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computer program abstracts

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EP – a program for determination of crystallite orientations from TEM Kikuchi and CBED diffraction patterns

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1. The crystallographic problem

Orientations of individual crystallites are of interest in many areas of research on polycrystalline materials (see *e.g.*, Kocks *et al.*, 1998). Analysis of Kikuchi patterns is one of the oldest and best established techniques of orientation determination. Convergent beam electron diffraction (CBED) patterns have the same geometry as Kikuchi patterns and can be used for determining orientations if a sufficient acquisition solid angle is available.

The program *EP* is a user interface linked with *KiKoCh* – an engine for pattern indexing and for determination of orientations. *EP* allows diffraction patterns to be loaded from bitmap files and the crystallite orientation to be obtained by marking lines with a mouse; in good quality patterns lines can be detected automatically. A similar system has been described recently by Zaefferer (2000).

2. Method of solution

The pattern indexing and orientation determination procedures contained in *KiKoCh* are based on principles described by Morawiec (1999). The user-provided data essential for the calculation are the microscope operating conditions and crystallographic data. The intensities of potential reflections are calculated based on the kinematic theory of diffraction. If an investigated material is not on a pre-existing list, information about atom locations in the unit cell must be provided.

The basic idea for the indexing procedure is to match the points of the reciprocal lattice calculated from the crystallographic data and the points of the lattice obtained from the diffraction pattern (*i.e.* the width and location of Kikuchi or CBED pairs). The orientation is obtained by calculating the rotation transforming the first set onto the second one in such a way that the discrepancy between the sets after the rotation takes its global minimum.

The automatic line detection is based on the Hough transform.

3. Software environment

EP is run using the Windows NT/00 operating systems. The user interface and structure-factor calculations are written in Visual Basic. *KiKoCh* and the routines for automatic line detection are written in Fortran 90 and have about 2500 and 500 lines of source code, respectively.

4. Hardware environment

The program is designed to work in a system with a digital camera attached to the microscope. However, numerous images obtained by scanning conventional films with Kikuchi patterns have also been analyzed. In a system with a digital camera and additional software for the control of pattern acquisition, *EP* is used at LETAM for the creation of high-resolution TEM orientation maps.

5. Program specification

EP could be used for indexing TEM Kikuchi or CBED patterns as well as for SEM electron backscattered diffraction (EBSD) patterns. However, it is more oriented towards TEM patterns. *EP* is robust in the sense that it is capable of handling poorly localized and spurious lines. In principle, the program is general: it can be applied to any crystal structure. However, only for relatively simple structures are the results immediate and can be obtained from a small number of lines. The use of 512 × 512 pixel images allows a relatively accurate localization of the lines which leads to precise relative orientation determination.

6. Documentation

A user manual is available at http://www.texture-anisotropy.org/Links/links.htm.

7. Availability

An educational version of the program with a limited set of patterns is available at http://www.texture-anisotropy.org/Links/links.htm. The complete system is distributed by LETAM.

References

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