NANO SCALE IMAGE ANALYSIS (NSIA)

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1. INTRODUCTION

Nanoscale materials (i.e. materials designed on the scale of 10^{-9} meters) have been growing in interest in recent years. This is due to the emergence of nanotechnology as a field of interest in technology and to the miniaturization limitations of current technology. Nanoscale-designed materials promise to have radically different properties than their bulk counterparts. For example, the photoluminescence properties of materials change significantly in nanomaterials. Widely discussed, carbon nanotubes have been either semiconducting or metallic and have vastly improved strength over any bulk carbon.

It is important, then, to be able to characterize the materials being used in order to fully understand the properties that they exhibit. A tool crucial to this characterization and understanding is the Transmission Electron Microscope (TEM). In order to view and understand the arrangements of atoms at an atomic scale, a high resolution transmission electron microscope is necessary. Furthermore, tools helping to analyze the images taken from the microscope could vastly enhance the ability of scientists to understand the phenomena that occur when designed at the nanoscale.

Crystalline materials are made up of atoms in specific sites within unit cells. These attributes of crystalline materials help define the many attributes that the bulk material shows. The size of these unit cells is on the order of only a couple of angstroms (10^{-10} meters) and so imaging them is somewhat of a challenge. This is solved through the use of a TEM in which resolutions up to one angstrom have been achieved. In a nanoscale world, the easy and reliable measurement of these properties of the crystals is vital to the characterization of the materials being used.

Lattice spacing determination in high resolution electron microscope images is a key way in which a material can be characterized and studied. The spacing of unit cells of atoms and the angles that the sides of the unit cells make are both techniques in characterizing a crystalline material. Also interesting are spaces in the crystal where this regularity breaks down. This can symbolize defects in the crystal structure, such as dislocations, point defects, and planar defects. Such defects can have a large impact on the properties of the material. In many cases, it can be difficult to see the presence of nanoscale particles without an aid.

When taking a low magnification, high resolution (500kx, 1.2 angstrom resolution) images, layers of atoms manifest themselves as a series of parallel lines. The separation between these lines can be used to determine the separation between the layers of atoms. This is important in determining several important factors about the material, including the crystallographic orientation and some mechanical properties. Most of the time, these lines are visible to the human eye and currently are measured by hand with a magnifying glass, after the pictures of the specimen have been developed, and after the specimen is no longer in the microscope. More and more, these microscopes have digital cameras installed on them, so the ability to make these measurements immediately, while the specimen is still in the microscope is an extremely useful tool to researchers. Knowing what you have already measured while you are still working on the microscope can lead to better analysis and an easier time of making all of the correct measurements. Moreover the visual scans are not very accurate and often miss hidden crystallographic orientations. Therefore, developing a tool to automate the process of determining the spacing and orientation of the lattice of atoms could be important to the development of the understanding of materials and their properties at the nanoscale.

Figure 1, shows the typical TEM image of the ZnS structure. The "linear" structure (parallel lines of different orientation) formed by an atomic lattice is clearly visible. The difference in orientation may come from the following sources: (i) different materials will have different orientation; (ii) often the layer that is below the surface can be seen, and this creates the additional orientation and (iii) different areas of the crystal can be oriented differently. Our primary goal is to detect this linear structure, or more specifically, to find the parallel lines, their relative orientations, and distances between parallel lines of the same direction. All this information is useful in the following important

I would like to thank Dr. Brani Vidakovic, without his help it would not be possible to create this toolbox. And I would like to thank Daniel Moore for providing the data.

