Designation: F 1811 – 97

Standard Practice for
Estimating the Power Spectral Density Function and Related Finish Parameters from Surface Profile Data[1]

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1. Scope

1.1 This practice defines the methodology for calculating a set of commonly used statistical parameters and functions of surface roughness from a set of measured surface profile data. Its purposes are to provide fundamental procedures and notation for processing and presenting data, to alert the reader to related issues that may arise in user-specific applications, and to provide literature references where further details can be found.

1.2 The present practice is limited to the analysis of one-dimensional or profile data taken at uniform intervals along straight lines across the surface under test, although reference is made to the more general case of two-dimensional measurements made over a rectangular array of data points.

1.3 The data analysis procedures described in this practice are generic and are not limited to specific surfaces, surface-generation techniques, degrees of roughness, or measuring techniques. Examples of measuring techniques that can be used to generate profile data for analysis are mechanical profiling instruments using a rigid contacting probe, optical profiling instruments that sample over a line or an array over an area of the surface, optical interferometry, and scanning-microscopy techniques such as atomic-force microscopy. The distinctions between different measuring techniques enter the present practice through various parameters and functions that are defined in Sections 3 and 5, such as their sampling intervals, bandwidths, and measurement transfer functions.

1.4 The primary interest here is the characterization of random or periodic aspects of surface finish rather than isolated surface defects such as pits, protrusions, scratches or ridges. Although the methods of data analysis described here can be equally well applied to profile data of isolated surface features, the parameters and functions that are derived using the procedures described in this practice may have a different physical significance than those derived from random or periodic surfaces.

1.5 The statistical parameters and functions that are discussed in this practice are, in fact, mathematical abstractions that are generally defined in terms of an infinitely-long linear profile across the surface, or the "ensemble" average of an infinite number of finite-length profiles. In contrast, real profile data are available in the form of one or more sets of digitized height data measured at a finite number of discrete positions on the surface under test. This practice gives both the abstract definitions of the statistical quantities of interest, and numerical procedures for determining values of these abstract quantities from sets of measured data. In the notation of this practice these numerical procedures are called "estimators" and the results that they produce are called "estimates".

1.6 This practice gives "periodogram" estimators for determining the root-mean-square (rms) roughness, rms slope, and power spectral density (PSD) of the surface directly from profile height or slope measurements. The statistical literature uses a circumflex to distinguish an estimator or estimate from its abstract or ensemble-average value. For example, $\hat{A}$ denotes an estimate of the quality A. However, some word-processors cannot place a circumflex over consonants in text. Any symbolic or verbal device may be used instead.

1.7 The quality of estimators of surface statistics are, in turn, characterized by higher-order statistical properties that describe their "bias" and "fluctuation" properties with respect to their abstract or ensemble-average versions. This practice does not discuss the higher-order statistical properties of the estimators given here since their practical significance and use are application-specific and beyond the scope of this document. Details of these and related subjects can be found in References (**1–10**)[2] at the end of this practice.

1.8 Raw measured profile data generally contain trending components that are independent of the microtopography of the surface being measured. These components must be subtracted before the difference or residual errors are subjected to the statistical-estimation routines given here. These trending components originate from both extrinsic and intrinsic sources. Extrinsic trends arise from the rigid-body positioning of the part under test in the measuring apparatus. In optics these displacement and rotation contributions are called "piston" and "tilt" errors. In contrast, intrinsic trends arise from deliberate or accidental shape errors inherent in the surface under test, such as a circular or parabolic curvature. In the absence of a-priori information about the true surface shape, the intrinsic shape

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[1] This practice is under the jurisdiction of ASTM Committee F-1 on Electronicsand is the direct responsibility of Subcommittee F01.06 on Silicon Materials and Process Control.

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[2] The boldface numbers in parentheses refer to the list of references at the end of this practice.

error is frequently limited to a quadratic (parabolic) curvature of the surface. Detrending of intrinsic and extrinsic trends is generally accomplished simultaneously by subtracting a detrending polynomial from the raw measured data, where the polynomial coefficients are determined by least-squares fitting to the measured data.

