Systematic Quantitative Characterization of Surface Nanostructures by Scanning Probe Microscopy of Thin-Films

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ABSTRACT

In this paper we present a new methodology to characterize surface nanostructures of thin films. The methodology focuses on isolating nanostructures and extracting quantitative information such as their shape and size. This methodology employs two distinct approaches. The first, which we call the overlay approach, proceeds by systematically considering the data rasters that constitute the scanning probe image in both vertical and horizontal directions. The second approach, based on Fuzzy Logic, relies on a Fuzzy Inference Engine to classify the surface points. Once classified, these points are then clustered into surface structures. We have applied both approaches to characterize organic semiconductor thin films deposited on various substrates. In this paper we present results based on Atomic Force Microscopy (AFM) data of pentacene films deposited on mica and characterized by both methods. The present results are discussed and compared along with the challenges of the two approaches.

Keywords: fuzzy logic, atomic force microscopy, characterization, nanostructures.

1 INTRODUCTION

Advanced characterization techniques are becoming increasingly important especially at the nanoscale. Conventional characterization methods focus on computing statistical metrics of the whole surface such as RMS, surface roughness, average height, etc. [1, 2]. However, these methods typically lack the ability to identify surface features with adequate precision. For instance, the Laplacian technique is useful at identifying the edges of surface structures but the resulting image often does not correlate well with the surface morphology as evident upon visual inspection [3]. Still other common surface analysis techniques require intervention in the form of a threshold value, thus introducing a potential source of error in the analysis.

In order to characterize a surface precisely, it is essential to recognize individual surface features and structures [4]. We have developed a generally applicable methodology that is able to isolate individual surface structures and then collect statistical information about each of them. The methodology can be achieved by two approaches. In the overlay approach we consider the height and derived gradient data in the horizontal and the vertical directions separately. The two sets of the intermediate classification data from the previous step are overlaid to form a complete representation of the surface. The second approach uses a Fuzzy Inference Engine (FIE) to classify each of the surface points. These points are then clustered into structures based on the FIE output. Both of our approaches are independent of feature size, and do not require any data-dependent threshold. Furthermore, both can be extended to process other types of Scanning Probe Microscopy (SPM) measurements.

2 THE OVERLAY APPROACH

The first approach we consider is based on processing height and slope data along the scan lines and in the direction perpendicular to them separately. This enables the identification of features such as up-hills, down-hills and flat areas (bottoms and tops) in each direction [4]. The data for this processing are then overlaid to develop a more concrete classification of areas. Finally, a clustering algorithm sweeps the data to organize neighboring structure points into structures.

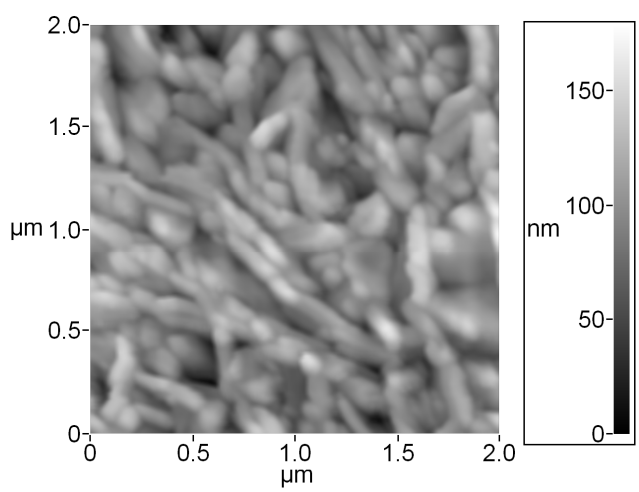

Figure 1: Image of pentacene on mica substrate.

2.1 Data Filtering & Trend Extraction

AFM Data are typically noisy, so a separate noise reduction step is necessary. We do this by using a moving-average filter, once vertically and then horizontally. This will capture the main trend on the surface. After the filtering step, two data sets are constructed by extracting the slope information in both dimensions, which identifies flat areas in each dimension.

