ARCHIVES OF METALLURGY AND MATERIALS
Volume 50 2005 Issue 1

A. MORAWIEC*, M. BIEDA*

ON ALGORITHMS FOR INDEXING OF K-LINE DIFRACTION PATTERNS[1)]

ALGORYTMY DO INDEKSOWANIA OBRAZÓW DYFRAKCYJNYCH KIKUCHI'EGO

Thanks to the progress in computer control of electron microscopes and in microscope cameras there is a strong trend towards automatic analysis of electron diffraction patterns. Such analysis allowed for creation of fully automatic orientation imaging — an important technique of investigation of polycrystalline materials. Two essential parts of the analysis are the indexing of the patterns and the determination of orientations. We are particularly concerned with systems using transmission electron microscopy (TEM) and Kikuchi patterns; with small solid angle covered by these patterns, indexing is a challenging problem. The indexing procedures are expected to be fast and reliable even in the presence of experimental errors in geometric parameters of the patterns. The first step towards optimal indexing is to formalize the problem. It is shown that indexing can be reduced to matching two sets of points: "Two point sets $\mathcal{G}$ and $\mathcal{H}$ are given. Determine a rotation carrying the largest subset of $\mathcal{G}$ to a position approximating a subset of H". Some new algorithms solving this problem are proposed. They are based on the generalized Hough transform with the rotation space as the parameter space. In the simplest case, a pair of points - one point from each set — contributes to rotations along a curve in the rotation space. After contributions are made by all pairs, the cell in the rotation space which received the largest number of contributions is considered to represent the orientation of the crystallite. Once the orientation is known, one can easily assign Miller indices to reflections.

Keywords: Transmission electron microscopy; Diffraction; Pattern matching; Generalized Hough transform.

Dzięki postępowi w komputerowym sterowaniu mikroskopami elektronowymi i unowocześnieniu kamer do tych mikroskopów istnieje silna tendencja do rozwijania automatycznej analizy elektronowych obrazów dyfrakcyjnych. Taka analiza pozwala na tworzenie w pełni automatycznych map orientacji — ważnej techniki badania materiałów polikrystalicznych. Dwiema istotnymi kwestiami w tej analizie jest indeksowanie obrazów dyfrakcyjnych i wyznaczanie orientacji. Szczególnym wyzwaniem jest indeksowanie obrazów dyfrakcyjnych Kikuchi'ego powstałych w transmisyjnym mikroskopie elektronowym. Procedury in-

* INSTYTUT METALURGII I INŻYNIERII MATERIAŁOWEJ IM. A. KRUPKOWSKIEGO,PAN, 30-059 KRAKÓW, UL. REYMONTA 25
[1)] invited lecture

deksujące powinny być szybkie i skuteczne nawet w przypadku błędów eksperymentalnych wpływających na parametry geometryczne tych obrazów. Formalne ujęcie problemu jest pierwszym krokiem do zoptymalizowania procedur indeksujących. Pokazano, że problem może zostać sprowadzony do porównania dwóch zbiorów punktów: „Dane są dwa zbiory G i H. Zadaniem jest wyznaczenie obrotu, który przekształca największy podzbiór zbioru G w podzbiór zbioru H z pewnym błędem aproksymacji". Zaproponowano nowe algorytmy rozwiązujące ten problem. Bazują one na uogólnionej transformacie Hougha z przestrzenią obrotów jako przestrzenią parametrów. W najprostszym przpadku, para punktów — po jednym z każdego zbioru — głosuje na obroty położone wzdłuż krzywej w przestrzeni obrotów. Po tym jak każda para „oddała" swój głos, przyjmuje się, że komórka w przestrzeni obrotów, która uzyskała największą liczbę głosów reprezentuje orientację krystalitu. Jeżeli znana jest orientacja łatwo można przyporządkować refleksom indeksy Millera.

1. Introduction

One of the important aspects of the investigation of polycrystalline materials is the determination of the topography of crystallites. This can be done by measurements of local orientations. There are a number of methods to determine crystal orientations from electron diffraction patterns. Particularly suitable for that purpose is the family of the so-called K-line diffraction patterns [1] which comprises: X-ray Kossel patterns, Kikuchi patterns, convergent beam electron diffraction (CBED) patterns, electron backscattering diffraction (EBSD) patterns and channeling patterns.

