Chemical contrast user guide

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These scripts and functions have been created by Gabriele Bertolini with the purpose of making simple and clear the data analysis performed for the scientific article:... and showed in its supplementary information.

Note: Matlab 2015a or new versions and the NanoLib library are needed to run these codes. In future the functions will be integrated in the NanoLib library under the folder NanoLib/sxm/op.

Contents

1 Scripts

The following scripts will be described:

1. Code2CreateSfemBorder.m;

2. Code2CreateStmBorder.m;

3. Code2GetContrast.m;

4. Code2GetProfileLine.m;

5. Code2GetResolution.m;

All of these scripts are structured in the same way. First is asked to the user to add the path of the NanoLib library, the path of the Functions folder, and to choose which file has to be open. Following, the file is loaded using the function loadProcessedSxM of the NanoLib library(see NanoLib user guide section 2.2.3). The index i of the channel desired is given by the function getChannel(see NanoLib user guide section 4.0.4) and so the data of that channel are easily found in file.channels(i).data . At this point one of the function in the folder Functions is called using as input the data of the channel chosen.

1.1 Code2CreateSfemBorder

This script opens a sxm file and applies **CreateStepBorder** function either to a Current map or to a Secondary electron map("Current" or "Channeltron" channels).

1.1.1 Function CreateStepBorder

This function acts as following:

- Plots alldata matrix using the colormap defined by nanonisMap (Nano-Lib/op/nanonisMap.m).
  Note: The x and y axis are in pixels and the origin is top/left corner(matrix representation).

- Allows the user to select the region of interest(roi) inside the image loaded by clicking and dragging the mouse. When double click the fit starts.

- Fits to every scan line inside the roi the step function $-A * tanh(B * (x - C) - D$ with $A, B, C, D > 0$; the fit parameter C is x coordinate of the inflection point of the tanh function i.e. the position of the step

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in a scanline. The y coordinate is the scan line index. All of these x, y coordinates define the points of the border line between W and C regions. **Note:** The shape of the function used for the fit defines an up/down step from left to right.

- Asks to the user whether to save the border points in a txt file.

- Plots the border line points as a green line.

- Creates a figure where only the roi is visible.

1.2   Code2CreateStmBorder

This script opens a sxm file and applies **CreateFreeHandBorder** function to a topography map("Z" channel).

1.2.1   Function CreateFreeHandBorder

This function acts as following:

- Plots alldata matrix using the colormap defined by nanonisMap (NanoLib/op/nanonisMap.m).
  Note: The x and y axis are in pixels and the origin is top/left corner(matrix representation).

- Allows the user to draw a border inside the image loaded by clicking and dragging the mouse.

- When double click on the line, the x and y coordinates of those points are saved in the txt file typed.

1.3   Code2GetContrast

This script opens a sxm file and applies **GetContrast** function either to a Current map or to a Secondary electron map(Current or Channeltron channels).

1.3.1   Function GetContrast

This function acts as following:

- Plots alldata matrix using the colormap defined by nanonisMap (NanoLib/op/nanonisMap.m).
  Note: The x and y axis are in pixels and the origin is top/left corner(matrix representation).

- Lets the user to draw a first region A inside the image loaded by clicking and dragging the mouse.

- Lets the user to draw a second region B inside the image loaded by clicking and dragging the mouse.

- Plots the histogram of the values for the two regions. A normal distribution might justify a total contrast calculation.

- Plots the histogram of the contrast for every line. If the line doesn't contain values for one of the two regions, then that scan line is not counted for the histogram and the contrast calculation.

- The contrast per line and the total contrast is calculated as following: Contrast $= |(A - B)/(A + B)|$ where A and B are the mean values of the regions.

- The mean values of the two regions and the total contrast are shown in the title of the "Contrast per line" figure.

1.4   Code2GetProfileLine

This script opens a sxm file and applies **GetProfileLine** function to a topography map("Z" channel).

1.4.1   Function GetProfileLine

This function acts as following:

- Plots alldata matrix using the colormap defined by nanonisMap (Nano-Lib/op/nanonisMap.m).
  Note: The x and y axis are in pixels and the origin is top/left corner(matrix representation).

- Lets the user draw the line and drag or modify it after created.

- Plots the line profile and upload it every time the drawn line is moved or modified. **Note:** The intensity of the line is not explicit but it has the same units of the data.

1.5   Code2GetResolution

This script opens a sxm file and applies **GetResolution** function to a topography map(Z channel).

1.5.1 Function GetResolution

This function acts as following:

- Plots alldata matrix using the colormap defined by nanonisMap (Nano-Lib/op/nanonisMap.m).
  Note: The x and y axis are in pixels and the origin is top/left corner(matrix representation).

- Lets the user load two text files which are supposed to contain two set of points inside the image representing the borders the user wants to compare.

- Plots the borders from the files.

- The code starts to compare for every line the x position of the of the first border with the x' position of the second border, creating the histogram called "reshist" of the displacement. Those scan line that do not contain points of one of the two borders are excluded.

- When one of the two borders is dragged the histogram is updated.

- The total shift between the two borders and the standard deviation is shown in the title of the reshist figure.

- Gives to the user the possibility to rotate one of the borders respect to a point chosen using the button present on top of the Data figure.