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DEVCOM ARMY RESEARCH LABORATORY

Using MATLAB to Calculate Parameters from Data Collected by Atomic Force Microscopy

by Wendy L Sarney

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14. ABSTRACT

This report describes the typical roughness parameters calculated by atomic force microscopy software and explains their physical meaning. We demonstrate MATLAB code that also calculates roughness parameters, the maximum peak height, the maximum valley depth, and the average particle width along a line profile at the height of the mean plane.

15. SUBJECT TERMS

atomic force microscopy; roughness; particle size; grain size; surface; Photonics, Electronics, and Quantum Sciences

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1. Introduction

This report discusses using MATLAB (MATLAB 2021) to calculate key surface parameters from data collected by atomic force microscopy (AFM). The code shown in this report finds the arithmetic mean height (R_a), root mean square height (R_q), the mean particle width, the maximum height above the mean surface plane (p_{max}), and the maximum depth below the mean surface plane (v_{max}). This MATLAB code can be used with any AFM that outputs line profiles in a .csv file.

1.1 Atomic Force Microscopy

AFM is a high-resolution imaging technique that characterizes a sample's surface topography. The specific resolution depends on the measurement mode selected, the room and sample (air vs. ambient) environment, and tip used (Gan 2009). The vertical resolution is related to the temperature, T, and the spring constant, k, of the cantilever:

$$\Delta z = \sqrt{\frac{4k_B T}{3k}} \tag{1}$$

where k_B is the Boltzmann constant (Butt and Jaschke 1995). The lateral resolution depends on the tip radius, the vertical resolution, and the difference in height of neighboring features, expressed as (Bustamante et al. 1997):

$$d = \sqrt{2R}(\sqrt{\Delta z} + \sqrt{\Delta z + \Delta h}). \tag{2}$$

From Eq. 2 we can see the vertical resolution is always better than the lateral resolution, and that there is less lateral resolution in rough samples.

The tip used to collect the data in this demonstration is Bruker's OTESPA-R3 AFM probe with a 7–10 nm tip radius and spring constant of 26 N/m (Bruker 2022). The lateral resolution is around 7 nm and the vertical resolution is around 2 nm.

We used the Hitachi AFM 5300 in ambient mode (Hitachi 2022) with its accompanying software package.

1.2 MATLAB

MATLAB is a widely used numerical computing software package developed by MathWorks. AFM software can export a .csv file for the measured line profiles, which (along with Excel .xlsl files) can be opened and read by MATLAB code.

The Hitachi AFM software calculates most pertinent surface area and line scan numbers, but it does not calculate average particle widths. Since it is a “black box” and we do not have its source code, we need to verify our understanding of the calculations before relying on its outputs. Also, the particle width value is of particular interest for our experiments, and we needed a less arduous manner of estimating it than physically measuring numerous particle sizes in the AFM image.

2. Using MATLAB with AFM Data

In this demonstration, we examined a film of hafnium dioxide grown by atomic layer deposition. The film is on a titanium-platinum bottom electrode layer on a silicon substrate. The measurements were obtained in tapping mode, which is a noncontacting dynamic force mode.

2.1 AFM Images and Data

We collected a 2- × 2-µm topography image, as shown in 2- and 3-D renderings in Figs. 1 and 2.

