\mathbf{R}_5$ and they are $\sqrt{7}(3\sqrt{21}/14 + \sqrt{7}/14\mathbf{k})$. Therefore, the rotational axis is $[0 \ 0 \ \sqrt{7}/14]$, which means $\langle 001 \rangle$, crystallographically, with the minimum rotational angle $2\theta = 21.79^\circ$ due to $\cos \theta = 3\sqrt{21}/14$.

Because the orthogonal coordinate system is applied at this stage, it is converted to the index for the hexagonal lattice.

The change in expression for components according to the basis transformation corresponds to

$$(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)\mathbf{E}_h = (\mathbf{e}'_1\mathbf{e}'_2\mathbf{e}'_3),$$

$$\mathbf{E}_h^{-1} = \begin{pmatrix} 1 & \sqrt{3}/3 & 0 \\ 0 & 2\sqrt{3}/3 & 0 \\ 0 & 0 & \sqrt{6}/4 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \sqrt{7}/14 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \sqrt{42}/56 \end{pmatrix}.$$

Therefore, $[0 \ 0 \ \sqrt{42}/56]$, which means $\langle 001 \rangle$.

4. Conclusion

CSL relations have already been shown mathematically by using advanced mathematics. However, these are abstract, making them difficult for material engineers to understand their derivation. Therefore, in this study, a derivation of coincidence relations is attempted in order to enable material engineers to easily understand the derivation by using the hexagonal lattice as an example.

Scale rotation of the quaternion ($\mathbf{E}_R$) is applied in order to present the rotational matrix for CSL.

The matrix ($\mathbf{H}_i$) specifying the ΣN coincidence relation of a certain lattice system is expressed by a similarity transformation using the matrix comprising its PTVs ($\mathbf{E}_i$), i.e., $\mathbf{H}_i = \mathbf{E}_i^{-1}\mathbf{E}_R\mathbf{E}_i$.

Furthermore, based on the rational number property of the transformation matrix elements, the following formula is derived: $N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2$, $N_i \in \mathbb{N}^+$, $N : \Sigma$ value. Here, $(N_0N_1N_2N_3)$ is specified by the integrality (lattice point) and irreducibility (unit cell) among the elements. Finally, based on the polar form of this quaternion, the coincidence relation can be derived.

List of Abbreviations

GO: Grain-oriented silicon steel
 CSL: Coincidence site lattice
 PTVs: Primitive translation vectors
 ESL: Expanded-standard lattice

ERL: Expanded-rotated lattice

$\mathbf{E}_s$: The bases of the standard (orthogonal) coordinate system

$\mathbf{E}_R$: The operation of expansion and rotation of $\mathbf{E}_s$

$\langle hkl \rangle$: The equivalent directions of crystal

$[hkl]$: The specific direction of crystal

Appendix A

Various mathematical details and the definitions used are presented herein for non-specialists in mathematics.

A.1. Definitions

$\mathbb{N}$: The set of positive integers

$\mathbb{N}^+$: The set of non-negative integers

$\mathbb{Z}$: The set of integers

$\mathbb{Z}^\times$: The set of non-zero integers

$\mathbb{Q}$: The set of rational numbers

$\mathbb{Q}^\times$: The set of non-zero rational numbers

$\mathbb{R}$: The set of real numbers

$(m, n) = 1$: Two positive integers m and n are relatively prime

Appendix B. Lemma

Lemma B.1 (Scale rotation). $\mathbf{Q} = \mathbf{q}\mathbf{r}\mathbf{q}^*$ is equal to the vector that is formed by rotating vector $\mathbf{r}$ around $\mathbf{V}(\mathbf{q})$ by $2\arg(\mathbf{q})$ and expanding the length $|\mathbf{q}|^2$ -fold. Here, $\mathbf{q} = a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$, $\mathbf{V}(\mathbf{q})$ is the vector part of $\mathbf{q}$, $[a_1, a_2, a_3]$, and the rotated vector $\mathbf{r}$ can be described as $[u_1, u_2, u_3] = u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k}$. In addition, $|\mathbf{q}|^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2$, and a_i must be real numbers.

