Chapter 7

GBToolbox

All approaches to characterization of boundaries discussed in the preceding chapters have been implemented in a package of computer programs called *GBToolbox*. The software has been written in the Java programming language, therefore, it is expected to run on all platforms equipped with Java Runtime Environment; its source code consists of about 40,000 lines. It has been tested on Windows (XP, 7, and 8) and Linux operating systems. The package is distributed with a user-friendly graphical interface. In what follows, the modules of the package are briefly described. Most of the features of *GBToolbox* work for data representing materials of the cubic O_h, hexagonal D_{6h}, tetragonal D_{4h}, and orthorombic D_{2h} holohedral symmetries.

Characterization of a bi-crystal

The historically first module of *GBToolbox* provides a user with a set of tools for a comprehensive geometric characterization of an individual boundary. For a user-specified boundary, the module calculates the distances from that boundary to the nearest tilt, twist, symmetric, and 180°-tilt boundaries[14]. Moreover, it returns macroscopic parameters of the nearest characteristic boundaries and the corresponding equivalent representations of the user's boundary for which these distances are minimal: it provides the symmetry transformations C_1 and C_2 needed for obtaining those representations from the initial one and information whether inversion or grain-exchange symmetries must be applied. The misorientation of the boundary which is to be characterized can be input as

---

[14]By the distances, we also understand their approximations. Besides those, it is possible to compute Fortes tilt and twist angles; in some other modules, also the disorientation-based parameters can be determined. It is, however, passed over for brevity.
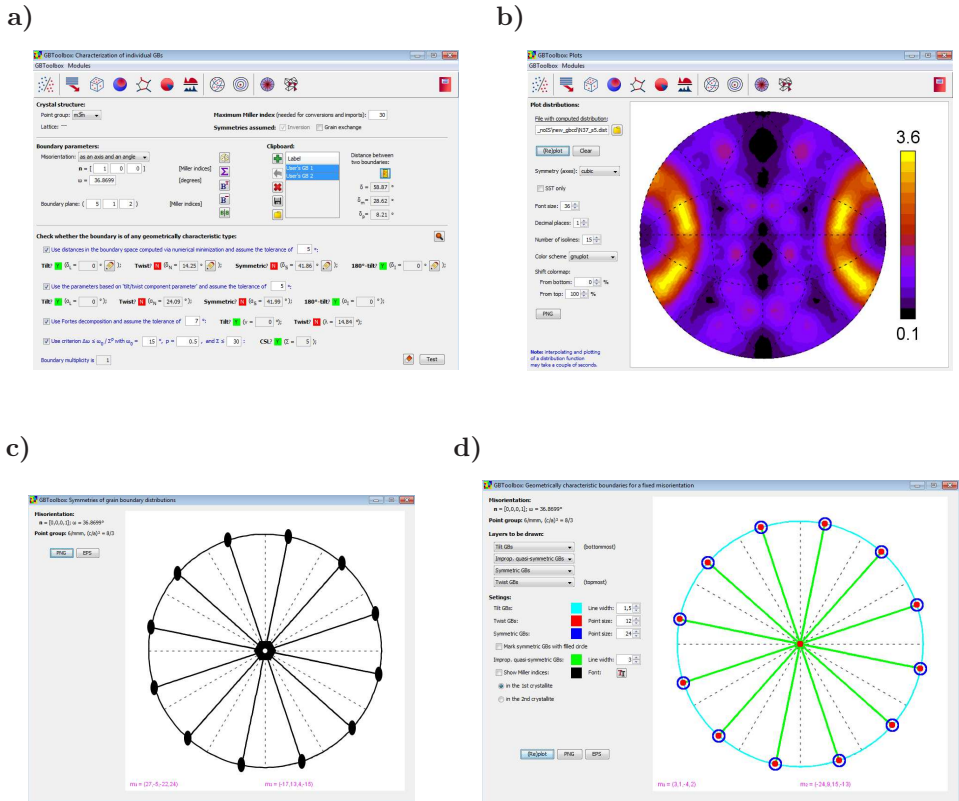
a)

b)

c)

d)

Figure 7.1: Screenshots taken from *GBToolbox*: *(a)* the module for characterization of bi-crystals, *(b)* the tool for previewing distributions saved in `dist`-files, and the windows showing diagrams with *(c)* symmetries of distributions and *(d)* locations of characteristic boundaries.

rotation axis and angle, Euler angles, a rotation matrix, a quaternion, or Rodrigues parameters. Conversions between these parameterizations are possible. The boundary plane is determined by its Miller indices. The user's boundary representation can be transformed to the representation with the smallest-angle misorientation. For completeness, the module also calculates the distance δ_m in the misorientation subspace to the closest coincidence site lattice boundary. Furthermore, a simple tool for comparing two boundaries is included; it is possible to calculate the distances δ, δ_m, and δ_p for two arbitrary boundaries. The boundary characterization can be performed with distinction of the grains or with grain-interchange symmetry allowed.

