

# Mathematical Tools that Connect Different Indexing Analyses <sup>†</sup>

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**Abstract:** As mathematical tools that can be commonly used for indexing analyses from different types of experimental patterns, we have recently developed (i) rules on forbidden  $hkl$ 's that can be used even when the space group and setting are unknown, (ii) an algorithm for error-stable Bravais lattice determination, (iii) generalization of the de Wolff figure of merit for powder diffraction (1D data) to data in higher-dimensions such as Kikuchi patterns (2D data) by electron backscatter diffraction (EBSD). In particular, (ii) could be used in a variety of situations, not just for indexing. It is explained how (i)–(iii) are used in the mathematical framework of our indexing algorithms.

**Keywords:** Bravais lattice; ab-initio indexing; figure of merit

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## 1. Introduction

Mathematical tools that can be commonly used in ab-initio indexing analyses are introduced herein. They were originally invented for powder diffraction [1], and subsequently applied to the indexing of Kikuchi bands in electron backscatter diffraction (EBSD) patterns [2]. “Ab-initio” means that the indexing is carried out without any prior information on the parameters and Bravais type of the unit cell.

In the case of powder diffraction, the values of  $d$ -spacings (hence, lengths of reciprocal-lattice vectors) are obtained from positions of diffraction peaks. In the EBSD case, the orientations of reciprocal-lattice vectors are provided from the positions of Kikuchi bands. Our indexing algorithms for them use a common mathematical framework shown in Figure 1. First, the parameters of the primitive cell are determined, because (i) simple rules of systematic absence are available, if only basis vectors of a primitive lattice are considered. Subsequently, (ii) Bravais-type (and centering) determination is carried out. This process can be error-stable enough to deal with unit-cell parameters containing large errors due to zero-point shifts (powder [3]) or projection-center shifts (EBSD [4]). We also (iii) generalized the idea of the de Wolff figure of merit  $M_n$  [5], which has been the most efficient indicator in powder indexing. The generalized one presents similar properties for EBSD patterns [2]. The developed software is now available on the web: Powder auto-indexing: <https://z-code.kek.jp/zrg/> (CONOGRAPH). EBSD ab-initio indexing: <https://osdn.net/projects/ebstd-conograph/>

In what follows, mainly the mathematics used for (ii) is discussed. Due to the limitation of the space, (i) and (iii) are only mentioned referring to published papers. The author believes that these theoretical results will be also useful in different analyses of crystallography.

