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A program for refinement of lattice parameters based on multiple convergent-beam electron diffraction patterns

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A package of computer programs for refinement of lattice parameters based on convergent-beam electron diffraction (CBED) patterns has been developed. The package is intended to facilitate the measurement of local elastic strains. The strain or lattice parameters are determined by matching experimental and simulated central disks of CBED patterns. The kinematical simulation is used in the primary fitting. In some cases, further refinement by means of dynamical simulation can be applied. User-specified strain components, camera lengths and voltage can be fitted. The software is not limited to any particular material or structure. It is capable of simultaneous matching of multiple patterns originating from the same sample location. The use of a number of different strategies allows for the verification of results and for checking their reliability. Operation of the software is controlled *via* a Windows user interface.

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1. Introduction

Convergent-beam electron diffraction (CBED) is one of the promising techniques of electron crystallography (Holmestad *et al.*, 1999). In particular, CBED patterns can be used for the refinement of lattice parameters. The parameters are calculated by matching experimental and simulated patterns. A standard approach is to match the geometry of high-order Laue zone (HOLZ) lines present in the central disk of CBED patterns. The achievable accuracy in the determination of lattice parameters is estimated to be about 0.01% (*e.g.* Armigliato *et al.*, 2005). The main advantage of the CBED method is its very good nanoscale spatial resolution. This allows the correlation of variations in lattice parameters with locations in microstructures. The key application of the method is the measurement of local elastic strains. There is particular interest in strains in microelectronic devices (*e.g.* Frabboni *et al.*, 1999; Armigliato *et al.*, 2001; Akaogi *et al.*, 2004; Toh *et al.*, 2005). The technique has also been used for the analysis of strain in superalloys (*e.g.* Li & Wahi, 1995; Völkl *et al.*, 1998*a*; Schulze & Feller-Kniepmeier, 2000), around isolated precipitates (Yonemura *et al.*, 1998) and near interfaces in metal matrix composites (Heinrich *et al.*, 2001). The applicability of the method to the determination of local strains is impaired to a certain extent by thin foil stress relaxation and difficulties with quantitative assessment of its influence.

With the matching of HOLZ line geometries, there is another difficulty which affects lattice parameter determination. A given HOLZ line pattern can be simulated with a number of different sets of lattice parameters (Maier *et al.*, 1996), and the inverse problem of lattice parameter determination is ill-conditioned (Morawiec, 2005). This ('ambiguity') issue is addressed by reducing the number of free parameters, or by matching simultaneously multiple patterns originating from the same location.

The advancement of the CBED-based method is also hindered by the presence of dynamical effects in the diffraction patterns. They affect the accuracy of the results. In principle, the effects can be taken into account by fitting experimental and dynamically simulated patterns. Such fitting, however, is challenging in practice due to long computation times. Moreover, it is necessary to input additional parameters (foil thickness, tilt angles). The most common approach is to assume the so-called 'effective voltage approximation' (Lin *et al.*, 1989; Tomokiyo *et al.*, 1994), in which the dynamical effects are accounted for by an alteration of voltage.

There are numerous computer programs for the simulation of CBED patterns (*e.g.* Spence & Zuo, 1992; Li, 2005). However, programs that determine lattice parameters (or strain) from the patterns belong to a different category. Besides the simulation capability, they must contain routines for matching the simulated and experimental patterns. Usually, presentations of such procedures are subsidiary parts of accounts on applications of the CBED technique (*e.g.* Krämer *et al.*, 2000), and only a few publications are focused on the software itself (Völkl *et al.*, 1998*b*; Paczkowski *et al.*, 2003). Worth attention is the system described by Armigliato *et al.* (2005), which, according to the paper, is capable of automatic strain mapping for Si samples in some specific orientations.

Generally, it is not easy to compare the programs for obtaining lattice parameters or strain from CBED patterns because the problem has been seen from various perspectives. In effect, procedures may be disparate, even if their main objectives are similar.[1] Additionally, it is not really clear how reliable particular programs are. In most papers on the subject, a computational procedure is presented and then applied to a specific problem, without convincing

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[1] Take for instance procedures for strain determination; they could be limited to the calculation of the strain tensor components with the assumption of plane stress conditions (*e.g.* Li *et al.*, 1998), or the plane strain approximation (*e.g.* Toda, Ikarashi & Ono, 2000), or some other selected components could be determined (*e.g.* Toh *et al.*, 2005).

