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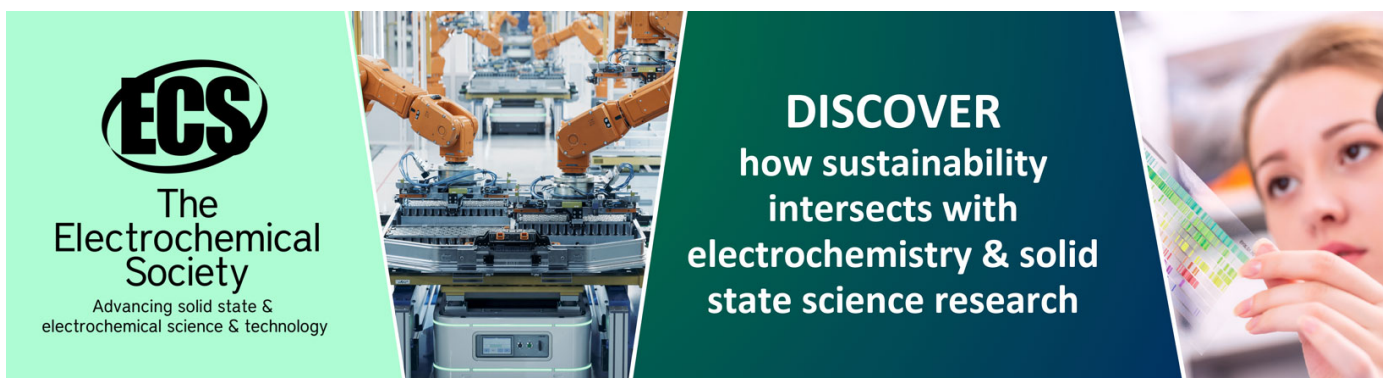
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Determination of orientations from monochromatic diffraction patterns as the constellation problem

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Abstract. Determination of crystal orientations from diffraction patterns is directly linked to pattern indexing. The problem of indexing can be seen as matching scattering vectors to vectors of the crystal reciprocal lattice. With known crystal structure, the simplest version of indexing is formulated as the (constellation) problem of matching vectors under rotations: given two sets X and Y of unit vectors, determine a rotation carrying the largest subset of X to a position approximating a subset of Y . It is shown that algorithms for solving the constellation problem establish a framework for several orientation determination methods. A class of these algorithms is based on accumulating contributions in the rotation space. A rotation with the largest accumulation is considered to solve the problem. The contributions can be made by n -tuples of vectors with n starting from 1. Formulas for the points of accumulation are given for arbitrary $n \geq 1$. Particularly simple turns out to be the case of 2-tuples. It has a potential of being robust, and it is easy to implement.

1. Introduction

Over the last two decades, automatic orientation imaging has become one of the most significant methods of investigating polycrystalline materials. That occurred thanks to the progress in orientation mappings carried out using mainly electron backscatter diffraction (EBSD) [1] and similar systems relying on transmission electron microscopy [2] or high-energy X-ray diffraction [3]. The orientation imaging is directly linked to indexing of diffraction patterns; orientation determination and indexing of patterns originating from known crystal structures are practically equivalent. As numerous patterns are being analyzed, the indexing algorithms need to be time efficient. Equally important is their robustness; indexing is expected to function properly despite errors in geometric parameters of the patterns and/or spurious reflections. Robustness is crucial in diffraction-based non-destructive grain shape reconstruction [3] when multiple crystallites contribute to recorded patterns. Indexing and orientation determination algorithms are as good as their ability to cope with imperfections of input data. For devising optimal algorithms, it is essential to express the problem in a formal way based on simple principles.

In pattern indexing and crystal orientation determination, the point is to match measured scattering vectors (differences between reflected and incident wave vectors) to low-index vectors of the crystal reciprocal lattice. From a computational perspective, indexing can be formulated as the so-called *largest common point set* (LCPS) problem; cf. [4]. In the simplest case, e.g., when EBSD bands are indexed, the magnitudes of the scattering vectors are unknown, and all involved vectors are assumed to be of unit magnitude. The corresponding restricted case of LCPS is referred to as the *constellation problem* [5]: given two sets X and Y of unit vectors, determine



a rotation carrying the largest subset of X to a position approximating a subset of Y . Solving this problem involves both combinatorial matching (assignment) and continuous alignment. In a strict formulation of the constellation problem, a given maximum distance between the matched vectors is allowed. In indexing, such a distance is difficult to specify, or it may vary widely because experimental errors depend on the scattering vector and the direction in space. The heuristic procedures considered below are suitable for solving cases with unspecified distance thresholds, but they do not provide any theoretical guarantee of the quality of the output. In that respect, they are similar to the softassign matching algorithm proposed in [6].

