Crystals 2020

sciforum

Conference Proceedings Paper

Mathematical tools that connect different indexing analyses

Ryoko Oishi-Tomiyasu[1,*]

[1] Institute of Mathematics for Industry, Kyushu University; tomiyasu@imi.kyushu-u.ac.jp
* Correspondence: tomiyasu@imi.kyushu-u.ac.jp;

Received: date; Accepted: date; Published: date

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) 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. 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/ebsd-conograph/

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

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 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].

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

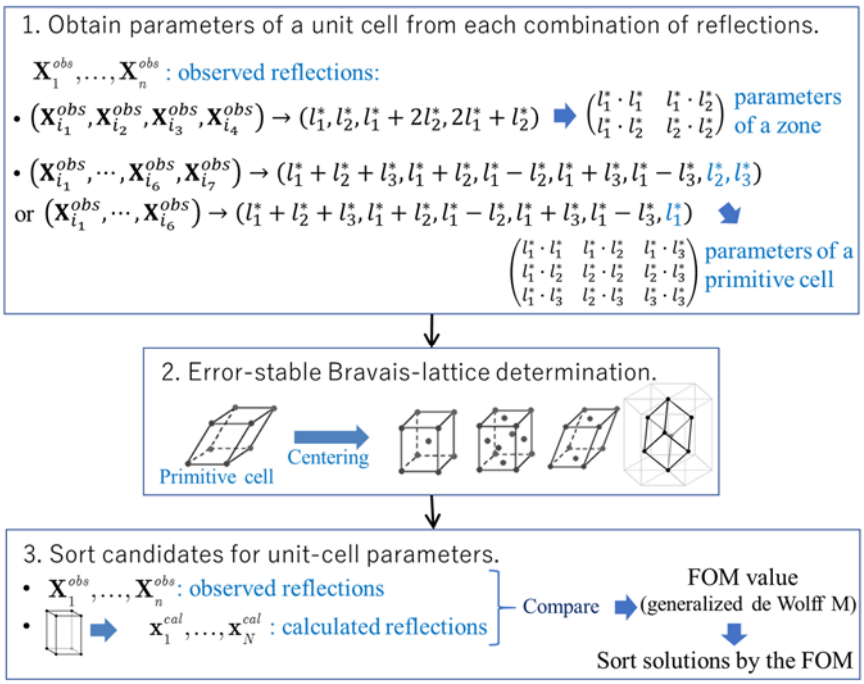

Figure 1. Common mathematical framework of our indexing algorithms

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 $v_1,\ldots,v_N$ of an *N*-dimensional(*N*-D) lattice *L* is associated to a quadratic form:

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

where $\mathbf{x} = (x_1,\ldots,x_N)^T$ 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 ±1):

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

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

On the linear space $\mathcal{S}_N$ consisting of *N*-by-*N* symmetric matrices, an inner product is defined by $S \bullet T := \mathrm{Trace}(ST)$, 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 $S \mapsto gSg^T$.

The following is an overview of the lattice-basis reduction theory that discusses methods to provide the representatives for the orbits $GL_N(\mathbb{Z}) \backslash \mathcal{S}_N^+$. 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) $\mathcal{D}[g_1]\cap\mathcal{D}[g_2]=\varnothing$ for any $g_1 \neq \pm g_2 \in GL_N(\mathbb{Z})$, where $\mathcal{D}[g] \underset{def}{=} \{gSg^T : S\in\mathcal{D}\}$.

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)' $\mathcal{D}^{in}[g_1]\cap\mathcal{D}^{in}[g_2]=\varnothing$ for any $g_1 \neq \pm g_2 \in GL_N(\mathbb{Z})$.

(iii)' $\mathcal{D}\cap\mathcal{D}[g]\neq\varnothing$ for only finitely many $g\in GL_N(\mathbb{Z})$.

It is straightforward to see that any S in $\mathcal{D}^{in}$ satisfies $\mathrm{Stab}(S)=\{\pm 1\}$. 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:

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

From the definition, $\mathcal{D}_{S_0}[g]=\mathcal{D}_{S_0} \Leftrightarrow g^T\in \mathrm{Stab}(S_0)$ 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 SA, forbidden reflections are not exceptional, but occur considerably high rate. The rules of SA stated in International Tables depend on the space group and setting of atomic positions. Simpler rules of SA are required for developing algorithms that generally work.

