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Texture Analysis with MTEX – Free and Open Source Software Toolbox

F. Bachmann[1,a], R. Hielscher[2,b] and H. Schaeben[1,c]

[1]Geoscience Mathematics and Informatics, TU Bergakademie Freiberg, Germany

[2]Helmholtz Zentrum München, Neuherberg, Germany

[a]bachman1@mailserver.tu-freiberg.de, [b]ralf.hielscher@helmholtz-muenchen.de,
[c]helmut.schaeben@geo.tu-freiberg.de

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Abstract. The MATLAB™ toolbox MTEX provides a unique way to represent, analyse and interpret crystallographic preferred orientation, i.e. texture, based on integral ("pole figure") or individual orientation ("EBSD") measurements. In particular, MTEX comprises functions to import, analyse and visualize diffraction pole figure data as well as EBSD data, to estimate an orientation density function from either kind of data, to compute texture characteristics, to model orientation density functions in terms of model functions or Fourier coefficients, to simulate pole figure or EBSD data, to create publication ready plots, to write scripts for multiple use, and others. Thus MTEX is a versatile free and open-source software toolbox for texture analysis and modeling.

Introduction

The general concept of the toolbox as outlined in the abstract may be illustrated by Fig. 1.

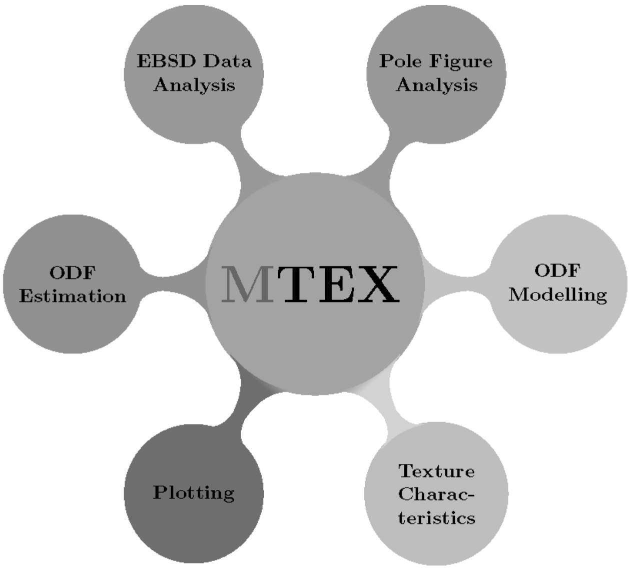

Figure 1. General concept of the MATLAB™ toolbox MTEX for texture analysis

MTEX features a novel unique method for the estimation of an orientation density function from diffraction pole figure intensities or from EBSD data classified by phase. An orientation density function is approximated by a non-negative linear combination of non-negative kernels, which are sufficiently well localized in spatial and frequency domain, more specifically with functions which are unimodal radially symmetric in spatial domain and with Fourier coefficients which vanish smoothly and sufficiently fast.

For the resolution of the inverse problem to determine an orientation density function from given experimental pole figure data this approach is justified by the general solution of the Darboux differential equation [1] governing the pole density function corresponding to an orientation density function. The pole density function has been recognized as mean of the totally geodesic Radon transfom of the orientation density function [2, 3], experimental pole figure data may be seen as its discrete values. Since the Radon transform is a linear integral transformation, it is applied to each term in the linear combination individually. Thus, experimental pole figure data are fitted by a non-negative linear combination of means of totally geodesic Radon transforms of the kernels. The best fit is determined as a solution of a constrained non-linear minimization problem and numerically found by a version of the conjugate gradient method.

The corresponding algorithm applies discretisation with radially symmetric basis functions centered at a given grid which may be irregular. The kernel itself is approximated by a finite Fourier series expansion. The series is finite either by truncation or by the special choice of the de la Vallée Poussin kernel [4 5, 6, 7], which is the default kernel of MTEX because of its unique mathematical properties. Then fast Fourier techniques for the sphere and the rotation group are applied to guarantee satisfying performance. For a comprehensive exposition of the MTEX approach to determine an orientation density function from experimental pole figure data the reader is referred to [8]. The mathematics MTEX is based on is presented in [7, 9]. The MTEX approach is especially well suited for sharp textures and high spatial resolution pole figures measured with respect to arbitrarily scattered specimen directions, e.g., with an area detector. Moreover, it allows for multi-scale representation of the orientation and the pole density function, respectively, cf. [10].