This paper describes a common framework for a number of indexing algorithms. Approaches which at first sight may look different, turn out to be based on similar foundations. We demonstrate that a number of these algorithms can be seen as an accumulation of contributions, i.e., a form of the generalized Hough transform with the abstract rotation space (or the symmetry induced fundamental region [7]) as the parameter space. The contributions can be made by individual vectors (one vector from each set), and in this case accumulation takes place along continuous curves in the rotation space; with two or more vectors from each set, accumulation takes place at discrete points in the rotation space. At the end, the rotation with the largest total accumulation is considered to solve the problem. We list straightforward formulas for the points of accumulation, and we check optimality of these points. The advantage of the considered methods lies in their robustness and conceptual simplicity. The algorithms are relatively easy to implement. We show that particularly simple is the case when pairs of vectors are matched.

Further on, X and Y contain unit vectors bound to a fixed center of rotation. The vectors are represented by column matrices with Cartesian components. Given a non-zero square matrix A , the symbol $\mathcal{O}(A)$ denotes the special orthogonal matrix closest to A in the sense that it minimizes the distance $\|A - \mathcal{O}(A)\|^2$; see [7]. For a non-zero vector x , the symbol $O(x, \omega)$ denotes the special orthogonal matrix representing the rotation by the angle ω about the axis determined by x .

2. Accumulation in the rotation space

One of the strategies for indexing of bands in EBSD patterns is known as 'triplet indexing' [1]. Inter-band angles are compared to angles following from known crystal structure. Based on each band triplet, potential crystal orientations are determined, and each of these orientations gets a vote. The orientation with the largest number of votes is considered to solve the problem. For a more formal description, instead of the angles, we use vectors. If a triplet of linearly independent vectors x_i of X ($i = 1, 2, 3$) is rotated to form the triplet $y_i (= R x_i)$ of Y , the special orthogonal matrix R representing the rotation can be expressed as

$$R = [y_1 \ y_2 \ y_3] [x_1 \ x_2 \ x_3]^{-1}. \quad (1)$$

In indexing, the (normalized scattering) vectors x_i of X are affected by errors, the match between (normalized reciprocal lattice) vectors y_i and the rotated x_i is only approximate, and the matrix $[y_1 \ y_2 \ y_3] [x_1 \ x_2 \ x_3]^{-1}$ needs to be adjusted to satisfy orthogonality conditions; e.g., one can use $R^{(3)} = \mathcal{O}([y_1 \ y_2 \ y_3] [x_1 \ x_2 \ x_3]^{-1})$. Now, similarly to [1], to determine the rotation carrying the largest subset of X to a subset of Y , all triplets from X and from Y are considered, and each pair of triplets contributes to a point in the rotation space. Assuming exact congruence between the largest matching subsets of X and Y , the rotation relating them gets the largest number of contributions, and the problem is reduced to locating a maximum of the contributions.

This 'triplet indexing' can be generalized to higher order procedures by employing n -tuples of vectors. To make such a generalization, one needs a formula calculating the rotation best matching large vector sets (and a clear understanding of what the "best matching" really means). Let $n \geq 3$, and let the rank of the involved matrices be equal to 3. In analogy to eq.(1) and

definition of $R'^{(3)}$, the rotation matrix can be obtained from

$$R'^{(n)} = \mathcal{O}([y_1 \ y_2 \ \dots \ y_n] [x_1 \ x_2 \ \dots \ x_n]^+) , \quad (2)$$

where the superscript $+$ denotes the generalized (Moore–Penrose) inverse. This solution is optimal in the sense that $R'^{(n)}$ is the special orthogonal matrix closest to the matrix $A = [y_1 \ y_2 \ \dots \ y_n] [x_1 \ x_2 \ \dots \ x_n]^+$ which in turn minimizes $\sum_{i=1}^n (y_i - Ax_i)^2$; cf. [8]. Less involved and more suitable is the solution given by

$$R^{(n)} = \mathcal{O}([y_1 \ y_2 \ \dots \ y_n] [x_1 \ x_2 \ \dots \ x_n]^T) ; \quad (3)$$

it is optimal in the sense of spherical regression, i.e., one can show that the above $R^{(n)}$ is the special orthogonal matrix minimizing the sum $\sum_{i=1}^n (y_i - R^{(n)}x_i)^2$.

In matching based on large n , additional vectors sharpen the criteria for the congruence of given subsets. On the other hand, using higher order n -tuples increases the computational costs. To avoid combinatorial explosion, n needs to be kept small. Moreover, numerical experiments show that with error affected data, higher order n -tuples do not really improve the quality of indexing; cf. [9]. This draws attention to indexing based on $n < 3$, i.e., on individual vectors ($n = 1$) or pairs of vectors ($n = 2$).

