

New developments of computer-aided crystallographic analysis in transmission electron microscopy

Stefan Zaefferer

Fachbereich Materialwissenschaft, Technische Universität Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany. Correspondence e-mail: zaeffer@forzpub.tu-darmstadt.de

A new computer program for on-line crystallographic analysis in transmission electron microscopy (TEM) is presented. The program is based on the fast on-line determination of single-crystal orientations from Kikuchi and spot patterns. Spot patterns, which are particularly useful in the case of highly deformed metals, are analyzed by a new digital image processing procedure. This procedure improves the precision and ease of the orientation measurement. The program permits the on-line measurement of glide systems characterized by the Burgers vector and the crystallographic line direction of dislocations and their glide planes. The determination of twin systems, based on the misorientation calculation for any crystal structure, is included as well. The possibility of determining the foil thickness permits the complete crystallographic characterization of interfaces. Finally, the program facilitates the discrimination of phases and includes the fit of the lattice parameters a , b and c from diffraction patterns. The new procedures are described in detail. Application examples are given for all functions.

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1. Introduction

Transmission electron microscopy (TEM) is one of the most important tools for studies in materials science. It does not only allow the observation of the microstructure inside a material, but also the quantification of the character of microstructural elements, such as crystallographic symmetry of phases, the orientation of grains, Burgers vectors and the line direction of dislocations, twin systems, types of interfaces, and so on, by the analysis of diffraction patterns. Furthermore, TEM allows the determination of the chemical composition of very small regions in combination with energy dispersive X-ray analysis (EDX) or electron energy loss spectrometry (EELS).

Two research projects on the determination of deformation mechanisms in titanium alloys and on the recrystallization mechanisms in Fe–36%Ni have been carried out by the author; both required extensive crystallographic studies with TEM. Therefore, a universal computer program for the evaluation of electron diffraction patterns and their application to crystallographic problems was created (C programming language, DOS/Windows operating system), in order to facilitate and speed up the quantitative crystallographic work employing TEM in the normal diffraction mode. The program is based on the fast on-line determination of individual crystal orientations from electron diffraction patterns. It subsequently permits the on-line determination of Burgers vectors,

the type and glide plane of dislocations and the determination of twinning systems. It has also been applied to crystallographic analyses of phases and interfaces in TiAl intermetallic alloys and in Al_2O_3 .

The main features of the program are as follows.

(i) On-line orientation determination from Kikuchi and spot patterns of any crystal structure. The program uses new algorithms for the indexing and orientation calculation which allow Kikuchi and spot patterns to be treated for all crystal structures in a similar way. Even patterns containing only one zone axis and complicated spot patterns are included in one single procedure.

(ii) A digital image processing procedure is used to determine the intensity and positions of spots in a spot pattern from highly deformed materials. This considerably improves the accuracy and ease of orientation determinations from spot patterns.

(iii) Support for work in the diffraction mode of the microscope by simulating the crystal tilt in a double-tilt or rotation-tilt sample holder. These features are, together with the possibility to display the stereographic projection, particularly helpful for tilt experiments.

(iv) On-line determination of the Burgers vector and crystallographic line direction of dislocations. From these values, the dislocation type (screw, edge or mixed) and the slip plane are calculated.

(v) Calculation of misorientations between crystals of any crystal symmetry for the determination of twinning systems.

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