2.2 Flat Points & Regions Identification

At this stage of analysis we identify all flat areas. We define flatness by requiring that the point-to-point variation does not exceed a small cutoff angle. All flats correspond to either tops of structures, or valleys between structures, as shown in Fig. 3a. Next, we find the average slope for the areas marked as non-Flat. Using that information we can decide whether the scan line is going upward or downward. Flats falling after a downhill are not considered to be part of any structure. Flats coming after an uphill will be recognized as part of the structure, which we augment to include half of the uphill before and half of the down hill after. We use this range of expansion to approximate the actual structure size. The points so identified we call Potential Structure Points (PSP), as shown in Fig. 3b.

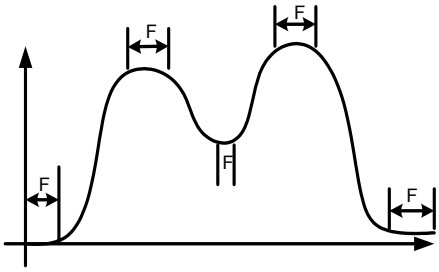

Figure 3a: Flat areas identified in each direction.

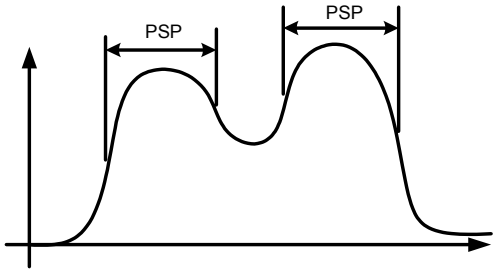

Figure 3b: Potential Structures Points (PSPs) in each direction.

2.3 Merge Horizontal & Vertical Data

Continuing, we merge the horizontal and vertical data together. Only points that are recognized in both directions as Potential Structure Points (PSPs) are regarded to be Structure Points (SPs), as shown in Fig. 4.

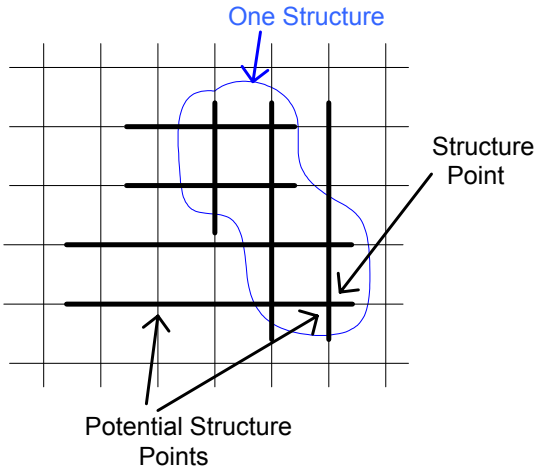

Figure 4: Overlaying vertical and horizontal data.

2.4 Points Grouping

Once data points are recognized as Structure Points (SPs), we sweep the grid to group neighboring SPs assigning an identifier unique for each structure, as shown in Fig. 5. This allows us to compute the area of each structure by counting its constituent SPs. We can also characterize the expanse of the structure by constructing an encompassing envelope, shown by the red border in Fig, 5.

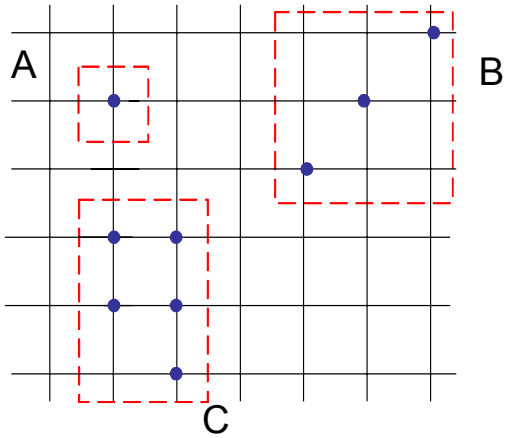

Figure 5: Grouping neighboring points into a structure. A, B, and C are the unique identifiers corresponding to the three structures shown.

3 THE FUZZY LOGIC APPROACH

In order to eliminate the need for data-dependent filtering and other arbitrary intervention we developed an alternative approach that employs a Mamdani fuzzy logic system to classify the surface points. This approach carries with it the advantage of being inherently insensitive to anomalous data. The inputs to the fuzzy system are the

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height and derived gradient information available for each point in the data set, while the output of the system is a topographical categorization of each point, as shown in Fig. 6. The fuzzy rule set decides the category of each point based on the membership of the current point and its surrounding neighbors. This allows them to be classified as part of either an uphill, downhill, top, or bottom. Once the tops are identified, we employ the series of steps described below to reconstruct the surface structures.