1.9 Although surfaces and surface measuring instruments exist in real or configuration space, they are most easily understood in frequency space, also known as Fourier transform, reciprocal or spatial-frequency space. This is because any practical measurement process can be considered to be a "linear system", meaning that the measured profile is the convolution of the true surface profile and the impulse response of the measuring system; and equivalently, the Fourier-amplitude spectrum of the measured profile is the product of that of the true profile and the frequency-dependent "transfer function" of the measurement system. This is expressed symbolically by the following equation:

$$A_{\text{meas}}(f_x) = A_{\text{true}}(f_x) \cdot T(f_x)$$

where:

A = the Fourier amplitudes,

$T(f_x)$ = instrument response function or the measurement transfer function, and

f_x = surface spatial frequency.

This factorization permits the surface and the measuring system to be discussed independently of each other in frequency space, and is an essential feature of any discussion of measurement systems.

1.10 Figure 1 sketches different forms of the measurement transfer function, $T(f_x)$:

1.10.1 Case (*a*) is a perfect measuring system, which has $T(f_x) = 1$ for all spatial frequencies, $0 \leq f_x \leq \infty$. This is unrealistic since no real measuring instrument is equally sensitive to all spatial frequencies. Case (*b*) is an ideal measuring system, which has $T(f_x) = 1$ for $LFL \leq f_x \leq HFL$ and $T(f_x) = 0$ otherwise, where *LFL* and *HFL* denote the low-frequency and high-frequency limits of the measurement. The range $LFL \leq f_x \leq HFL$ is called the bandpass or bandwidth of the measurement, and ratio *HFL/LFL* is called the dynamic range of the measurement. Case (*c*) represents a realistic measuring system, since it includes the fact that $T(f_x)$ need not be unity within the measurement bandpass or strictly zero outside the bandpass.

1.11 If the measurement transfer function is known to deviate significantly from unity within the measurement bandpass, the measured power spectral density (*PSD*) can be transformed into the form that would have been measured by an instrument with the ideal rectangular form through the process of digital "restoration." In its simplest form restoration involves dividing the measured *PSD* by the known form of $|T(f_x)|^2$ over the measurement bandpass. Restoration is particularly relevant to measuring instruments that involve optical microscopes since the transfer functions of microscope systems are not unity over their bandpass but tend to fall linearly between unity at $T(0) = 1$ and $T(HFL) = 0$. The need for, and methodology of digital restoration is instrument specific and this practice places no requirements on its use.

1.12 This practice requires that any data on surface finish parameters or functions generated by the procedures described herein be accompanied by an identifying description of measuring instrument used, estimates of its low- and high-frequency limits, *LFL* and *HFL*, and a statement of whether or not restoration techniques were used.

1.13 In order to make a quantitative comparison between profile data obtained from different measurement techniques, the statistical parameters and functions of interest must be compared over the same or comparable spatial-frequency regions. The most common quantities used to compare surfaces are their root-mean-square (rms) roughness values, which are the square roots of the areas under the *PSD* between specified surface-frequency limits. Surface statistics derived from measurements involving different spatial-frequency ranges cannot be compared quantitatively except in an approximate way. In some cases measurements with partially or even nonoverlapping bandwidths can be compared by using analytic models of the *PSD*s to extrapolate the *PSD*s outside their measurement bandwidth.

1.14 Examples of specific band-width limits can be drawn from the optical and semiconductor industries. In optics the so-called total integrated scatter or TIS measurement technique leads to rms roughness values involving an annulus in two-dimensional spatial frequencies space from 0.069 to 1.48 μm^{-1}; that is, a dynamic range of 1.48/0.069 = 21/1. In contrast, the range of spatial frequencies involved in optical and mechanical scanning techniques are generally much larger than this, frequently having a dynamic ranges of 512/1 or more. In the latter case the subrange of 0.0125 to 1 μm^{-1} has been used to discuss the rms surface roughness in the semiconductor industry. These numbers are provided to illustrate the magnitudes and ranges of *HFL* and *LFL* encountered in practice but do not constitute a recommendation of particular limits for the specification of surface finish parameters. Such selections are application dependent, and are to be made at the users' discretion.

