Roughness Spectroscopy

P. Fraundorf
Physics & Astronomy, U. Missouri-StL,
St. Louis, MO, USA
(March 1, 2004)

Optical interferometry, as well as confocal light, stereopair scanning electron, scanning tunneling amd scanning force microscopies, may all produce topographic maps of surfaces. We show here that by decomposing the height variance of such images into an integral over log[spatial period or frequency] that a quantitative fingerprint of second moment statistics emerges which is useful for comparison over a broad range of sizes and specimens. The results have a natural direct-space interpretation, even though two-dimensional and azimuthally-averaged one-dimensional power spectra serve as a starting point for the analysis. Some limiting surface types, and several effects of noise on experimental scanning tunneling microscope images, illustrate.

05.70.Ce, 02.50.Wp, 75.10.Hk, 01.55.+b

I. INTRODUCTION

Topographic images of surfaces contain specific data on the position of may individual surface elements. They also contain information on statistical properties of the surface, such as the height mean and standard deviation. Standard deviation is related to the expected value for height squared, and is therefore called a "second moment" statistic. Although a complete picture of second moment statistics for a surface is contained in its power spectrum, the frequency-space representation is unwieldy when roughness measurements on size scales ranging over more than two orders of magnitude are considered. We describe here an intuitive strategy, the spectral decomposition of variance on a log[period] scale, which is useful for providing a physical picture both surface roughness, and constraints on roughness, over many orders of magnitude in size.

II. LOG-SCALE DECOMPOSITION OF VARIANCE

Modern microscopes can provide maps of specimen topography on size scales reaching from centimeters to Angstroms. The two common methods for displaying information about roughness (or the second moment statistics of any property in space, for that matter) are the Fourier power spectrum, and its direct space transform: the autocorrelation function or interferogram. Unfortunately, for a surface exhibiting lateral structure over this eight-decade range of sizes, both the power spectrum per unit frequency and the autocorrelation function per unit period will find most of the information they contain pressed into the plot's origin. This suggests that power could be plotted in units of log[*period*]. Rather than add this logarithmic constraint as yet another element of abstraction in the analysis of power spectra, a paradigm shift is recommended.

Any given topographic map (e.g. a 128×128 image containing information on size scales ranging over two orders of magnitude) will contain some average level of vertical fluctuations. These fluctuations can be characterized (in 2nd-moment terms) by the rms variation σ_h in height across the image. The question we pose is simple: Over what lateral size scales is this rms variation distributed? More specifically, how many nm of rms fluctuation, per decade in the range of lateral sizes, does the map contain for spatial periods throughout the range represented in the image? A plot of this quantity versus log[period] would by inspection let us estimate the rms variation for a map covering any range of sizes included in the range covered by the plot.

Except for changes in variable, the shift requires no departure from the signal processing (power spectrum) approach mentioned above. This is because Parseval's theorem describes of simple decomposition of height-squared (or variance for maps of zero mean height) as a function of $\log[frequency] \equiv -\log[period]$. We begin by defining a "unit-normalized" continuous Fourier transform:

$$H[u,v] \equiv \frac{1}{W^2}\int_{-\frac{W}{2}}^{+\frac{W}{2}} dx \int_{-\frac{W}{2}}^{+\frac{W}{2}} dy \times h[x,y]e^{-2\pi i(ux+vy)}$$

over a square field in x,y of side W. This definition gives H the same units as h (in our case length or height in the vertical direction), and in effect assumes that h goes to zero (the vertical origin value) outside the square field. The resulting inverse transform is:

$$h[x,y] = W^2 \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} dv \times H[u,v] e^{+2\pi i(ux+vy)}$$

and the Parseval relation:

$$\frac{1}{W^2} \int_{-\frac{W}{2}}^{+\frac{W}{2}} dx \int_{-\frac{W}{2}}^{+\frac{W}{2}} dy \, |h[x,y]|^2 = W^2 \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} dv \, |H[u,v]|^2 .$$

