Generative Topographical Interpretation of AFM Data

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Abstract

Atomic Force Microscopy (AFM) provides unprecedented access to the topography of nanomaterials, **(Binnig et al., 1986)** yet raw data often suffers from sensor artifacts and high-frequency noise, necessitating manual analysis. This report talks about "Nano-Constellations," an automated computer vision pipeline designed to treat atomic peaks as a "stellar map." By implementing asymmetric cropping to eliminate edge-noise and utilizing Delaunay Triangulation for structural reconstruction, we transform raw TiO_2 intensity data into a 3D geometric web. The results demonstrate a high-fidelity 3D reconstruction that allows for perspective flipping and real-time visualization of interatomic strain. This insight provides a scalable alternative to commercial software for high-throughput semiconductor quality control.

Methods

The computational workflow for the Nano-Constellation pipeline was developed using Python's scientific stack, with image processing implemented via scikit-image (**Vander Walt et al., 2014**). The process is divided into three distinct phases:

Image Pre-processing and Asymmetric Normalization

Raw AFM scans of TiO_2 surfaces frequently exhibit "border artifacts," characterized by high-intensity sensor saturation (the "yellow wall") on the right-hand margin. To ensure peak detection accuracy, an asymmetric crop was applied, Horizontal Axis: 5% removed from the left, 15% removed from the right and Vertical Axis: 5% removed from the top, 10% removed from the bottom. The remaining data was normalized using Min-Max scaling to a range of [0,1] and enhanced via contrast-limited adaptive histogram equalization to distinguish subtle atomic peaks from the background substrate.

Feature Extraction (The "Stellar" Localization)

Individual atomic positions were identified using a peak local maxima algorithm. To account for the physical size of the TiO_2 atoms, a minimum distance constraint (dmin =15 pixels) was enforced to prevent redundant detections. The coordinates (x,y) of these features serve as the nodes for the subsequent geometric mapping.

Geometric Lattice Reconstruction (Delaunay Triangulation)

To understand the physics of the crystal surface, we utilized **Delaunay Triangulation**. This ensures that for every set of three atoms, the circumcircle of the resulting triangle is empty of other points.(**Delaunay B., 1934**)

Results and Discussion

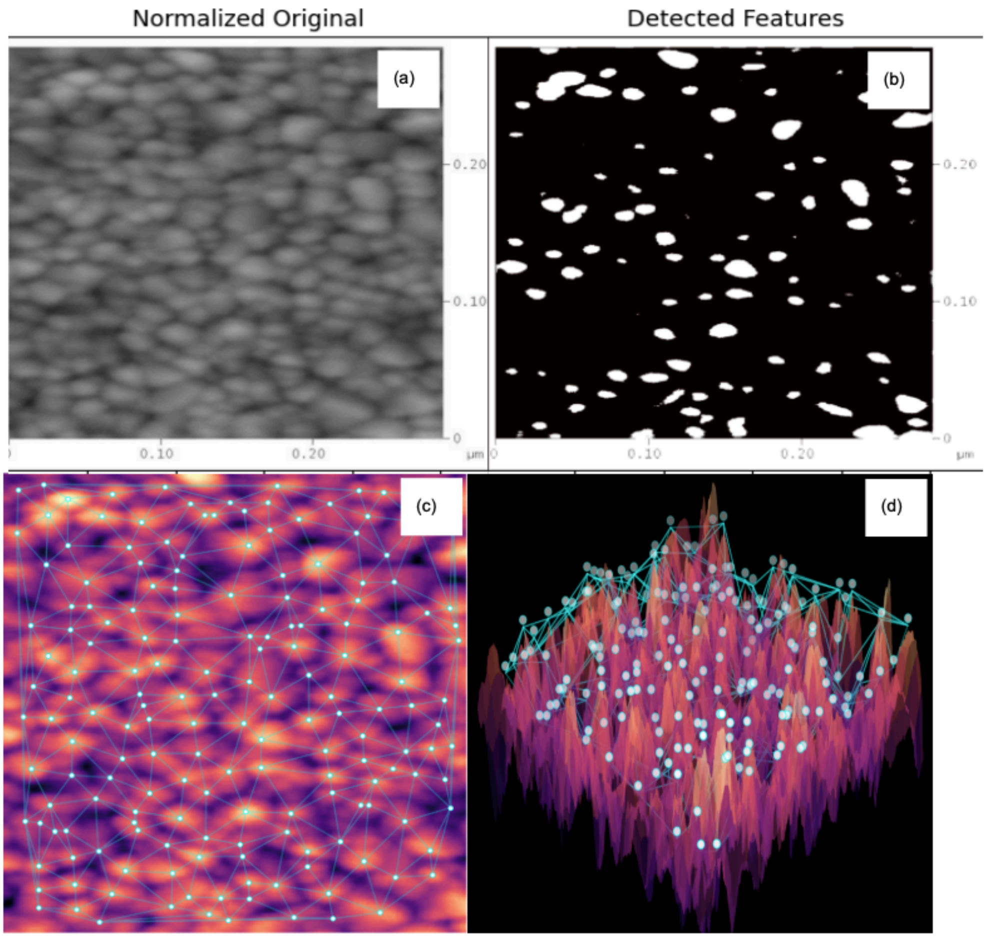

Figure 1: Multimodal Surface Analysis. (a) Normalized scan; (b) features detection; (c) Geometric lattice mesh; (d) 3D topographic view.
Using Interpretable data Figure 1 shows (a) is the original TiO_2 AFM image, (b) are the individual bright spots identified by the peak_local_max function on the processed image. Each white dot corresponds to a detected TiO_2 particle or a high-intensity site on the surface. The Nano-Constellation pipeline successfully resolved the TiO_2 surface into a structured geometric mesh (c). By visualizing the lattice in a 3D perspective (d), we identified that the highest regions of strain (deviations in bond length) were correlated with surface impurities.

References

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