National Research Council

NRC·CNRC Canada

National Institute for Nanotechnology

qEELS

User Manual

Version 1.1

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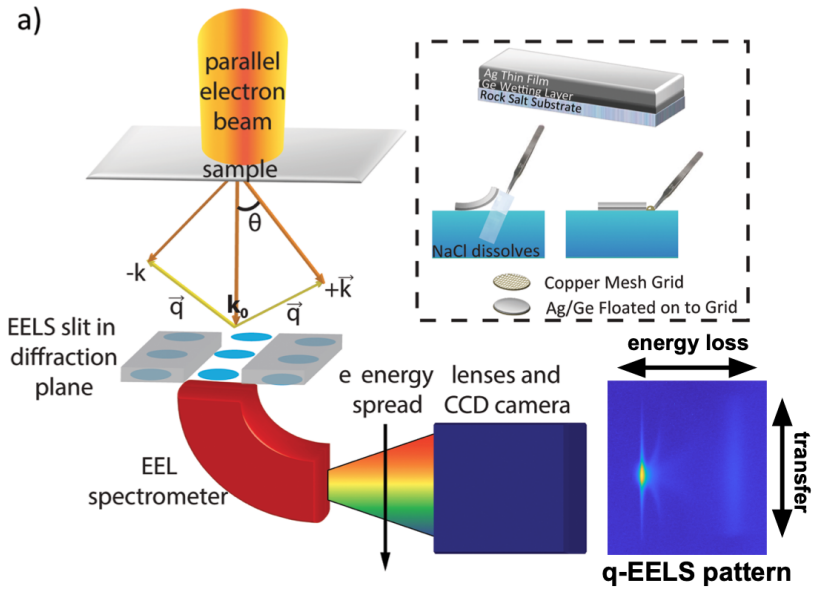
1. Introduction

qEELS is a software that was developed initially in MATLAB by Dr. Misa Hayashida with the National Research Council's National Institute for Nanotechnology at the University of Alberta. The software was translated to Python by students at the University of British Columbia.

1.1. Overview

Momentum-resolved electron energy loss spectroscopy (q-EELS) in a transmission electron microscope.



ACS Photonics 2017, 4, 4, 1009−1014

This software package calibrates energy loss axis (eV/pixel) and transfer axis (microrad/pixel) by fitting peaks of surface plasmon and bulk plasmon in q-EELS patterns. The results are downloadable in csv format.

1.2. User Groups

National Research Council of Canada nanotechnology researchers at the University of Alberta.

2. Getting Started

2.1. Licensing & Cautions

Note the following licenses associated with this software:
National Research Council of Canada :
https://nrc.canada.ca/en/research-development/intellectual-property-licensing
Python:
https://docs.python.org/3/license.html
Matplotlib:
https://matplotlib.org/stable/users/project/license.html
NumPy/SciPy:
https://numpy.org/doc/stable/license.html

When using this software, ensure to follow the National Research Council of Canada's Intellectual Property policy.

2.2. Set-up Considerations

The qEELS software uses tools that users need to download on their machine. If you want to download and run the software on your machine, you must verify that your machine has permission to download Python and batch files required. If you are unsure if your machine has permission, please contact your IT support service.

3. Installation Guide

Use the following guides to install qEELS on your Windows machine.

3.1. Windows Install

1. A compatible version of **Python** (Python >=3.9) must be installed.
    a. See: https://www.python.org/downloads/windows/
2. Extract the full source code to a folder on your machine.
    a. Go to the GitHub repository, and click the green button that says "Code" then **Download Zip.**
    b. Extract the zip file. (Unzip the file)
    c. See: https://github.com/UBCO-COSC-499-Summer-2022/matlab-to-python-application-translation-project2-nrc.git
3. Navigate into the **qEELS folder**.
4. Run the `install.py` file in the folder with Python. This installs the software.
    a. You can do this by right clicking on the file and click **with Python.**
5. Run the `main.py` file in the folder with Python. This runs the software.
    a. You can do this by right clicking on the file and click **with Python.**

3.2. Mac/Linux Install

1. A compatible version of Python (Python >=3.9) must be installed.
    a. Using a package manager such as `brew` or `apt` is recommended.
        i. `brew install python@3.9`
        ii. `sudo apt install python3.9`
2. Install supporting libraries for Tcl/Tk.
    a. `brew install python-tk`
    b. `sudo apt install python3-tk`
3. Extract the full source code to a folder on your machine.
    a. Go to the GitHub repository, and click the green button that says "Code," then click **Download Zip.**
    b. Go to the GitHub repository, and click the green button that says "Code" then **Download Zip.**
    c. Extract the zip file. (Unzip the file)
    d. See: https://github.com/UBCO-COSC-499-Summer-2022/matlab-to-python-application-translation-project2-nrc.git
4. Navigate into the **qEELS folder**.
5. Run the `install.py` file in the folder with Python. This installs the software.
    a. You can do this by right clicking on the file and click **with Python.**
6. Run its `main.py` file in the folder with Python. This runs the software.
    a. You can do this by right clicking on the file and click **with Python.**

3.3. Executables

The user can also run qEELS using an executable file (EXE file). Executables are easily run on Windows machines. Simply download the file onto your machine, double-click on the file in your directory, and the software will begin.

4. System Organization & Navigation

In the qEELS main window, there are two main areas; where the image is displayed and where the controls and results are. To the right of the window is where the image is displayed and to the left is where users will upload the image, select features, view results, and save.