The proof is omitted.

Lemma B.2. Σ -value, N , is expressed as $N = |\mathbf{q}|^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2$.

Proof. From (5), the absolute value of quaternion $\mathbf{q}$ is $|\mathbf{q}| = \sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2}$. Therefore, as the length of each PTV of $\mathbf{E}_i$ is extended $|\mathbf{q}|^2$ -fold by applying Lemma B.1, its volume is expanded from $\det[\mathbf{E}_i]$ to $(|\mathbf{q}|^2)^3 \det[\mathbf{E}_i]$.

On the other hand, the volumes of ERL and ESL are $\det[N\mathbf{E}_i]$ and $\det[N\mathbf{R}\mathbf{E}_i]$, respectively, and finally $N^3 \det[\mathbf{E}_i]$. Therefore, $N^3 = |\mathbf{q}|^6$, i.e., $N = |\mathbf{q}|^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2$. In addition, the volume of CSL is $\det[\mathbf{C}\mathbf{E}_i] = N \det[\mathbf{E}_i]$ based on the definition of CSL. $\square$

Lemma B.3. The squares of coefficients of the quaternion applied for CSL, a_i^2 , are rational numbers.

Proof. a_i is a real number, and N is a natural number satisfying $a_0^2 + a_1^2 + a_2^2 + a_3^2 = N$, based on Theorem.

When $a_i \neq 0$: If a_i^2 is an irrational number, there is an irrational number with the opposite sign (< 0), which is a_j^2 ($i \neq j$). However, a_i and a_j are real numbers, and thus, $a_j^2, a_i^2 \geq 0$, which is a contradiction.

When $a_i = 0$: Zero is included as it is a rational number. $\square$

Lemma B.4. When m is the product of different prime numbers, an arbitrary rational number “ a ”, which is not zero, is uniquely expressed by the product of square number b^2 and square-free integer m , as $a = b^2m$ ($b \in \mathbb{Q}^\times$, m is a square-free integer) according to factorization into prime factors of a . In this case, $\mathbb{Q}(\sqrt{a}) = \mathbb{Q}(\sqrt{m})$.

Proof. Since $r + s\sqrt{a} = r + sb\sqrt{m}$, the right-hand side is $t + u\sqrt{m} = t + u\sqrt{a/b^2} = t + (u/b)\sqrt{a}$, ($r, s, t, u \in \mathbb{Z}$).

Therefore, the fields for $r + sb\sqrt{m}$ and $t + (u/b)\sqrt{a}$ match. $\square$

Lemma B.5. The coefficients of the quaternion are expressed as $a_i = N_i\sqrt{m_i}$ (m_i is a square-free integer, $N_i \in \mathbb{N}^\times$).

Proof. Since a_i^2 is a rational number, based on Lemmas B.3 and B.4, it can be expressed as $a_i^2 = N_i^2m_i := (L_i/M_i)$, $a_i = N_i\sqrt{m_i} = \pm \sqrt{L_i/M_i}$, $(L_i, M_i) = 1$, $M_i \neq 0$, and there are certain restrictions, as $L_i, M_i \in \mathbb{Z}$, $L_iM_i \geq 0$; the same sign, L_i and M_i are non-negative, as the part within the square root is non-negative.

Furthermore, each element of (9) is an integer; thus, the square member is expressed as

$$\begin{aligned} H_{33} &= L_0/M_0 - L_1/M_1 - L_2/M_2 + L_3/M_3 \\ &= \{L_0M_1M_2M_3 - L_1M_0M_2M_3 - L_2M_0M_1M_3 \\ &\quad + L_3M_0M_1M_2\}/(M_0M_1M_2M_3). \end{aligned}$$

For H_{33} to be an integer for an arbitrary integer $L_i = N_i^2m_i$, its denominator $(M_0M_1M_2M_3) = \pm 1$ is the sufficient condition. Because M_i is a positive integer, $(M_0M_1M_2M_3) = +1$. Therefore, $M_i = 1$.