Given individual orientation measurements an orientation density function is determined by non-parametric kernel density estimation where the measurements are the centres of the kernels to be superposed [11]. Here, fast Fourier transform provides the numerics for fast summation of functions defined on the sphere or the rotation group.

Once an orientation density function has been determined with either kind of data, MTEX provides functions to compute various properties of the estimated orientation density function as Fourier C-coefficients, modal orientation, mean orientation, volume portions, texture index, entropy, etc., which are of interest. Choosing the Dirichlet kernel for this estimation, unbiased estimates of the Fourier C-coefficients up to any reasonably given finite order may be computed.

MTEX also features function to model an orientation density function and its corresponding pole density functions in terms of model functions including uniform, unimodal and fibre distributions or in terms of Fourier C-coefficients. An overwiev of workflows is displayed in Fig. 2.

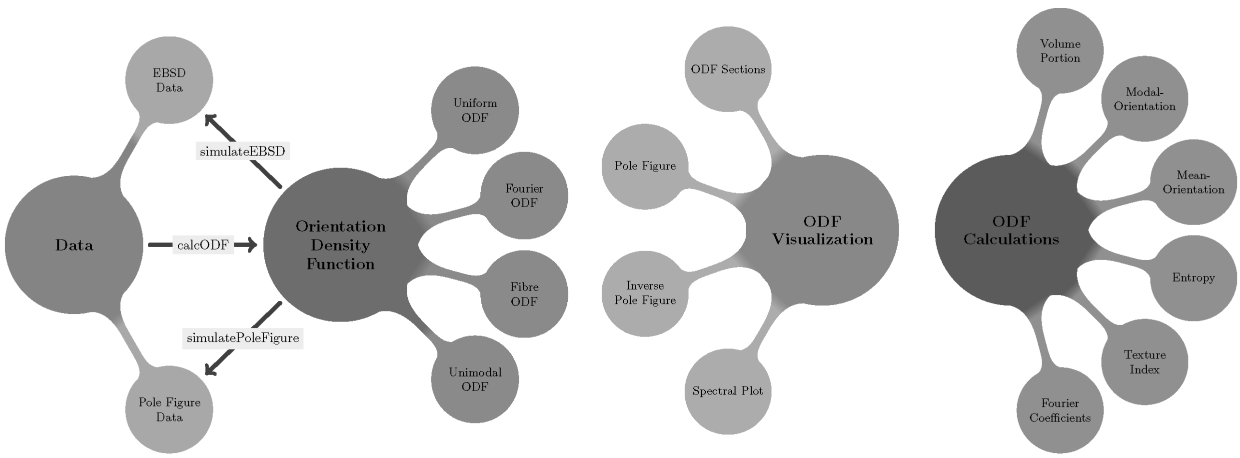

Figure 2. Workflows in MTEX

Functions and Features of MTEX in Greater Detail

Analysis and Visualization of Crystallographic Geometries. MTEX allows to define arbitrary crystal and specimen symmetries with arbitrary geometries using the class symmetry. Miller indices may be plotted in various spherical projections, the angle between two directions given in terms of Miller indices can be calculated or all crystallographically equivalent directions can be computed. MTEX applies embedding of rotations into the sphere of unit quaternions, a subset of the skew field of real quaternions. However, there are methods to convert them into Euler angles (Bunge's or Matthies' and Roe's convention, respectively), Rodrigues parameters, matrices or angle-axis parametrization. Quaternions can be applied to Miller indices, orientation density functions, pole figure data, and EBSD data to perform rotations.

Calculations with Model orientation density functionss. MTEX provides simple functions to define mathematical model orientation density functions, e.g., uniform orientation density function, unimodal orientation density function of several types, fibre orientation density functions of several types, or any superposition of them. In particular the MTEX toolbox already contains some popular standard orientation density functions as the "Santa Fe" and the "MIX 2" sample orientation density functions.