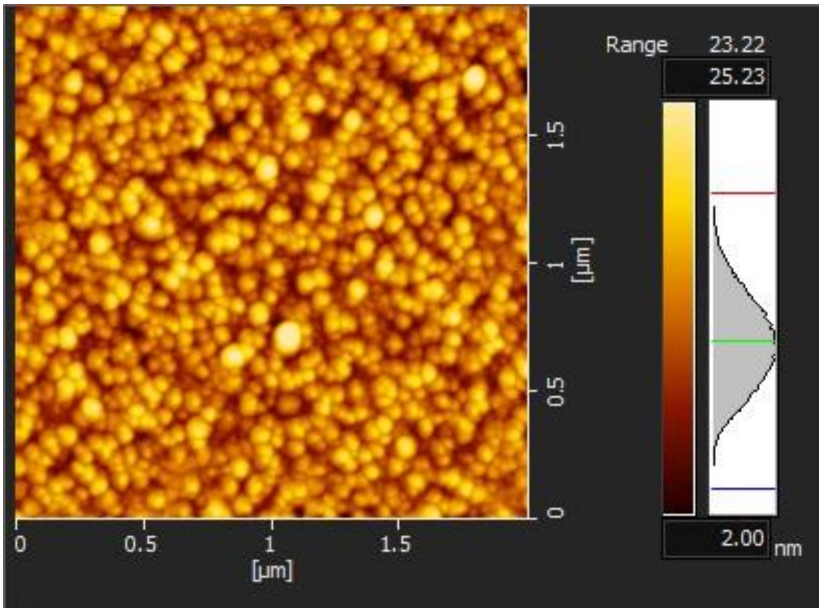

Fig. 1 Rendering of the sample’s surface topography in 2-D

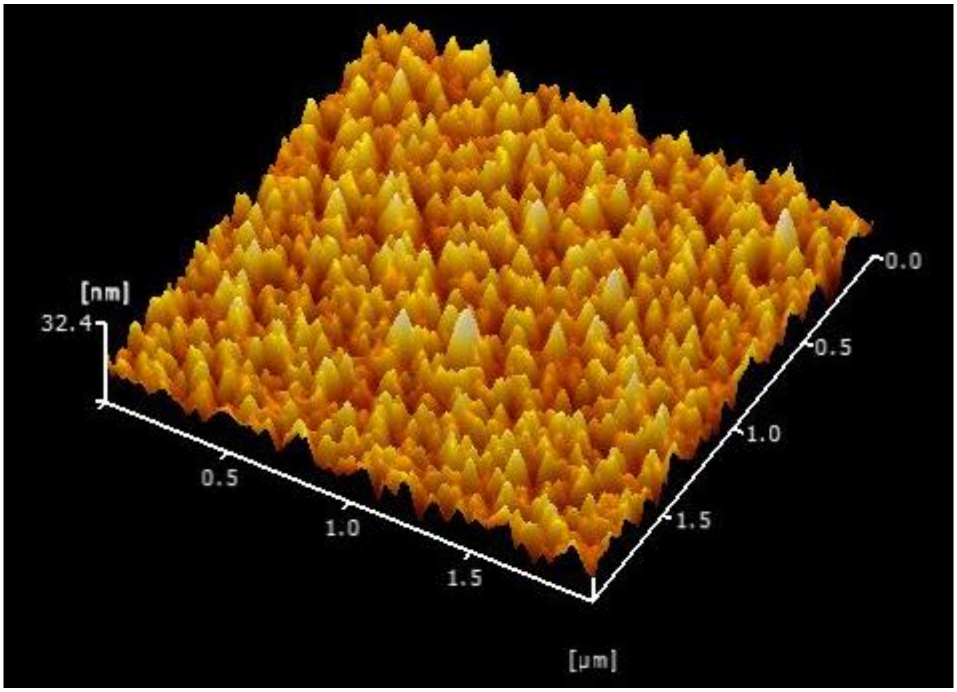

Fig. 2 Rendering of the sample's surface topography in 3-D

Line profiles are created through the AFM software's GUI by drawing a line of any length or orientation onto the image. Since this image indicates our sample is fairly uniform, we drew six randomly oriented 2-μm lines. Sometimes certain crystals have surface features that are related to the crystallographic orientation of the underlying planes. To get truly characteristic roughness and particle size measurements over a mostly uniform area, it is important to collect profiles over multiple, randomly oriented lines. If the features are orientation specific, then the lines are drawn to correspond to the orientations of interest and the measurements must be qualified when reported. For instance, if particle size is measured along a specific orientation, we would state something like: "The average particle size is x nm along the [100] direction."

The software only allows three line profiles to be drawn at a time. To get six lines, we saved two sets of profiles. Each line profile has a corresponding .csv file containing two columns of numbers: one for the location on the line and the other for the measured height for that location. Each .csv file was opened in Microsoft Excel and extraneous text that cannot be understood by MATLAB was removed. The files were then saved as .xlsl files.

The measured roughnesses for the line profiles shown in Fig. 3(a,b) are listed in Table 1 as well as the mean value, the standard deviation (StDev) of the profiles from the mean, and the coefficient of variation (COV).

