# DIST: Defect Analysis and Statistics Toolbox

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## Defects Matter

For any electronic device, controlling defects present in the material is crucial for understanding its properties.

***Atomic defects*** occur when atoms in the crystal structure are removed or displaced, or when impurities are present.

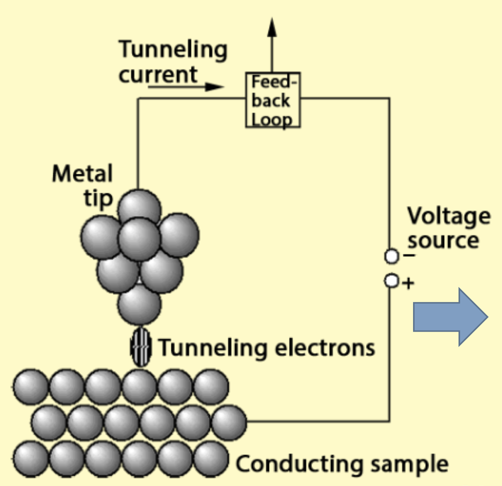
- Defects disrupt the crystal lattice, which alters how electrons propagate through a material. The conductivity of a material depends on its electron mobility.

***Single-layer (2D) Semiconductors***

- Many 2D semiconductors have high electron mobility, making them applicable for fast transistors.
- Defects have a greater effect on the properties of single-layer materials.
- Knowing how defects alter the electronic properties of a material allows us to develop methods for tailoring 2D materials.

### How do we characterize defects?

- **Scanning Tunneling Microscopy** (STM) generates atomically resolved images of the surfaces of materials.

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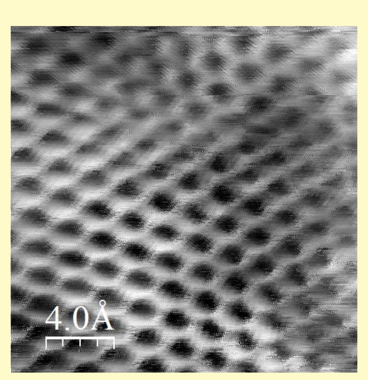


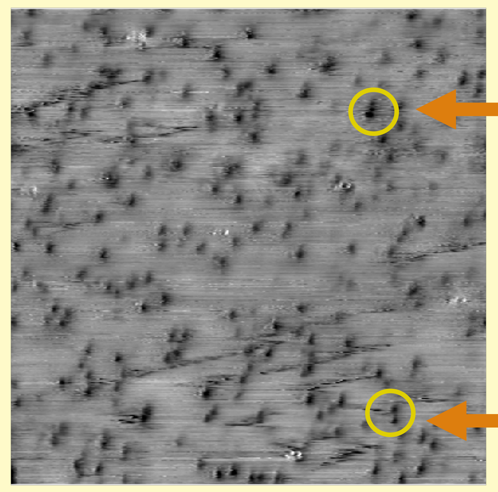

***Above:*** *STM image of graphene. The hexagonal lattice structure is clear in this image. Dark spots indicate places with no atoms.*

***Left:*** *STM image of MoTe2. The large white circles and small black dots are two types of atomic defects. The spots occur because of changes in the charge density on the sample.*

**Using STM images, we can characterize defects in a sample by counting them and calculating their shape, size, and height in the material.**

## The Challenge!

***How long would it take you to count all the black dots in this STM image? What if you had to count them in 20 images?***



All of these are atomic defects we care about analyzing!

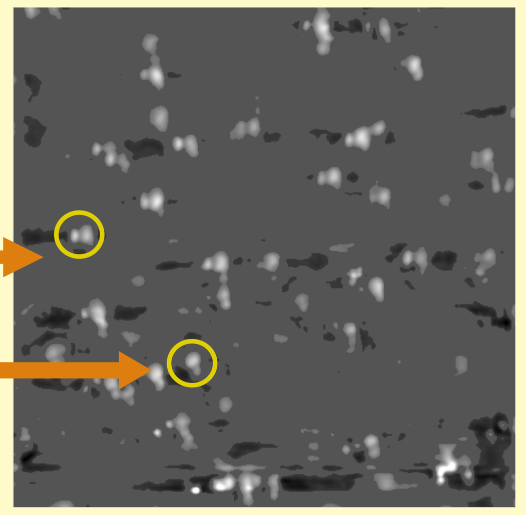
***DIST processes images to make defects stand out, and automatically identifies and locates them.***