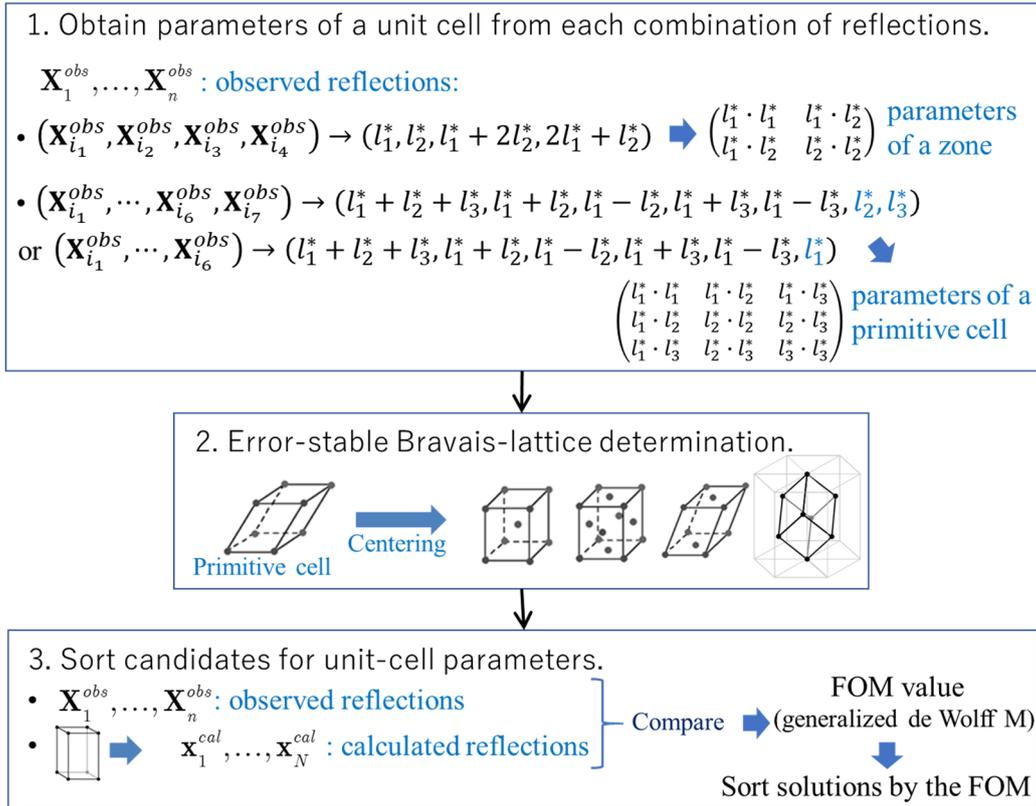


Figure 1. Common mathematical framework of our indexing algorithms.

1.1. Notation

We summarize the notation and symbols used in the article. The inner product of the Euclidean space  $\mathbb{R}^N$  is denoted by  $u \cdot v$ , and the Euclidean norm  $u \cdot u$  is denoted by  $|u|^2$ . Any basis  $v_1, \dots, v_N$  of an  $N$ -dimensional ( $N$ -D) lattice  $L$  is associated to a quadratic form:

$$f(x_1, \dots, x_N) = |x_1 v_1 + \dots + x_N v_N|^2 = \mathbf{x}^T S \mathbf{x}, \tag{1}$$

where  $\mathbf{x} = (x_1, \dots, x_N)^T$  is a vector, and  $S$  is the symmetric matrix with  $v_i \cdot v_j$  in the  $(i, j)$ -entry.  $S$  is also the Gramian (or metric tensor [6]) of  $L$ . The stabilizer of  $S$  is defined as the following subgroup of  $GL_N(\mathbb{Z})$  (=the group of integral matrices with the determinant  $\pm 1$ ):

$$\text{Stab}(S) = \{g \in GL_N(\mathbb{Z}) : g S g^T = S\}. \tag{2}$$

The Gramians  $S_1, S_2$  belong to the same Bravais type, if  $\text{Stab}(S_1), \text{Stab}(S_2)$  are conjugate in  $GL_N(\mathbb{Z})$  (i.e., there exists  $\sigma \in GL_N(\mathbb{Z})$  such that  $\sigma \text{Stab}(S_1) \sigma^{-1} = \text{Stab}(S_2)$ ) [7].

On the linear space  $\mathcal{S}_N$  consisting of  $N$ -by- $N$  symmetric matrices, an inner product is defined by  $S \bullet T := \text{Trace}(ST)$ , which makes  $\mathcal{S}_N$  the metric space (the distance between  $S$  and  $T$  equals  $(S - T) \bullet (S - T)$ ). The subset of  $\mathcal{S}_N$  consisting of all the positive definite symmetric matrices is denoted by  $\mathcal{S}_N^+$ . The action of  $GL_N(\mathbb{Z})$  on  $\mathcal{S}_N^+$  is given by  $S \mapsto g S g^T$ .

The following is an overview of the lattice-basis reduction theory that discusses methods to provide the representatives for the orbits  $GL_N(\mathbb{Z}) \setminus \mathcal{S}_N^+$ . Namely,  $\mathcal{D} \subset \mathcal{S}_N^+$  is the subset that fulfills the following (i), (ii):

- (i)  $\mathcal{S}_N^+ = \bigcup_{g \in GL_N(\mathbb{Z})} \mathcal{D}[g]$ ,
- (ii)  $\mathcal{D}[g_1] \cap \mathcal{D}[g_2] = \emptyset$  for any  $g_1 \neq \pm g_2 \in GL_N(\mathbb{Z})$ , where  $\mathcal{D}[g] \stackrel{def}{=} \{gSg^T : S \in \mathcal{D}\}$ .

As the boundaries of  $\mathcal{D}$  are prone to complications, overlaps of the boundary  $\partial\mathcal{D} := \mathcal{D} \setminus \mathcal{D}^{in}$  ( $\mathcal{D}^{in}$ : set of interior points of  $\mathcal{D}$ ) are frequently allowed. In such a case,  $\mathcal{D}$  should satisfies (i) and the following (ii)' and (iii)':

- (ii)'  $\mathcal{D}^{in}[g_1] \cap \mathcal{D}^{in}[g_2] = \emptyset$  for any  $g_1 \neq \pm g_2 \in GL_N(\mathbb{Z})$ .
- (iii)'  $\mathcal{D} \cap \mathcal{D}[g] \neq \emptyset$  for only finitely many  $g \in GL_N(\mathbb{Z})$ .