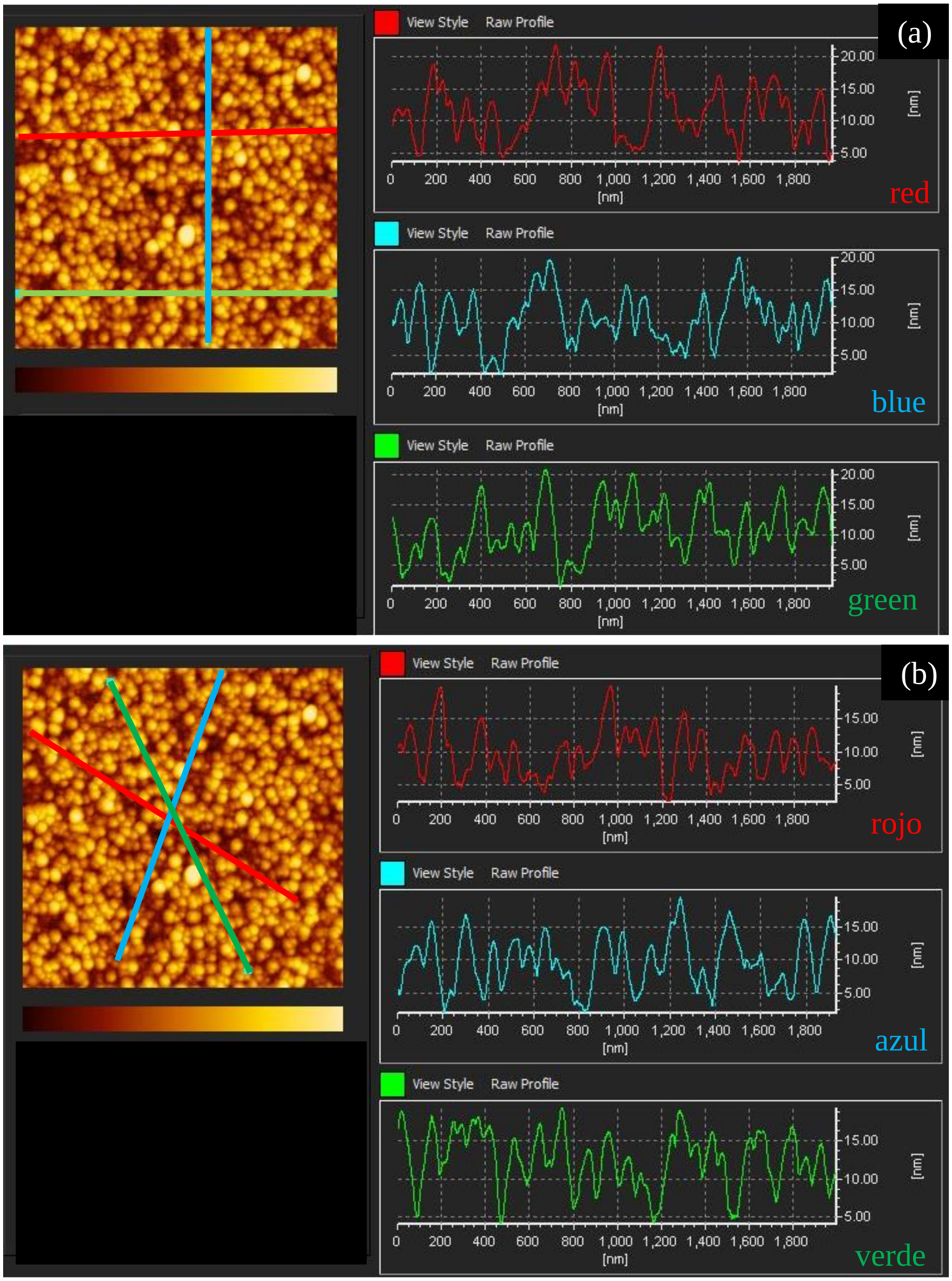

Fig. 3 (a) Line profiles indicated by the red, blue, and green lines on the AFM image. (b) Line profiles indicated by the red, blue, and green lines on the AFM image. To avoid redundancy, the .csv files and data tables refer to the lines by Spanish color names: rojo, azul, and verde.

Table 1 **Roughness measurements from AFM software**

	Line profile	R_a (nm)	R_q (nm)
	red	3.6	4.2
	blue	3.1	3.8
	green	3.4	4.1
	rojo	2.8	3.5
	azul	3.3	3.9
	verde	2.9	3.5
Statistics	Mean	3.2	3.8
	StDev	0.3	0.3
	COV	9.6%	7.6%

Physical Meaning of Measured Parameters

A schematic of a surface profile is shown in Fig. 4. The location of the mean plane is found by averaging the y values of the profile at each measured *x*. The R_a is equal to average of the absolute values of the difference of each measured y from the position of mean plane:

$$R_a = \frac{1}{L}\int_0^L z(x)dx\ . \tag{3}$$

The R_q is described by the standard deviation of the heights along the line:

$$R_q = \sqrt{\frac{1}{L}\int_0^L z^2(x)}\, dx. \tag{4}$$

Both R_a and R_q are used to describe surface roughness. The R_a is less sensitive to the presence of a few large peaks or valleys than the R_q. Therefore, the data in Table 1 show that the R_q is greater than the R_a. The more uniform the roughness across the profile, the more similar the R_a and R_q measurements.