Import, Analysis, and Visualization of Integral Diffraction Data. MTEX's import wizzard supports a wide range of pole figure formats including, e.g., the XRDML format. However, it is also easy to use one of the generic methods to import data of an initially unsupported format. It is emphasized that the data may be arbitrarily scattered over the pole sphere. Fig. 3 dsiplays experimental pole figures with intensities measured at an irregular, adaptively locally refined grid. Once the data are imported, there are various methods to analyse, edit and plot them.

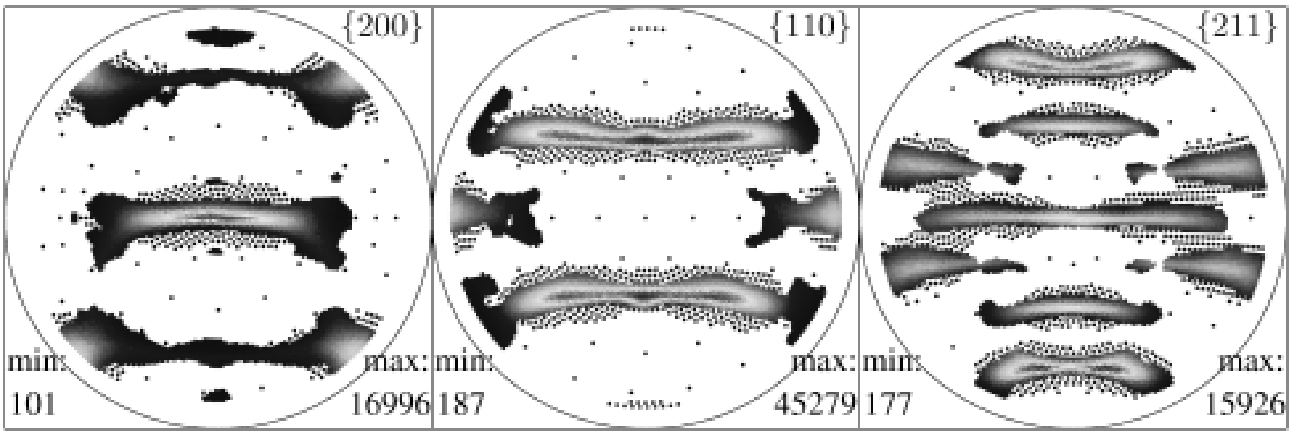

Figure 3. X-ray diffraction data measured at an irregular adaptively locally refined grid

Import, Analysis, and Visualization of Individual Orientation Data (EBSD). MTEX also provides an import wizzard for EBSD data. This interface allows to extract orientation and phase data from almost arbitrary ASCII files, cf. Fig. 4 and Fig. 5. EBSD data may be used for non-parametric orientation density function estimation, Fourier coefficient estimation, etc. In fact, all methods available for orientation density functions may be applied to orientation density functions estimated from EBSD data. In particular it is possible to compare orientation density functions estimated from EBSD data with those estimated from pole figure data using the command *calcerror*. Another useful command in MTEX is *simulateEBSD* which allows to simulate EBSD data for a given orientation density function.

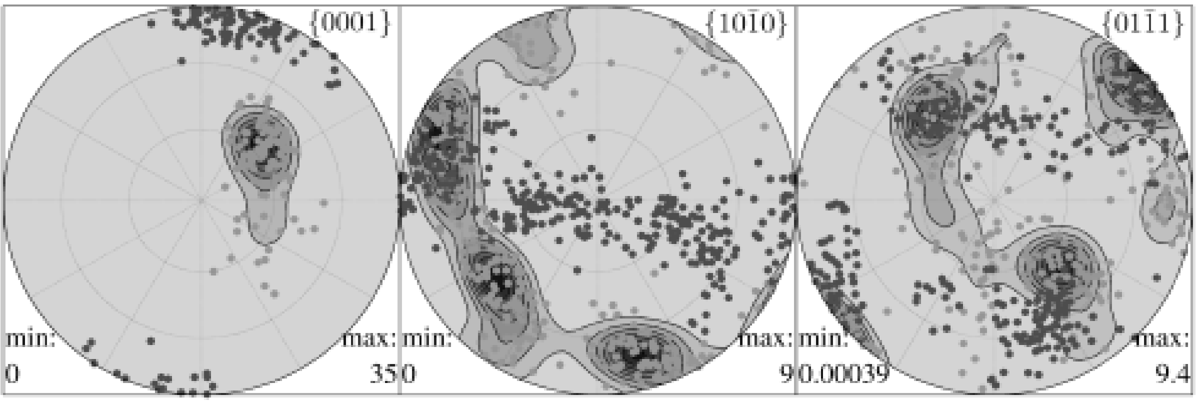

Figure 4. Pole density functions recalculated from Neutron diffraction data overlaid with two different EBSD data sets.

