Manual

The reference and technical notes of this plugin:

Y. Wang, U. Salzberger, W. Sigle, Y Eren Suyolcu, P. A van Aken, Oxygen octahedra picker: A software tool to extract quantitative information from STEM images, Ultramicroscopy, **168**, 46(2016).

Another application (examples) of these scripts can be found in [ACS Applied Materials & Interfaces **8**, 6763 (2016)].

Please kindly cite my publication in using this Plugin. If you have any questions or suggestions in using this plugin do not hesitate to contact me: y.wang@fkf.mpg.de , yi.cnrs@gmail.com (Yi WANG).

Installation:

1. Copy this plugin to the Gatan/Plugins folder,

2. Lunch DigitalMicrograph – the script will appear in the "Custom" menu.
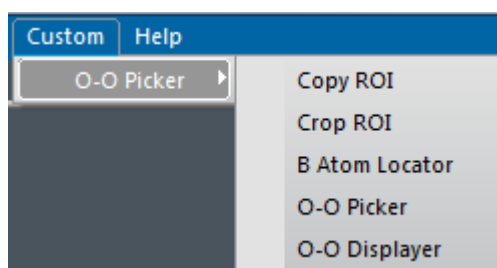
(This script will work with GMS 2.x and 3.x. If you use lower version of GMS, e.g GMS1.x, please contact me for the right version of Plugin.)

5 scripts were inlcuded in this Plugin: Copy of ROI, Crop of ROI, B atom locator, O-O picker, and O-O displayer.

Please ensure HREM mouse tool 👁 has been installed. (HREM Research - HREM Mouse Tool: http://www.hremresearch.com/Eng/plugin/plugin005/index.html)

How to work:

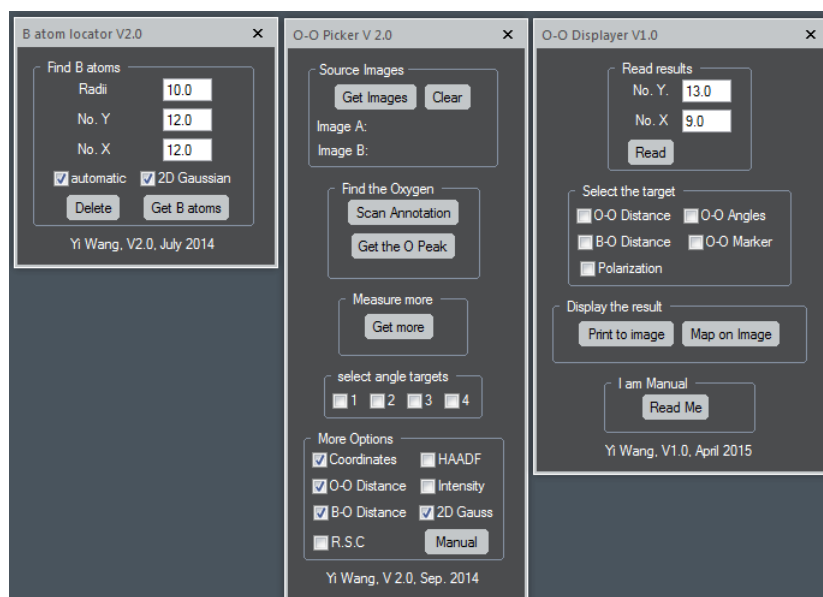The user interface of the scripts:

Figure 1 the User interface of B atom locator, O-O picker and O-O displayer.

