Quantitative AFM / STM Image analysis
Basics of Image Processing
--before quantitative analysis
The Nature of “Raw” AFM / STM data
The Nature of “Raw” AFM / STM data:
2D matrix of topography
Remove the “Background” of an Image
Background Tilt and Bow
Higher Order Plan Fitting to Remove Background
Inter-line Background Offset
Inter-line Background Offset & Line Leveling
Line Leveling Caused Art Effect
Exclusion of Points From Leveling
Exclusion of Points From Leveling
Now we are ready for Quantitative Analysis
Quantitative Analysis of an Image
--There is rich information in the topography images
Quantitative Analysis of an Image

Topography image

- Grain detection and statistics
  - Number of grains: 1022
  - Height: Mean, 66.7 nm
  - Equilibrium diameter: Mean, 0.207 μm
  - Mean diameter: Mean, 0.242 μm
- Analysis of Individual Grains
  - Grain coverage detection

- BFO-LSMO-STO March 22nd sample 10x10 micron scan grain analysis and statistics

- Statistics over all grains - Binarized image analysis:
  - Number of grains: 2000
  - Total area occupied by grains: 55.7 μm² (62.7%)
  - Density of grains: 235.5 grains/μm²
  - Grain parameters:
    - Area: Mean, 0.0028 μm²
    - Orientation: 4.55 °
Quantitative Analysis of an Image

Topography image

Data analysis report
Measurement of Smoothness/Roughness
---The mathematics of roughness

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_a, R_{ass}, R_{y(i)}$</td>
<td>arithmetic average of absolute values</td>
<td>$R_a = \frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>$R_q$</td>
<td>root mean squared</td>
<td>$R_q = \sqrt[2]{\frac{1}{n} \sum_{i=1}^{n} y_i^{2/2}}$</td>
</tr>
<tr>
<td>$R_v$</td>
<td>maximum valley depth</td>
<td>$R_v = \min y_i$</td>
</tr>
<tr>
<td>$R_p$</td>
<td>maximum peak height</td>
<td>$R_p = \max y_i$</td>
</tr>
<tr>
<td>$R_{z(i)}$</td>
<td>Maximum Height of the Profile</td>
<td>$R_{z(i)} = R_p - R_v$</td>
</tr>
<tr>
<td>$R_{sk}$</td>
<td>skewness</td>
<td>$R_{sk} = \frac{1}{nR_q^{2}} \sum_{i=1}^{n} y_i^{3}$</td>
</tr>
<tr>
<td>$R_{ku}$</td>
<td>kurtosis</td>
<td>$R_{ku} = \frac{1}{nR_q^{4}} \sum_{i=1}^{n} y_i^{4}$</td>
</tr>
<tr>
<td>$R_{zDIN}, R_{rel}$</td>
<td>average distance between the highest peak and lowest valley in each sampling length, ASME Y14.3M - 1996 Surface Texture Symbols</td>
<td>$R_{zDIN} = \frac{1}{s} \sum_{i=1}^{s} R_{zi}$, where $s$ is the number of sampling lengths, and $R_{zi}$ is $R_z$ for the $i^{th}$ sampling length.</td>
</tr>
<tr>
<td>$R_{zJIS}$</td>
<td>Japanese Industrial Standard for $R_z$, based on the five highest peaks and lowest valleys over the entire sampling length.</td>
<td>$R_{zJIS} = \frac{1}{5} \sum_{i=1}^{5} R_{pi} - R_{o(i)}$, where $R_{pi}, R_{oi}$ are the $i^{th}$ highest peak, and lowest valley respectively.</td>
</tr>
</tbody>
</table>

Peak to valley & root mean square are most commonly used parameter to describe surface roughness.
Measurement of Smoothness/Roughness
--measured by peak to valley height $\Delta z$
Measurement of Smoothness/Roughness
--measuring the root mean square

\[ R_q = \sqrt{\frac{1}{n} \sum_{i=1}^{n} y_i^2} \]

\[ x_{\text{rms}} = \sqrt{\frac{1}{n} (x_1^2 + x_2^2 + \ldots + x_n^2)} \]
Measurement of Smoothness/Roughness

--The problem of peak to valley height $\Delta z$ and why use RMS

These two samples has similar Peak to valley height, but obviously has different roughness. The peak to valley height roughness does not take into account the weight of the entire surface, only consider the difference between the upper and lower most data points. RMS takes into account all the surface topography contribution.
Measurement of Smoothness/Roughness

--RMS roughness

ISO 25178
Height Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sq</td>
<td>56.0 nm</td>
</tr>
<tr>
<td>Ssk</td>
<td>-0.033</td>
</tr>
<tr>
<td>Sku</td>
<td>2.20</td>
</tr>
<tr>
<td>Sp</td>
<td>145 nm</td>
</tr>
<tr>
<td>Sv</td>
<td>160 nm</td>
</tr>
<tr>
<td>Sz</td>
<td>304 nm</td>
</tr>
<tr>
<td>Sa</td>
<td>47.3 nm</td>
</tr>
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</table>