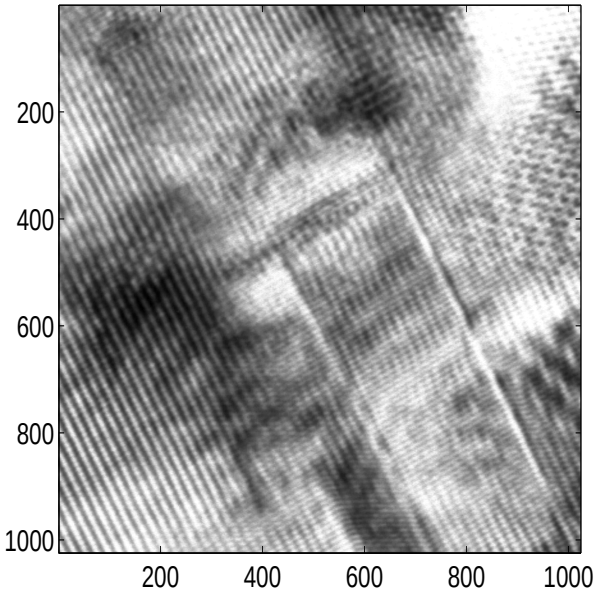

FIGURE 1. Example of the TEM image of the ZnS structure. Parallel lines formed by an atomic lattice are clearly visible. They form approximately 30° angle with the y-axis.

applications. First of all, by knowing of the relative orientation of different materials we can learn more about the crystallographic structure of the interfaces of the materials. Second, the knowledge of the orientation of the surface layer and the layers below it, coupled with diffraction pattern and images at higher resolution, can give us signature of the material, its structure and properties. Finally by learning the distances between parallel lines the distance between atoms, the lattice spacings can be determined.

For this purpose a new method of identifying crystallographic orientations, and determining lattice spacings was developed. For more details on the method, see the companion paper "*Linear Feature Identification and Inference in Nano-scale Images*", available at Jacket's Wavelets page `http://www.isye.gatech.edu/~brani/wavelet.html`.

The method is implemented in the MATLAB toolbox NSIA. This manual provides installation and step-by-step instructions for the toolbox.

2. INSTALLATION

In order to install MATLAB toolbox `NSIA`, unzip all the required files into your MATALAB "work" folder (for example `c:\matlab6p5\work\nsia`). Next, create a temporary folder `c:\matlab6p5 \work\nsia\temp`. The name of the MATLAB root folder can be arbitrary, however the structure `\work\nsia` and `\work\nsia\temp` must be preserved. Finally, add a path to MATLAB. This can be done by opening MATLAB and going to `File`. Click onto `Set Path...`, and then `Add Folder...`. Select your NSIA folder, and save. This last step can be avoided if one makes `c:\matlab6p5\work\nsia` the "current directory" every time before starting the program.

3. GETTING STARTED

3.1. **Main Menu (Figure 2).** Figure 2 shows the start menu of the program. It consists of six buttons:

(1) "`Select Image`": This button opens the "Image Selection" window (shown in Figure 3) which allows one to open an image file and select a region of interest.
(2) "`Hough Transform`": This button opens the "Hough Transform" window (shown in Figure 4) which performs the Hough transformation of the selected image.
(3) "`Analysis`": This button opens the "Analysis" window (shown in Figure 5) which detects various orientations and estimates the distance between lines formed by an atomic lattice.

(4) "`Convert to meters`": This button opens the "Convert to meters" window (shown in Figure 6) which allows the conversion of average distance detected in the analysis stage to meters.
(5) "`CDWT`": This button opens the "CDWT" window (shown in Figure 7) which performs a continuous directional wavelet transformation along the detected direction/orientation of the selected image.
(6) "`Close`": This button closes the application.

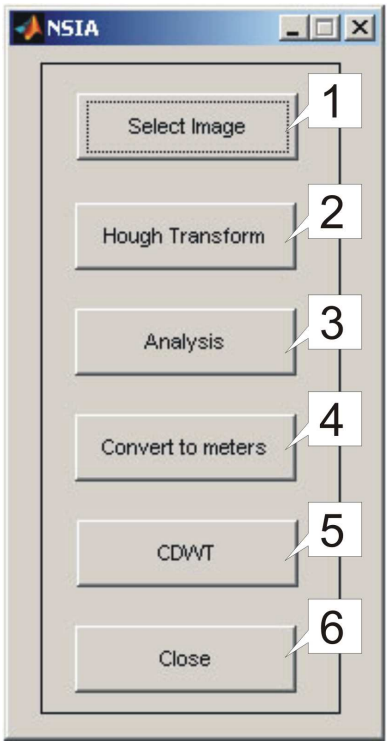

FIGURE 2. Main menu.