Preparing your ADF and ABF images: (a) If necessary, you can use the two additional scripts to "ROI" and crop your images: The "Copy ROI" script can be used to clone the position of ROI to another image, the "Crop ROI" script will create new image from the ROI on the foremost image and copy all the tags and calibration. (b) Since the scripts will take the annotation as the input, please remove the scale bars of your input images.
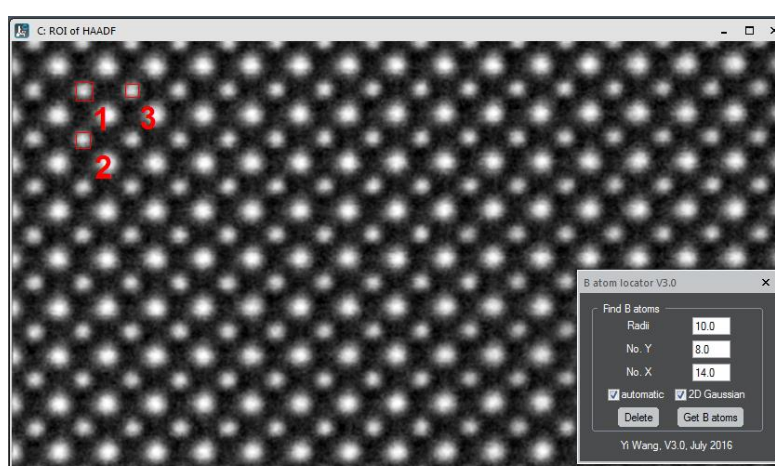

Figure 2 the setting and inputs of the B atom navigator program.

B atom locator

(1) Using HREM mouse tool selects three B atomic columns on the ADF image, as shown in Figure 2.

(2) Input proper radii of the atomic column in pixels. Input the number of unit cell (No. X) that you would like to search along horizontal direction, and the number of unit cell (No. Y) along vertical direction. The "automatic" option works for ABO_3 structure (for more complicated structure uncheck "automatic" the program will work column by column manually).

(3) Press "Get B atoms".

    a) If "automatic" is checked, the program will search all the B atoms in area defined by No.Y and No. X

    b) If "automatic" is unchecked, the program will search B atoms column by column. The program will ask you to confirm the order of the column (Figure 3, the number is used to order the result in the Tag file and it will update automatically. If the number/order is correct, just press Ok). Press "Ok", it will start to search B atomic column.
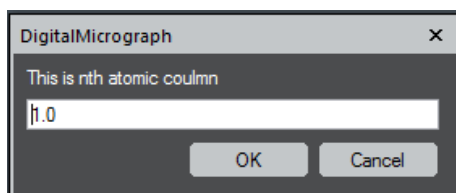

Figure 3 window for updating the order of coulmn for writing the tag file.

(4) The result will be marked on the ADF image and a table named "Coordinates of B" will appear (don't close this table, save it and don't rename, the next program will this table as one of the input files).

Oxygen-octahedral Picker

(1) Using HREM mouse tool selects four Oxygen atomic columns of the first octahedral on the ABF image, as shown in Fig.4. (Please keep the "Coordinates of B" table open.)
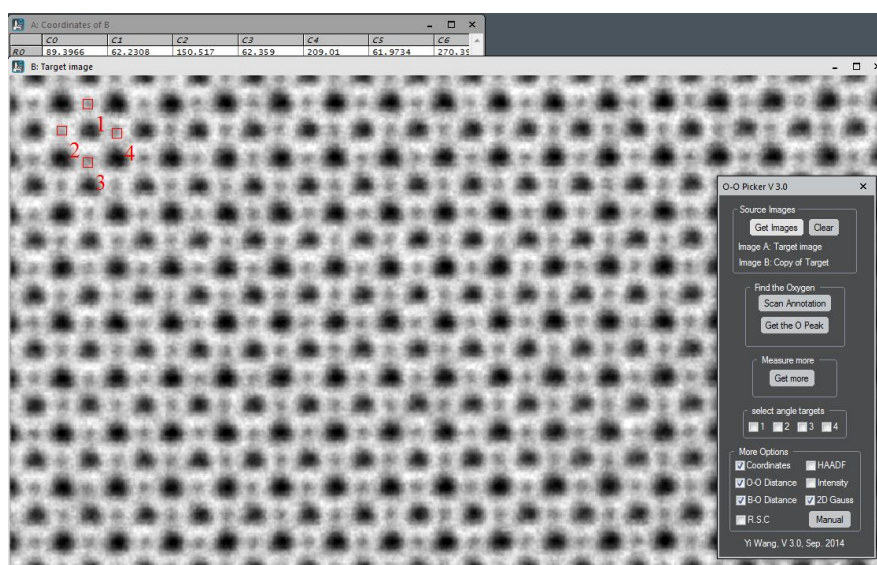

Figure 4 the setting and inputs of the O-O picker script.