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* $l_1^*, l_2^*, l_1^*+2l_2^*, 2l_1^*+l_2^*$ *corresponds 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^*.

Theorem1 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 that some combinations of observed reflections correspond to $l_1^*, l_2^*, l_1^*+2l_2^*, 2l_1^*+l_2^*$, for some 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

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

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

$$\begin{pmatrix} l_1^* \Big/ \left| l_1^* \right| & 2l_2^* \Big/ \left| l_2^* \right| & -\left(l_1^* + 2l_2^* \right) \Big/ \left| l_1^* + 2l_2^* \right| \end{pmatrix} \mathbf{x} = 0 \quad (6)$$

In both of Eq.(5), (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 Eq.(7). The remaining length (or direction) of $2l_1^* + l_2^*$ can be used to remove unlikely solutions quickly.

$$\begin{pmatrix} l_1^* \cdot l_1^* & l_1^* \cdot l_2^* \\ l_1^* \cdot l_2^* & l_2^* \cdot l_2^* \end{pmatrix} \quad (7)$$

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, in *CONOGRAPH*, $l_1^* \pm l_2^*$, $l_1^* \pm l_3^*$, $l_1^* + l_2^* + l_3^*$ and either of l_1^* or $\left\{ l_2^*, l_3^* \right\}$ are assigned to various combinations of observed reflections. See Figure 5 of [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}? In practice, 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] (the computation time is rapidly augmented as *n* increases). However, if $S^{obs} \neq \hat{S}$, no matter how close S^{obs} is to $\hat{S}$, $g \in \mathrm{Stab}(S^{obs})$ is not generally true for any $1 \neq g \in \mathrm{Stab}(\hat{S})$. As a result, it is only possible to estimate likely ones as $\mathrm{Stab}(\hat{S})$. It is common in libraries developed by mathematicians (e.g., *Magma* [13]) that the parameters of a lattice cannot be entered in floating-type numbers. For this reason, error-stable methods have been investigated in mathematical crystallography.

This determination can be done by step 1 & 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: if $S^{obs} \in \mathcal{D}$, then $\hat{S} \in \cup_{g \in H_0} \mathcal{D}[g]$.

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

Table 1. Outline of error-stable Bravais lattice determination methods[1]

Prepared sets in codes	1. For a domain $\mathcal{D}$ that fulfills (i), (ii)′, (iii)′ in Section 1.1, and its topological closure $\overline{\mathcal{D}}$, let G_0 be the finite set consisting of all $g \in GL_N(\mathbb{Z})$ with $\overline{\mathcal{D}} \cap \overline{\mathcal{D}}[g] \neq \varnothing$. For each finite group G_k ($k = 1,\ldots,m$) contained in G_0, prepare the set of linear subspace L_k consisting of all $S \in \mathcal{S}_n$ with $\mathrm{Stab}(S) \supset G_k$. (Namely, $L_1,\ldots,L_m$ are *lattice characters* [6].) 2. Finite set H_0 consisting of operations g for which $\mathcal{D}[g]$ may contain $\hat{S}$ when S^{obs} is in $\mathcal{D}$.
Input parameters	Gramian S^{obs} (assume $S^{obs} \in \mathcal{D}$ by exchanging the basis)
Step 1	For any $g \in H_0$, if $S_2^{obs} = g^{-1}S^{obs}\left(g^{-1}\right)^T$ is close to the domain $\overline{\mathcal{D}}$ within the error of S^{obs} (*i.e.*, nearly reduced), do the following; for each L_k ($k = 1,\ldots,m$), calculate $S \in L_k$ close to S_2^{obs} *e.g.*, by projecting S_2^{obs} on L_k. If S_2^{obs} and S are close to each other within the error, store g, S in the array for the Bravais type of L_k.
Step 2	Output the stored g, S after removing duplicates.

[1] 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]. H_0 must contain G_0, because all the non-triclinic S belong to the boundary of the Niggli-reduced domain. Hence, the computation time of the method of Table 1 is roughly estimated as $|H_0| \times m \geqq 168 \times 42 = 7056$. This is a little time consuming, if it is applied to multiple primitive cells generated in the indexing process.

The methods of Andrews & 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).

Use of the Delaunay reduced domain was proposed Burzlaff & 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.

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

Question 2: Under which assumption on the error size of S^{obs}, is it possible to output all the S with $S^{obs} \approx S$ and $\mathrm{Stab}(S) = \mathrm{Stab}(\hat{S})$?

