LiberTEM: Development of the pipeline for crystallography analysis including GUI development

About me

I am a third year student of Electrical Engineering faculty of RWTH Aachen. My master thesis with the topic “Efficient quantification of feature shifts in pixelated scanning transmission electron microscopy data” was written under the supervision from Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Image processing department of RWTH Aachen. One of the goals of my thesis was the development of the algorithm for region clustering of the phase change materials. I’ve decided to apply for GSoC this year, because I wanted the algorithms, developed during my master thesis, to be integrated in LiberTEM and make them accessible for material scientists without programming knowledge.

Details:

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2. University: RWTH Aachen

   Program: Electrical Engineering, Information Technology and Computer Engineering

   Year: 3

   Expected graduation date: 2019-09-30

Code contribution

Fluctuation electron microscopy (FEM) is the analysis of statistical variations in diffraction from small volumes [1]. FEM analysis in STEM can be done by calculation of standard deviation over a ring for each frame (second moment dark field image). FEM UDF is accessible via Python API.

https://github.com/LiberTEM/LiberTEM/pull/313

1. J.M Gibson, M.M.J Treacy, Atom pair persistence in disordered materials from fluctuation microscopy, Ultramicroscopy, Volume 83, Issues 3–4, 2000, Pages 169-178

Project information

1. Sub-org name: LiberTEM
2. Project Abstract:

Developing of the pipeline for crystallography analysis including GUI development

3. Detailed description:

Phase-change materials (PCM) are some of the most promising materials for data-storage applications. PCM are already used in rewriteable optical data storage and offer great potential as an emerging non-volatile electronic memory by storing information as a difference in electrical resistivity.

Distinguishing between amorphous and crystalline regions can be hard in microstructure analysis with 4-D-STEM because of low contrast between them during two most common method of visualization: bright and dark field imaging. But clustering of PCM regions (amorphous, crystalline phases with different lattice orientation) can gain information about a correlation between electrical properties of the material and its structure

Project include:

· Implementing of UDF for crystal/amorphous regions clustering;

· Implementing of UDF for clustering of regions with different lattice orientation, based on non-zero order diffraction peaks detection;

· Development of Graphical user interface (GUI) for full crystallography analysis.

4. Weekly timeline

○ **Community Bonding** (May 7-26): Getting familiar with GUI basics, literature and libraries overview.

○ **Week 1** (May 27-31): Implementing of a UDF for distinguishing of crystalline and amorphous regions:

· Deleting of outliers and frames preprocessing (such a deleting of non-zero order diffraction peak for each frame)

· Integration of frames over a ring in Fourier space

· Segmentation of the image, based on calculation of Crystallinity map and bright field image (clusters: membrane, crystalline regions of phase change materials (PCM), and amorphous regions of PCM.

· Writing tests

○ **Week 2** (June 3): Implementing of a UDF for feature vector forming based on blob (non-zero order diffraction peaks) finding:

· Calculation of standard deviation of frames from the region of interest (crystalline regions)

· Peak finding and creating of the binary mask with highlighted peaks (all possible positions of non-zero order diffraction peaks)

· Creating a criterion about the decision if the highlighted pixels, which were calculated in the previous step, at each frame are blobs

· Forming of a feature vector for each frame, which will be used for crystalline regions clustering

· Writing tests

○ **Week 3** (June 10): Writing of documentation for written UDFs and submission of them

○ **Week 4** (June 17): Testing of clustering functions + integration of developed functions into Web API

○ **Week 5** (June 24): Fixing of a small GUI issue (ex. Otsu based thresholding of the image+ User defined thresholding of the image)

○ **Week 6** (July 1)- **Week 7** (July 8): Developing of a GUI version which supports multichannel thresholding:

· Thresholding will be done based on bright field image and crystallography map, which calculation in UDF was integrated in week 3
· Options: User defined threshold or Otsu's thresholding method
· Input images: bright field image, crystallinity map
· Input parameters: Threshold levels (or option to calculate them with Otsu method)
· Output: the image with 3 clusters:
- Membrane (high intensity on bright field image, low intensity on crystalline map)
- Amorphous regions of PCM (low intensity on bright field image, low intensity on crystalline map)
- Crystalline regions of PCM (low intensity on bright field image, high intensity on crystalline map) + Fraction calculation (%) of amorphous phase of PCM

○ **Week 8** (July 15)- **Week 9** (July 22): Development of GUI for blob finding and clustering
· Calculation of SD image of frames, which belongs to crystalline region
· Finding the peaks on SD image and deleting of outliers, by setting of a ring mask (to mask the zero order diffraction peak out) to reduce the number of pixels to check
· Setting of a blob/not blob decision criterion (reference frame, tolerance value, region of integration for given pixel (given possible position of non-zero order diffraction peak)
· Visualization of the detection to estimate the precision of a peak finding for each frame, feature vector forming
· Set number of clusters (or automatic calculation of them) and clustering method
○ **Week 10** (July 29): Debugging of implemented GUIs and handling of edge cases

○ **Week 11** (August 5): Testing of the GUIs of already processed dataset with known behavior of the output. Bugs fixing.

○ **Week 12** (August 12): Documentations writing.

○ **Final week** (August 19): Submitting of the project