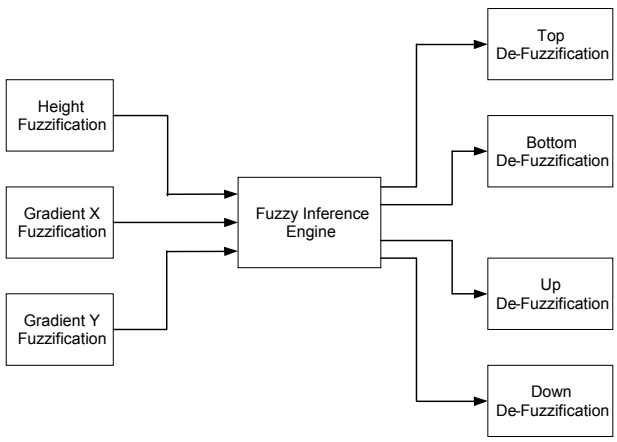

Figure 6: A block diagram for the fuzzy engine.

3.1 Points Classification Engine

The height (H), the gradient in the horizontal direction (G_x) and that in the vertical direction (G_y), are fuzzified based on different membership functions. For H we have three membership functions, viz., Large, Medium & Small. Similarly, for G_x and G_y, there are also three membership functions -Positive, Negative and Zero. The data are processed by determining the membership of each point in these three input classes prior to being passed to the FIE.

The FIE consists of an embedded a set of rules that classify each point into four output variables. The result of applying the rules contained in the FIE is a membership ranking of each point in each of the output variables.

These results are aggregated and de-fuzzified using a True-False membership function. The variable with the largest membership ranking will determine the classification of the current point.

3.2 Clustering of Tops of Structures

Once individual points are classified, the tops of structures are clustered based on their proximity to each other. In Fig. 7, each structure top is distinguished by a randomly assigned color. Due to artifacts in the measurement and the fuzzy nature of the algorithm, false tops appear. For this particular specimen which is 2µm x 2µm, tops of size less than 15 nm x 20 nm are considered to be clearly anomalous and are thus removed, as illustrated in Fig. 8.

The size of the tops that we removed is not determined by the physical size, rather is chosen relative to the specimen size.

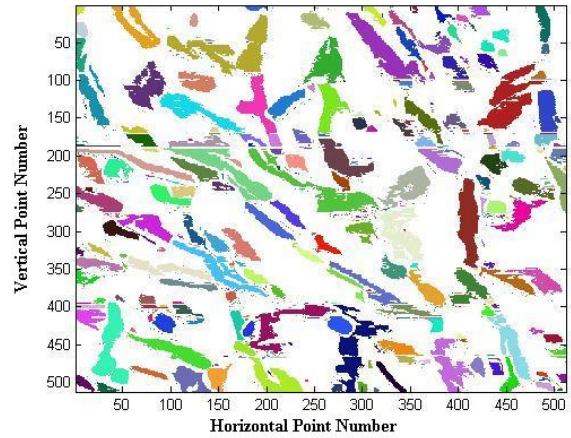

Figure 7: Top points clustered to show tops of structures using the 2 µm x 2 µm scan shown in Fig. 1.

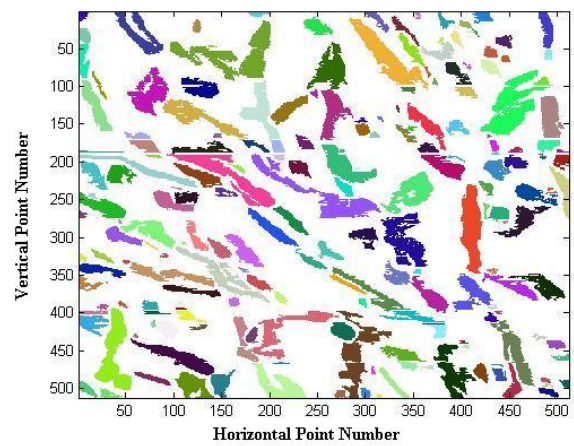

Figure 8: Tops of structures with anomalous tops removed using the 2 µm x 2 µm scan shown in Fig. 1.