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

- $S_0 = I_3$ (3×3 identity matrix): if $\mathcal{D}$ is the Niggli-reduced domain,

$$\mathcal{D}_{I_3} = \bigcup_{g \in \mathrm{Stab}(I_3)} \mathcal{D}\left[g^T\right] \tag{8}$$

- $S_0 = A_3$ in Eq.(4): if $\mathcal{D}$ is the Delaunay-reduced domain,

$$\mathcal{D}_{A_3} = \bigcup_{g \in \mathrm{Stab}(A_3)} \mathcal{D}\left[g^T\right] \tag{9}$$

By the choice of S_0, $\mathcal{D}_{S_0}$ can include non-triclinic L_k in the interior distant from its boundary $\partial\mathcal{D}_{S_0}$. In such a case, if $\hat{S}$ is in L_k and *Venkov-reduced* with regard to S_0, $S^{obs} \approx \hat{S}$ is also in the interior of $\mathcal{D}_{S_0}$. As a result, it is not necessary to consider the nearly-reduced. H_0 may be set to $\{1\}$ if the Venkov reduction is used.

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 **Question 2**):

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

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

Theorem 3. [Theorem 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 } holds)**
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[1]	A_3	Yes	⋯ Table 5 in [19]
Rhombohedral	A_3	conditionally yes[2]	64 (16) ⋯ Table 6 in [19]
Base-centered monoclinic	A_3	conditionally yes[2]	69 (21) ⋯ Table 8 in [19]

[1] 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.

[2] This is yes, if the software user only needs the S closest to S^{obs} among those with the Bravais type B.

There are only 5 Bravais types in Table 2, because it is straightforward to classify unit cells after the centering determination (i.e., conventional unit cells) into higher-symmetric Bravais types.

In Table 2, if H_0 ={ 1 }, the number of operations required for the error-stable determination is same as the exact case. Therefore, contrary to our intuition, it is possible to output S with $S^{obs} \approx S$ and $\mathrm{Stab}(S) = \mathrm{Stab}(\hat{S})$ very 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 $\hat{S}$.

3.1. Computation results

The implemented program is used in our indexing software [1,2]. It was also used to build a database of quadratic forms [20]. In [2], indexing analysis was carried out for EBSD patterns with projection-centers shifted as follows (z: the camera length).

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

The software succeeded in indexing of orthorhombic—cubic cells in most of the cases. Among them, there were only a few failures due to errors in Bravais-lattice determination (see Tables 4,5 and Figure 9 in [2] for more details).

5. Discussion

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

Prior to such theoretical results, software developers of indexing analysis had to develop case-by-case algorithms or heuristics to deal with the symmetries by themselves. 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 to obtain reliable and efficient analytical methods in short time.

Funding: This study was financially supported by the PREST (JPMJPR14E6) and JST Mirai (JPMJMI18GD)

Acknowledgments: We would like to extend our gratitude to Mr. R. Taniguchi and Mr. S. E. Graiff-Zurita of Kyushu University, who helped us in coding the software, and performing the computation.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Oishi-Tomiyasu, R. Robust powder auto-indexing using many peaks. *J. Appl. Cryst.*, **2014**, *47*, 593—598. doi.org/10.1107/S1600576714000922
2. Oishi-Tomiyasu, R., Tanaka, T., Nakagawa, J. Distribution rules of systematic absence and generalized de Wolff figure of merit applied to EBSD ab-initio indexing. https://arxiv.org/abs/2003.13403.
3. Dong, C.; Wu, F.; Chen, H. Correction of zero shift in powder diffraction patterns using the reflection-pair method. *J. Appl. Cryst*. **1999**, *32*, 850-853. doi:10.1107/S0021889899007396