One then can write for the mean height (which can be conveniently set to zero in most applications):

$$\langle h \rangle \equiv \frac{1}{W^2} \int_{-\frac{W}{2}}^{+\frac{W}{2}} dx \int_{-\frac{W}{2}}^{+\frac{W}{2}} dy \times h[x,y] = H[0,0]$$

and for the resulting rms roughness σ_h we can write:

$$\begin{aligned} \sigma_h^2 + \langle h \rangle^2 = \langle h^2 \rangle &\equiv \frac{1}{W^2} \int_{-\frac{W}{2}}^{+\frac{W}{2}} dx \int_{-\frac{W}{2}}^{+\frac{W}{2}} dy \, |h[x,y]|^2 \\ &= W^2 \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} dv \, |H[u,v]|^2 \\ &= \int_0^{\infty} df \times R_f^2 = \int_{-\infty}^{+\infty} d(\lg f) \times f \ln(10) R_f^2 \end{aligned}$$

where the discrete azimuthally-averaged roughness function R_f^2 is written in terms of an azimuthal average of Fourier coefficients as

$$R_f^2 \equiv \frac{1}{2\pi} \int_0^{2\pi} d\phi \left(2\pi f W^2 \, |H[f,\phi]|^2 \right) .$$

As in the usual case when height data is available over a discrete set of equally-spaced intervals (e.g. a square of N intervals on a side), the discrete transform becomes (in this case assuming periodic behavior outside the image field):

$$H_{lm} \equiv \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} h_{jk} e^{-2\pi i(jl+km)/N^2} \forall (l,m) = 0, N-1.$$

The corresponding inverse transform is

$$h_{jk} = \sum_{l=0}^{N-1} \sum_{m=0}^{N-1} H_{lm} e^{+2\pi i(jl+km)/N^2} \forall (j,k) = 0, N-1,$$

and Parseval's relation becomes

$$\frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} |h_{jk}|^2 = \sum_{l=0}^{N-1} \sum_{m=0}^{N-1} |H_{lm}|^2 .$$

In this discrete case, our estimate of mean height becomes

$$\langle h \rangle \equiv \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} h_{jk} = H_{00}.$$

The rms roughness then obeys:

$$\begin{aligned}\sigma_h^2 + \langle h\rangle^2 = \langle h^2\rangle &\equiv \frac{1}{N^2}\sum_{j=0}^{N-1}\sum_{k=0}^{N-1}|h_{jk}|^2 \\ &= \sum_{l=0}^{N-1}\sum_{m=0}^{N-1}|H_{lm}|^2 \\ &\simeq \sum_{n=0}^{\frac{N}{2}} R_n^2 \simeq \sum_{n=1}^{\frac{N}{2}} \Delta(\lg n)\times n\ln(10)R_n^2\end{aligned}$$

where the discrete azimuthally-averaged roughness function R_n^2 is written in terms of the azimuthally-averaged power $\left\langle |H_n|^2 \right\rangle$ corresponding to physical frequency $f = \frac{n}{W}$, as

$$R_n^2 \equiv 2\pi n \left\langle |H_n|^2 \right\rangle .$$

Here W is again the physical field width of the image, and the Nyquist critical (maximum non-aliased) frequency detectable in the data is $f_c \equiv \frac{N}{2W}$.

The quantity $R_{\mathrm{lg}} \equiv \sqrt{f\ln(10)R_f^2} \simeq \sqrt{n\ln(10)R_n^2}$ for frequency $f = \frac{n}{W}$, as you can see from the equations above has units of height. It is also independent of the units chosen to measure lateral distance. The total rms roughness in a high resolution map whose mean height has been set to zero, which contains data covering several decades of lateral size, is equal to the square root of the sum of the squares of the value that R_{lg} takes within each of those decades. This is because a decrease in lateral period, or increase in frequency, by a factor of 10 corresponds to $\Delta(\lg f) = \Delta(\lg n) = 1$. Hence R_{lg} is a spectral index for roughness with a very simple direct-space interpretation. We examine it more carefully below.

III. EFFECTS OF CHANGING SAMPLE SIZE

IV. SUMMARY

ACKNOWLEDGMENTS

This work has benefited indirectly from support by the U.S. Department of Energy, the Missouri Research Board, as well as Monsanto and MEMC Electronic Materials Companies. It has benefited most, however, from the interest and support of students at UM-St. Louis.