1.15 The limits of integration involved in the determination of rms roughness and slope values from measured profile data are introduced by multiplying the measured *PSD* by a factor equal to zero for spatial frequencies outside the desired bandpass and unity within the desired bandpass, as shown in Case (*b*) in Fig. 1. This is called a top-hat or binary filter function. Before the ready availability of digital frequency-domain processing as employed in this practice, bandwidth limits were imposed by passing the profile data through analog or digital filters without explicitly transforming them into the frequency domain and multiplying by a top-hat function. The two processes are mathematically equivalent, providing the data filter has the desired frequency response. Real data filters, however, frequently have Gaussian or *RC* forms that only approximate the desired top-hat form that introduces some ambiguity in their interpretation. This practice recommends the determination of rms roughness and slope values using top-hat windowing of the measured *PSD* in the frequency domain.

1.16 The *PSD* and rms roughness are surface statistics of particular interest to the optics and semiconductor industries because of their direct relationship to the functional properties of such surfaces. In the case of rougher surfaces these are still valid and useful statistics, although the functional properties of such surfaces may depend on additional statistics as well. The ASME Standard on Surface Texture, B46.1, discusses additional surface statistics, terms, and measurement methods applicable to machined surfaces.

1.17 The units used in this practice are a self-consistent set of SI units that are appropriate for many measurements in the semiconductor and optics industry. This practice does not mandate the use of these units, but does require that results expressed in other units be referenced to SI units for ease of comparison.

1.18 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

E 284 Terminology Relating to Appearance of Materials[3]

E 1392 Practice for Angle Resolved Optical Scatter Measurements on Specular or Diffuse Surfaces[4]

F 1048 Test Method for Measuring the Effective Surface Roughness of Optical Components by Total Integrated Scattering[4]

2.2 *ANSI Standard:*

ANSI/ASME B46.1 Surface Texture (Surface Roughness, Waviness and Lay)[5]

3. Terminology

3.1 *Definitions: Introduction—This section provides the definitions of special terms used in this practice, and includes the mathematical definitions of different profile statistics in terms of continuous, infinitely-long profiles. The corresponding estimators of those statistics based on linear, sampled, finite-trace-length data are given in Section 5. Definitions of terms not included here will be found in Terminology E 284, Practice E 1392, Test Method F 1048 or ANSI/ASME B46.1.*

3.2 *aperture averaging, local averaging, data averaging*—As used here, aperture and local averaging mean that an estimate of the power spectral density function (*PSD*) is "smoothed" by replacing its value at a given spatial frequency by its average over a local frequency range using a particular weighting function. Data averaging means the numerical averaging of statistical estimates of the PSD, the mean-square surface roughness or the mean-square profile slope derived from different measurements, in order to obtain a single, composite result. For example, a rectangular or square array of measurements can be separated into a set of parallel profile measurements which can be analyzed separately and the results averaged.

3.2.1 *Discussion*—The averaged quantities must include the same range of surface spatial frequencies.

3.3 *bandwidth, bandwidth limits*—The range of surface spatial frequencies included in a measurement or specification. It is specified by a high-frequency limit (*HFL*) and a low-frequency limit (*LFL*).

3.3.1 *Discussion*—The bandwidth and the measurement transfer function over the bandwidth must be taken into account when measurements or statistical properties are compared. Different measuring instruments are generally sensitive to different ranges of surface spatial frequencies; that is, they have different bandwidth limits. Real bandwidth limits are necessarily finite since no measuring instrument is sensitive to infinitely-low or to infinitely-high surface spatial frequencies.

3.4 *bias error*—The average deviation between an estimate of a statistical quantity and its true value.

3.4.1 *Discussion*—The periodogram estimator of the power spectral density (*PSD*) given in this practice is a zero-bias or unbiased estimator of the *PSD*. On the other hand, local averaging of the periodogram can introduce bias errors in regions where the spectrum varies rapidly with frequency.

3.5 *deterministic profile, deterministic roughness*—A deterministic profile is a surface profile that is a known function of surface position, with no random dependencies on position.

3.5.1 *Discussion*—In contrast, a random profile is known only in terms of a probability distribution function.

3.6 *dynamic range*—The ratio of the high- to low-frequency limits of the bandwidth of a given measurement technique:

Dynamic range = HFL/LFL.

3.6.1 *Discussion*—This is a useful single-number characteristic of a measuring apparatus. It completely describes the measurement effects on surfaces with power-law power spectra.