(2) Press "Get Images", select input ABF image. If you want to use filtered image as a guide for improving atom locating, choose filtered ABF image as Guide image and the ABF image as Raw image (the final atomic column fitting will be performed on the Raw image). Otherwise, just set both images as the ABF image, as shown in Figure 5. Then, clik "Ok". The script will rename the image as "Target image" and creat a image with name of "Copy of Target image".
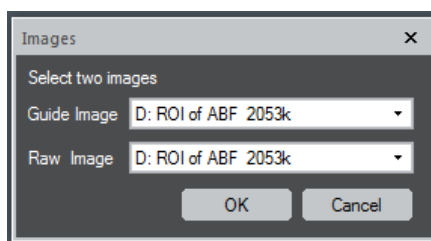

Figure 5 window for selecting the ABF images.

(3) Press "Scan annotation", input the radii of the Oxygen atomic column (Figure 6, for 2D Gaussian fitting the value should be no less than 5 pixels). In the output window, you will also have some text output giving you the format of the results (the unit of the results is pixel).
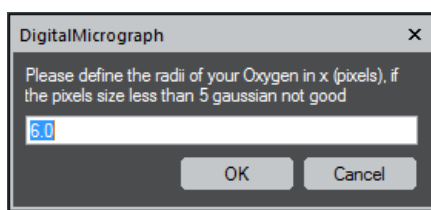

Figure 6 window for inputing the radii of O atomic column.

(4) Press "Get the O Peak", the scipt will search the 4 Oxygen atomic columns and the position will be marked on the "Copy of Targe image", as shown in Figure 7. Check whether the O atomic columns were located properly or not.
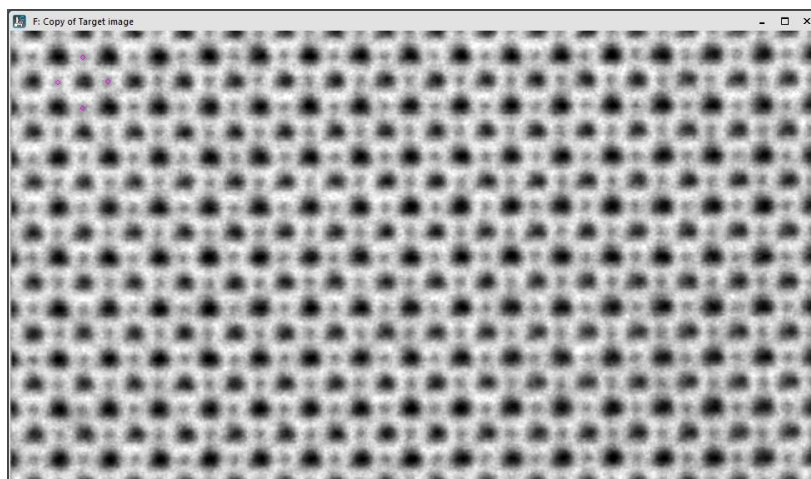

Figure 7 the result of intital 4 O atomic column locating.

(5) Press "Get more", the program will ask you to confirm the order of the column (similar to Figure 3, the number is used to order the result in the Tag file and it will update automatically. If the number/order is correct, just press Ok).

