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Geometric Phase Analysis (GPA) Manual

Acknowledgements + Motivation



This software is based on the following paper: M. Hytch, F. Snoeck, R. Kilaas, Ultramicroscopy **74** (1998) 131-146 All credit regarding the GPA method goes to them.

- The example image shown in this manual (the gate region of a a 45 nm CMOS structure) was recorded by V. B. Özdöl on the JEOL-ARM 1250 installed at the Max Planck Institute for Metals Research in Stuttgart.
- The primary reason for developing this software was the need to be able to compute strain maps from **complex wave functions** resulting from a high-resolution focal series reconstruction and data stacks (e.g. the raw data for a focal series reconstruction).

This tool has been tested using GMS 1.7 and should run on all newer versions of DM as well.

Installation



1. Download FRWRtools.gt1 and Transforms.dll and copy these files to the DM/PlugIns folder

2. Start DM – an additional menu item (see at right) which contains an item for the GPA analysis will appear.

| FRWRtools LARBED | | | | | |
|------------------|-----------------------------|--|--|--|--|
| | Copy Tags | | | | |
| | Acquire Foc. Series / EFTEM | | | | |
| | Align Series | | | | |
| | FRWR Setup | | | | |
| | Read Image | | | | |
| | Create Stack | | | | |
| | Volume Tools | | | | |
| | Complex Image | | | | |
| | FFT (real->complex) | | | | |
| | IFFT (complex->real) | | | | |
| | FFT (complex->complex) | | | | |
| | IFFT (complex->complex) | | | | |
| | Diffractogram | | | | |
| < | Geometric Phase Analysis | | | | |

Starting

- Load a high-resolution image, a high-resolution complex wave function, or a stack of highresolution images / wave functions.
- Ensure correct calibration (in nm)
- Rotate your image to ensure that the x-direction of your image is horizontal (e_{xx} is the strain along the horizontal axis, e_{yy}, along the vertical axis).
- For stacks: If the input data is a stack of images the analysis is done for the current slice and can be repeated for each slice by simply changing the slice and pressing the "Get Phase Maps" button again. Identical aperture positions and shapes will then be used for each slice.





Starting GPA

Click on "Geometric Phase Analysis"

8 additional images and a graphical user interface will appear.

The position of these images will be the same as when this programm was called for the last time. When running the tool for the first time you should move the windows to where you would like them to be (e.g. as shown to the right).

Closing GPAtool will close the 9 new windows. Calling it again will open the windows in their previous position again.





Position the circlular annotations in the diffractogram to the reflections you want to use for the analysis and press "Read Apertures". This will read the reciprocal space coordinates of the reflections of choice into the GUI (grain 1).

Lattice reflections



a* (1/nm): length of reciprocal lattice vector corresponding to the first reflection.

b* (1/nm): length of reciprocal lattice vector corresponding to the second reflection.

gamma (deg):angle between a* and b* in degree

theta (deg):angle of a* with the horizontal axis

| 🛱 GPA Tool | | | | | |
|--|--|---|--|--|--|
| GPA | | | | | |
| grain 1 a* (1/nm): 3.68106 b* (1/nm): 5.21336 gamma (deg): 90.1094 theta (deg): -90.1541 Resolution (nm): 1.0 | grain 2 a* (1/nm): > d* (1/nm): b* (1/nm): gamma (deg): theta (deg): Smoothing: 0.7 | 3.64425 5.26279 89.9852 -89.7558 | | | |
| Make strain matrix symmetric Color scale: -0.03 0.03 | | | | | |
| Set Apertures Read Apertures Get Phase Maps Refine G-vectors | | | | | |
| | | b* | | | |

Choosing alternative sets of reflections

You may push the current set of reflections to the coordinates in "grain 2" using the "->"button, reposition the apertures, and read their positions again into "grain 1".

This will now allow you to obtain strain maps for different aperture positions very easily (keeping all aother parameters the same) and also save their values when closing the program.

The "<->" button, for example, will exchange the extracted lattice parameters of the 2 "grains".

Note: only the values in "grain 1" are being used in the generation of the strain maps.





Resolution and smoothing

The parameter "resolution" defines the radius of the aperture used

"smooth" defines the outer fraction of the aperture radius which shall be reduced in amplitude by a cosine mask.

Matlab code:

% x is radial rec. space axis in 1/nm % res is the resolution in nm % s is the fractional smoothing

 $\begin{array}{ll} x &= 1/res^{*}[-1.5:0.01:1.5]; & & -1.5 \\ y &= zeros(size(x)); \\ y(find(abs(x) < 1/res)) = 1; \\ ind &= find((abs(x) > (1-s)/res) \& (abs(x) < 1/res)); \\ y(ind) &= 0.5^{*}(1+cos(pi^{*}(abs(x(ind))-(1-s)/res)^{*}res/s)); \\ plot(x,y); \end{array}$





Defining the reference area



B: diffractogram GPA Tool GPA grain 1 grain 2 a* (1/nm): 3.18857 3.68106 a* (1/nm): 3.18437 5.21336 b* (1/nm): b* (1/nm): <-> gamma (deg): 110.09 gamma (deg): 90.1094 <----145.28 theta (deg): theta (deg): -90.1541 Resolution (nm): 6.0 Smoothing: 0.7 Make strain matrix symmetric V Color scale: -0.03 0.03 Read Apertures Get Phase Maps Refine G-vectors Set Apertures G: phi_b* F: phi_a* - - X

Please define an area of perfect (unstrained) crystal by repositioning the region of interest defined in the phase image of refection a*.

Defining the reference lattice



Pressing "Refine G-vectors" will minimize the overall phase gradient within this ROI in both phase images and re-compute the strain maps.



The output



As shown in the paper by M. Hytch et al, the strain tensor can be shown as a symmetric matrix ($e_xy = e_yx$) by also defining a lattice rotation. scale_a^{*} and scale_b^{*} are the amplitude of reflections a^{*} and b^{*}.



(-1-11) and (111) reflections



The color scale limits were set to -0.03 and 0.03 in all 4 strain component maps using the "Color scale" settings in the GPA GUI.



(002) and (220) reflections





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Color scale: -0.05 .. 0.2