The p_{max} and v_{max} are equal to the height (or depth) of the highest peak and the deepest valley.

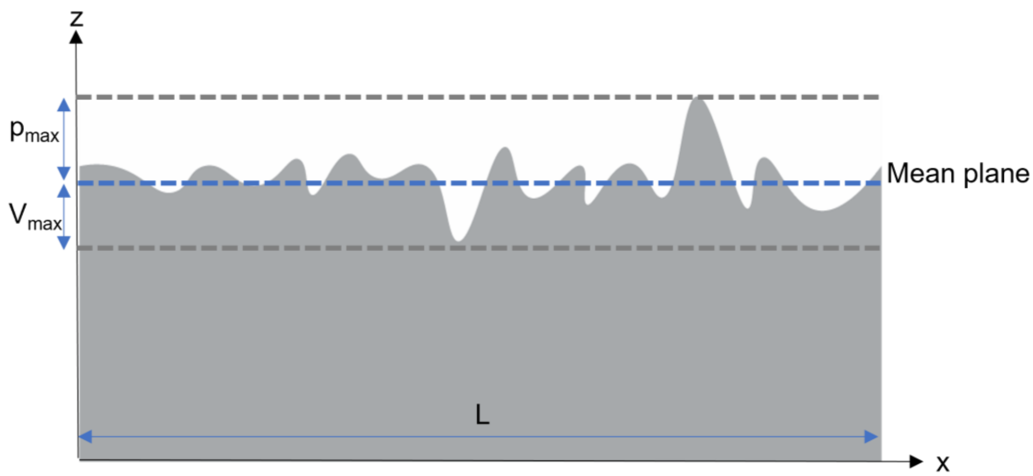

Fig. 4 Line profile with measured parameters

2.2 MATLAB Code

Sections 1–4 of the MATLAB code are shown in Fig. 5. As an example, it is calling the .xlsl file from the "azul" profile generated by the AFM software and shown in Fig. 3b. Section 1 includes the code for opening and reading the data.

In Section 2, we calculate the location of the mean plane as shown graphically in Fig. 4. We also find the height of the highest peak and the depth of the deepest valley.

In Section 3, MATLAB finds the local minima and maxima, which are the peaks and valleys of the data. We graph the profile and label the peaks and valleys in Section 4.

Sections 5 and 6 calculate the average particle width along the lateral direction at the height of the mean plane. The code locates the peaks and valleys and measures the average distance between peaks and the average distance between valleys. On average, the mean plane cuts the particles in half along the vertical dimension. Laterally, the average intersection between the mean plane and each side of the particle occurs halfway between the peak and the valley. Therefore, the average particle width should be approximately half the average distance between either the peaks or the valleys. We determined the particle size using both calculations and averaged the two values. Of all the measurements collected, this is the least accurate, but it is useful to compare across samples to determine either increasing or decreasing trends in particle size.

```matlab

% Wendy L. Sarney
% June 13,2022
% Program calculates AFM roughness and particle widths

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 1
% Read the line profile from the file
rawTable = readtable('azul.xlsx','Sheet','Sheet1');
x = rawTable.A; %: get the first excel column;
z = rawTable.B; %: get the second excel column;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 2
%Find height of the mean plane, tallest peak, deepest valley
mean_plane=mean(z);
p_max = max(z-mean_plane); %Find height of tallest peak
v_max = abs(min(z-mean_plane)); %Find depth of deepest valley

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 3
% Find the peaks and valleys
valley = islocalmin(z);
peak = islocalmax(z);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 4
% Plot the line profile
figure(1)
plot(x,z,'g-', x(peak), z(peak), 'b*',x(valley), z(valley), 'r*')
yline([mean(z)],'--') % plot the mean plane

xlabel('lateral distance along profile (nm)')
ylabel('height (nm)')
title("Line Profile")

legend('profile','localmax','localmin', 'mean plane')