'Manual' analysis of diffraction patterns is time consuming and prone to errors. Therefore, there is a trend towards fully automatic procedures. Such procedures allow for orientation mapping. The orientation mapping techniques were originated in mid-eighties using Kossel patterns [2]. Nowadays, orientation maps are created based on a step-by-step beam scan on computer controlled electron microscopes equipped with digital cameras. At each step, a diffraction pattern is acquired and indexed, and an orientation is determined. The automatically generated orientation maps complement conventional contrast images with quantitative information on grain orientations. Particularly successful are orientation mapping systems using scanning electron microscopy (SEM) and EBSD patterns. EBSD/SEM mapping is already a well established technique of characterization of polycrystalline materials [3, 4].

Here, we are focused on indexing applied to orientation mapping based on transmission electron microscopy (TEM) and Kikuchi patterns [5]. The approach is similar to that of SEM/EBSD systems. The resulting maps have relatively good spatial resolution and good accuracy in relative orientations. These two features are important for ultra-fine microstructure and sub-grain characterization. On the other hand, in the case of TEM, indexing is relatively complex because large Milller indices of the diffracting planes must be taken into account. The TEM orientation mapping provides results complementary to those of SEM/EBSD systems.

It must be mentioned that TEM orientation maps can also be obtained by the so-called 'Dark Field Scanning' with orientation at a given point determined from intensities corresponding to various incident beam directions [6]. Moreover, a mapping

system employing selected area diffraction (spot) patterns and template matching has been created recently [7]. These are time efficient approaches, which do not employ indexing procedures of the type described here. However, in both cases, the orientation accuracy is relatively low.

The standard analysis of *K*-line diffraction patterns is performed in two stages: line detection and indexing (Fig. 1). (In the case of Kossel patterns, the first stage is the detection of conics.) Line detection is done either 'manually' or by using automatic procedures. Although, automatic line detection is not a subject of this paper, we would like to note that for better performance of line detection algorithms, specific features of diffraction patterns must be taken into account, and therefore, dedicated programs are written for that purpose; to our knowledge, all currently maintained systems use the Hough transform, which is a robust, effective and easy to understand method based on an accumulation in the parameter space. A Kikuchi diffraction pattern shows deficit and excess lines. Therefore, separate lines are detected, and then lines with similar inclinations (i.e., nearly parallel) are grouped together to create line pairs. In the case of EBSP, large consolidation of images is used and usually diffraction bands are detected. Locations of line pairs or bands are used as an input for indexing.

Generally, indexing or assigning Miller indices to diffraction lines or bands can be performed without knowing the crystal structure or its orientation. Here, the term 'indexing' is used in a narrow sense, i.e., it is assumed that the structure of the material is known. Thus, it is also known, which reflections are forbidden and which are detectable. In principle, intensities of lines or bands can be used. In practice, it is sufficient to index diffraction patterns based on the geometry without using intensities of particular reflections, i.e., only the "on-off" case plays a role.

K-line diffraction patterns of different types have the same diffraction geometry, and the same principles are applicable for indexing in all these cases. Differences lie in the already mentioned type of input data (bands, line pairs, single lines) and in the solid angle covered by the detector. That angle is related to the sample-to-detector distance (effective camera length) and is relatively small for patterns originating from TEM. Roughly, the smaller the acquisition angle, the higher index reflections must be taken into account, and this has an influence on the reliability of the indexing results.

Orientation mapping is the most obvious reason for development in automatic indexing. However, there are other situations, in which automatic indexing is very useful. In particular, this concerns cases in which there is interest in solving single patterns, like in residual strain determination or in analysis of a specific interface.