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tests confirming its reliability. This approach disappoints because there is a straightforward way of performing such tests by running a program on simulated patterns for which the right answers are known. Moreover, we are not aware of any program for CBED-based lattice-parameter determination available for an independent evaluation.

This communication introduces a new package of programs, called *TEMStrain*, intended to facilitate the CBED-based refinement process. This paper presents the capabilities of the package, implemented procedures of refinement, and the method used to test the software.

2. Main features of the program

Briefly, *TEMStrain* is a Windows application that allows the simultaneous matching of multiple (up to ten) patterns. It is 'general', *i.e.* it is not limited to any particular material or structure. The software is capable of semi-automatic detection and indexing of HOLZ lines. It allows for fitting user-specified strain components, camera lengths and voltage. Besides standard strategies (based on distances between intersections of HOLZ lines), the program uses other schemes based directly on the analytic equation of the lines. The software is capable of dynamical simulation and refinement of parameters by matching experimental and dynamically simulated patterns. Last but not least, the program has a user-friendly interface (Fig. 1). Below, the most essential features and functions of *TEMStrain* are described in more detail.

2.1. Input and output

The program requires diffraction patterns in the form of 512 × 512 pixel 8-bit bitmap files. Other mandatory input data are reference lattice parameters, the approximate orientation of each pattern, approximate camera lengths (one per pattern), and voltage. Additionally, in some cases, foil thickness and tilt angles must be entered. Since in its general form the optimization problem of HOLZ line fitting is ill-conditioned (and the final outcome of the optimization process may depend on the starting values and the limits on optimization parameters), all initial (reference) values should be as accurate as possible, and parameter bounds should be narrow.

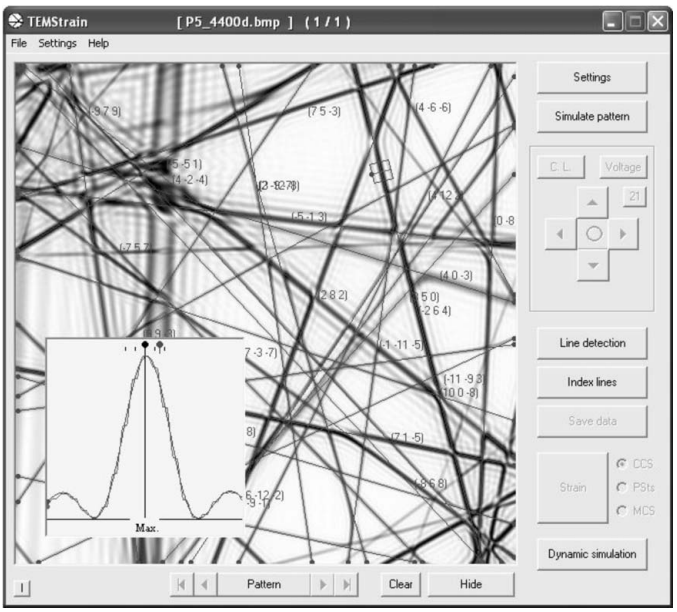

Figure 1
The main window of *TEMStrain*. The displayed pattern is used in the test described in §3. The picture in the lower left corner of the pattern shows a local profile of the indicated line; based on the profile, the line can be dragged to a proper place.

Relative deviations from reference values of lattice parameters, orientations, camera lengths, and voltages can be subject to fitting. If multiple patterns are used, the fitting concerns one set of lattice parameters (one strain tensor) and separate orientations, camera lengths, and voltages for each pattern. (In fitting of the voltage, a separate value ascribed to each pattern allows for considering 'effective voltages' of particular zones.) Most of the optimization parameters can also be fixed; this does not apply to orientation parameters.

In the output, one obtains new values of free optimization parameters. Strain can be obtained in three forms. The standard approach is to calculate (some or all) strain tensor components in a coordinate system linked to the crystal lattice. Another method is to calculate strain under the assumption of plane stress conditions. This option was developed to take into account thin-foil stress relaxation. In both the above cases, multiple patterns are allowed. Finally, with the ambiguity issue in mind, the strain components determinable from a given pattern can be calculated; they are given in the microscope coordinate system.

