KikSpot: software for simulation, analysis and indexing of TEM diffraction patterns, and for TEM-based orientation mapping

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Knowing individual crystal orientations is of a great interest in many areas of polycrystalline materials research. KikSpot is a software package for determination of crystal orientations using two types of TEM diffraction patterns: Kikuchi patterns and spot patterns. The package has the capability of handling automatically large collections of diffraction patterns, and this feature can be used to create orientation maps. The software also allows for analyzing individual patterns (in terms of indexing and orientation determination) in a fully automatic or semi-automatic way; the later refers to indexing and orientation determination preceded by manual detection of reflections.

KikSpot analyses the patterns based on user-provided information about microscope operating conditions (e.g., accelerating voltage, camera length) and crystallographic data for structures of investigated phases. (All crystallographic space groups and non-standard settings are allowed.) For both types of diffraction patterns, intensities of reflections are calculated using the kinematic approximation, but the methods of pattern indexing are different. Spot patterns are solved using the so-called “template matching” (Rauch & Dupuy, 2005). In this method, the crystal orientation is determined by comparing the experimental pattern to a set of simulated patterns (templates). The templates are calculated for a grid of orientations having user-defined resolution and limited by the crystal symmetry. The orientation corresponding to the simulated pattern with the highest correlation to the experimental pattern is considered to be a solution. In the case of Kikuchi patterns, the orientation is calculated from positions of Kikuchi lines (and both excess and deficient lines are used). The positions are obtained via Hough transform, the standard method of line detection in raster images. The detected lines are grouped into pairs based on their separations and locations, and each pair provides an experimental reciprocal lattice vector. These vectors are compared with the theoretical ones obtained from the known crystal structure, and the crystal orientation is calculated (Morawiec, 1999).

The package allows for some additional analyses of diffraction patterns (and this includes ring patterns) like measurement of *d*-spacings or inter-planar angles, and visualization of diffraction profiles coupled with phase identification. KikSpot also has a build-in crystallographic calculator.

The program runs under MS Windows family operating systems (XP, Vista, 7, 8.1) using .NET 4.0 Client Profile framework (freely available at microsoft.com).

References

Rauch, E.F., and Dupuy, L. (2005) Rapid diffraction patterns identification through template matching, Arch. Metall. Mater. 50, 87–99

Morawiec, A. (1999) Automatic orientation determination from Kikuchi patterns, J. Appl. Cryst. 32, 788–798