3.2. **"Image Selection" Window (Figure 3).**

(1) In this field the image is displayed.
(2) This filed displays the selected region.
(3) This allows the selection the size of the subimage in a pop-up menu. The "`Select`" button displays the crosshair which allows for the selection of a region of interest.
(4) "`Open Image`" starts the standard menu for opening files. It allows the selecting of JPG image from files on the hard drive. The "`Save`" button saves the selected subimage. The "`Close`" button closes the current window.

3.3. **"Hough Transform" Window (Figure 4).**

(1) The "`Load`" button loads the last saved subimage.
(2) This field displays an image.
(3) The "`Half Degree Step`" allows one to select $\Delta\theta = 0.5$ degrees in the Hough transform. This will increase sensitivity as well as computational time. The "`Hough Transform`" button performs the Hough transformation of the image.
(4) This field displays the Hough transformation of the image.
(5) The "`Save`" button saves the information required for the next step. The "`Close`" button closes the current window.

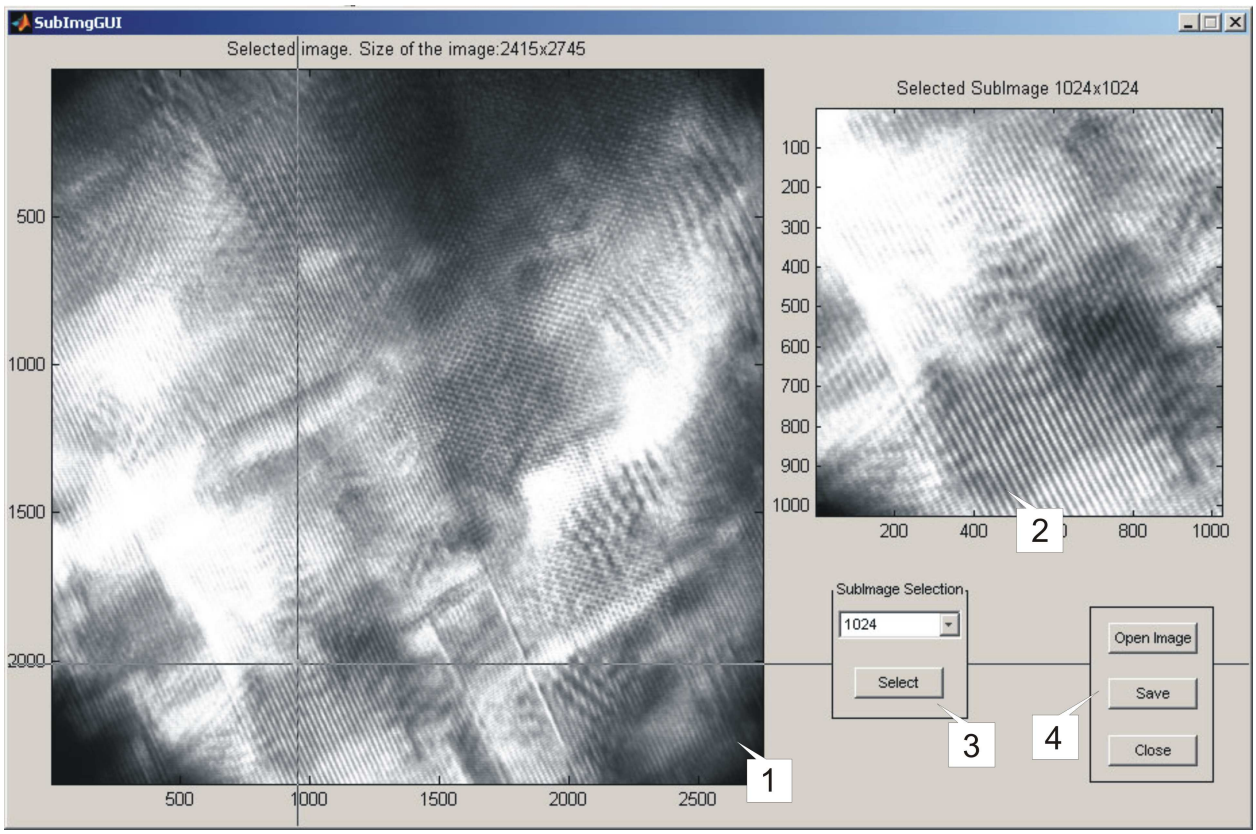

FIGURE 3. `Select Image` window.