2.2. Orientation, camera length and voltage

To alleviate dynamical effects, it is recommended to stay away from low-index zone axes. The software allows for arbitrary sample orientations. Since the patterns suitable for the refinement are recorded with large camera lengths, relatively good approximations of orientations are needed. High precision in orientations is crucial for indexing. In practice, we determine orientations fully automatically using the *EP* package (Fundenberger *et al.*, 2003) and patterns recorded at smaller camera lengths; then the orientations are fine-tuned manually. Camera lengths and voltage can also be adjusted manually. The voltage must be pre-calibrated using a reference sample because, within the kinematical approximation, a change of the radiation wavelength from λ to $(1 - \varepsilon)\lambda$ has the same effect on the geometry of HOLZ lines as the isotropic strain, $\varepsilon \times$ (identity matrix) (Morawiec, 2006).

2.3. Line detection and indexing

HOLZ lines in a CBED pattern can be marked manually using the computer mouse. In addition, the program allows the automatic detection of lines. The procedure for line detection is based on the Hough transform with the 'backmapping' of Gerig & Klein (1986). Moreover, the program performs an additional local search for a precise determination of peaks in the line parameter space (*cf* Krämer & Mayer, 1999). Despite that, with the automatic detection, the precision in location of some lines may be unsatisfactory. Therefore, human inspection is needed. Correction can be made using a tool that displays local profiles of intensities in directions perpendicular to HOLZ lines (Fig. 1).

The indexing procedure (ascribing Miller indices to lines marking HOLZ reflections) relies on the known orientations. In order to index a given marking line, say L, the program performs a search through reflections in a kinematically simulated diagram. If there is a reflection with the simulated line closer to L than a user-specified limit (and it is the closest of such simulated lines), then the Miller indices of this reflection are ascribed to L.

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Table 1
Results of the example test for particular strategies.

The 'true values' were used for dynamical simulation of the pattern. The fitting was initialized with the 'starting values'. The results are in the column of 'recalculated values'. The number [*n*] indicates that the corresponding starting value was a result of the preceding calculation numbered *n*. Lattice parameters are given in the form $(a, b, c / \alpha, \beta, \gamma)$ with *a*, *b* and *c* in Å, and α, β and γ in degrees. An extra insignificant digit is shown for better visualization of differences between results of particular approaches. Differences between variants of the strategies were negligible.

		Starting values	Recalculated values	True values
Voltage calibration; lattice parameters assumed to be known				
1	Strategy 1			
	Voltage	200.00 kV	199.22 kV	199.00 kV
	Camera length	1150.0 mm	1163.4 mm	1160.0 mm
2	Strategy 2			
	Voltage	200.00 kV	199.20 kV	199.00 kV
	Camera length	1150.0 mm	1163.7 mm	1160.0 mm
3	'Dynamical' refinement			
	Voltage	200.00 kV	199.00 kV	199.00 kV
	Camera length	1150.0 mm	1160.2 mm	1160.0 mm
Lattice-parameter determination; plane stress case				
4	Strategy 1			
	Voltage [1]	Fixed at 199.22 kV		199.00 kV
	Lattice parameters	$\begin{pmatrix}4.0050, 4.0050, 4.0700\\90.000, 90.000, 90.000\end{pmatrix}$	$\begin{pmatrix}4.0000, 4.0128, 4.0674\\89.970, 89.931, 89.954\end{pmatrix}$	$\begin{pmatrix}3.9999, 4.0132, 4.0669\\89.976, 89.924, 89.939\end{pmatrix}$
	Camera length [1]	1163.4 mm	1163.4 mm	1160.0 mm
5	Strategy 2			
	Voltage [2]	Fixed at 199.20 kV		199.00 kV
	Lattice parameters	$\begin{pmatrix}4.0050, 4.0050, 4.0700\\90.000, 90.000, 90.000\end{pmatrix}$	$\begin{pmatrix}3.9997, 4.0132, 4.0672\\89.970, 89.925, 89.950\end{pmatrix}$	$\begin{pmatrix}3.9999, 4.0132, 4.0669\\89.976, 89.924, 89.939\end{pmatrix}$
	Camera length [2]	1163.7 mm	1164.2 mm	1160.0 mm
6	'Dynamical' refinement			
	Voltage [3]	Fixed at 199.00 kV		199.00 kV
	Lattice parameters [4]	$\begin{pmatrix}4.0000, 4.0128, 4.0674\\89.970, 89.931, 89.954\end{pmatrix}$	$\begin{pmatrix}4.0001, 4.0132, 4.0670\\89.974, 89.930, 89.942\end{pmatrix}$	$\begin{pmatrix}3.9999, 4.0132, 4.0669\\89.976, 89.924, 89.939\end{pmatrix}$
	Camera length [4]	1163.4 mm	1163.4 mm	1160.0 mm