ISO 25178
Height Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sq</td>
<td>4.4 nm</td>
</tr>
<tr>
<td>Ssk</td>
<td>4.81</td>
</tr>
<tr>
<td>Sku</td>
<td>42.0</td>
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<tr>
<td>Sp</td>
<td>207 nm</td>
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<tr>
<td>Sv</td>
<td>43.7 nm</td>
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<tr>
<td>Sz</td>
<td>251 nm</td>
</tr>
<tr>
<td>Sa</td>
<td>9.41 nm</td>
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Topography (Layer 1 / 4)
In **statistics**, a **histogram** is a graphical representation of the **distribution** of data. It is an estimate of the **probability distribution** of a **continuous variable** and was first introduced by **Karl Pearson**. A histogram is a representation of tabulated **frequencies**, shown as adjacent **rectangles** or **squares** (in some situations), erected over discrete intervals (bins), with an area proportional to the frequency of the observations in the interval.
Histogram application in topography data analysis
--Statistical measurement of height
Histogram application in topography data analysis
--Statistical measurement of height

The effect of flattening of individual lines
Histogram application in topography data analysis
--Statistical measurement of height

The effect of proper three point leveling
Histogram application in topography data analysis

--Statistical measurement of height

A total view of surface roughness

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>c1</td>
<td>206</td>
<td>nm</td>
</tr>
<tr>
<td>c2</td>
<td>126</td>
<td>nm</td>
</tr>
<tr>
<td>c2 - c1</td>
<td>79.9</td>
<td>nm</td>
</tr>
<tr>
<td>Smr(c1)</td>
<td>35.1</td>
<td>%</td>
</tr>
<tr>
<td>Smr(c2)</td>
<td>76.8</td>
<td>%</td>
</tr>
<tr>
<td>Smr(c2) - Smr(c1)</td>
<td>41.6</td>
<td>%</td>
</tr>
</tbody>
</table>
Measurement of Smoothness/Roughness

--Histogram tells more than just the roughness

Histogram tells a very flat substrate height and varying crystal height distribution
Smart Use Of Histogram
--measuring of step height
Smart Use Of Histogram
--measuring monolayer coverage

Here the upper peak represent the higher “covered” area, and the lower peak represent the substrate exposed area. A 73% coverage can be read on the graphics.
Smart Use Of Histogram -- masking secondary data processing

1. Using height as mask threshold.
2. Apply the same mask to secondary data ©
3. Calculate statistics before and after masking.
Smart Use Of Histogram II
-- masking secondary data to study side dependency

1. Using height as mask threshold.
2. Apply the same mask to secondary data ©
3. Calculate statistics before and after masking.
4. Changing the threshold and repeat

Particle size < 50nm

50nm < Particle size < 100nm

100nm < Particle size < 200nm

200nm < Particle size < 500nm
Smart Use Of Histogram II
-- result without size sorting
Smart Use Of Histogram II
-- result with and without size sorting
Measuring particle size

Z is the only reliable measuring axis for nanoparticles
Measuring particle size
Using graining analysis package or peak counting statistics to measuring particles size distribution
Measuring particle size
--With peak counting statistics
Measurement of a step height

An average along the measuring line is the way to ensure accuracy
Measurement of a step height

Histogram can be used for properly leveled image
Measurement of a step height

Proper leveling is the key for successful measurement.
The Fourier transform, named for Joseph Fourier, is a mathematical transform that expresses a mathematical function of time as a function of frequency. For instance, the transform of a musical chord made up of pure notes without overtones, expressed as loudness as a function of time, is a mathematical representation of the amplitudes and phases of the individual notes that make it up. The function of time is often called the time domain representation, and the function of frequency is called the frequency domain representation. The inverse Fourier transform expresses a frequency domain function in the time domain.
2D Fourier Transform and its application in graphics

\[
F(x,y) = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} f(m,n)e^{-j2\pi \left(\frac{m}{M}x + \frac{n}{N}y\right)}
\]

\[
f(m,n) = \frac{1}{MN} \sum_{x=0}^{M-1} \sum_{y=0}^{N-1} F(x,y)e^{j2\pi \left(\frac{m}{M}x + \frac{n}{N}y\right)}
\]

2D FFT has wide use in image process, to identify periodic features

where \(f(m,n)\) is the pixel at coordinates \((m,n)\), \(F(x,y)\) is the value of the image in the frequency domain corresponding to the coordinates \(x\) and \(y\), and \(M\) and \(N\) are the dimensions of the image.
Measurement of surface periodicity with FFT
High Frequency Noise and FFT Filtering
FFT Filtering Used to Enhance Periodical Features
Measurement of surface texture

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropy</td>
<td>36.3 %</td>
<td></td>
</tr>
<tr>
<td>First Direction</td>
<td>71.5°</td>
<td></td>
</tr>
<tr>
<td>Second Direction</td>
<td>45.0°</td>
<td></td>
</tr>
<tr>
<td>Third Direction</td>
<td>53.6°</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropy</td>
<td>34.8 %</td>
<td></td>
</tr>
<tr>
<td>Periodicity</td>
<td>8.49 %</td>
<td></td>
</tr>
<tr>
<td>Period</td>
<td>0.505 μm</td>
<td></td>
</tr>
<tr>
<td>Direction of period</td>
<td>109°</td>
<td></td>
</tr>
</tbody>
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Summary

Basic Image Processing--From Raw Data to Quality Images

• The Nature of “Raw” AFM / STM data
• Removing the “Background” of an Image for quantitative analysis
• Application of histogram for data analysis
• FFT analysis and Filtering Used to Enhance Periodical Features
• Other stuff
Questions?