Indexing procedures are expected to be general (applicable to arbitrary crystal symmetries and structures), robust and fast. There are a number of different algorithms used for indexing [8–11]. All of them were created based on a 'trial and error' search for an approach that gives satisfactory results. On the other hand, the ideal situation would be to formalize the indexing problem and to index the patterns by an algorithm proven to be optimal. The goal of this paper is to present an unknown formal side of indexing. It will be shown that an approach similar to Hough transform can be used for solving the indexing problem. This new heuristic approach turns out to be

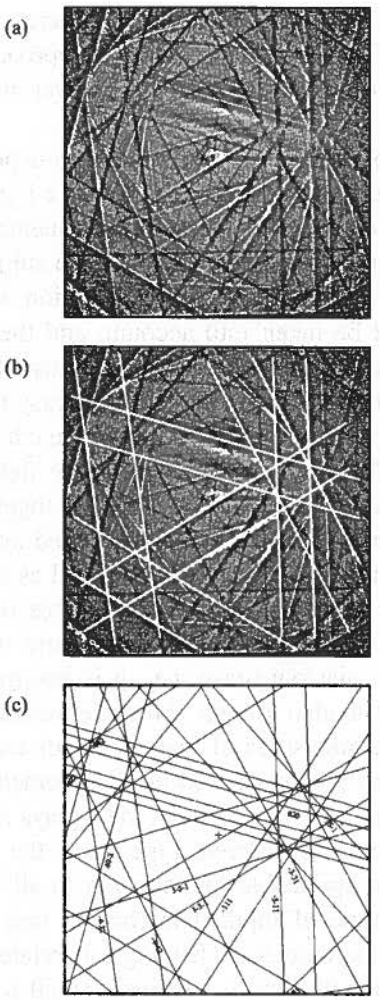

Fig. 1. Illustration of main stages of K-line patter analysis. The corrected K i k u c h i pattern (courtesy of E. Bouzy, Univ. De Metz) shown in (a) is subject to line detection (b). The detected lines are a basis for indexing (c)

a generalization of some existing indexing procedures and it allows for a perspective view on the indexing in general. It is also instructive because it explains indexing based on the well understood procedure of H o u g h transform.

2. Formal aspects of indexing and orientation determination

Generally, indexing is performed by matching geometric features of the diffraction pattern in the sample reference frame with the corresponding features obtained

from crystallographic data. More precisely, reciprocal lattice vectors acquired from an experimental pattern are matched with vectors calculated from crystallographic data.

It is convenient to represent the data in two Cartesian reference frames, one attached to the sample, the other one — to the crystal:

— For a given K i k u c h i pair, the coordinates of the reciprocal lattice vector $\boldsymbol{g}$ in the sample reference frame can be calculated directly from parameters of detected lines or bands based on the Kossel cone equation[1] $\boldsymbol{g} \cdot \boldsymbol{g} = \pm 2\boldsymbol{k} \cdot \boldsymbol{g}$, where $\boldsymbol{k}$ represents the wave vectors of reflected beam. See Fig. 2.

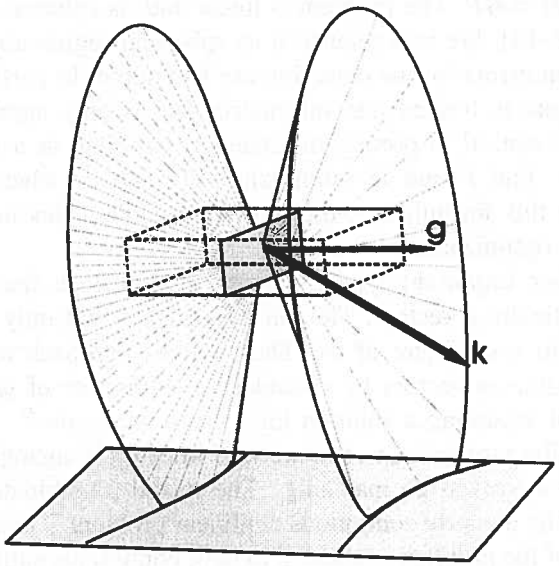

Fig. 2. Schematic illustration of K o s s e l cones and the geometry of K-line diffraction patterns

— In the crystal coordinate system, the Cartesian coordinates of the reciprocal lattice vector $\boldsymbol{h}$ corresponding to the reflecting plane $\boldsymbol{h}^*=(h\ k\ l)$ are given by $\boldsymbol{h} = A^{-1}(\boldsymbol{h}^*)^T$, where the (ij) element of A is the j-th Cartesian component of the i-th direct lattice basis vector.