3.3 Linking of Uphill and Downhill Points

In the previous step we have clustered the tops of the structures. Now, we are left with points that are classified as bottom, uphill and downhill points. While the bottom points are not considered to be associated with any structure, the uphill and downhill points must be linked. The linking algorithm searches in all four grid directions to find the closest structure top. While searching, if a bottom is encountered before reaching a top, then that direction is not pursued as a possible direction to link to. Among the remaining directions the one which has the shortest distance

to the top will be selected. Thus, each point will be linked to one of its neighboring points, leading to the closest top. However, if a point is surrounded by bottoms from all directions, that point will not be connected to any other point.

3.4 Structure Growth

Now that the algorithm has identified tops, grouped them together, disregarded bottoms, and linked up- and down hills, next, the data are swept to group those links which lead to a top. Once such a chain of links is found, we follow the path of the chain till it terminates at the top and associate this chain with that particular top.

4 RESULTS

Previously in this paper we have described two distinct approaches for characterizing nanostructured thin films. In this section we compare the results obtained using each of these approaches.

Figure 10 shows the concluding results obtained using the overlay approach and Fig. 11 shows those for the Fuzzy Logic approach. In both figures, each individual surface structure is assigned a randomly generated color to distinguish it from surrounding structures. A close comparison of these two figures and the original AFM data in Fig.1 makes it evident that the Fuzzy Logic approach can isolate structures without blurring together multiple structures. Furthermore, the Fuzzy Logic approach is robust to entire classes of data anomalies, such as the raster discontinuities which frequently occur due to substrate hysteresis or to instrument vibration.

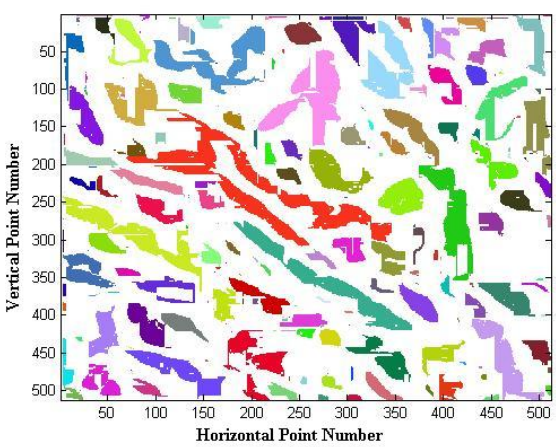

Figure 10: Structures recognized using the overlay approach for the 2 µm x 2 µm scan shown in Fig. 1.

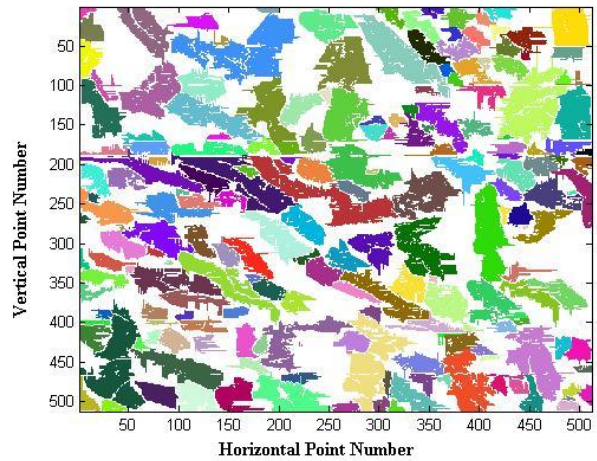

Figure 11: Structures recognized using the fuzzy logic approach for the 2 µm x 2 µm scan shown in Fig. 1.

5 CONCLUSION

In conclusion, we have presented the development and results of two approaches to analyze surface nanostructures. Both of the approaches developed are independent of the shape and size of the surface features. We have applied these two approaches to analyze AFM data for nanostructured thin films and demonstrated fast and precise recognition of different types of structures. A comparison of the results obtained employing the two approaches reveals that the Fuzzy Logic approach yields more precise structure boundaries.

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