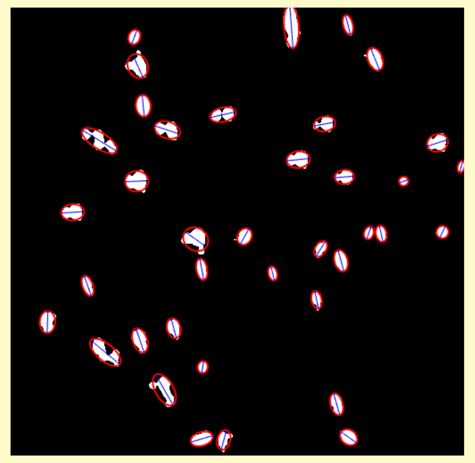
***How long would it take now?***

The defects are much more obvious against a uniform background.

***Could you calculate the precise orientation of all the dumbbell shapes in this image?***

These two defects have the same shape but are pointing in different directions.





***DIST isolates identified defects to automatically compute statistics like shape, orientation, and area.***

## Our Approach

**Start:** Raw image **(1)**

Reduce background noise **(2)**

Add height-based contours **(3)**

Filter contours/shape matching **(4)**

Identify defects **(5)**

Allow user correction **(6)**

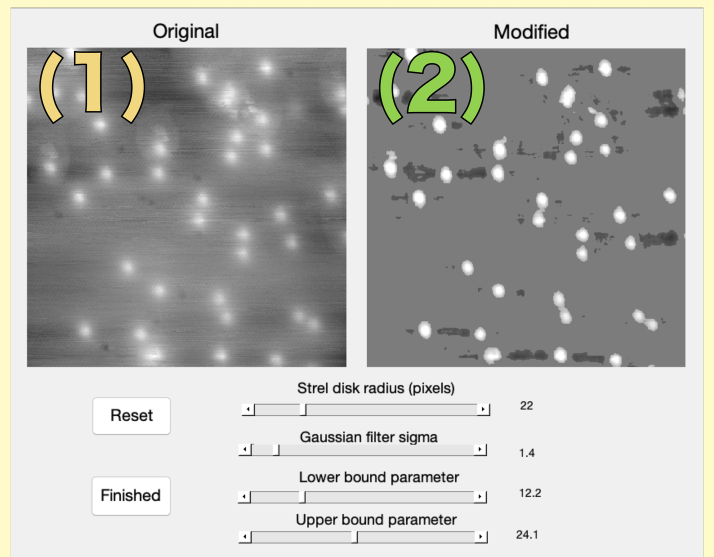
**End:** Output defect statistics **(7)**

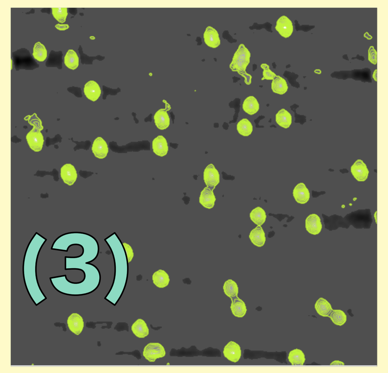
## DIST Development

- Needed a way to automatically identify and analyze defects in STM images.
- Used MATLAB's built-in contour generation function to isolate bright and dark extrema.
- Wrote algorithms to reduce background noise, filter contours, and compare shapes of different defects.
- Challenge: each image is different and requires different processing depending on the size and density of defects.

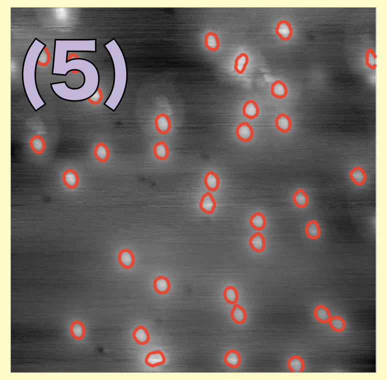
**Right:** Solution to background noise.

- Created a user interface that allows for flexible processing
- Sliders make for fast and easy alterations
- Processed image updates as you change the settings
- **Lower and upper parameters** determine the range of pixel values that are set to the mean pixel value of the image.