For a given pattern, one has two figures: $\mathcal{G}$ — composed of all g vectors related to detected reflections, and $\mathcal{H}$ — composed of all $\boldsymbol{h}$ vectors related to potentially detectable reflections in the pattern. The indexing is done by matching $\boldsymbol{g}$ vectors with $\boldsymbol{h}$ vectors, or more precisely, by determining a subfigure of $\mathcal{H}$ which is congruent to $\mathcal{G}$. Let the matrices $\boldsymbol{G}$ and $\boldsymbol{H}$ be built of all available vectors $\boldsymbol{g}$ and $\boldsymbol{h}$, respectively, as matrix columns. Apart from experimental errors, there exists a rotation transforming vectors of $\mathcal{G}$ on certain vectors in $\mathcal{H}$. Thus, there exist a proper orthogonal matrix $\boldsymbol{O}$ such that

$$\boldsymbol{O} \cdot \boldsymbol{G} = \boldsymbol{H} \cdot \boldsymbol{P};$$

[1] The relationdhip follows directly from the Laue equation.

$\boldsymbol{P}$ is an unknown rectangular matrix with zero entries everywhere except the value of 1 at each entry (mn) such that the m-th $\boldsymbol{h}$ vector corresponds to the n-th $\boldsymbol{g}$ vector (i.e., there is exactly one '1' in each column). The matrix $\boldsymbol{P}$ represents the assignment (indexing) problem and $\boldsymbol{O}$ corresponds to the orientation determination problem.

Once $\boldsymbol{O}$ is known, it is straightforward to determine $\boldsymbol{P}$ by comparing columns of $\boldsymbol{OG}$ with $\boldsymbol{H}$. And vice versa, knowing $\boldsymbol{P}$, one can determine $\boldsymbol{O}$: Assuming that the assignment is known, there is a standard procedure for matching vectors; the issue is equivalent to the (Procrustes) problem of getting the 'best' orthogonal matrix $\boldsymbol{O}$ transforming $\boldsymbol{G}$ on $\boldsymbol{H'} = \boldsymbol{HP}$. The problem is linear and its solution has been described numerous times [12–16]. We will refer to it as spherical regression.

It is obvious that errors in line detection are inevitable. In particular, the accuracy of the line parameters is limited and the matrix $\boldsymbol{OG}$ is only approximately equal to $\boldsymbol{HP}$. Therefore, it is natural to portray the indexing problem as a modification of the Procrustes problem: find $\boldsymbol{P}$ and $\boldsymbol{O}$ minimizing $|\boldsymbol{HP}-\boldsymbol{OG}|^2$, where $|\cdot|$ denotes the Frobenius norm. In this formulation, the indexing problem lies in combinatorial $(\boldsymbol{P})$ and continuous $(\boldsymbol{O})$ optimization.

However, another important type of errors are spurious lines or bands. These errors lead to illegitimate g vectors. This, in turn, means that only a part of $\mathcal{G}$ can be actually congruent to a subfigure of $\mathcal{H}$. The simplest approach to this complication is to eliminate spurious g vectors by considering subfigures of $\mathcal{G}$, and to use some additional criteria of accepting a solution for a given subfigure.[2)]

For solving similar problems in computerized imaging Rangarajan, Chui and Bookstein [17] proposed a 'softassign matching'. The mixed (combinatorial + continuous) problem is replaced by a purely continuous nonlinear problem. The matrix representing combinatorial part of the problem is allowed to have continuous entries but its evolution in the optimization process is guided by additional constraints and barrier functions.

