## Manual (script version)

-----System Requirement-----

- 1. Cuda GPU (4GB memory or more)
- 2. CPU calculation is also supported (2016b and later version), but it is slow (~10-30s/pattern).
- 3. Matlab 2016a and later version
- 4. For Pascal GPU, Matlab 2017a and later version is required.

### main\_PACBED\_identify\_demo.m

-----FUNCTION-----

- 1. Align a series of PACBEDs
- 2. Measure their thickness and tilt values

-----HOW TO RUN-----

- 1. Contact Prof. LeBeau (imlebeau@ncsu.edu) to get all large network files before run the code
- 2. Setup network name correctly in the load NN model for PACBED section
- Setup input data in the load data section, you can call file\_load function for direct input from image files
- 4. Setup parameters in the PACBED alignment section
- 5. Setup parameters in the thickness/tilt measurement section
- 6. Run code (recommend Run Section)

-----OUTPUT-----

- Output thickness/tilt measurement are in thickness\_determine and tilt\_determine variables, respectively
- Aligned images are in img\_out cell.
  Call Img\_series\_Looper(img\_out, name\_list) to view
- 3. Center, shift and rotation angle of PACBEDs can be found in para\_in cell

### main\_PACBED\_identify\_4D\_STEM\_demo.m

-----FUNCTION-----

- 1. Align PACBEDs from 4D-STEM
- 2. Measure their thickness and tilt values

-----HOW TO RUN-----

- 1. Contact Prof. LeBeau (<a href="mailto:imlebeau@ncsu.edu">imlebeau@ncsu.edu</a>) to get all large network files before run the code
- Setup network name correctly in the load NN model for PACBED section
- 3. Setup input data in the load database section
- 4. Setup parameters in the PACBED alignment section
- 5. Setup parameters in the thickness/tilt measurement section
- 6. Run code (recommend Run Section)

-----OUTPUT-----

 Output thickness/tilt measurement are in thickness\_determine and tilt\_determine variables, respectively

- 2. Run Display thickness/tilt map section to visualize the result
- Aligned images are in img\_align\_cell cell.
  Call Img\_series\_Looper(img\_align\_cell, name\_list) to view
- 4. Center, shift and rotation angle of PACBEDs can be found in 'para\_in' cell

# main\_Hybrid\_CNN\_LSF\_demo.m -----FUNCTION------

- 1. Align PACBEDs using CNN
- 2. The thickness and tilt measurement serves as initial input to LSF
- 3. Fast LSF to measure PACBED thickness and tilt

### -----HOW TO RUN-----

- 1. Contact Prof. LeBeau (<a href="mailto:jmlebeau@ncsu.edu">jmlebeau@ncsu.edu</a>) to get all large network files and simulations before run the code
- 2. Setup LSF search range in the LSF Parameter Setup section
- 3. Setup network name correctly in the CNN load NN model for PACBED section
- 4. Setup input data in the 'load data' section, you can call **file\_load** function for direct input from image files
- Setup parameters in the CNN Image alignment and thickness/tilt measurement from CNN section
- 6. Setup parameters in the LSF get tilt label number and its neighbour list section
- 7. Run code (recommend Run Section)

### -----OUTPUT-----

- Output CNN thickness/tilt measurement are in the thickness\_determine\_CNN and tilt\_determine\_CNN variables, respectively
- 2. Output LSF thickness measurement is in the thickness\_determine\_LSF variable
- 3. Output LSF tilt measurement (component along [100] and [010] direction, amplitude, azimuth angle) are in the tilt\_HG, tilt\_r, and tilt\_azimuth variables.
- 4. Run Look at the best match and the difference section to visualize the result
- 5. Final and intermediate result from LSF can be found in data\_out cell

If you find this software package is useful, please cite:

Weizong Xu, James M. LeBeau, A Deep Convolutional Neural Network to Analyze Position Averaged Convergent Beam Electron Diffraction Patterns, arXiv: 1708.00855, 2017.

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