2.4. Pattern simulation

The main procedures of *TEMStrain* rely on the geometry of the HOLZ lines. For calculating locations of the lines, the program essentially makes use of what Ewald (1969) called 'geometric theory of diffraction'. Kinematical theory is needed only to decide whether a given line should be taken into account or not. For this purpose, structure factors are computed using the table of Waasmaier & Kirfel (1995), for X-ray relativistic form factors, and the Mott formula (*e.g.* Doyle & Cowley, 1974). The Debye–Waller temperature factor is set to zero. The dynamical simulations are carried out using the Bloch wave scheme (*e.g.* Jones *et al.*, 1977). Fourier coefficients of the superposition of atomic potentials are calculated from the structure factors of the kinematical theory. Absorption is neglected.

2.5. Computational strategies

As already mentioned, the strain or lattice parameters are calculated by fitting features of experimental patterns to corresponding features of simulated patterns. The patterns are matched by minimization of pre-defined objective functions. For the actual optimization, we use *MINUIT* (version 94.1, CERN Program Library D506; see James, 1998).

The principal tasks of the program are performed by using kinematically simulated patterns. In this kinematical framework, essentially two variations of two different strategies are available. If the fitting converges, results of variants of a given strategy are usually similar. The first strategy is based on matching distances between intersections of HOLZ lines. One variant of this approach relies on matching the ratios of these distances to an average distance (Zuo, 1992); the ratios do not depend on camera lengths. In the second variant, the camera lengths are subject to fitting (Morawiec, 2006). In both cases, the number of intersection points taken into account depends on a user-controlled 'domain' of these points defined by the maximal distance of the points from the pattern centre, and by minimal and maximal intersection angles. The orientations are determined in a separate step by finding the 'the best rotation relating two sets of vectors' (see *e.g.* Morawiec, 2004, and references therein). The first set consists of wavevectors pointing to line intersections in the experimental pattern, and the second one contains the wavevectors pointing to corresponding intersections in patterns simulated with the updated lattice parameters (and camera lengths if the first variant is used).

The second strategy is the 'K-line equation-based scheme' (KLEBS) using directly the underlying algebraic equation of HOLZ lines (Morawiec, 2007). The parameters are determined by minimizing sums of squared deviations of experimentally determined left-hand sides of the equation from the exactly known right-hand sides. The orientation parameters are subject to fitting alongside other free parameters. A variant of this strategy uses a linearized form of the 'K-line equation'.

In order to improve the reliability of results, the above procedures should be combined. In the case of inconsistencies, one can try to resolve them by performing dynamical simulations for each of the potential results. The program calculates the (Spearman's) rank correlation coefficient between the experimental and the simulated pattern. A comparison of the coefficients may indicate the best result. Furthermore, after convincingly reliable results are obtained by the 'kinematical' fitting, a further refinement based on dynamically simulated patterns is possible. There is no matching of intensities in this case, but we use fitting of distances between short segments of selected HOLZ lines (*cf.* Zuo *et al.*, 1998; Kim *et al.*, 2004). However, the performance of the latter approach is less than spectacular. It can be attempted for high-quality experimental patterns and only if the starting values of the optimization parameters are already close to their true values. Tests indicate improvement of the results in cases with a small number of parameters. If that number is large, the fitting of dynamically simulated patterns frequently terminates in local minima without any significant improvement with respect to the outcome of the 'kinematical' approach. Moreover, such 'dynamical' refinement is a very slow process.[2] With multiple runs and multiple patterns, the execution times may easily become prohibitive. In this situation, the fitting based on dynamical simulation is recommended for a small number of parameters and only after the best possible job was done using the combination of strategies employing the kinematical approach.

The reliability of these procedures has been tested on simulated patterns. With the determination of all lattice parameters from a

[2] The time needed for dynamical simulation strongly depends on the number of beams involved and the resolution. Using a typical personal computer, a rough approximation or a small fragment of a pattern can be calculated within seconds, but a 'reasonably' good simulation of a full pattern may take hours or days. An optimization process with numerous parameters (lattice parameters, camera lengths, orientation parameters) must call such simulations many times (of the order of 10^3).

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single pattern, the optimization problem is ill-conditioned, and even if more patterns are used, the results may be erroneous. Our experience based on tests utilizing dynamically simulated patterns is that one needs to be accurate with input data and very scrupulous in marking the HOLZ lines. Even if the resulting parameters lead to an apparently perfect fit between the experimental and simulated patterns, one should remain sceptical and double-check each detail. Results need to be confirmed by applying a number of computational approaches (with various combinations of patterns, diverse sets of marking lines, changing starting and bounding values of parameters, *etc.*) and by visual inspection.