3.4. **"Analysis" Window (Figure 5).**

(1) The "`Load`" button loads the last selected image. The "`Close`" button closes the current window and saves the results required for the next step.
(2) The "`Plot Image`" button displays the image in field (7).
(3) The controlled parameters field allows to change parameters to increase sensitivity of the method.
(4) The "`Detect`" button performs the analysis of the image and detects parallel lines formed by an atomic lattice, and measures the distance between them. The results of the analysis are displayed in (5) and (6).
(5) This displays the plot of the energy function, with circles representing detected angles/orientations of the parallel lines.
(6) This field lists the results of the analysis (detected orientation, number of parallel lines, average distance between the lines and standard deviation of the distances). Selecting particular orientation and clicking the "`Plot`" button will plot lines of this orientation over the image in field (7), graph of the distances between the lines in field (8), and display the histogram of the distances in the field (9).
(7) This field displays the image under investigation.
(8) This field displays the graph of the distances between the lines.
(9) This field displays the histogram of the distances between the lines.
(10) This is the control over calculation of the average distance between the lines. There are three possible choices in the pop-up menu: standard average, trimmed average, and winsorized average. Upper and lower quantiles for the trimmed and winsorized averages are shown in corresponding fields. Select the desired method in the menu, enter the values of the quantiles if necessary, and click the "`Recalculate Avg.`" button to get the results.
(11) This is the control over the elimination of the close lines. Select the "`Eliminate Close Lines`" option together with the number of pixels in the pop-up menu, and click the "`Detect`" button to get the results.