Allowing for spurious vectors is an integral part of a certain issue considered in computational geometry. The 'largest common point set' problem is usually formulated in terms of point sets and in a more general framework: Given two point sets $\mathcal{G}$ and $\mathcal{H}$ and a positive number ε determine the largest subset of $\mathcal{G}$ such that there is an isometry carrying $\mathcal{G}$ to a position in which each point of the subset is not further than ε from a point of $\mathcal{H}$ (e.g., [18]). There is a considerable interest in the 'largest common point set' problem because of its applications to determination of structural similarities in macromolecules and recognition of molecules. What matters here is that with the isometry being a proper rotation and points of $\mathcal{G}$ and $\mathcal{H}$ identified with their position vectors bound to the fixed center of rotation, the largest common point set problem is actually a mathematical formulation of the indexing problem. The term 'constellation problem' is sometimes used to describe point matching (e.g., [19]). However, it fits

[2)] Formally, $\boldsymbol{P}$ must be allowed to have some zero columns, and one needs to rewrite our basic equation as $\boldsymbol{OG'} = \boldsymbol{HP}$, where the matrix $\boldsymbol{P'}$ is like the identity matrix except that 1's on the diagonal of $\boldsymbol{P'}$ are allowed to be replaced by zeros if they correspond to spurious line paris or bands. The optimization procedure needs a modification because one must minimize the number of zero columns in $\boldsymbol{P}$ and $\boldsymbol{P'}$.

better the limited case with isometric transformations limited to rotations, and we use it in this narrow sense.

3. Indexing as the generalized Hough transform

There is an approach to the indexing/orientation determination problem, which provides a family of solutions and sheds some light on indexing in general. The methods can be seen as heuristic solutions to the constellation problem. They are based on rating orientations by making an accumulation in the orientation space.

Accumulation along curves

Let $\underline{g}$ and $\underline{h}$ denote normalized vectors $\boldsymbol{g}$ and $\boldsymbol{h}$, i.e., $\underline{g} = \boldsymbol{g} / |g|$ and $\underline{h} = \boldsymbol{h} / |\boldsymbol{h}|$. Given $\boldsymbol{g}$ and $\boldsymbol{h}$, the accumulation is made at all rotations transforming $\underline{g}$ on $\underline{h}$. There is a relatively easy way to calculate the parameters of such rotations. Let $\boldsymbol{R}(\boldsymbol{x}, \omega)$ be the special orthogonal matrix of the rotation by the angle ω about the axis determined by $\boldsymbol{x}$. It can be shown that for $\underline{g} + \underline{h} \neq \boldsymbol{0}$, the matrix

$$\boldsymbol{O}(\omega) = \boldsymbol{R}(\underline{g} + \underline{h}, \pi)\boldsymbol{R}(\boldsymbol{g}, \omega),$$

carries $\underline{g}$ on $\underline{h}$, i.e. $\boldsymbol{O}(\omega)\underline{g} = \underline{h}$; see, e.g., [20]. For ω given by the numbers between 0 and 2π, the rotations corresponding to $\boldsymbol{O}(\omega)$ cover a closed curve in the parameter space. Rotations on this curve are potential solutions to the indexing problem. If the considered $\boldsymbol{h}$ actually matches the considered $\boldsymbol{g}$, one of these rotations is a true solution. In reality, the $\boldsymbol{g}$ vector may correspond to a different vector of $\mathcal{H}$, and this means that all other vectors of this set must be taken into account. Ultimately, all pairs of vectors — one vector from $\mathcal{G}$ and one from $\mathcal{H}$ — are used to make the accumulations along corresponding curves in the rotation space.

Congruent subsets of $\mathcal{G}$ and $\mathcal{H}$ lead to accumulation along curves intersecting at one point corresponding to the rotation caring one subset onto the other one. Since we are looking for the largest matching subsets of $\mathcal{G}$ and $\mathcal{H}$, it is enough to locate the maximum in the accumulator space; the maximum corresponds to the parameters of the sought rotation. This approach to orientation determination and indexing can be seen as a form of the generalized Hough transform.

The above argumentation is based on the assumption of an exact congruency between the largest matching subsets of $\mathcal{G}$ and $\mathcal{H}$. When the match is only approximate, the curves do not intersect at a point but are located at some distances from the optimal rotation. This can be taken into account by replacing the sharp curves by smooth distributions. Von Mises-Fisher distribution is suitable for this purpose [21].