(6) The program will ask you that do you want to refine the B atom locating (Figure 8) on ABF image or no (0 use result from ADF, 1 will refine the B atom position on ABF image), the default setting is 0. If you choose 1, in the next window the program will ask you to define the radii of B atomic column.
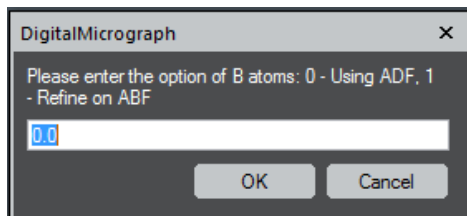

Figure 8 window for the option refine the B atomic column locating.

(7) Then, the program will take the pre-located B atomic column positions as a guide to detect all the octahedra along the column on the ABF image, the results will be marked on the "Copy of Targer image" (Figure 9). On the "Target image", the program will move the the square annotations to the next column.
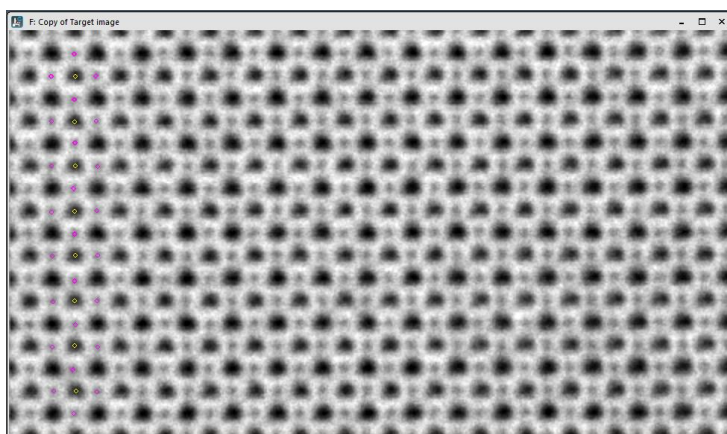

Figure 9 the result of located O atomic columns.

(8) Check whether the square annotations were pleaced on the next column properly or no. Repeat steps 4 and 5 for other columns.

The final results provided by this software are: (in the Notes window) the coordinates of detected atomic columns, (in the Results window) the atomic column intensities, the distances between the atomic columns, and the angles between selected atomic columns, based on the selection of the user. These results are also stored in the Tag file of "Copy of Target image".

Read and displace the result

This part is not yet well documented; please let me know if you have trouble in using it.

(1) Select the "Copy of Target image", input the correct No. Y and No. X, and then press "Read", the program will read the result stored in the Tag file and also print into the result window.

(2) Press the "Print to image", the program will print all result into image.

(3) Select the options, i.e., O-O marker and Polarization; press "Map on the image" the program will mark the oxygen octahedra (Figure 10) or polarization on the image.
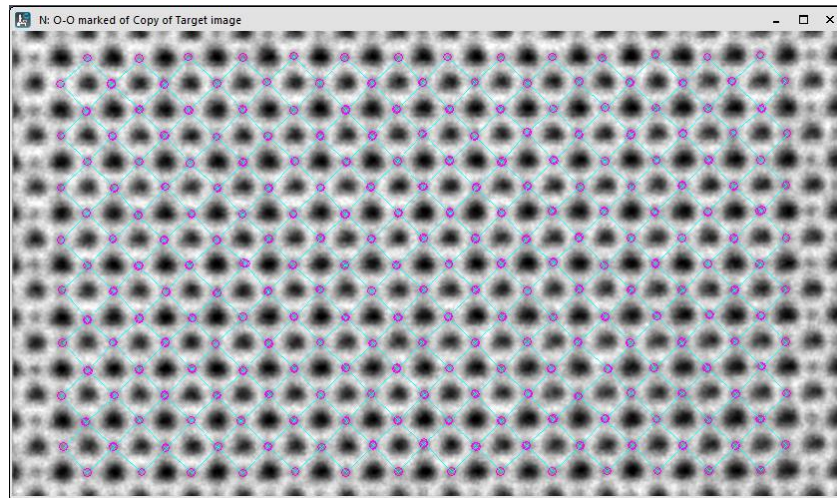

Figure 10 the result of map the oxgyen octahedra on the image.