It is straightforward to see that any  $S$  in  $\mathcal{D}^{in}$  satisfies  $\text{Stab}(S) = \{\pm 1\}$ . Thus, all the  $S$  with non-triclinic Bravais types belong to the boundary of  $\mathcal{D}$ . The following are the definitions of Venkov [8] and Delaunay reductions used in Section 3; for any fixed  $S_0 \in \mathcal{S}_N^+$ , define  $\mathcal{D}_{S_0}$  by:

$$\mathcal{D}_{S_0} := \{S \in \mathcal{S}_N^+ : S \bullet S_0 \leq (gSg^T) \bullet S_0 \text{ for any } g \in GL_N(\mathbb{Z})\}. \tag{3}$$

From the definition,  $\mathcal{D}_{S_0}[g] = \mathcal{D}_{S_0} \Leftrightarrow g^T \in \text{Stab}(S_0)$  holds. If  $S$  belongs to  $\mathcal{D}_{S_0}$ ,  $S$  is *Venkov-reduced* with regard to  $S_0$ . In particular,  $S$  is *Selling-reduced*, if  $S$  belongs to  $\mathcal{D}_{A_N}$ , where  $A_N$  is the symmetric matrix with 2 in the diagonal entries and 1 in the other entries.

$$A_N(i, j) = \begin{cases} 2 & i = j, \\ 1 & i \neq j. \end{cases} \tag{4}$$

## 2. Determination of the Primitive Lattice

For some types of systematic absence (SA), the ratio of forbidden reflections is not small, but considerably high rate. The rules of SA stated in International Tables depend on the space group and setting of atomic positions. Simple rules of SA are useful for developing algorithms that generally work, if they are available.

In order to obtain such simple rules, only basis vectors of the primitive lattice are considered herein.  $L^*$  is the reciprocal lattice of the crystal lattice  $L$ .  $\{l_1^*, l_2^*\}$  is a *primitive set*, if it is a subset of some basis  $l_1^*, l_2^*, l_3^*$  of  $L^*$ .

**Theorem 1.** (Theorem 2, [9]) *Regardless of the type of SA, there are infinitely many primitive sets  $\{l_1^*, l_2^*\}$  of  $L^*$  such that none of  $l_1^*, l_2^*, l_1^* + 2l_2^*, 2l_1^* + l_2^*$  correspond to an extinct reflection due to the SA. Furthermore, there exist infinitely many 2D sublattices  $L_2^*$  of  $L^*$  such that  $L_2^*$  is expanded by such  $l_1^*, l_2^*$ .*

Theorem 1 is not true, if  $l_1^*, l_2^*, l_1^* + 2l_2^*, 2l_1^* + l_2^*$  are replaced e.g., by  $l_1^*, l_2^*, l_1^* + l_2^*, l_1^* - l_2^*$  (vectors in Ito's formula [10]:  $2\left(\left|l_1^*\right|^2 + \left|l_2^*\right|^2\right) = \left|l_1^* + l_2^*\right|^2 + \left|l_1^* - l_2^*\right|^2$ ). The theorem assures us that

some combinations of observed reflections correspond to  $l_1^*, l_2^*, l_1^* + 2l_2^*, 2l_1^* + l_2^*$ , for some two vectors  $l_1^*, l_2^*$  contained in a basis of  $L^*$ . In the powder case, the inner product  $l_1^* \cdot l_2^*$  is computed by

$$l_1^* \cdot l_2^* = \left( |l_1^* + 2l_2^*|^2 - |l_1^*|^2 - 4|l_2^*|^2 \right) / 4 = \left( |2l_1^* + l_2^*|^2 - 4|l_1^*|^2 - |l_2^*|^2 \right) / 4. \tag{5}$$

Similarly, in the EBSD case, the direction  $l^* / |l^*|$  of the reciprocal-lattice vector  $l$  are obtained from the coordinates of Kikuchi bands. The vector-length ratio  $|l_1^*| : |l_2^*| : |l_1^* + 2l_2^*|$  can be calculated from the directions of  $l_1^* / |l_1^*|, l_2^* / |l_2^*|, (l_1^* + 2l_2^*) / |l_1^* + 2l_2^*|$  by solving the linear equation.