```

Fig. 5 Sections 1–4 of MATLAB code

```matlab
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 5
% Find distance between valleys

xminimas=x(valley); % Find the location of the valleys
xmaximas=x(peak); % Find the location of the peaks

for p=1:numel(xminimas)-1
    differences(p) = xminimas(p+1)-xminimas(p); %Find the distance between adjacent valleys
end

Mean_particle_size1=mean(differences)/2; % Find the average distance between the valleys
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 6
%Find distances between peaks
for p=1:numel(xmaximas)-1
    differences(p) = xmaximas(p+1)-xmaximas(p);
end
Mean_particle_size2=mean(differences)/2;

Mean_particle_size=(Mean_particle_size1+Mean_particle_size2)/2;
```

Fig. 6 Sections 5 and 6 of MATLAB code

Figure 7 shows Sections 7–9 of the MATLAB code. Section 7 calculates R_a and Section 8 calculates R_q. Section 9 directs the code to display the calculations.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 7
%Find arithmetic mean height

Roughness=abs(z-mean_plane); % Difference in height at each x relative to average plane

Ra=mean(Roughness); %Arithmetic mean height

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 8
%Find RMS roughness

RMS=std(z);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 9
% Output

fprintf("The arithmetic mean height Ra is %.1f nm\n", Ra)

fprintf("The RMS roughness is %.1f nm \n", RMS)

fprintf("The mean particle width is  %.0f nm \n", Mean_particle_size)

fprintf("The maximum height is %.1f nm above the mean plane\n",p_max)
fprintf("The minumum height is %.1f nm below the mean plane\n", v_max)

```

Fig. 7 Sections 7–9 of the MATLAB code

3. Outputs of the MATLAB Code

When the code is executed using the "azul" data file, the command window gives the outputs shown in Fig. 8 along with the profile shown in Fig. 9.

```
Command Window
>> AFMProfile
The arithmetic mean height Ra is 3.3 nm
The Rv is 3.9 nm
The mean particle width is  24 nm
The maximum height is 9.8 nm above the mean plane
The minumum height is 7.9 nm below the mean plane
>>
```

Fig. 8 Command window generated by MATLAB

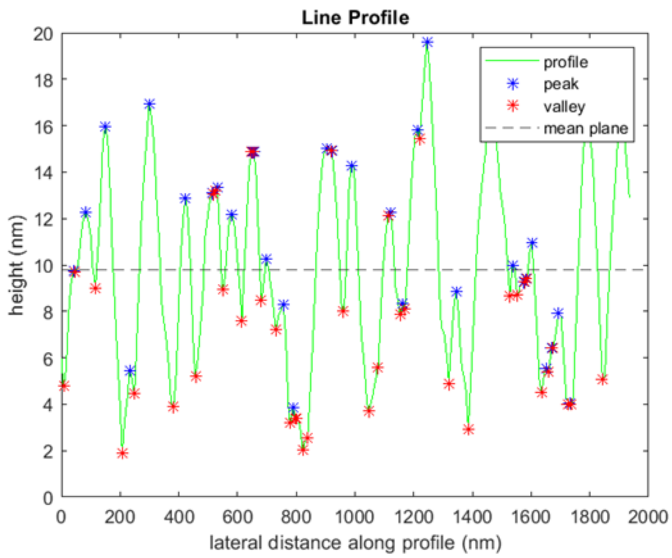

Fig. 9 Line profile generated by the MATLAB code

We can see that the R_a and R_q of 3.3 and 3.9 values generated by the MATLAB code are the same as that calculated by the AFM software shown in Table 1. The particle size of 24 nm is reasonable when compared to measurements made directly onto the image in Fig. 1.

4. Conclusion

The MATLAB code in this software calculates roughness parameters identical to those produced by the Hitachi AFM software. Furthermore, it calculates the lateral particle width along the height of the mean plane. This code can be used for any AFM software that outputs .csv files.

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List of Symbols, Abbreviations, and Acronyms

2-D	two-dimensional
3-D	three-dimensional
AFM	atomic force microscopy
ARL	Army Research Laboratory
COV	coefficient of variation
DEVCOM	US Army Combat Capabilities Development Command
GUI	graphical user interface
p_{max}	maximum height above the mean surface plane
R_a	arithmetic mean height
R_q	root mean square height
StDev	standard deviation
v_{max}	maximum depth below the mean surface plane

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