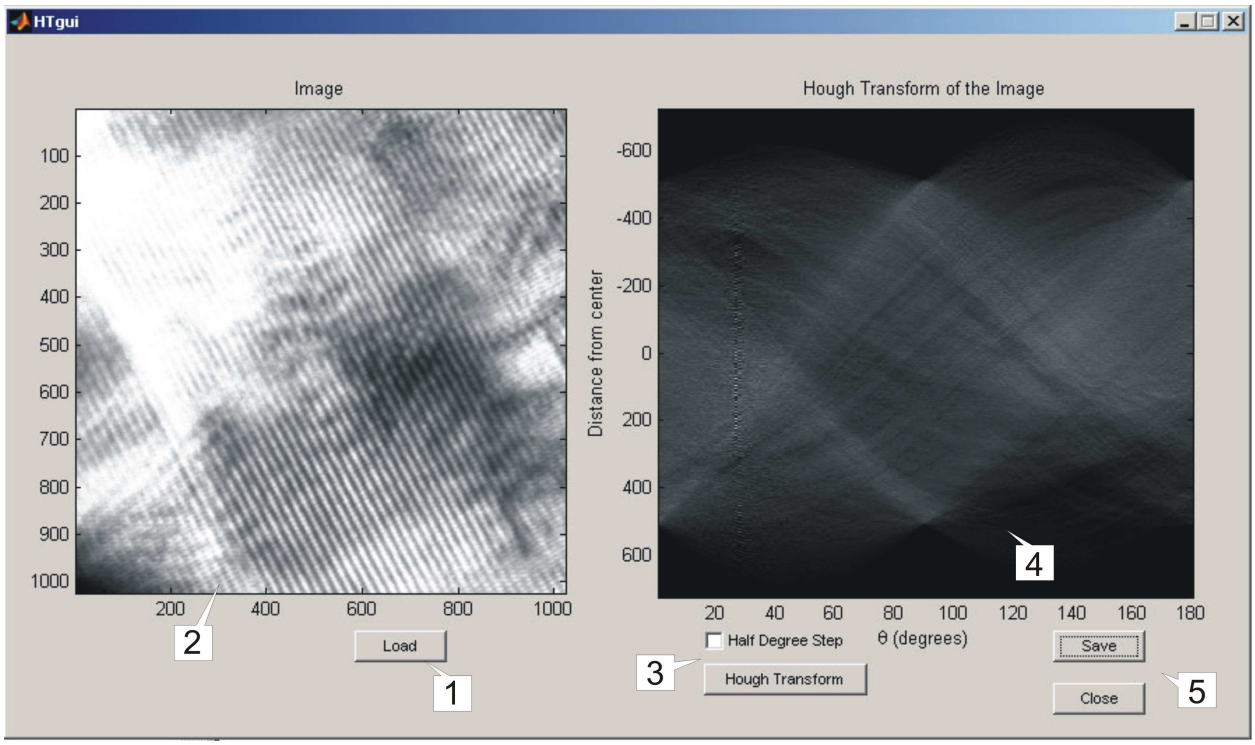

FIGURE 4. `Hough Transform` window.

3.5. **"Convert to meters" Window (Figure 6).**

(1) The "`Load`" button loads the results from the previous step of the analysis. The "`Calculate`" button converts the results to meters.
(2) This menu allows the selection of the resolution at which the image was originally scanned.
(3) This menu allows the selection the magnification of the microscope used.
(4) This field displays the results.

3.6. **"CDWT" Window (Figure 7).**

(1) The "`Load`" button loads the image under investigation (displayed in field (4)). The "`Save`" button saves the results of the continuous directional wavelet transformation on the hard drive. The "`Close`" button closes current window.
(2) This is a list of all detected orientations. Select the desired orientation by clicking on it.
(3) Select the scale of the wavelet transformation by sliding the rule or entering the value in a field. The "`CDirWT`" button performs the transformation.
(4) This field displays the image under investigation.
(5) This field displays the results of the wavelet transform.

4. STEP-BY-STEP INSTRUCTIONS.

- Type "nsia" in the MATLAB command line (`>>nsia`) in order to start the program. Figure 2 shows the start menu. To make a full analysis one needs to go through each of the steps.
- Analysis starts with the loading of the image and selection of a subimage of interest. Click `Select Image` button (Figure 2.(1)). "Image Selection" window shown in Figure 3 will appear.
- Click the `Open Image` button (Figure 3.(4)). The standard menu for opening file will appear (currently the program works only with JPG format). Select the desired file. The field Figure 3.(1) will display the selected image.