The first step is to upload a **PRZ image** by clicking the **Upload Image** button. This button opens a popup window to upload the image into the software. The image will be displayed on the right. In the **Average Pixel, Micro rad/Pixel upper, Micro rad/Pixel lower,** and **EV/Pixel** boxes, the initial values will now be displayed.

Prerequisite: Images that are to be uploaded to this software should be formatted on your machine as "_____.prz." The image needs to be of a **q-EELS pattern** obtained from a transmission electron microscope.

To perform contrast adjustment on the image, use the **Contrast Adjustment** sliders. The **Contrast Min** slider adjusts the lightest areas in the image. The **Contrast Max** slider adjusts the darkest areas in the image. As contrast is adjusted, the results are shown in the image.

The next step is to indicate the **bulk plasmons** and **surface plasmons** on the image. First, select the pair of Bulk Plasmon points on the image. Select the **Bulk Plasmon 1** radio button and indicate its location by clicking on the image. Change the location by rec-clicking or adjusting manually in the **X** and **Y** boxes. After finishing, select the **Bulk Plasmon 2** radio button and indicate its location by clicking on the image. Change the location of the point by re-clicking or adjusting manually in the **X** and **Y** boxes. A box will appear going around these two points. Adjust the size of the box by typing the amount of pixels desired into the **Width** box. **Repeat** these steps for **Surface Plasmon Upper 1 and 2,** and again for **Surface Plasmon Lower 1 and 2**.

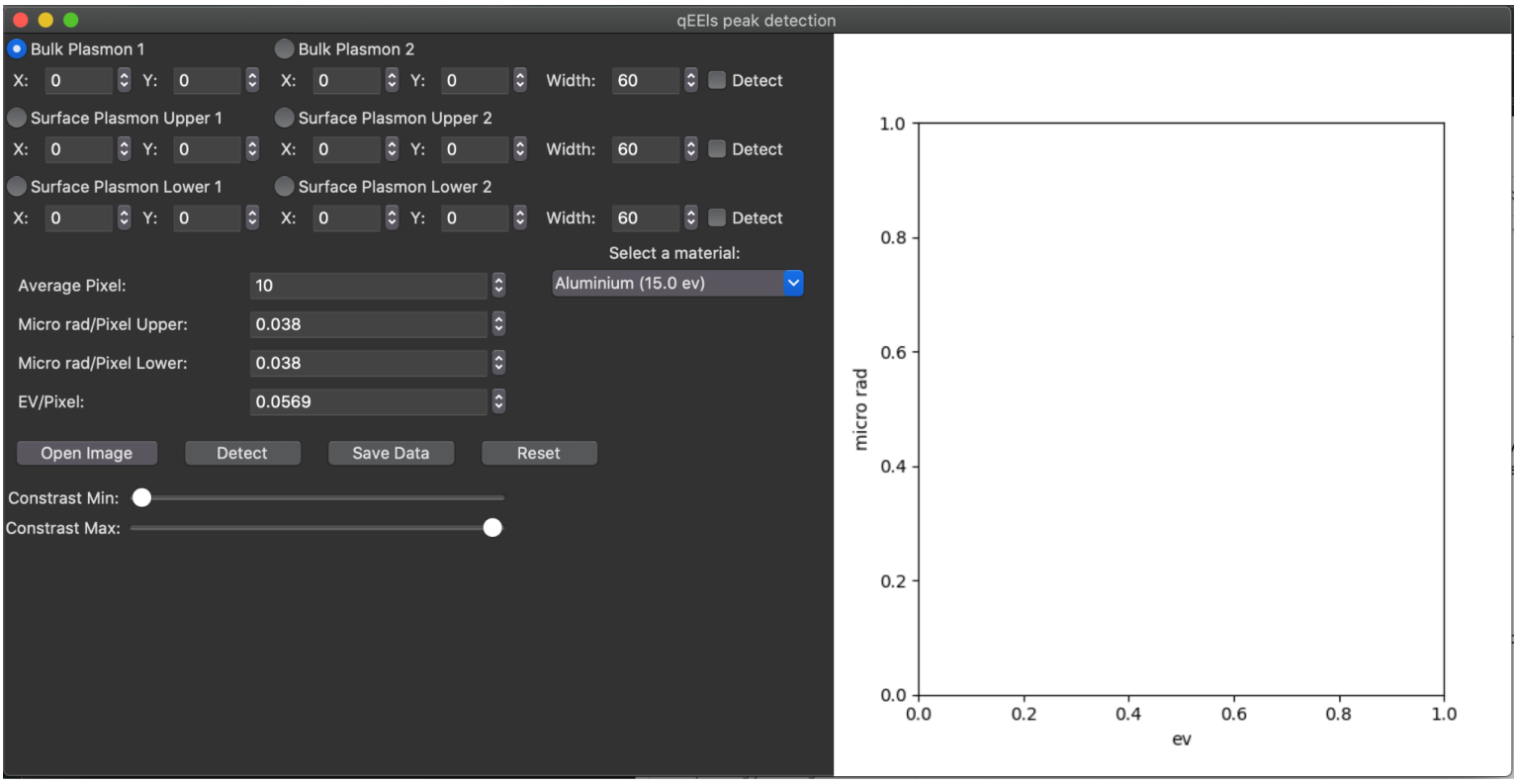
Indicate the material type using the **material type** listbox. The material type is the material that the image is measuring. Click on the material of the image from the list of 6 materials.

Now select which points to detect by selecting the **Detect** selection box to the right of each pair of points.