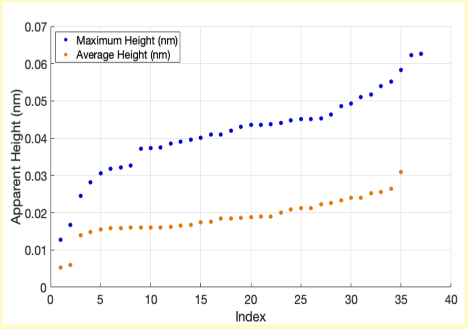


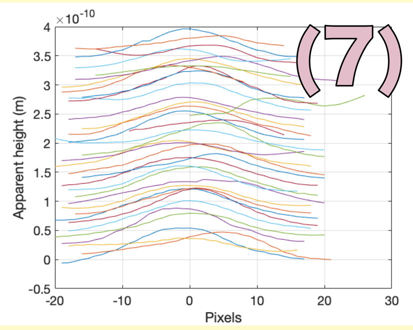




**Left:** User decides on bright or dark defects, then contours are generated around all the extrema




**Left:** The contours remaining after shape comparison and filtering are the identified defects. The user can add or delete contours that were incorrectly identified.



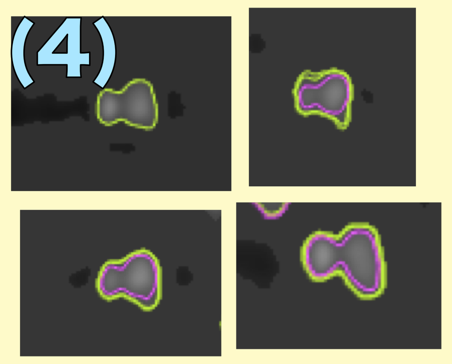




**Left:** Line profiles from identified defects. Each line represents a cross section of a defect.

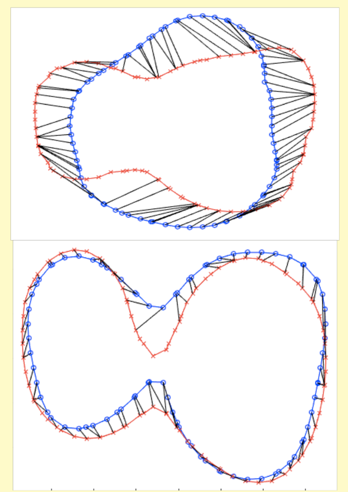
**Right:** Plot of apparent heights of defects. Apparent height data tells the user how deep in the material the defects are.

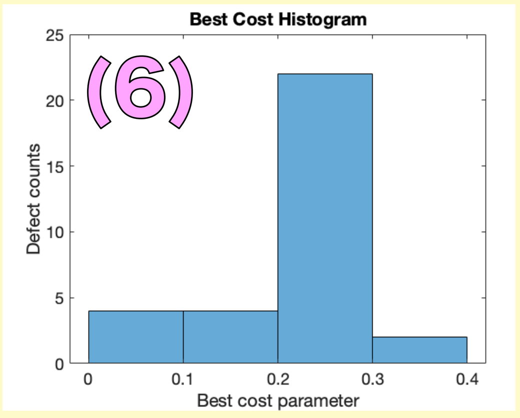
## Advanced Features

**Top left:** user-selected template contour. The purple plots indicate the best-matching shape out of a group of (green) nested contours.




**Right:** the template shape (red) is being compared to a second shape (blue). The lines indicate the distance between matching vertices of the contours.






**Above:** histogram of results of shape-matching. Y-axis is defect count. Lower values on the x-axis indicate a better similarity factor between template and contour. From here a user can filter defects based on shape similarity.

## Future Work

Moving forward, we will transfer the entirety of the program into a MATLAB GUI (as seen under *DIST Development*). We will also be improving the program's generality, so that it can be used with images outside of STM.

MATLAB has included some new region-of-interest (ROI) features and tools that may aid in isolating defects in images and shape comparisons. We hope to implement the changes to make the toolbox smoother and easier to use. Additionally, we are going to implement batch-processing features for analysis of multiple images at once.

**References**

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[2] Das Sarma, S., Adam, S., et al. (2011). Electronic transport in two- dimensional graphene. *Reviews of Modern Physics*, *83*(2), 407–470. https://doi.org/10.1103/RevModPhys.83.407
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[4] O. van Kaick, G. Hamarneh, H. Zhang, P. Wighton "Contour Correspondence via Ant Colony Optimization" (Pacific Graphics 2007), pp. 271-280, 2007. http://dx.doi.org/10.1109/PG.2007.56