3.7 *detrended profile, $Z_d(x)$*—The raw or measured profile

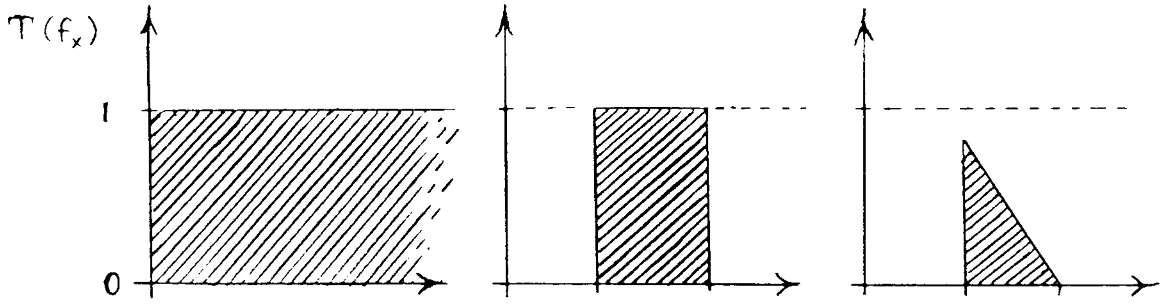

FIG. 1 Different Forms of the Measurement-Transfer or Instrumental-Response Function as a Function of Spatial Frequency, f_x.

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[3] *Annual Book of ASTM Standards*, Vol 06.01.

[4] *Annual Book of ASTM Standards*, Vol 10.05.

[5] Available from the American National Standards Institute, 11 W. 42 nd St., 13th Floor, New York, NY 10036.

after removing instrumental and surface trends. The detrended profile is the input for the statistical estimation routines described in Section 5.

3.7.1 *Discussion*—If the parametric form of the trend is known, its least-squares-fitted form can be subtracted from the measured profile data. Otherwise a generic power-series form can be used. This practice describes the procedures for removing a zero-, first- or second-order polynomial in the trace distance. A zero-order polynomial removes piston; a first-order polynomial removes piston and tilt; and a second-order polynomial removes piston, tilt and quadratic curvature. In each case the detrended data set has zero mean. The coefficients of constant and linear terms correspond to the rigid-body orientation of the part being measured and need not be recorded. However, the coefficient of the quadratic term represents the intrinsic curvature of the surface being measured and should be recorded.

3.8 *ensemble, ensemble-average value*—An "ensemble" is an infinitely large collection (infinite ensemble) of quantities, the properties of which are governed by some statistical distribution law. For example, surface profiles, and rms roughness values. An "ensemble average value" is the value of a particular surface parameter or function averaged over the appropriate distribution functions. The ensemble average value of the quantity A is denoted by $<A>$.

3.8.1 *Discussion*—Estimates of ensemble-average quantities based on a finite collection of measurements (finite ensemble) can deviate from their infinite-ensemble values by fluctuation and bias errors.

3.9 *estimator, estimated value, or estimate*—An estimator is an algorithm or mathematical procedure for calculating an "estimate" the ensemble-average value of a roughness statistic from a finite set of measured profile data.

3.9.1 *Discussion*—In this practice a circumflex is used to distinguish estimators and estimates from the corresponding ensemble-average quantities (see also 1.6).

3.10 *fast fourier transform or FFT*—An algorithm for calculating the Fourier transform (discrete Fourier transform or *DFT*) of a set of numerical data. It is now ubiquitous and can be found in any computer data analysis package (see 5.4.2 for details).

3.10.1 *Discussion*—The discovery of the *FFT* is generally attributed to Cooley and Tukey, although it was used and reported in the earlier literature by a number of others, including Gauss, two centuries before.

3.11 *finish parameters and functions*—Numbers or functions that characterize surface height fluctuations. Their values and forms may vary depending on the bandwidth of surface frequencies that they contain, and the shapes of the transfer functions of the measurement instruments involved. These quantities are represented by their ensemble-average values derived from measurements using specific estimation routines.

3.11.1 *Discussion*—In general, the finish parameters and functions of an area are different from those of profiles taken across the surface. In the case of surfaces that are statistically isotropic, however, the area and profile statistics have a one-to-one relationship. Except for incidental remarks, this practice is concerned exclusively with the properties of surface profiles.