Now click the **Detect** button below. A diagram will appear where on the image, showing the calculated energy loss axis and transfer axis. In the **Average Pixel, Micro rad/Pixel upper, Micro rad/Pixel lower,** and **EV/Pixel boxes**, the results will now be displayed. Download the results in csv format by clicking the Save Data button. Restart the entire process using the **Reset** button.

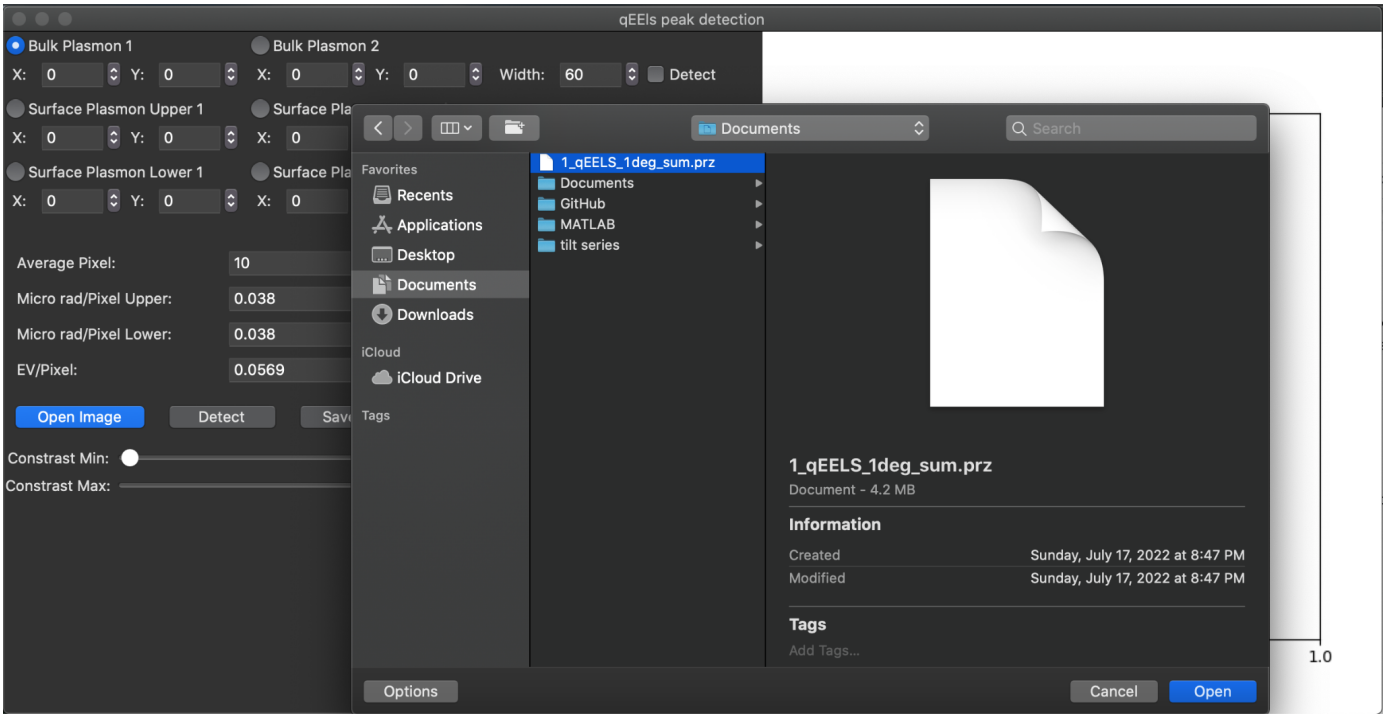
5. Step-by-Step Guide

The qEELS main window:

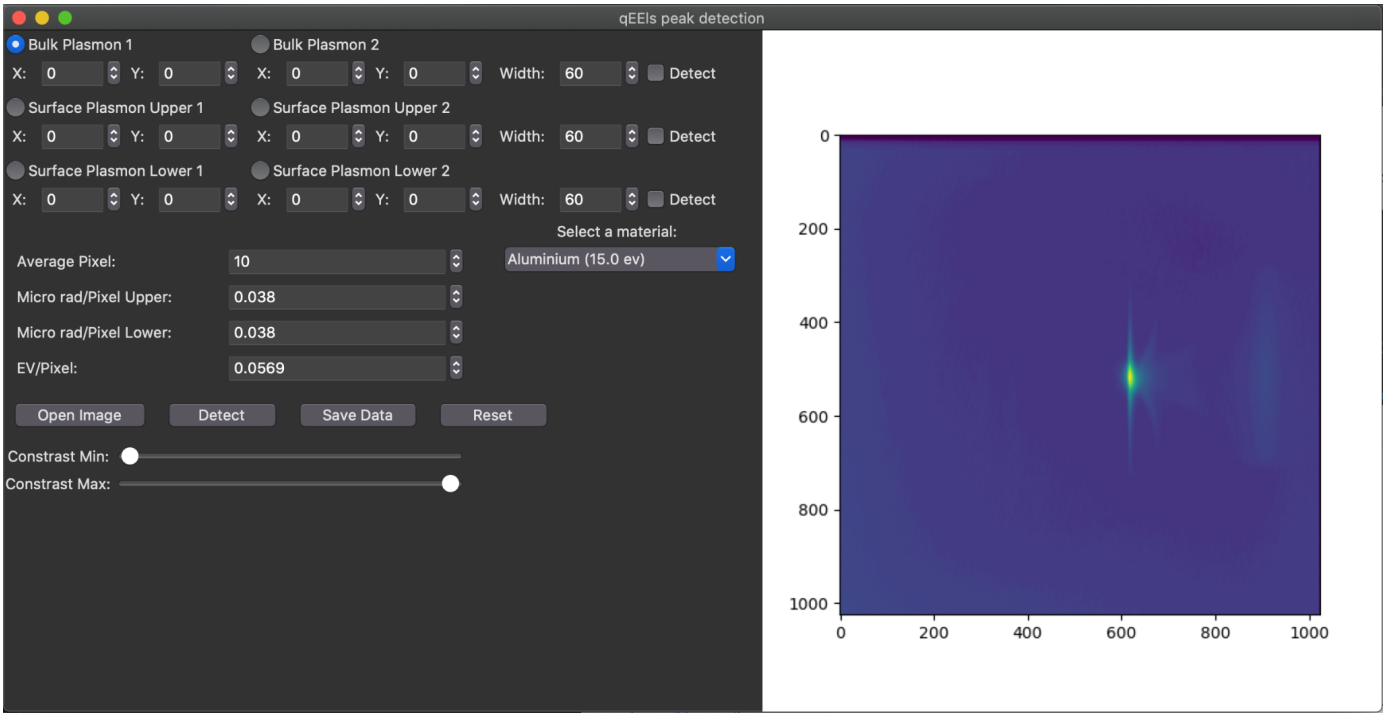


This is the qEELS main window. To the right is where the image is displayed and to the left is where users will upload the image, select features, view results, and save.

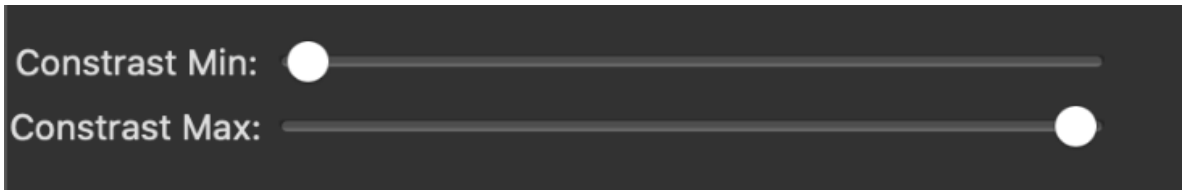
1. Uploading your image



1. Click on the **Open Image** button in the Main Window.
2. In the popup window, navigate to where the first image is stored on the device.
3. Click **open**. The image will appear in the Main Window.