$$\left( l_1^* / |l_1^*| \quad 2l_2^* / |l_2^*| \quad -(l_1^* + 2l_2^*) / |l_1^* + 2l_2^*| \right) \mathbf{x} = 0 \tag{6}$$

In both Equations (5) and (6), the lengths (or directions) of  $l_1^*, l_2^*, l_1^* + 2l_2^*$  are sufficient to obtain the matrix (or the ratio of its components) in Equation (7). The remaining length (or direction) of  $2l_1^* + l_2^*$  can be used to remove unlikely solutions quickly.

$$\begin{pmatrix} l_1^* \cdot l_1^* & l_1^* \cdot l_2^* \\ l_1^* \cdot l_2^* & l_2^* \cdot l_2^* \end{pmatrix} \tag{7}$$

Theorem 2 is a 3D version of Theorem 1.

**Theorem 2.** (Theorem 4 in [9]) *Regardless of the type of SA, there are infinitely many bases  $\langle l_1^*, l_2^*, l_3^* \rangle$  of  $L^*$  such that the following hold:*

- (a) *the reflections of  $\pm l_1^* + l_2^* + l_3^*$  are not forbidden.*
- (b) *For both  $i = 2, 3$ , (i) none of the reflections of  $ml_1^* + (m - 1)(-l_1^* + l_i^*)$  are forbidden for any integer  $m$ , or (ii) none of the reflections of  $ml_i^* + (m - 1)(l_1^* - l_i^*)$  are forbidden for any integer  $m \geq 0$ .*

As a result, CONOGRAPH assigns  $l_1^* \pm l_2^*, l_1^* \pm l_3^*, l_1^* + l_2^* + l_3^*$  and either of  $l_1^*$  or  $\{l_2^*, l_3^*\}$  to various combinations of observed reflections. See [2] for the EBSD case.

### 3. Bravais-Lattice Determination from Unit-Cell Parameters Containing Large Observation Errors

#### 3.1. Theoretical Background

After the parameters of the primitive cell are obtained in the indexing process, it is necessary to convert them into parameters of the conventional cell. For a Gramian matrix  $S^{obs}$  extracted from observed data, how can one estimate the Bravais type of the unknown true value  $\hat{S}$  of  $S^{obs}$ ? The error can be observational errors or rounding errors of floating-point numbers [11].

If  $S^{obs}$  is exact (i.e.,  $S^{obs} = \hat{S}$ ), the symmetry group of  $n$ -by- $n$   $S^{obs}$  can be determined e.g., by the method of [12]. However, if  $S^{obs} \neq \hat{S}$ , no matter how close  $S^{obs}$  is to  $\hat{S}$ ,  $g \in \text{Stab}(S^{obs})$  is not generally true even if  $1 \neq g \in \text{Stab}(\hat{S})$ . As a result, it is only possible to estimate likely ones as  $\text{Stab}(\hat{S})$ . For this reason, error-stable methods have been investigated in mathematical crystallography.

This determination can be done by step 1 and 2 in Table 1 by using a finite set  $H_0$  with the following property, where  $\mathcal{D}$  is a domain that fulfills (i), (ii)', (iii)' in Section 1.1.

$$H_0: \text{if } S^{obs} \in \mathcal{D}, \text{ then } \hat{S} \in \bigcup_{g \in H_0} \mathcal{D}[g].$$

Namely,  $H_0$  is a finite set containing all  $g \in GL_N(\mathbb{Z})$  such that  $g^{-1}S^{obs}(g^{-1})^T$  is nearly reduced (i.e., close to  $\mathcal{D}$ ) for some  $S^{obs}$  that belongs to  $\mathcal{D}$ .