3.12 *fluctuation error*—A general term denoting the deviation of a quantity from its mean, average or detrended value. Fluctuation errors are usually measured in terms of their mean-square or rms values.

3.12.1 *Discussion*—For example, R_q is the rms fluctuation error in the surface height and Δ_q is the rms fluctuation error in the profile slope. In turn, the estimates of R_q and Δ_q have their own fluctuation errors. The magnitudes of these higher fluctuation errors not discussed in this practice.

3.13 *high-frequency limit, HFL, 1/micrometers*—The highest spatial frequency contained in a profile data set or specification. The *HFL* of a measurement is determined by the details of the measurement process, and its value in specifications is determined by the user.

3.13.1 *Discussion*—If the sampling interval in the measurement process is D, the extreme value of the *HFL* is given by the Nyquist criterion: HFL = ½D. However, other electrical, mechanical, or optical filtering mechanisms may further limit the *HFL*. Examples of such mechanisms are: the stylus tip radius, projected measurement pixel size, optical resolution, and electrical and digital filters, all of which contribute to the high-frequency roll-off of the instrument transfer function. If the Nyquist frequency is used to determine the *HFL*, care should be taken to determine that the true *HFL* is not reduced by these additional mechanisms.

3.14 *intrinsic surface or finish parameters*—Surface parameters such as the rms roughness or rms slope that contain all surface spatial frequencies from zero to infinity.

3.14.1 *Discussion*—Intrinsic parameters are statistical abstractions that cannot be measured or estimated directly since real measurements are sensitive to only limited ranges of surface spatial frequencies. They can, however, be inferred from real measurements by augmenting measurements with a-priori information about very low and very high spatial frequencies contained in physically-based models of the *PSD*s of the surfaces involved. All measured finish parameters are finite but their corresponding intrinsic values need not be. The important distinction between intrinsic and measured (bandwidth limited) finish parameters is not always made in the literature.

3.15 *impulse response*—The impulse response of a profile-measuring system is the measured shape of an impulse or infinitely-sharp ridge lying perpendicularly to the profile direction. In the case of a linear measuring system the impulse response is the Fourier transform of the system transfer function.

3.15.1 *Discussion*—The impulse response of a perfect measuring system would be an infinitely sharp spike or delta function. In contrast, the impulse response of real measuring systems has a finite width.

3.16 *isotropic surface, statistically-isotropic surface*—A surface whose intrinsic finish parameters and functions are independent of the rotational position of the surface about its surface normal.

3.16.1 *Discussion*—The rms roughness of profiles taken across an isotropically rough surface is independent of the profile directions, and equals the rms roughness of the surface area. The rms slope of an isotropically rough surface is also independent of the profile direction and equals $1/\sqrt{(2)}$ of the rms area gradient. The one-dimensional or profile power spectrum of an isotropic surface is also independent of the direction of the profile on the surface, and is related to the two-dimensional spectrum of the surface area by an integral transform. Examples of this are given in 3.37.

3.17 *linear systems, linear measurement system*—A signal-processing concept more precisely described as a linear, shift-invariant system. For the present purposes, a linear measurement of the surface profile is the true profile convolved with the impulse response of the measuring system, or equivalently, the Fourier amplitude spectrum of the measurement is the true amplitude spectrum times the measurement transfer function as indicated in 1.9.

3.17.1 *Discussion*—All practical measurement systems are taken to be linear over their operating ranges.

3.18 *low-frequency limit, LFL, 1/micrometers*—The lowest spatial frequency contained in a profile data set or specification.

3.18.1 *Discussion*—The minimum *LFL* in a profile measurement is the reciprocal of the length of the surface profile. The estimated value of the *PSD* at this value of the *LFL* is generally attenuated by the detrending process. To avoid this effect the lowest practical *LFL* is sometimes taken to be 3 to 5 times the reciprocal of the scan length. The *LFL* in surface specifications is determined by the user.