That is, $a_i = \pm\sqrt{L_i} = N_i\sqrt{m_i}$ ($N_i \in \mathbb{N}^\times$, m_i is square-free, $L_i \in \mathbb{N}^+$). $\square$

Lemma B.6. The only quaternions that satisfy $\mathbf{r} : [U_1, U_2, U_3] = \mathbf{r} \cdot [u_1, u_2, u_3] = \mathbf{q}\mathbf{r}\mathbf{q}^*$ for an arbitrary vector $\mathbf{r} : [u_1, u_2, u_3]$ are $\mathbf{q} = \pm 1$.

Proof. Since $\mathbf{r} = \mathbf{q}\mathbf{r}\mathbf{q}^*$ is calculated as

$$\begin{aligned} U_1 &= \{u_1(a_0^2 + a_1^2 - a_2^2 - a_3^2) - 2a_0a_3u_2 + 2a_0a_2u_3 \\ &\quad + 2a_1a_2u_2 + 2a_1a_3u_3\}, \\ U_2 &= \{u_2(a_0^2 - a_1^2 + a_2^2 - a_3^2) + 2a_0a_3u_1 + 2a_2a_3u_3 \\ &\quad - 2a_0a_1u_3 + 2a_1a_2u_1\}, \\ U_3 &= \{u_3(a_0^2 - a_1^2 - a_2^2 + a_3^2) - 2a_0a_2u_1 + 2a_1a_3u_1 \\ &\quad + 2a_0a_1u_2 + 2a_2a_3u_2\}, \end{aligned}$$

therefore,

$$\begin{aligned} u_1 &= 1, & u_2 &= 0, & u_3 &= 0, \\ u_1 &= 0, & u_2 &= 1, & u_3 &= 0, \\ u_1 &= 0, & u_2 &= 0, & u_3 &= 1 \end{aligned}$$

hold; then ($\because \mathbf{r}$ is an arbitrary vector).

$$\begin{aligned} (a_0^2 + a_1^2 - a_2^2 - a_3^2) &= 1, & (a_0^2 - a_1^2 + a_2^2 - a_3^2) &= 1, \\ (a_0^2 - a_1^2 - a_2^2 + a_3^2) &= 1; \text{ therefore,} \\ a_0^2 &= 1, & a_1^2 &= a_2^2 = a_3^2 = 0 \quad \therefore \mathbf{q} = \pm 1. \quad \square \end{aligned}$$

Lemma B.7. The rotation $\mathbf{R}(\mathbf{u}, \theta)$ is expressed by using unit quaternions $\mathbf{q}(\mathbf{V}(\mathbf{q}), \theta/2)$ and $-\mathbf{q}(\mathbf{V}(\mathbf{q}), \theta/2)$,

$$\mathbf{V}(\mathbf{q})\mathbf{V}(\mathbf{q}) = 1 \text{ as } \mathbf{R}(\mathbf{u}, \theta) = \mathbf{q}\mathbf{r}\mathbf{q}^* = (-\mathbf{q})\mathbf{r}(-\mathbf{q})^*,$$

indicating the same rotation.

Proof. Since the unit quaternions $\mathbf{q}$ and $\mathbf{q}_1$ indicate the same rotation, $\mathbf{q}\mathbf{r}\mathbf{q}^* = \mathbf{q}_1\mathbf{r}\mathbf{q}_1^*$, therefore, applying $\mathbf{q}^*$ from the left and $\mathbf{q}$ from the right, $\mathbf{q}$ is the unit quaternion, and thus $\mathbf{q}\mathbf{q}^* = 1$,

$$\mathbf{q}^*\mathbf{q}\mathbf{r}\mathbf{q}^*\mathbf{q} = (\mathbf{q}^*\mathbf{q}_1)\mathbf{r}(\mathbf{q}^*\mathbf{q}_1)^* = \mathbf{Q}\mathbf{r}\mathbf{Q}^*.$$

Meanwhile, based on Lemma B.6, $\mathbf{q}^*\mathbf{q}_1 = \pm 1$, and therefore applying $\mathbf{q}$ from the left, $\mathbf{q}\mathbf{q}^*\mathbf{q}_1 = \pm \mathbf{q}$ $\therefore \mathbf{q}_1 = \pm \mathbf{q}$.