The procedure for accumulating contributions based on individual vectors ($n = 1$) was described in [4]. Given two vectors x_1 and y_1 in X and Y , respectively, we look for all rotations transforming x_1 on y_1 . Assuming that $x_1 \neq -y_1$, these rotations are represented by the matrices $R^{(1)}(\omega) = O(y_1, \omega) O(x_1 + y_1, \pi)$, and they constitute an ω -parameterized geodesic in the rotation space. Each pair from $X \times Y$ contributes to rotations located on one of these lines. As above, the rotation relating the largest matching subsets of X and Y gets the largest number of contributions, and again, the problem is reduced to locating a maximum of the contributions. A variant of this approach was implemented by Schmidt [10].

The unexplored case of $n = 2$ turns out to be particularly interesting. It is in a sense elemental among those providing discrete solutions. Eqs.(2–3) cannot be directly extended to get rotations matching 2-tuples. (When the rank of $[x_1 \ x_2 \ \dots \ x_n]$ is smaller than 3, the Moore–Penrose inverse gives A satisfying $y_i = Ax_i$ and minimizing $\|A\|^2$ [8], but $\mathcal{O}(A)$ is generally distant from the best rotation matrix carrying x_i on y_i . Also eq.(3) is inconvenient because of complications with calculating the special orthogonal matrix closest to a singular matrix.) The simplest way of circumventing this problem is to use eqs.(2–3) for $n = 3$ with the third linearly independent vector, say x , formed from x_1, x_2 , and a corresponding vector y analogously constructed from y_1, y_2 . The simplest choice is to use the cross products $x = x_1 \times x_2$ and $y = y_1 \times y_2$; with these vectors, the matrices $[x_1 \ x_2 \ x]^T$ and $[x_1 \ x_2 \ x]^{-1}$ are generally different, but eqs. (2) and (3) lead to the same result

$$R^{(2)} = \mathcal{O}([y_1 \ y_2 \ y][x_1 \ x_2 \ x]^T) = \mathcal{O}([y_1 \ y_2 \ y][x_1 \ x_2 \ x]^{-1}) = [r_1^y \ r_2^y \ r_3^y][r_1^x \ r_2^x \ r_3^x]^T, \quad (4)$$

where r_1^x, r_2^x and r_3^x represent normalized versions of $x, x_1 + x_2$ and $x_1 - x_2$, respectively, and the r_i^y vectors are defined in analogous way. The essential point is that $R^{(2)}$ given by eq.(4) also transforms the pair x_1, x_2 to the position closest to that of y_1, y_2 in the sense of spherical regression. Moreover, with the last part of eq.(4), the computation of this optimal rotation matrix involves only elementary steps.

As in all accumulation-based methods, at the end, one needs to determine the locations of maxima in the accumulator space. Since the match between vectors is only approximate, some tolerance must be allowed. A straightforward way to evaluate the contributions is by partitioning the rotation space into equivolume bins of size linked to the accuracy of experimental data and the resolution of resulting orientations. The center of the bin with the largest accumulation

is the sought rotation matching the largest subsets of X and Y . With this approach, extra measures are needed to take account of contributions distributed in neighboring bins.

Instead of binning, cluster analysis can be implemented. One of the methods is to use a list of potential solutions: Every new rotation obtained from eqs.(2–4) is compared to already saved potential solutions. If the rotation deviates from a given solution by a misorientation angle smaller than a threshold, a ranking number of that solution is increased, and the solution is corrected by taking a weighted average [11] of the solution and the new rotation. Otherwise, the rotation is appended to the list as a new potential solution. Clearly, this approach is more suitable for resolving the discrete cases ($n \geq 2$) than the continuous one ($n = 1$).

With $n \geq 2$, some of the matchings can be omitted by assuming that the vectors x_i can match y_i only if the angles between vectors of the n -tuples differ by less than a threshold; if not, the n -tuples are rejected as a possible match. (This is particularly simple when $n = 2$: the vectors x_1 and x_2 can match y_1 and y_2 only if the angle between x_1 and x_2 is close to that between y_1 and y_2 .) This approach links the indexing methods described above to methods in which measured angles between scattering vectors are compared to angles between reciprocal lattice vectors with potential solutions scored according to the number of good matches. Thus, in essence, these methods also use a form of accumulation, but the accumulator space and the way of contributing are not explicitly identified.

3. Final remarks

An inspection of the field (including ab initio indexing) shows that robust solutions to the indexing problem are based on various forms of accumulation. They differ by the nature of contributions, the parameter space, and the methods of collecting and counting the contributions. Depending on demands, one may use various combinations of these forms; in particular, to improve reliability of indexing, one may apply multiple contributions of different types and various methods of counting the contributions. Moreover, as the orientation determination via accumulation can be seen as the generalized Hough transform, its reliability can also be improved by adapting known enhancements of that transform [12].

For brevity, we considered only the constellation problem (LCPS problem limited to rotations), with all vectors having the same magnitude, but it is worth noting that the described procedures can be relatively easily generalized to matching vectors with arbitrary magnitudes.

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