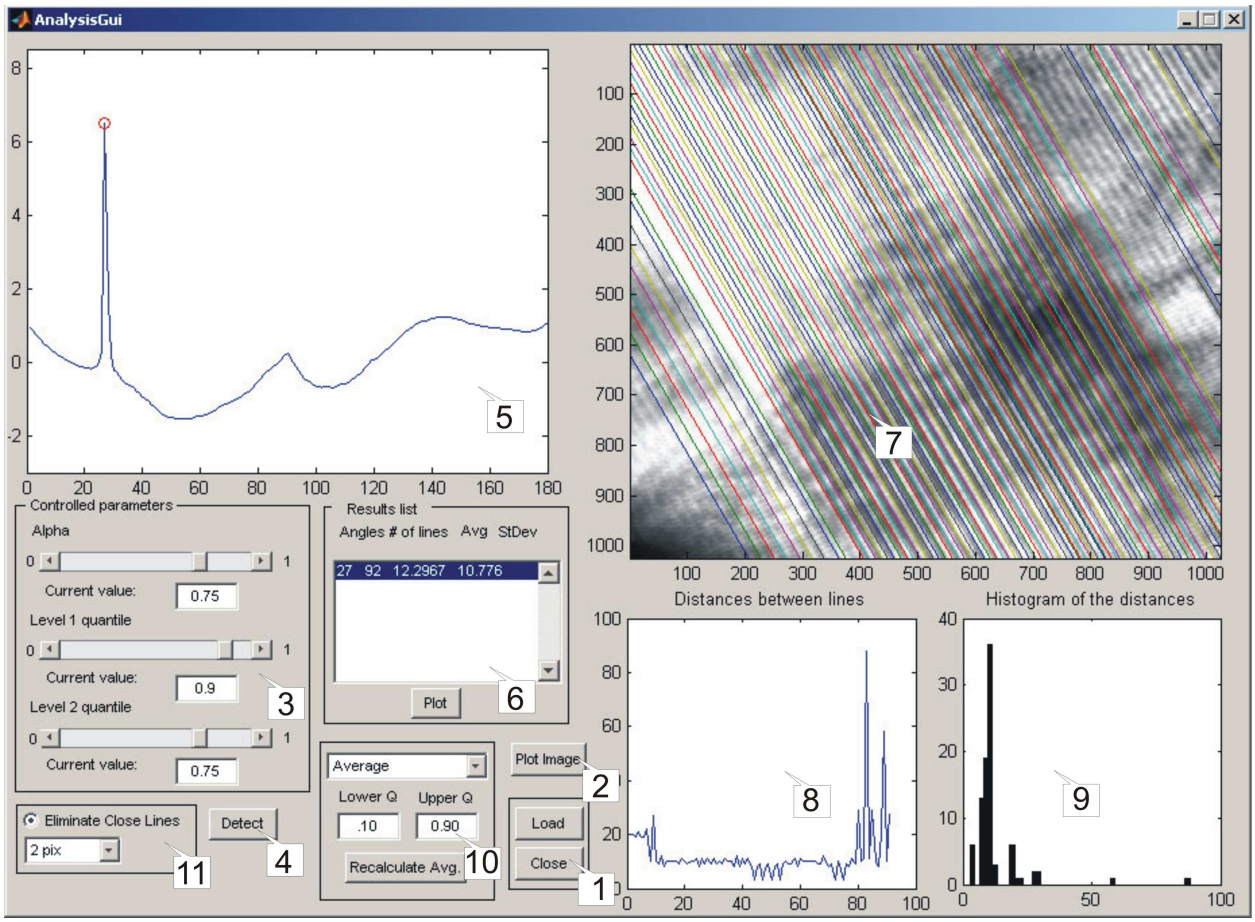

FIGURE 5. `Analysis` window.

- Select the subimage size in the pop-up menu Figure 3.(3). The available sizes are 256×256, 512×512, 1024×1024, 2048×2048 and 4096×4096. The larger the subimage size, the longer it will take to run the analysis. The recommended subimage size is 1024×1024.
- Click the `Select` button Figure 3.(3). The crosshair appears, click on the region of interest. The filed Figure 3.(2), will display the selected region. This step can be repeated until desired region is selected.
- Then satisfied with the selected subimage, click `Save` and `Close` buttons (Figure 3.(4)). This will save the selected subimage and close this window.
- Click the `Hough Transform` button (Figure 2.(2)). The "Hough Transform" window shown in Figure 4 will appear.
- Clicking on the `Load` button (Figure 4.(1)) the last selected subimage will be loaded and shown in (Figure 4.(2)).
- Now one has an option of selecting "Half degree step" (Figure 4.(3)). This will increase sensitivity as well as calculation time. It is not recommend to select this option during the first run. If the procedure, however, fails to detect orientations, one can select this option in a second run. Click the `Hough Transform` button. This is the longest computational step in the program. Upon completion, the Hough transform of the image will be displayed in (Figure 4.(4)).
- Click the `Save` and `Close` buttons to save the results and close the window (Figure 4.(5)).
- Click the `Analysis` button (Figure 2.(3)). The "Analysis" window shown in Figure 5 will appear.
- Click the `Load` button (Figure 5.(1)). This loads the previously saved information.
- Click the `Plot Image` button (Figure 5.(2)) to display the image under investigation.