Therefore, $\mathbf{q} = a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$ and $-\mathbf{q} = -a_0 - \mathbf{i}a_1 - \mathbf{j}a_2 - \mathbf{k}a_3$ indicate the same rotation. $\square$

Lemma B.8. When m_i and m_j are not relatively prime for two rational numbers $a_i = b_i^2m_i$, $a_j = b_j^2m_j$ in Lemma B.4, the expression can be formed as $a_i = nb_i^2M_i$, $a_j = nb_j^2M_j$ using $(M_i, M_j) = 1$, and thus $\mathbb{Q}(\sqrt{a_i \cdot a_j}) = \mathbb{Q}(\sqrt{M_i \cdot M_j})$ holds.

Proof. $\mathbb{Q}(\sqrt{a_i \cdot a_j}) = \mathbb{Q}(\sqrt{b_i^2nM_i \cdot b_j^2nM_j}) = \mathbb{Q}(b_ib_jn\sqrt{M_i \cdot M_j}) = \mathbb{Q}(\sqrt{M_i \cdot M_j})$. $\square$

Lemma B.9. For $a_i = b_i^2m_i$ and $a_j = b_j^2m_j$, the adjoint element for the extension field is $\sqrt{m_i m_j}$,

especially, when $a_i = a_j$, it is $\sqrt{a_i \cdot a_j} \in \mathbb{Q}$ and when $(a_i, a_j) = 1$, it is $\sqrt{m_i m_j}$.

Proof. Based on Lemma B.8, for rational number $a_i = b_i^2m_i$, $\mathbb{Q}(\sqrt{a_i}) = \mathbb{Q}(\sqrt{m_i})$. Therefore,

- When $a_i \equiv 0, a_j \equiv 0 \pmod{n}$, $\sqrt{a_i a_j} = \sqrt{nb_i^2m_i \cdot nb_j^2m_j} = nb_ib_j\sqrt{m_i m_j} = \mathbb{Q}(\sqrt{m_i m_j})$.
- Similarly, when $(a_i, a_j) = 1$, $\sqrt{a_i a_j} = \sqrt{b_i^2m_i \cdot b_j^2m_j} = b_ib_j\sqrt{m_i m_j} = \mathbb{Q}(\sqrt{m_i m_j})$. $\square$

Lemma B.10. For the congruence equation, when

$$\begin{aligned} a &\equiv b \pmod{m} \quad \text{and} \quad c \equiv d \pmod{m}, \\ a + c &\equiv b + d \pmod{m}, \\ a - c &\equiv b - d \pmod{m}, \quad \text{and} \\ ac &\equiv bd \pmod{m} \text{ hold.} \end{aligned}$$

The proof is omitted.

Lemma B.11. There are 12 elements of rotational symmetry in the hexagonal lattice, which are expressed by using unit quaternions as follows:

$$\begin{aligned} \mathbf{R}_1 &: \sqrt{3}/2 + 1/2\mathbf{k}, & \mathbf{A} &: \mathbf{i}, \\ \mathbf{R}_2 &: 1/2 + \sqrt{3}/2\mathbf{k}, & \mathbf{B} &: +1/2\mathbf{i} + \sqrt{3}/2\mathbf{j}, \\ \mathbf{R}_3 &: \mathbf{k}, & \mathbf{C} &: -1/2\mathbf{i} + \sqrt{3}/2\mathbf{j}, \\ \mathbf{R}_4 &: 1/2 - \sqrt{3}/2\mathbf{k}, & \alpha &: \mathbf{j}, \\ \mathbf{R}_5 &: \sqrt{3}/2 - 1/2\mathbf{k}, & \beta &: +\sqrt{3}/2\mathbf{i} + 1/2\mathbf{j}, \\ \mathbf{R}_6 &: 1, & \gamma &: -\sqrt{3}/2\mathbf{i} + 1/2\mathbf{j}. \end{aligned}$$

Lemma B.12. Expression based on symmetry of the hexagonal lattice: permutation of N_i .