**Table 1.** Outline of error-stable Bravais lattice determination methods <sup>1</sup>.

<b>Prepared sets in codes</b>	<p>1. For a domain <math>\mathcal{D}</math> that fulfills (i), (ii)', (iii)' in Section 1.1, and its topological closure <math>\overline{\mathcal{D}}</math>, let <math>G_0</math> be the finite set consisting of all <math>g \in GL_N(\mathbb{Z})</math> with <math>\overline{\mathcal{D}} \cap \overline{\mathcal{D}[g]} \neq \emptyset</math>. For each finite group <math>G_k</math> (<math>k = 1, \dots, m</math>) contained in <math>G_0</math>, prepare the set of linear subspace <math>L_k</math> consisting of all <math>S \in \mathcal{S}_n</math> with <math>\text{Stab}(S) \supset G_k</math>. (Namely, <math>L_1, \dots, L_m</math> are lattice characters [6].)</p> <p>2. Finite set <math>H_0</math> consisting of operations <math>g</math> for which <math>\mathcal{D}[g]</math> may contain <math>\hat{S}</math> when <math>S^{obs}</math> is in <math>\mathcal{D}</math>.</p>
<b>Input parameters</b>	Gramian $S^{obs}$ (assume $S^{obs} \in \mathcal{D}$ by exchanging the basis)
<b>Step 1</b>	For any $g \in H_0$ , if $S_2^{obs} = g^{-1}S^{obs}(g^{-1})^T$ is close to the domain $\overline{\mathcal{D}}$ (i.e., nearly reduced), do the following; for each $L_k$ ( $k = 1, \dots, m$ ), calculate $S \in L_k$ closest to $S_2^{obs}$ by projecting $S_2^{obs}$ on $L_k$ . If $S_2^{obs}$ and $S$ are close to each other, store $g, S$ in the array for the Bravais type of $L_k$ .
<b>Step 2</b>	Output the stored $g, S$ after removing duplicates.

<sup>1</sup> The same calculation can be done, even if  $\mathcal{D}$  is replaced by a union of finitely many  $\mathcal{D}[g]$  such as the Venkov reduced domain  $\mathcal{D}_{S_0}$ . The only difference is that  $L_k$  may not be in the boundary of  $\overline{\mathcal{D}}$ .

If  $\mathcal{D}$  is the Niggli-reduced domain (Chap.9.2.2, [6]),  $G_0$  in Table 1 consists of 168 elements. The number  $m$  of lattice characters  $L_k$  is 42, after two triclinic cases are excluded (Table 9.2.5.1 [6]). From the definition,  $H_0$  must contain  $G_0$ , hence, the computation time of the method of Table 1 is roughly estimated as  $|H_0| \times m \geq 168 \times 42 = 7056$ . This is a little time consuming if it is applied to multiple primitive cells generated in the indexing process.

The methods of Andrews and Bernstein [14,15] are basically same as this Niggli-reduced case, although it is not assured that their heuristics can always generate all the necessary operations (in their method, 25 operations in [16] are used to generate the elements of  $H_0$ ).

The use of the Delaunay reduced domain was proposed Burzlaff and Zimmermann [17,18]. This reduces the number of lattice characters from 44 to 30. However,  $H_0$  is set to  $\{1\}$  in their method, so it can basically handle only the exact case.

Thus, the following are the problems, in order to develop a faster and more reliable Bravais-lattice determination method.

**Q1:** Which reduction method minimizes the computation time for Table 1?

**Q2:** Under which assumption on the error size of  $S^{obs}$  is it possible to output all the  $S$  with  $S^{obs} \approx S$  and  $\text{Stab}(S) = \text{Stab}(\hat{S})$ ?

Our idea for **Q1** was to use the following Venkov-reduced domain  $\mathcal{D}_{S_0}$  as  $\mathcal{D}$  in Table 1.

- $S_0 = I_3$  ( $3 \times 3$  identity matrix).
- $S_0 = A_3$  in Equation (4).

By the choice of  $S_0$ ,  $\mathcal{D}_{S_0}$  include non-triclinic  $L_k$  in the interior distant from its boundary  $\partial\mathcal{D}_{S_0}$ . If  $\hat{S}$  is in  $L_k$  and  $\mathcal{D}_{S_0}$ ,  $S^{obs} \approx \hat{S}$  is also in the interior of  $\mathcal{D}_{S_0}$ . As a result,  $\hat{S}$  and  $S^{obs}$  are both reduced with regard to the same basis. In this case, it is not necessary to consider the nearly-reduced case (namely,  $H_0$  may be set to  $\{1\}$ ).

Based on this idea, the author proved that error-stable determination is possible under the following condition **C** on the error size of  $S^{obs}$  [19] (This is an answer to **Q2**):

**C:** for any 3-by-3 symmetric matrix  $T$  and  $0 \neq \mathbf{v} \in \mathbb{Z}^n$ , if  $\hat{S} \cdot T \geq \mathbf{v} \hat{S} \mathbf{v}^T / 2$ ,  $S^{obs} \cdot T > 0$  also holds.