Preparing data sets for analysis

In order to investigate of boundary data sets, parameters of boundaries need to be extracted from the experimentally collected 3D orientation maps. *GBToolbox* was *not* designed for this purpose, but it is capable of importing boundary networks already reconstructed using *DREAM.3D* program and reading its output files. The reconstructed boundaries are modeled by meshes of triangular segments with local boundary parameters ascribed to each of those segments (cf. Chap. 4). The imported meshes are stored in `gbdat` files. Each line of such a file contains a list of values characterizing one segment: Euler angles (in total, six) corresponding to (average) orientations of the adjacent grains, two spherical angles describing the boundary normal (expressed in the laboratory reference frame), area of the segment, and a number which tells us how many segments constitute a given boundary. Additional import options can be selected. A user can exclude boundaries belonging to surface grains (i.e., those which are cut and not fully contained within the analyzed map). One can also exclude borders of each boundary (narrow strips built of mesh segments directly neighboring triple lines); cf. Chap. 4. Furthermore, *QSlim* program (Garland and Heckbert, 1997) may be run in batch and utilized for mesh simplification: boundary surfaces can be approximated by other meshes which consist of smaller numbers of segments. The `gbdat` files are the input files for further analyses.

The created input files can be supplemented with the distances to the nearest tilt, twist, symmetric, and 180°-tilt boundaries. The distances are calculated for each mesh segment and they are appended to the corresponding lines of `gbdat` files. Such a processing of the input files is essential, e.g., for estimation of the fractions of geometrically characteristic boundaries in the considered

set(s).

We have also seen that, in some cases, it is interesting (or even essential) to analyze different subsets of the data. *GBToolbox* allows for excluding boundaries of specified parameters (within assumed tolerances) from existing `gbdat` files.

Data sets filled with random boundaries are often used as reference data sets corresponding to the data with no anisotropy. *GBToolbox* allows for creating `gbdat` files containing random boundaries generated according to the model of uniformity determined by the distance function δ.

Analysis of boundary data sets

Another module of *GBToolbox* allows for analysis of the boundary networks saved in `gbdat` files; multiple files can be opened if a data set was split into several files. If the `gbdat` files have been previously processed so that they contain the distances to the nearest tilt, twist, symmetric, or 180°-tilt boundaries, then the fractions of boundaries which are classified to these (one or multiple) groups can be easily estimated; cf., e.g., Tab. 5.1. *GBToolbox* includes the first implementation of the new approach for computation of grain boundaries distributions based on kernel density estimation[15]. If predefined limiting radii ρ_m and ρ_p are used, the distributions will be normalized (and expressed in multiples of random distribution) automatically. Other limiting radii can be specified, but in that case, the distributions need to be normalized manually using a provided tool. The computed distribution will be saved in a text file with the extension `dist`. These files consist of five columns. The first two numbers are coordinates corresponding to stereographic projection of boundary normal, the next two are zenith and azimuth angles representing that normal (in the crystallite reference frame), and the last value is the value of the distribution. During the normalization procedure an additional `dist` file is created. It contains the errors of the distribution.

To help in exploration of boundary distributions, a module for identification of symmetries of sections through the distributions for a given misorientation has been added. It displays the corresponding symmetry axes and mirror lines; cf. Fig. B.1. Similar module which instantly locates all tilt, twist, symmetric, and 180°-tilt boundaries for a fixed misorientation (using the analytical

---

[15]For cross-check purposes, the distributions of boundary populations can also be computed using the partition-based method. The same applies to boundary-plane distributions averaged over misorientations.

method) is provided; see Fig. B.2. As was already explained, the locations of (near-)characteristic boundaries can also be read from the distributions of the distances to the nearest geometrically characteristic boundaries. The capability of obtaining such distributions is also added to *GBToolbox*. The program computes the distances for boundaries with a fixed misorientation and boundary normals forming a dense grid of directions; the results are saved to `dist`-format files. Eventually, a module for rough location of the maxima in the distributions is provided for testing; see Sec. 8.2.

Also the distributions of boundary planes can be computed with *GBToolbox* using a method adapting the kernel density estimation technique. Populations (given in MRD) of particular boundary planes can be considered from different viewpoints. One can consider boundary planes averaged over misorientations in both crystallite and laboratory reference frames (as in Sec. 6.3). There is also the idea of analyzing the distributions of boundary normals expressed in the second crystallite assuming a fixed normal in the first grain. In other words, we consider functions of four macroscopic parameters averaged over the fifth degree of freedom. Although *GBToolbox* allows for computing the distributions of the latter type, they are not discussed in this dissertation.

Visualization tools

GBToolbox has also been equipped with a simple plotting tool that displays contour graphs based on data stored in `dist` files. Depending on its type, a distribution can be plotted on a hemisphere or can be restricted to the standard stereographic triangle. Also, some other basic tools are provided: a user can set the density of isolines, choose colors representing function values, adjust legend font size, and export the obtained plots to `png` graphic files. With *GBToolbox* it is also possible to prepare `vtk` files containing mesh segments of boundaries with user-specified parameters. Such files can be displayed using, e.g., *ParaView* package (Henderson et al., 2004); see Fig. 4.2.