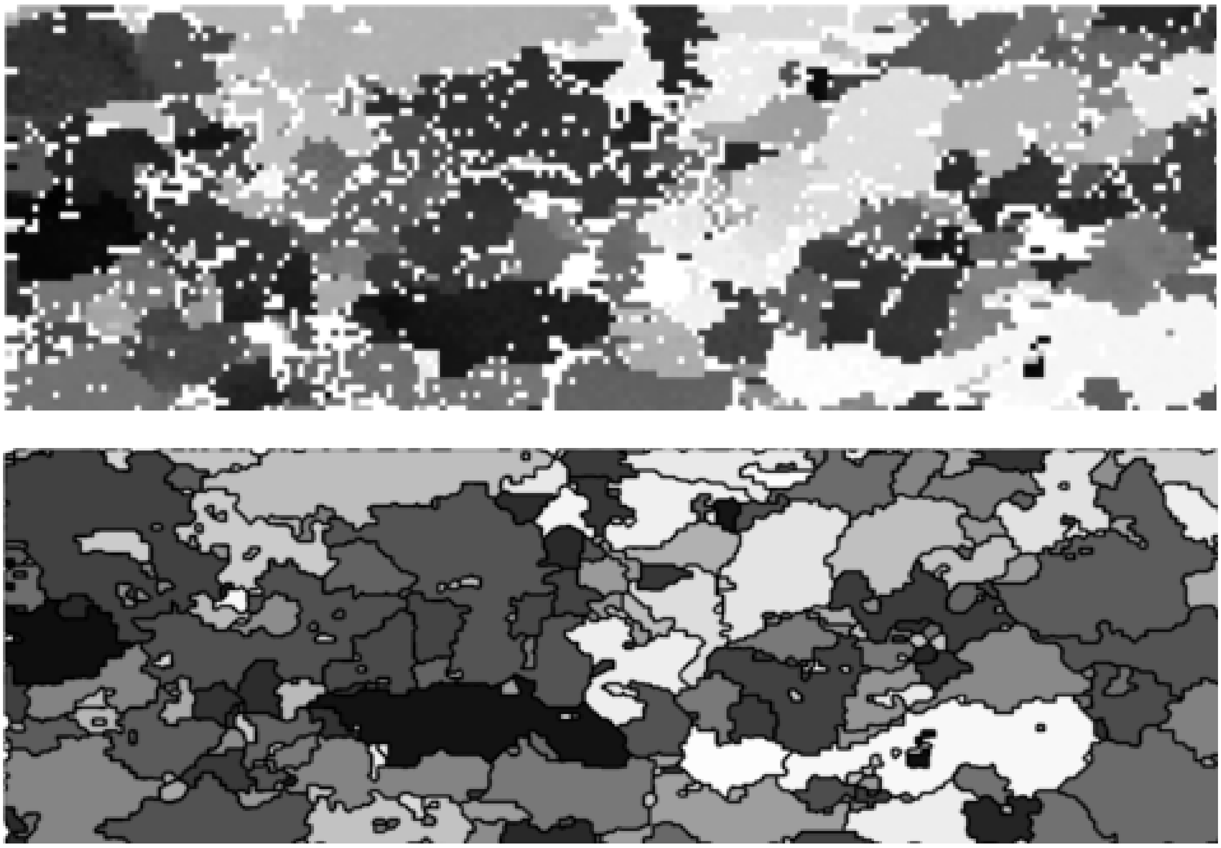

Figure 5. Raw EBSD data, spatially indexed and RGB-colour coded (top), and grains according to MTEX's explicit mathematical grain model (bottom)

Recovering Orientation Density Functions. One of MTEX major functions is *calcODF* which recovers an estimate of the orientation density function from pole figure or EBSD data according to a novel method based on a discretization of the space of orientation density functions by uniodal radially symmetric functions and on their fast spherical Fourier transform. The kernel may be chosen from a set including the de la Vallée Poussin kernel (default), von Mises – Fisher, Gauss – Weierstrass, Abel – Poisson, Dirichlet kernel and others. The algorithm has proven to be stable and applies in particular to very sharp textures with low crystal symmetry.