Proof. Based on (10), $m_i m_j = 1 = 1 \times 1, 2 = 1 \times 2, 3 = 1 \times 3, 6 = 2 \times 3 = 1 \times 6, m_i \in \mathbb{N}$ is satisfied only by $(m_0, m_1, m_2, m_3) = (1263) = (2136) = (6312) = (3621)$. Because $a_i = N_i\sqrt{m_i}$ based on Lemma B.5,

$$\begin{aligned} N &= a_0^2 + a_1^2 + a_2^2 + a_3^2 = \Sigma(N_i\sqrt{m_i})^2, \quad i = 0-3, \\ (N_0)^2 &+ (\sqrt{2}N_1)^2 + (\sqrt{6}N_2)^2 + (\sqrt{3}N_3)^2, \\ (\sqrt{2}N_0)^2 &+ (N_1)^2 + (\sqrt{3}N_2)^2 + (\sqrt{6}N_3)^2, \\ (\sqrt{6}N_0)^2 &+ (\sqrt{3}N_1)^2 + (N_2)^2 + (\sqrt{2}N_3)^2, \\ (\sqrt{3}N_0)^2 &+ (\sqrt{6}N_1)^2 + (\sqrt{2}N_2)^2 + (N_3)^2. \end{aligned}$$

However, the form of the formula does not change even when N_i is substituted, and thus, $N = a_0^2 + a_1^2 + a_2^2 + a_3^2$ is a symmetric polynomial; they are all

intrinsically the same and expressed as

$$N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2. \quad (\text{B.1})$$

In addition, these four expressions are included in the symmetry operation in Lemma B.11. $\square$

Lemma B.13. *Expression based on symmetry of hexagonal lattice: sign for N_i .*

Proof. For the sign of N_i that satisfies $N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2$, considering Lemmas B.7 and B.11, only the following two cases are independent:

$$\begin{aligned} \mathbf{q} &= N_0 + \sqrt{2}N_1\mathbf{i} + \sqrt{6}N_2\mathbf{j} + \sqrt{3}N_3\mathbf{k} = \sqrt{N}\{\cos(\theta/2) \\ &\quad + h/R\sin(\theta/2)\mathbf{i} + k/R\sin(\theta/2)\mathbf{j} + l/R\sin(\theta/2)\mathbf{k}\}, \\ \mathbf{q}^* &= N_0 - \sqrt{2}N_1\mathbf{i} - \sqrt{6}N_2\mathbf{j} - \sqrt{3}N_3\mathbf{k} = \sqrt{N}\{\cos(-\theta/2) \\ &\quad + h/R\sin(-\theta/2)\mathbf{i} + k/R\sin(-\theta/2)\mathbf{j} \\ &\quad + l/R\sin(-\theta/2)\mathbf{k}\} : R^2 = h^2 + k^2 + l^2. \end{aligned}$$

These are conjugate to one another and are rotations in reverse directions around the same axis (the right-hand side system is specified first), and one of the two must therefore be omitted. Here, θ is the rotation angle and $\theta/2$ is an argument. Finally, the formula $N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2$, $N_i \in \mathbb{N}^+$ is derived. $\square$

Appendix C. Minimum Rotational Angle

CSL relation is identified with the minimum rotational angle and rotational axis. For identification, basis transformation should be considered, i.e., the “different expressions with the same lattice point alignment”. The discrimination among expressions is formed by using coordinate transformation. According to the basis transformation of the lattice system, there are 12 different expressions for the hexagonal lattice (Lemma B.11). Among these, the coordinate system is rotated under fixing the lattice (the elements of CSL formation), in order to obtain the minimum rotation angle, which is achieved by a rotation operation using the unit quaternion. Table 3 lists the equivalent expressions.

Contribution

This work is a collaboration and completed by discussion by both the authors. They contributed to all

contexts. Both authors have read and approved the final manuscript.

Competing Interests

The authors declare that they have no competing interests.

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