2.6. Platform, language, documentation and availability

The program has been developed and tested under the Windows XP operating system. The source code is written in Fortran 90 (key computations) and Visual Basic 6 (user interface). For documentation, HTML-formatted help for *TEMStrain* can be called from the program itself. An installation package (4.9 Mbyte .exe file) can be obtained by contacting LETAM or the author.

3. A simple example test

This section illustrates the performance of the program and demonstrates the method of testing it. Most tests were carried out on dynamically simulated patterns. Here, for brevity, we use the same pattern for two purposes. One is the calibration of voltage based on known lattice parameters. The other function is to determine the lattice parameters with the voltage assumed to be known.

The pattern shown in Fig. 1 was dynamically simulated for the ordered γ phase of TiAl crystal in the orientation $\sim [11\,\bar{7}\,15]$ under the assumption of plane stress conditions. The fitting was based on 30 marking lines with absolute values of Miller indices up to 12. Example results of the voltage calibration are listed in the upper part of Table 1. Using the voltage and camera length from that step, the lattice parameters were calculated in the plane stress approximation (*i.e.* three independent lattice-related parameters plus orientation and camera length are subject to fitting). Results are given in the lower part of Table 1. An attempt to obtain all six lattice parameters (*i.e.* without the plane stress assumption) failed because of the 'ambiguity problem'; it leads to large discrepancies between results of different strategies and their variants.

The results of Table 1 are in a sense representative but they were obtained for particular program settings (parameter bounds, domains of the intersection points, required tolerance of the objective function at the minimum, *etc.*). With different settings, the results would be slightly different (The dispersion of results for different starting conditions is of the same magnitude as for different methods.)

It must be emphasized that the test pattern was influenced by dynamical effects but free from other experimental 'distortions'. Analysis of real experimental patterns is not that easy, the optimization process does not converge so well, and, of course, a real study always has an element of uncertainty because true results are not known. The point of using *TEMStrain* is to 'bracket' reliably the range of acceptable lattice parameters.

4. Final remarks

Further interest in the determination of lattice parameters in the submicrometre scale, especially in terms of local elastic strains, is certain. Among a number of fields concerned with these issues, the most prominent area yearning for a reliable high-resolution strain determination method is microelectronics, with a variety of strain-related issues.[3] This interest is a driving force in the development of tools for local strain determination. Besides the CBED-based approach, X-ray microdiffraction (*e.g.* MacDowell *et al.*, 2001; Phillips *et al.*, 2004), micro-Raman spectroscopy (*e.g.*, DeWolf & Maes, 1998; Gustafson *et al.*, 2006) and electron backscatter diffraction (*e.g.* Keller *et al.*, 2004; Wilkinson *et al.*, 2006) have also been considered. The CBED technique is not free from difficulties, but has the important advantage of very good spatial resolution, beyond the reach of other methods. Therefore, its suitability for a reliable local lattice-parameter and strain determination will definitely be explored further. On the experimental side, high-quality CBED patterns are becoming more accessible due to the popularity of CCD cameras and a growing number of energy filters, but much remains to be done on the side of computations and interpretation. *TEMStrain* is a computational tool intended to facilitate CBED-based measurements. We actually see it as a benchmark for future, more comprehensive and more robust programs analyzing CBED patterns.

The package has some limitations. With its relative generality, allowing for diffraction patterns with diverse features, full automation of the lattice-parameter determination and strain mapping are not achievable, and refinement by *TEMStrain* is still a time-consuming and tedious process. Moreover, the program is applicable only to simple patterns, in which a HOLZ reflection is a line without splitting; the latter effect appears in the case of variations of lattice parameters or strain gradients (Clément *et al.*, 2004; Benedetti *et al.*, 2006). Finally, it must be stressed that testing was limited to simple structures with small unit cells. On the other hand, *TEMStrain* combines a number of useful capabilities, from easy adjustment of orientations, through straightforward detection and indexing of HOLZ lines, to direct accessibility of dynamically simulated patterns. The most important feature of this software is that the reliability of the results can be verified by comparing the output from a number of different strategies available in the package.

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[3] Local strain fields in electronic devices lead to the formation of crystal defects and ultimately to degraded functioning of circuit elements. On the other hand, in 'strained silicon technology', strain is used to affect the electronic band structure in order to increase carrier mobility in channel regions of devices; for a review see Lee *et al.* (2005).

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