A simpler way of locating the maximum is to partition the accumulator space into cells, and to take the center of the cell with the largest accumulation as the matching rotation. The resolution of the method is linked to the cell size, and the latter must be related to the level of experimental errors. The partitioning of the parameter space is

a bit complicated because the (rotation) space is curved and cannot be parameterized without some singularities. Moreover, the accumulation must be scaled by the 'invariant volume' of the cells. Therefore, some parameterizations (e.g., the so-called isochoric parameters [22]) turn out to be convenient while other parameter sets (e.g., Euler angles, which are affected by 'gimbal lock') are not.

Since normalized vectors $\underline{g}$ and $\underline{h}$ were used in the above considerations, $\boldsymbol{g}$ and $\boldsymbol{h}$ with considerably different magnitudes are taken into account as a possible match. This can be easily avoided: Knowing the bandwidth or a distance between a pair of Kikuchi lines, one can estimate the magnitudes of $\boldsymbol{g}$ vectors, and the magnitudes of $\boldsymbol{h}$ vectors are directly available. If the difference in magnitudes is beyond certain threshold, the pair $\boldsymbol{g}$ and $\boldsymbol{h}$ may be rejected as a possible match. For many pairs, this rejection step allows for skipping the accumulation in the parameter space.

In the above considerations, it was assumed that $\underline{g} \neq -\underline{h}$, i.e., there was no accumulation at some rotations by π. Frequently, such rotations can be excluded as possible solutions based on some additional arguments. (For instance, the largest rotation angle necessary to describe all orientations of a cubic crystal is 62.8°.) If there are no such arguments, one can match $\mathcal{H}$ to $\mathcal{G}$ transformed by a known rotation so the cases with $\underline{g} \approx -\underline{h}$ are avoided.

Matching pairs of vectors

Now, let us take a step forward. Instead of using one vector from each set, one may take a pair (or doublet) and determine a rotation carrying a doublet from $\mathcal{G}$ on a doublet from $\mathcal{H}$. This makes sense only if the doublets are approximately congruent. Congruency can be checked by comparing vector magnitudes and the angle between the vectors. If the doublets differ too much, they are not accepted as a possible match; otherwise, accumulation is made in the rotation space at the rotation determined by the fore mentioned spherical regression. This is again a form of the generalized Hough transform. This time, the accumulation is made not along curves but at points of the accumulator space. After considering all different doublets from $\mathcal{G}$ and $\mathcal{H}$, a solution of the indexing problem is obtained by locating the maximum in the accumulator space. As in the previous case, this can be done by partitioning the parameter space or by using smooth (von Mises-Fisher) distributions.

A considerably more convenient alternative approach is to create a list of potential solutions. A rotation determined from two doublets is appended to the list only if it differs by a threshold from each of the already saved solutions. If the rotation is close to one of the solutions, the accumulation ascribed to that solution is increased, and the solution is corrected by taking the weighted average [23] of the solution and the rotation.

Higher order procedures

Two doublets already determine a point in the rotation space. Thus, adding new vectors to such doublets and using triplets, quadruplets (generally, n-tuples) can only sharpen criteria for the congruence of the considered subsets. The procedures of order one and

two, which were described above, are in a sense elemental in comparison to higher order procedures involving n-tuples (with $n > 2$).

Such higher order procedures have been already applied to indexing. A third order 'voting' has been used for indexing diffraction patterns in one of the EBSD systems [8]. Moreover, there is a relation between some of the strategies used for indexing K i k u c h i patterns [9] and the approach with highest possible order n equal to the number of vectors in $\mathcal{G}$; in this case, one begins with all determined g vectors and uses the rejection step to reach the solution.

It is worth noting that the reliability of results depends on the order n. For instance, we have compared reliability of the third and the fourth order procedures by applying them to simulated Kikuchi patterns. The former turned out to be better. This indicates that it might be even better to use the second order. It is planned to verify this indication.