Calculating Texture Characteristics. MTEX offers functions to compute a wide range of texture characteristics like the modal orientation, mean orientation, entropy, texture index, Fourier coefficients, and volume portion in the neighbourhood of a given orientation for any mathematical model orientation density function or any computed orientation density function. Furthermore, arbitrary orientation density functions can quantitatively be compared indepently of being model orientation density functions, orientation density functions estimated from pole figure data or estimated from EBSD data.

Creating Publication Ready Plots. Based on state-of-the-art MATLAB™ plotting routines, MTEX allows to create professional plots of pole figure data, pole and inverse pole density functions, and orientation density function in several sections including plain φ_1 – sections (Fig. 6), σ – sections, and others. There are also many plotting options to adjust the plots to the specific standards of the journal of your choice. Plots may be saved in any image format, e.g., as pdf, jpg, png, eps, tiff, bmp.

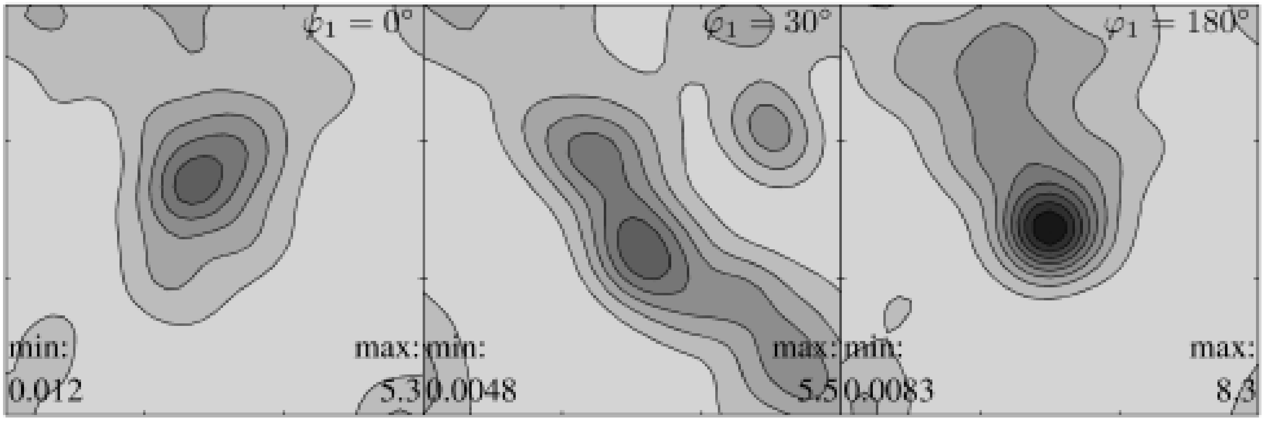

Figure 6. Orientation density function plotted in conventionally plain φ_1 - sections

Writing Scripts for multiple Use. Using the MTEX toolbox it is easy to write scripts for special jobs as to import pole figure data, preprocess them, compute an orientation density function, postprocess it, store it to a given location and finally create several plots. Such scripts can then be applied to batch process many similar data sets. Examples of scripts are included in the help.

Comprehensive Documentation. MTEX comes with over 500 pages of help explaining the mathematical concepts, the philosophy behind MTEX, and the syntax and use of all 300 functions available in MTEX. Furthermore, the documentation includes numerous examples and tutorials concerning major issues as orientation density function estimation, data import, calculation of texture characteristics, orientation density function and pole figure plotting, and many more.

Availability. An implementation of the algorithm is available as free and open source MATLAB™ toolbox MTEX and may be downloaded from http://code.google.com/p/mtex/.

Moreover, MTEX is not just a software toolbox but also a research project open to any party wishing to contribute to set out in a joint effort for a new standard of mathematical and numerical texture analysis.

Summary

The reader is invited to join the free and open source project MTEX.

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