4. Ram, F.; Zaefferer, S.; Jäpel, T.; Raabe, D. Error analysis of the crystal orientations and disorientations obtained by the classical electron backscatter diffraction technique. *J. Appl. Cryst.*, **2015**, *48*, 797–813. doi:10.1107/S1600576715005762
5. de Wolff, P. M. A Simplified Criterion for the Reliability of a Powder Pattern Indexing. *J. Appl. Cryst.* **1968**, *1*, 108--113. doi:10.1107/S002188986800508X
6. Hahn, T. *et.al.* International Tables for Crystallography Vol.A, 5th ed.; Publisher: Springer, **2005**.
7. Michel, L. Symmetry, invariants, topology. iv. fundamental concepts for the study of crystal symmetry. *Physics Reports*, **2001**, *341*, 265--336.
8. Venkov, B. A. On the reduction of positive quadratic forms. *Izv. Akad. Nauk SSSR Ser. Mat.*, **1940**, *134*, 37--52.
9. Oishi-Tomiyasu, R. Distribution rules of systematic absences on the Conway topograph and their application to powder auto-indexing. *Acta Cryst.*, **2013**, *A69*, 603–610. doi:10.1107/S0108767313021740
10. Ito, T. A general powder *X*-ray photography. *Nature*, **1949**, *164*, 755—756. doi:10.1038/164755a0
11. Grosse-Kunstleve, R. W.; Sauter, N. K.; Adams, P. D. Numerically stable algorithms for the computation of reduced unit cells. *Acta Cryst.*, 2004, A60, 1—6. doi:10.1107/S010876730302186X
12. Plesken, W.; Souvignier, B. B. Computing isometries of lattices. *J. Symbolic. Comput.*, **1997**, *24*, 327--334. doi:10.1006/jsco.1996.0130
13. Bosma, W.; Cannon, J.; Playoust, C. The Magma algebra system. I: The user language. *J. Symbolic Comput.*, **1997**, *24 (3-4)*, 235—265. doi:10.1006/jsco.1996.0125
14. Andrews, L. C.; Bernstein, H. J. Lattices and reduced cells as points in 6-space and selection of bravais lattice type by projections. *Acta Cryst.*, **1988**, *A44*, 1009--1018. doi:10.1107/S0108767388006427
15. Andrews, L.C.; Bernstein, H. J. The geometry of Niggli reduction: BGAOL--embedding Niggli reduction and analysis of boundaries. *J. Appl. Cryst.* **2014**, *47(1)*, 346—359. doi:10.1107/S1600576714014460
16. Gruber, B. The relationship between reduced cells in a general Bravais lattice. *Acta Cryst.*, **1973**, *A29*, 433--440. doi:10.1107/S0567739473001063
17. Burzlaff, H.; Zimmermann, H. On the metrical properties of lattices. *Z. Kristallogr.*, **1985**, *170*, 247--262. doi:10.1524/zkri.1985.170.14.247
18. Zimmermann H.; Burzlaff, H. Delos--a computer program for the determination of a unique conventional cell. *Z. Kristallogr.*, **1985**, *170*, 241--246. doi:10.1524/zkri.1985.170.14.241
19. Oishi-Tomiyasu, R. Rapid bravais-lattice determination algorithm for lattice parameters containing large observation errors. *Acta Cryst. A.*, **2012**, *68*, 525--535. doi:10.1107/S0108767312024579
20. Oishi-Tomiyasu, R. Positive-definite ternary quadratic forms with the same representations over Z. *Int. J. Number Theory*, **2020**, *16(7)*, 1493--1534.
21. de Wolff, P. M. Detection of simultaneous zone relations among powder diffraction lines. *Acta Cryst.*, **1958**, *11*, 664—665. doi:10.1107/S0365110X58001729
22. Visser, J. W. A fully automatic program for finding the unit cell from powder data. *J. Appl. Cryst.*, **1969**, *2*, 89—95. doi:10.1107/S0021889869006649
23. Kohlbeck, F.; Horl, E.M. Trial and error indexing program for powder patterns of monoclinic substances. *J. Appl. Cryst.*, **1978**, *11*, 60—61. doi:10.1107/S0021889878012716
24. Boultif, A.; Louër, D. Powder pattern indexing with the dichotomy method. *J. Appl. Cryst.*, **2004**, *37*, 724—731. doi:10.1107/S0021889804014876
25. Dingley, D. J.; Wright, S. I. Determination of crystal phase from an electron backscatter diffraction pattern. *J. Appl. Cryst.*, **2009**, 42, 234—241. doi:10.1107/S0021889809001654
26. Li, L.; Ouyang, S.; Yang, Y.; Han, M. EBSDL: a computer program for determining an unknown Bravais lattice using a single electron backscatter diffraction pattern. *J. Appl. Cryst.*, **2014**, *47*, 1466—1468. doi:10.1107/S160057671401382X
27. Li, L.; Han, M. Determining the Bravais lattice using a single electron backscatter diffraction pattern. *J. Appl. Cryst.*, **2015**, *48*, 107—115. doi.org/10.1107/S1600576714025989