Namely, **C** excludes only the case:  $\mathbf{v}^T S \mathbf{v} / 2 \leq \hat{S} \cdot T \approx S^{obs} \cdot T \leq 0$  (if  $L$  is the crystal lattice with the Gramian  $\hat{S}$ , the half of the squared-length of some non-zero vector in  $L$  is observed as a non-positive value). Hence, **C** assumes that the error of  $S^{obs}$  is not extraordinary large. Under this condition, the following is proved:

**Theorem 3.** (Theorems 1–4 in [19]) For a given  $S^{obs} \in \mathcal{D}_{S_0}$ , assume that  $\hat{S}$  belongs to the Bravais type  $B$ , in addition to **C**. In this case,  $\hat{S}$  belongs to the  $V_B$ , a union of finitely many linear subspaces in Table 2.

**Table 2.**  $B, S_0, V_B$  in Theorem 1.

Bravais Type $B$	$S_0$	$H_0 = \{1\}$ ?	The Number of Linear Subspaces $V_B$ (The Number When $H_0 = \{1\}$ )
Primitive monoclinic	$I_3$	Yes	3 (3) ... Table 3 in [19]
Face-centered orthorhombic	$A_3$	Yes	3 (3) ... Table 4 in [19]
Body-centered orthorhombic <sup>1</sup>	$A_3$	Yes	... Table 5 in [19]
Rhombohedral	$A_3$	conditionally yes <sup>2</sup>	64 (16) ... Table 6 in [19]
Base-centered monoclinic	$A_3$	conditionally yes <sup>2</sup>	69 (21) ... Table 8 in [19]

<sup>1</sup> As for the face-centered case, our method simply uses the fact that  $S^{obs}$  has the face-centered symmetry if and only if the inverse of  $S^{obs}$  has the body-centered symmetry. <sup>2</sup> If  $H_0 = \{1\}$ , the number of steps can be reduced to the same number as the case when  $S^{obs}$  is exact.  $H_0 = \{1\}$  also holds even for rhombohedral and base-centered case, by adding another condition to those of Theorem 3 [19].

After the centering types of the unit cell are classified to those in Table 2, it is straightforward to classify them into higher-symmetric Bravais types.

Therefore, contrary to our intuition, regardless of the magnitude of the error in  $S^{obs}$ , it is possible to output  $S$  with  $S^{obs} \approx S$  and  $\text{Stab}(S) = \text{Stab}(\hat{S})$  generally, without increasing the computation time at all. However, the error of  $S^{obs}$  affects the distance between the output  $S$  and its true value  $\hat{S}$ .

### 3.2. Computation Results

The implemented program is used in our indexing software [1,2]. In [2], indexing analysis was carried out for EBSD patterns with large projection-center shifts as follows ( $z$ : the camera length).

$$\frac{\Delta x}{z}, \frac{\Delta y}{z}, \frac{\Delta z}{z} = 0, \pm 0.005, \pm 0.01, \pm 0.02 \quad (10)$$

Nevertheless, Bravais-lattice determination failed only for a small number of cases among them (see Tables and Figure in [2] for more details).

## 4. Discussion

The theorems presented in Sections 2 and 3 hold true for any symmetry types the crystal structures can have. Our error-stable Bravais-type determination is mathematically guaranteed, even for parameters containing large error. Although the number of operations  $|H_0| \times m \geq 168 \times 42 = 7056$  cannot be decreased as long as the Niggli reduction is used, it can be reduced from 7056 to 154 (58, conditionally) by using the Venkov reduction for  $I_3$  and  $A_3$ . However, other reduction methods (or  $S_0$ ) might be able to provide a faster method. No studies have been reported for lattices of dimensions more than 3.

As ab-initio indexing software for powder diffraction patterns, *ITO* [21,22], *TREOR* [23], and *DICVOL* [24] are well known. EBSD ab-initio indexing have been also studied in [25–27], although more accurate methods for band extraction and projection center identification are also needed for this indexing analysis.

From a theoretical point of view, the two indexing analyses have much in common. This suggests that updating the mathematical crystallography is effective in obtaining reliable and efficient analytical methods in a short time.

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