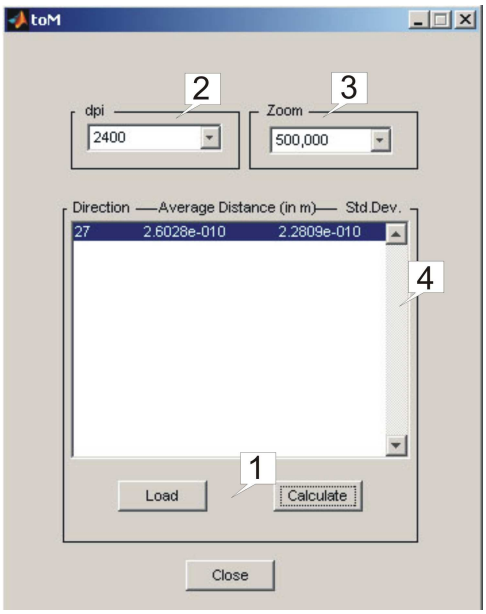

FIGURE 6. `Convert to meters` window.

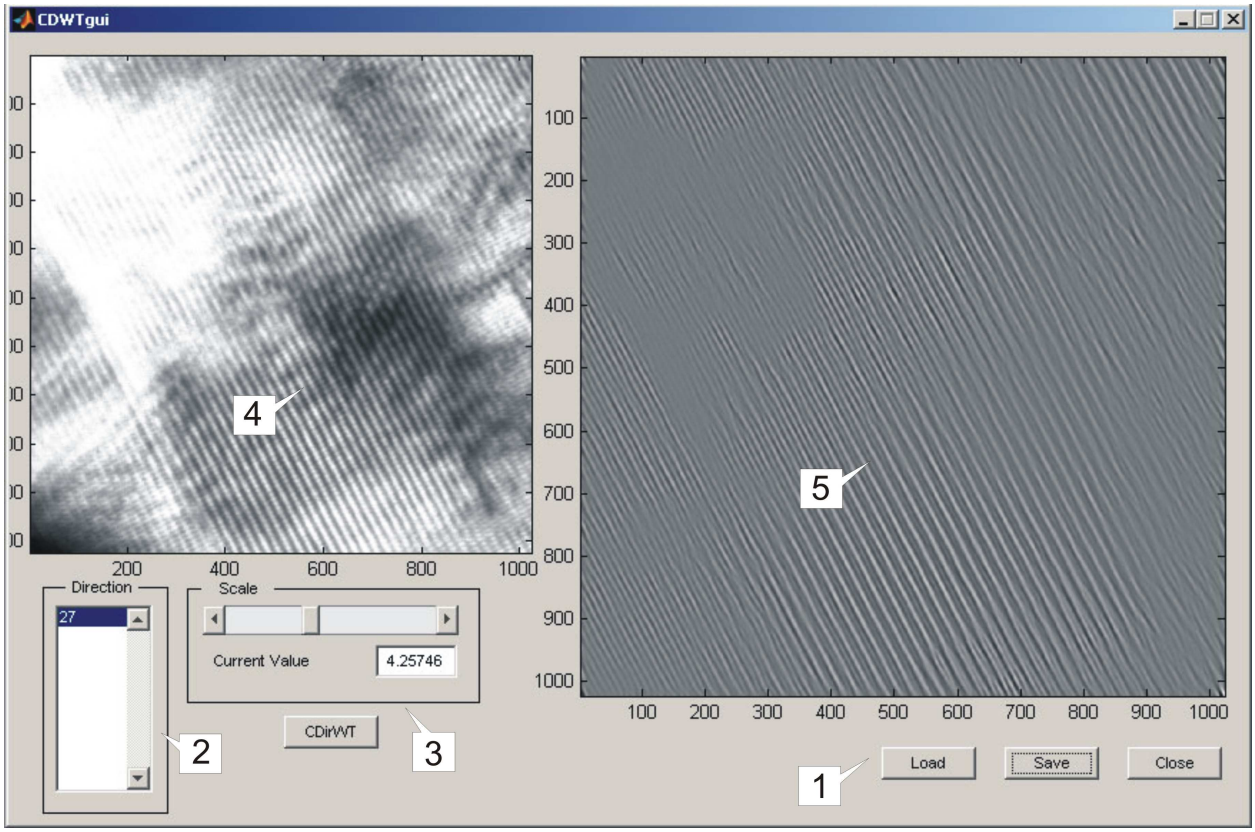

FIGURE 7. `CDWT` window.