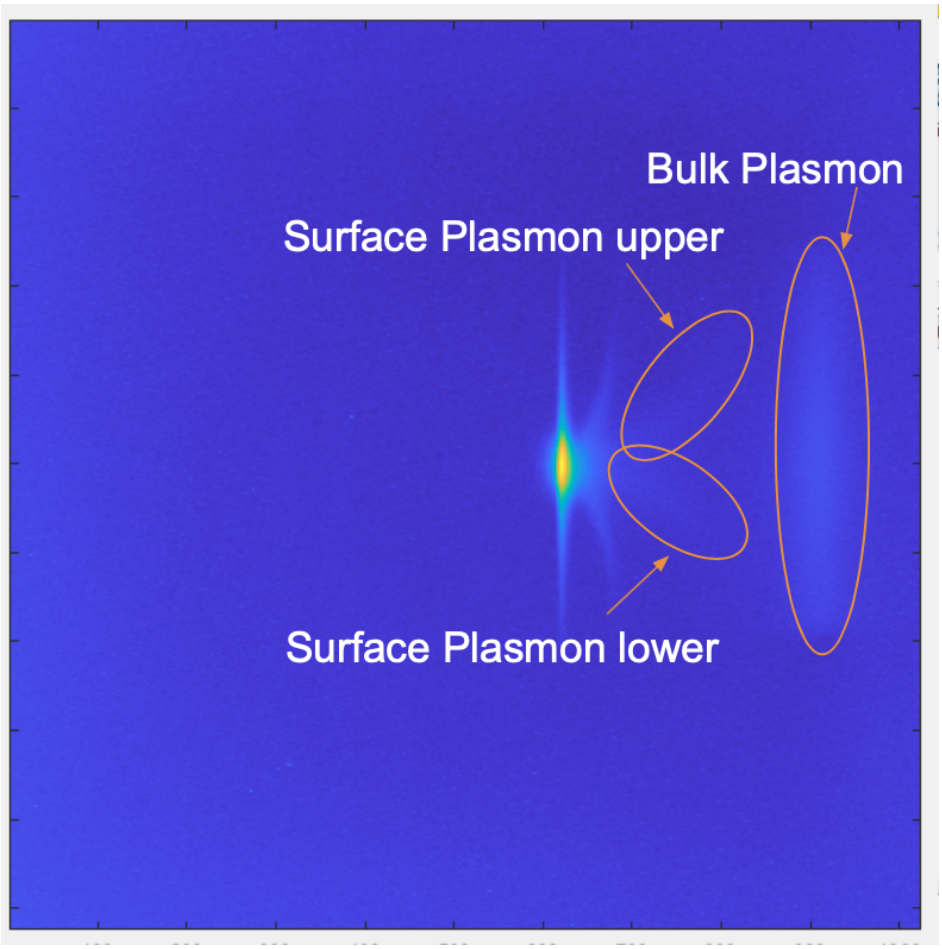
Perform Contrast Adjustment



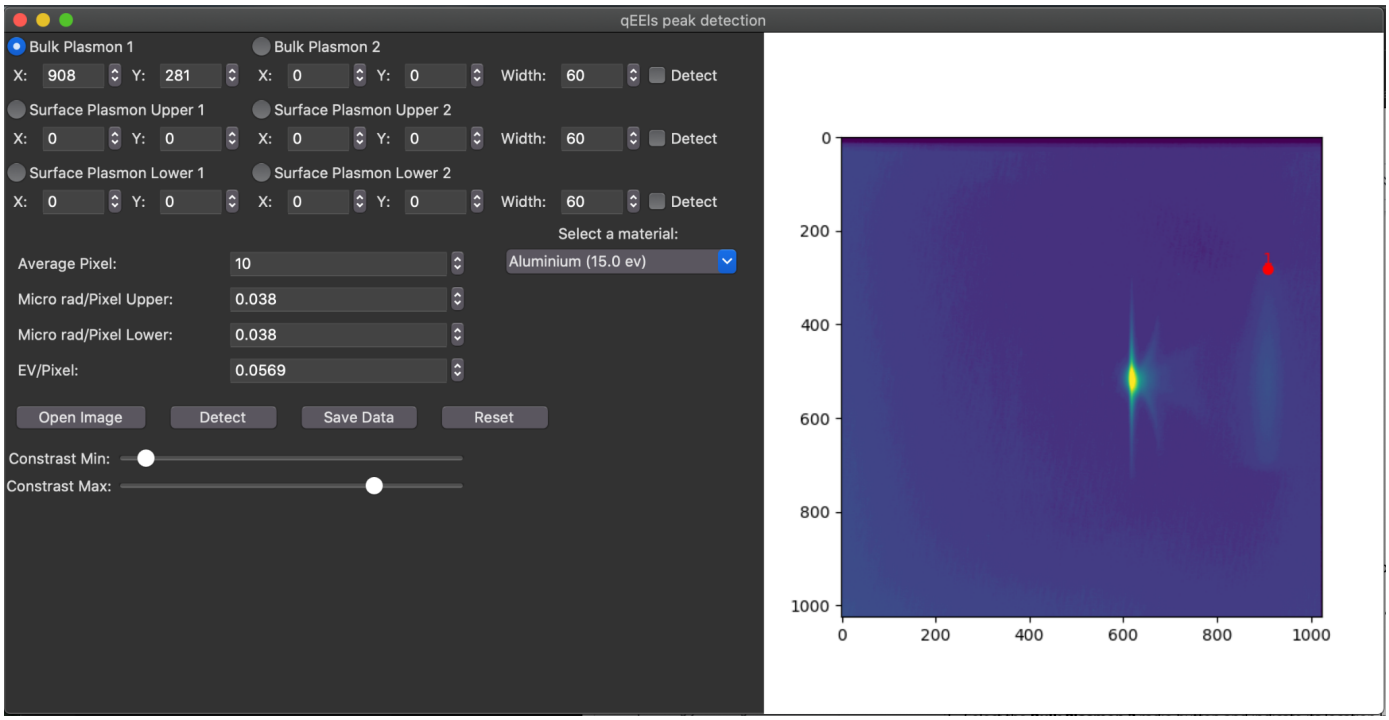
- Use these sliders to adjust contrast.

2. Indicate location of features

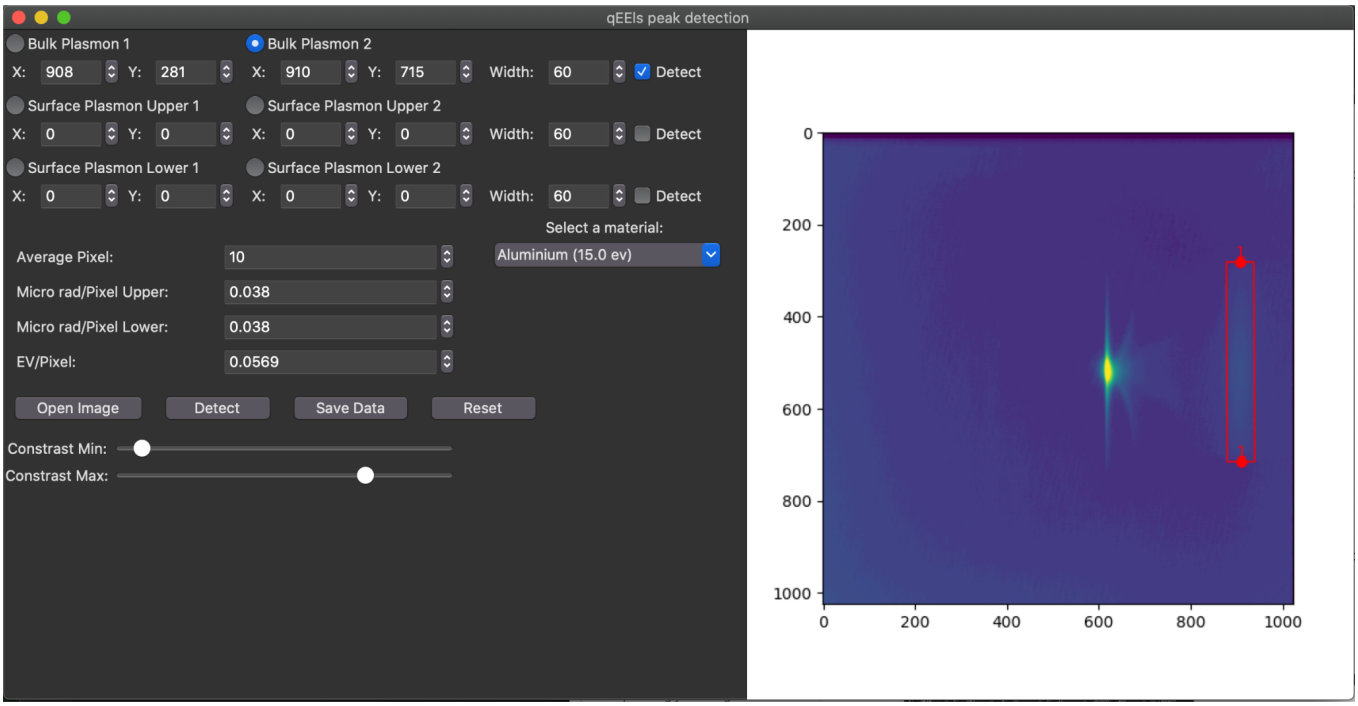
Purpose of this software is to detect peaks similar to in the displayed image:



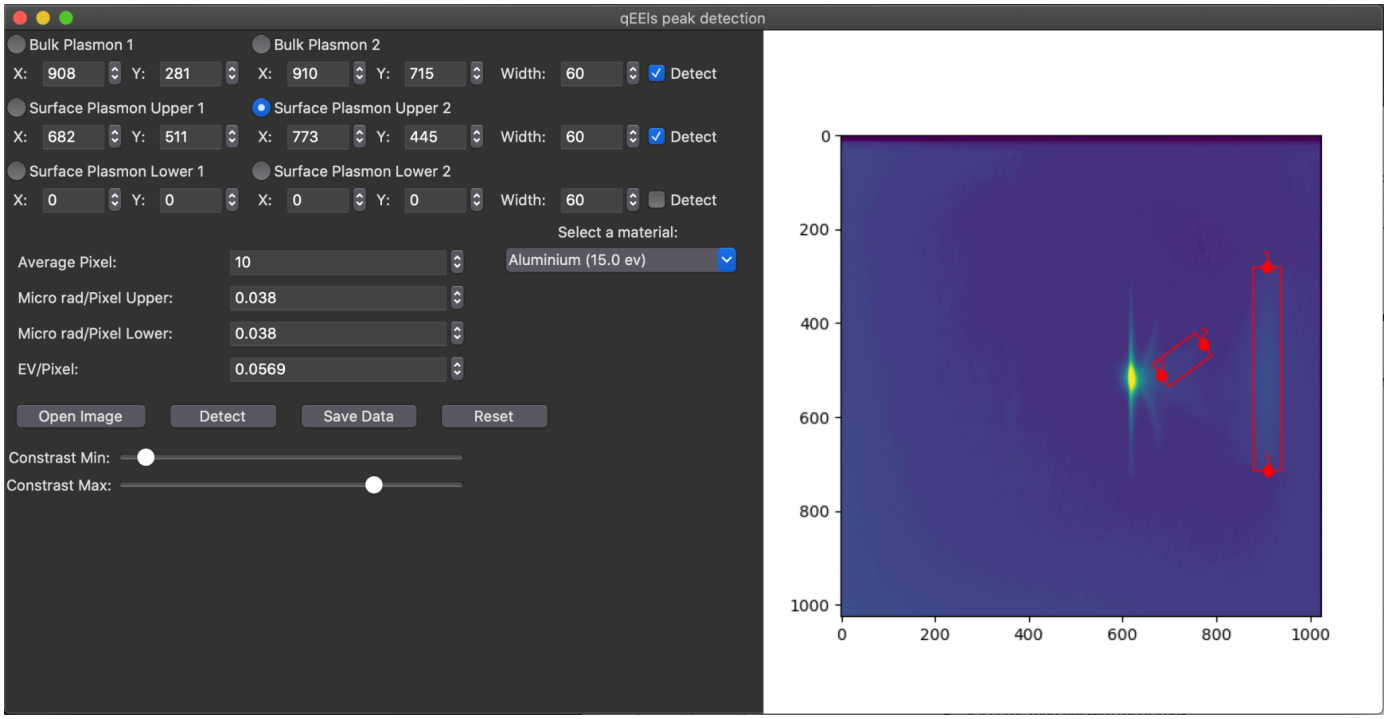
1. Select the **Bulk Plasmon 1** radio button and indicate its location by clicking on the image.
2. Change the location by rec-clicking or adjusting manually in the **X** and **Y** boxes.



