TEM*Strain* – a software package for elastic strain determination from CBED patterns

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Abstract – A package of computer programs facilitating lattice parameter refinement or strain determination from convergent beam electron diffraction (CBED) patterns will be presented. The software works in conventional way, i.e., by matching experimental and simulated central disks of CBED patterns. It is capable of simultaneous matching of multiple patterns originating from the same sample location. The main fitting procedures rely on kinematical simulation but the program has also an option with dynamical simulation, and the correlation between experimental and dynamically simulated patterns can be calculated. The package contains a number of different computational strategies. This feature allows for verification of results.

Introduction

The convergent beam electron diffraction (CBED) is known to be applicable to refinement of lattice parameters or determination of elastic strains [1]. The parameters or strains are obtained by matching experimental and simulated central disks of CBED patterns. The most common approach is to match distances between intersections of high order Laue zone (HOLZ) lines present in the central disks. The technique has the important advantage of very good nanoscale spatial resolution, beyond the reach of other methods. Current developments in the field of high resolution strain measurements are driven by interests in strains in microelectronic devices.

However, the CBED technique is not free of difficulties. Because of the usage of thin foil, stress relaxation is expected, and a quantitative assessment of the relaxation is complicated. Moreover, the CBED patterns contain dynamical effects affecting the accuracy of results. Last not least, the results may be ambiguous; Maier *et al.* [2] made it clear that a solution obtained from a single pattern cannot be unique because a CBED pattern can be simulated by a number of different lattice parameters (or more formally, the problem of lattice parameter determination is ill–conditioned [3]).

The issue of "ambiguity" is usually addressed by reduction of the number of free parameters. Another approach is to use multiple experimental CBED patterns originating from the same location, and to match them simultaneously to patterns simulated with one set of lattice parameters.

TEM*Strain*

Dealing with multiple patterns corresponding to various foil orientations is complicated. Therefore a new package of computer programs called TEM*Strain* has been developed. It is intended to facilitate the analysis of CBED patterns and the calculation of strains. The package allows for simultaneous matching of up to ten patterns. It is not limited to any particular material or structure, and it works for arbitrary sample orientations. (In practice, orientations are determined automatically using another program and patterns with smaller camera lengths.) TEM*Strain* is capable of fitting user specified strain components, camera lengths and voltage. The package contains routines for dynamic simulation of diffraction patterns by the Bloch wave method [1].

TEM*Strain* is equipped with a Windows user interface (Fig. 1). HOLZ lines in a CBED pattern can be marked manually with a computer mouse, or they can be detected automatically. The automatic line detection uses the Hough transform and the so–called "backmapping" [4]. However, in the case of automatic line detection, a human verification of the outcome is needed. The indexing of patterns is based on the approximately known orientations.

Strains can be calculated in three different settings. The basic approach is to obtain strain tensor components in a Cartesian coordinate system linked to the crystal lattice. The second one is to get strain under the assumption of plane stress conditions. In both cases, multiple patterns can be used.

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Moreover, strain components determinable from a given pattern can be calculated from that pattern; they are calculated in the microscope coordinate system.

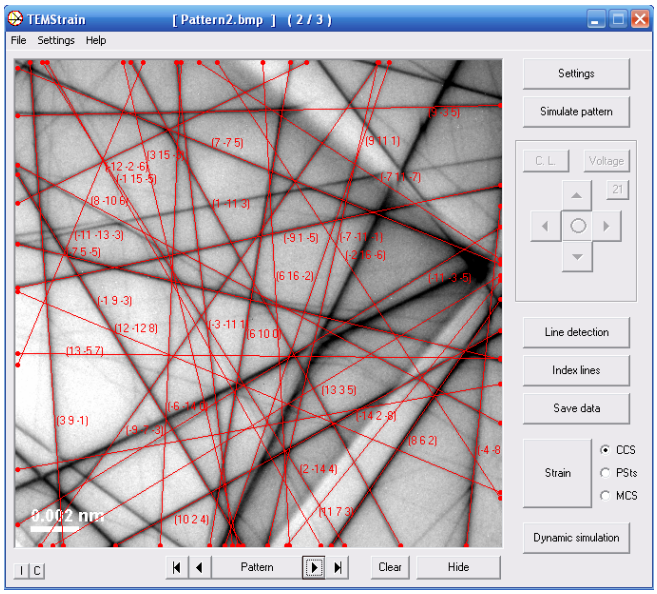

Fig. 1. The user interface of TEM*Strain*

A number of different computation methods are used for matching the patterns. The primary fitting procedures are based on kinematically simulated patterns with two main strategies. The first one matches distances between intersections of HOLZ lines or ratios of these distances [5]. The number of intersection points is controlled by a user who can change a "domain" of these points (bounded by the maximal distance of the points from the pattern center, and by minimal and maximal intersection angles). The second strategy is the "K–line equation based scheme" (KLEBS) [6]. It uses directly the algebraic equation of HOLZ lines. For better reliability of results, these strategies should be combined. Moreover, inconsistencies can be resolved by performing dynamical simulations and by comparing the (Spearman's) rank correlation coefficient between experimental and simulated patterns. A further refinement is possible by matching elements of experimental and dynamically simulated patterns. However, the performance of the latter approach is less than spectacular and the computing process is very slow.

TEM*Strain* has capabilities of a number of other programs for CBED based strain determination. The most important feature is that a user can verify reliability of results by comparing the output from different strategies available in the package. An installation package of the current version of TEM*Strain* is available on request.

References

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