- Click the `Detect` button (Figure 5.(4)). For the first run it is recommended to run the analysis with the default parameters. A graph will appear in Figure 5.(5) with circles representing detected angles . Information about

the detected angles, number of detected lines in each direction as well as the average distance between the lines of the same orientation will be listed in the "Results list" Figure 5.(6).

- One can select any detected direction and using the `Plot` button (Figure 5.(6)), draw all the lines of the selected direction. A graph which shows the distances (Figure 5.(8)) as well as the histogram of the distances (Figure 5.(9)) will also appear.
- One can change the controlled parameters in order to detect additional directions by sliding the bars or entering the parameter value manually (Figure 5.(3)). After changing the parameters, click the `Detect` button again.
- It is also possible to change the way average distance are calculated in the pop-up menu.Usual average, trimmed average (enter the lower and upper percentages for the trimming), or winsorized average can be calculated (Figure 5.(10)).
- When all desired orientation are found, it is recommended to improve the results by elimination of the close lines. The reason for this is that in the real life images the lines are almost never straight and always discontinuous. This creates the problem of close lines, when a single line generates several broken segments which are getting detected as several lines. This introduces large errors into the analysis of the distances between the lines. The elimination of the closes can be done in two steps. First select `Eliminate Close Lines` (Figure 5.(10)). Next, in a menu below select 3pix, 2pix or 1pix, and click the `Detect` button again. This step takes some time. It will through all detected lines of all detected directions, finding the lines with distances between which are less that 3 pixels, 2 pixel or 1 pixel, eliminating insignificant ones. This step significantly improves results.
- Close the window by clicking the `Close` button. It will automatically save information required for the next step.
- To conversion of distances from pixels to meters. Click the `Convert to meters` button (Figure 2.(4)). The "Convert to meters" window shown in Figure 6 will appear.
- Click the `Load` button (Figure 6.(1)).
- Select the resolution at which the image was originally scanned in the pop-up menu (Figure 6.(2)), and select the magnification of the microscope used (Figure 6.(3)).
- Click `Calculate` to get the results.
- The final step is CDWT, which stands for Continuous Directional Wavelet Transformation. This feature will help to see the structure of layers. Click the `CDWT` button (Figure 2.(5)).
- Click the `Load` button (Figure 7.(1)). The image under investigation will appear in Figure 6.(4)), as well as all detected directions in Figure 6.(2).
- Select the desired direction from the list (Figure 6.(2)). Select the scale of the wavelet transformation (Figure 6.(3)). The recommend the scale to is around 4-8.
- Click on the `CDirWT` button (Figure 6.(3)) to get the results. The filed in Figure 6.(5) will display the wavelet transformation along the specified direction.
- Click on the `Save` button, to save the results. The results will be saved in CWTDdata.mat file in `...\nsia\temp` folder.

5. COMMENTS

The following functions are from the WaveLab toolbox for the MATLAB.

Available at `http://www-stat.stanford.edu/~wavelab/`.

ancov.m, downdyadhi.m, downdyadlo.m, dyad.m, dyadlength.m, fwt_po.m, fwt_stat.m, fwt_ti.m, iconv.m iwt_po.m, iwt_stat.m lshift.m, makeonfilter.m, mirrorfilt.m, packet.m, reverse.m, rshift.m, shapeasrow.m, shapelike.m, ti2stat.m, updyadhi.m, updyadlo.m, upsample.m

And the following functions are from YAWTB toolbox.

Available at `http://www.fyma.ucl.ac.be/projects/yawtb/index.php`.

cauchy2d.m, cwt_2d.m, getopts.m, list_elem.m, yapuls.m, yawopts.m.

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