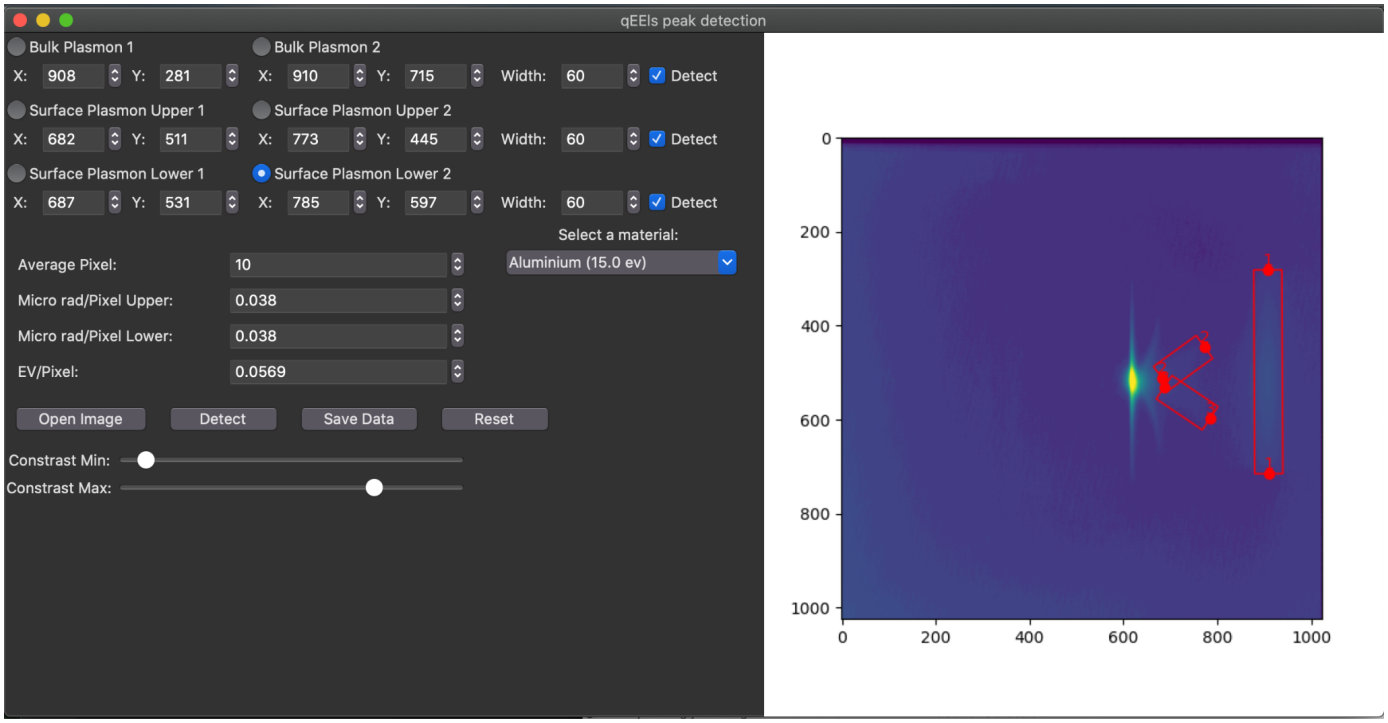
3. Select the **Bulk Plasmon 2** radio button and indicate its location by clicking on the image.
4. Change the location of the point by re-clicking or adjusting manually in the **X** and **Y** boxes.

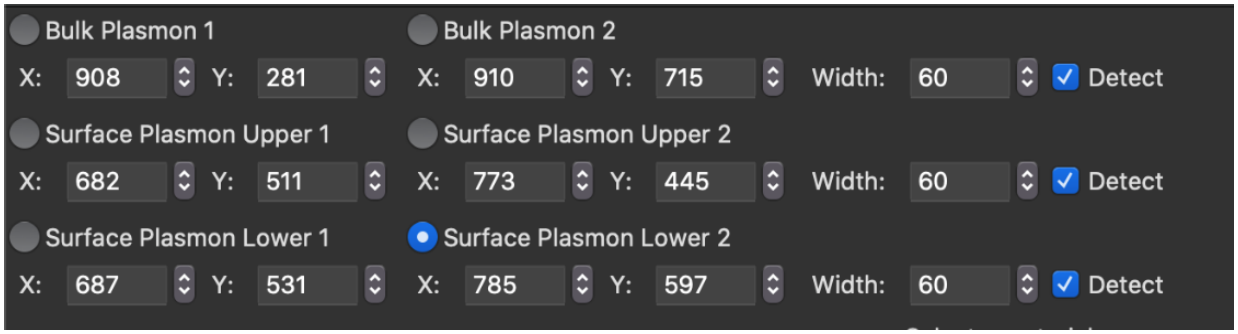


- Repeat these steps for surface plasmon upper 1 and surface plasmon upper 2:



- Repeat these steps for surface plasmon lower 1 and surface plasmon lower 2:



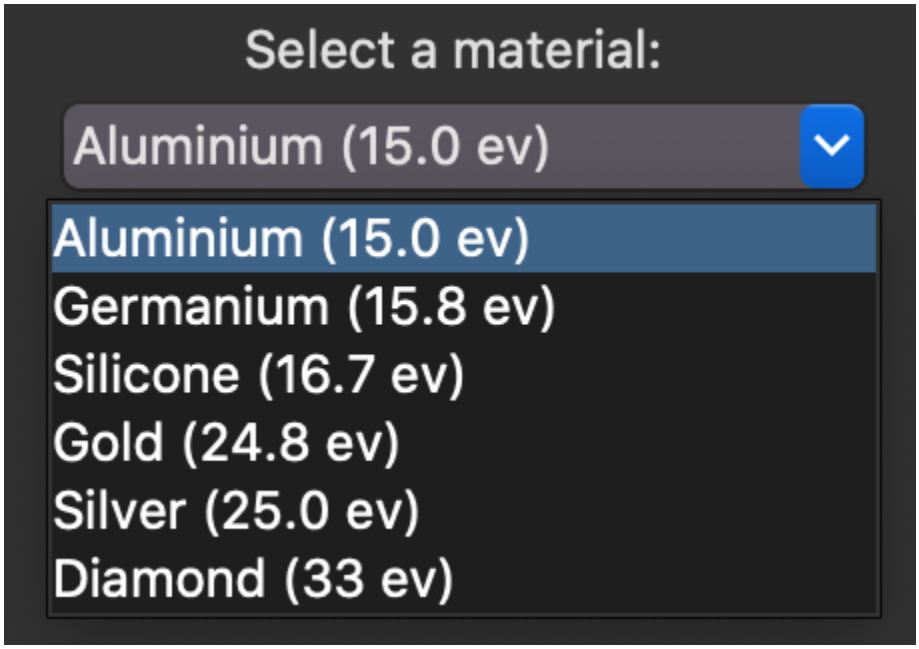


- Below each radio button, the **X and Y location** is displayed for the point selected on the image.
- Edit the X and Y of the point by typing into the box or using the up and down arrows.
- Adjust the size of the box drawn on the image using the **Width** box, type into the box or use the up and down arrows.
- The **Detect** selection box is used for selecting which pairs of points to calculate.