4. Final remarks

Automatic indexing of K-line diffraction patterns is essential for further development of local texture analysis. It is believed that there is a room for improvement of the reliability of the existing indexing procedures. This is particularly important in the cases of low symmetry materials, and poor quality patterns. It is proposed to formalize the indexing problem and search for its optimal solution. As a possible approach, we suggest application of various forms of the generalized Hough transform. Some of them turn out to be already applied in existing systems but those of lowest order have not been tested yet.

One may speculate about future developments in automatic indexing. Within the framework described above, besides the verification of the applicability of the low order schemes, some other steps can be envisioned. E.g., the current path form a pattern to an orientation consists of the line or band detection and indexing. Since both steps are based on accumulation, one may consider skipping the intermediate stage of line detection and making the accumulation directly in the orientation space.

Moreover, applying template matching, analogous to that of R a u c h [7], to indexing of K-line patterns seems to be feasible but there are a number of concerns, which must be taken into account. First, K-line patterns are much more complex than spot patterns and their signal-to-noise ratio is much lower. Moreover, variability of K-line patterns with orientation is much stronger than that of spot patterns. On the other hand, the template matching may be appealing because the approach is conceptually very simple.

There is also an issue of indexing K-line diffraction patterns, in which only one of the lines of the pair can be detected and the other one is out of view. This is usually the case for K o s s e l and CBED patterns, and may occur for K i k u c h i patterns if they are collected with large camera lengths. There is no problem with indexing K o s s e l patterns because the curvature of conics allows for the determination of parameters of the diffracting plane. However, the case of K i k u c h i or CBED patterns is complex.

We are not aware of any automatic method of indexing directly such patterns from single lines.

REFERENCES

[1] J.M. Cowley, Diffraction Physics, North-Holland, Amsterdam (1981).
[2] Y. Inokuti, C. Maeda, Y. Ito, Metall. Trans. **A16**, 1613-1623 (1985).
[3] B.L. Adams, S.I. Wright, K. Kunze, Metall. Trans. **A24**, 819- 831 (1993).
[4] R.A. Schwarzer, Micron **28**, 249-265 (1997).
[5] J.J. Fundenberger, A. Morawiec, E. Bouzy, J.S. Lecomte, Ultramicroscopy **96**, 127-137 (2003).
[6] S.I. Wright, D.J. Dingley, In: Proc. EUROMAT **4**, 253-258 (1999).
[7] E. Rauch, This volume, (2005).
[8] S.I. Wright, J.Computer-Assisted Microsc. **5**, 207-221 (1993).
[9] A. Morawiec, J. Appl. Cryst. **32**, 788-798 (1999).
[10] S. Zaefferer, J. Appl. Cryst. **33**, 10-25 (2000).
[11] A. Morawiec, J.J. Fundenberger, E. Bouzy, J.S. Lecomte, J. Appl. Cryst. **35**, 287 (2002).
[12] J.K. MacKenzie, Acta Cryst. **10**, 61-62 (1957).
[13] G. Wahba, J.L. Farrell, J.C. Stuelpnagel, SIAM Rev. **8**, 384- 386 (1966).
[14] W. Kabsch, Acta Cryst. **A32**, 922-923 (1976).
[15] W. Kabsch, Acta Cryst. **A34**, 827-828 (1978).
[16] M.A. Stephens, Biometrika **66**, 41-48 (1979).
[17] A. Rangarajan, H. Chui, F.L. Bookstein, In: Duncan, J., Gindi, G. (Eds.), Information Processing in Medical Imaging, Springer, Berlin, pp.29-42 (1997).
[18] C. Ambühl, S. Chakraborty, B. Gärtner, In: ESA, Lecture Notes in Computer Science, Vol. 1879, Springer, Berlin, pp.52-64 (2000).
[19] D.E. Cardoze, L.J. Schulman, In: Proc. 39th Annual Symposium on Foundations of Computer Science, pp.156-165 (1998).
[20] A. Morawiec, Orientations and Rotations, Springer, Berlin (2004).
[21] M.J. Prentice, J. R. Statist. Soc. **B48**, 214-222 (1986).
[22] F.C. Frank, Metall. Trans. **A19**, 403-408 (1988).
[23] M. Moakher, SIAM J. Matrix Anal. Appl. **24**, 1-16 (2002).

Received: 24 January 2005.