3. Detect fitted peaks

Material Selection

- Select the material with this drop down menu.

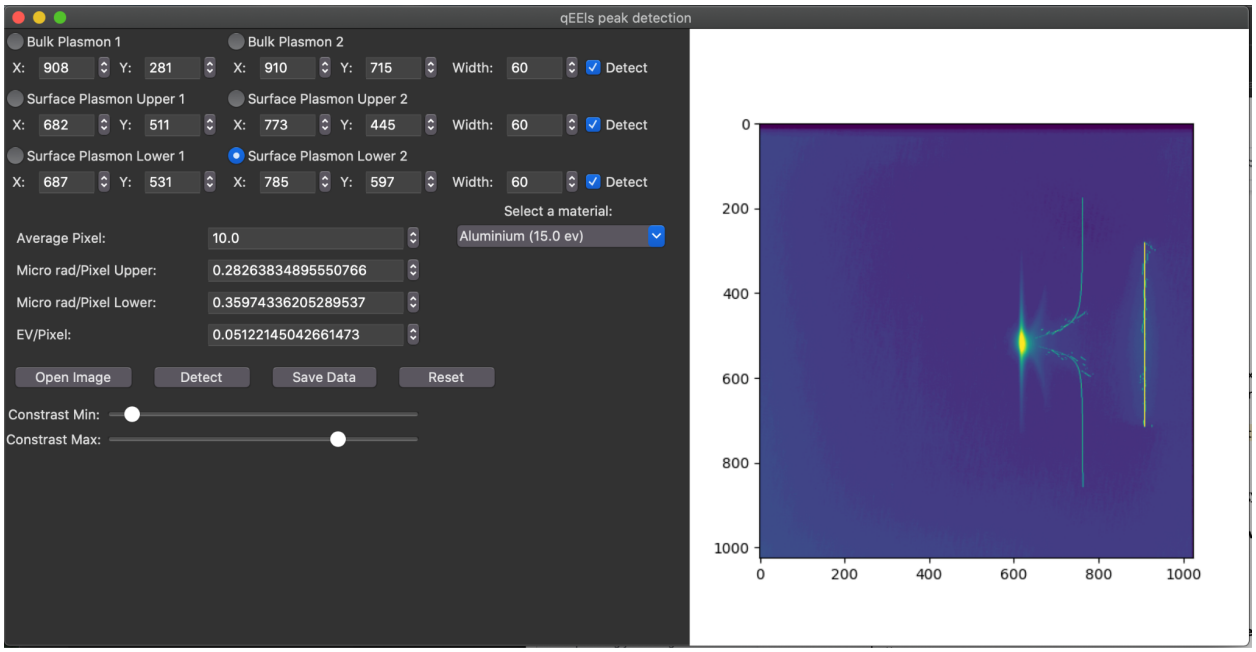


Detection

1. Select which points to detect by selecting the **Detect** selection boxes.
2. When ready for calculating detection, click the main **Detect** button.

4. Calibrated energy loss axis and transfer axis

- A diagram will appear on the image, showing the calculated energy loss axis and transfer axis.
- In the **Average Pixel, Micro rad/Pixel upper, Micro rad/Pixel lower,** and **EV/Pixel boxes**, the results are displayed.



- Download the results in csv format by clicking the **Save Data** button.
- Restart the entire process using the **Reset** button.

6. Troubleshooting and Support

6.1. Error Messages

- Incorrect Python version - Ensure that you have the correct Python version. There might have been an old version of Python already installed on your machine. In your Command Prompt, run:
    - `python --version`
- Python not installed in PATH - Ensure that Python is installed in the proper location on your machine. If the following runs and displays the correct version of Python, you have correctly installed it on your PATH variable. In your Command Prompt, run:
    - `python --version`
- Batch not running - Download the file on your machine and double-click on the file to start. If using Command Prompt, ensure that you are navigated to your batch file.

6.2. Support

If you are using qEELS and notice there are errors, inconsistencies, or need other additional assistance, please contact Dr. Misa Hayashida at the National Institute for Nanotechnology with the National Research Council of Canada at the University of Alberta.

Appendix A - Record of Changes

Record of Changes:

Version	Date DD/MM/YYYY	Author	Description of Changes
1.0	13/07/2022	Jasmine Mishra	Creation of User Manual.
1.1	14/08/2022	Jasmine Mishra	Finished adding all requirements

Appendix B - Notes to the Author

This document is a User Manual for qEELS. The final document should be delivered in an electronically searchable format. The manual should stand on its own with all elements explained for readers.

When modifying this document, the author should note that:

- When significant changes are made to the software, this document needs updating.
    - Note modifications made to this document in Appendix A.
- This document uses Open Sans font for accessibility and readability.
- Headings are left aligned, bolded, and size 18 font (except appendixes).
- There is a 12 font soft space between paragraphs and headings except Step-by-Step Guide.
- Keep consistent styling.