3.19 *mean-square profile roughness, R_q^2, nanometers squared*—The ensemble-average value of the square of the height of the detrended profile:

$$R_q^2 = \lim_{L \to \infty} \frac{1}{L}\int_{-L/2}^{+L/2} dx\,(Z_d(x))^2 = \int_0^{+\infty} df_x\; S_1(f_x)$$

where:

$Z_d\,(x)$ is the detrended surface profile, and

$S_1(f_x)$ is its power spectral density.

The optics literature uses the symbol σ for R_q.

3.19.1 *Discussion*—The intrinsic value of the mean-square roughness of an isotropically-rough surface area equals the mean-square roughness of any profile across it. The rms roughness, R_q, is distinct from the arithmetic-average roughness, R_a. The two are only related through a specific height-distribution function. For example, for a Gaussian height distribution,

$$R_a = \sqrt{(2/\pi)}\; R_q = 0.798\; R_q\,.$$

3.20 *mean-square profile slope, Δ_q^2, units of choice*—The average value of the square of the slope of the detrended profile:

$$\Delta_q^2 = \lim_{L \to \infty} \frac{1}{L}\int_{-L/2}^{+L/2} dx \left(\frac{dZ_d}{dx}\right)^2 = \int_0^{+\infty} df_x S_1(f_x) \cdot (2\pi f_x)^2$$

3.20.1 *Discussion*—This expression assumes that the average slope has been removed in the detrending process. The integrand in the frequency integral on the right can be viewed as the slope power spectral density. The mean-square surface slope of an isotropically-rough two-dimensional surface is half the mean-square gradient of the surface itself.

3.21 *measured profile parameters and functions*—Quantities derived from detrended profile data that include the bandwidth and transfer function effects of the particular measurement system used.

3.21.1 *Discussion*—Measured parameters and functions can be used for comparing surfaces quality providing the same measurement system is used in all cases. In order to compare quantitative measurements made by different measurement systems, or to estimate intrinsic surface properties, the system bandwidths and transfer functions must be taken into account. In the early literature, measurement systems were taken to be "perfect" in the sense of 1.10.1, and the effects of their bandwidths and transfer functions were ignored.

3.22 *Nyquist frequency, 1/micrometers*—The spatial frequency equal to the reciprocal of twice the sampling interval. See 3.13.1.

3.22.1 *Discussion*—The Nyquist frequency represents the highest undistorted frequency involved in a series of uniformly-spaced profile measurements. Higher-frequency components in the surface appear at lower-frequencies through the process of aliasing. Unless the effects of aliasing are removed by anti-aliasing mechanisms in the measurement process, they will corrupt the measured spectrum immediately below the Nyquist frequency. In that case the *HFL* should be taken to be a factor of 3 to 5 below the Nyquist frequency.

3.23 *periodic roughness, periodic random roughness*—Purely periodic roughness is deterministic. Periodic random roughness is modified version of purely periodic roughness that has a definite fundamental spatial frequency but random variations in its phase or amplitude.

3.23.1 *Discussion*—The power spectra of periodic and periodic random roughness appear as isolated peaks in the power spectral density function. This pattern is distinct from the broad variations appearing for purely random surfaces. Random surfaces can be viewed as periodic surfaces with a broad distribution of fundamental periods.

3.24 *periodogram estimator, periodogram estimates*—The periodogram is the particular estimator for the power spectral density discussed in this practice. It is proportional to the square magnitude of the discrete Fourier transform of the detrended data set. Periodogram estimates are estimates of particular finish parameters that are derived from the periodogram estimate of the power spectrum.

3.25 *power spectral density, PSD or power spectrum*—A statistical function that shows how the mean-square $(\text{rms})^2$ of a given quantity is distributed among the various surface spatial frequencies inherent in the profile height.

3.25.1 *Discussion*—The two conventional measures of surface roughness, R_a and R_q do not carry any information about the transverse scale of the surface roughness. That is, they are independent of how much the surface profile is squeezed or stretched parallel to the surface plane. The *PSD* is the simplest statistic that carries that important additional information.

(1) *profile or one-dimensional PSD of the surface height, micrometers-cubed*—This quantity has the units of μm^3, and is a function of the spatial frequency, f_x, in units of inverse micrometers, μm^{-1}. It is defined as follows:

$$S_1(f_x) = \lim_{L \to \infty} \left\langle \frac{2}{L}\left| \int_{-L/2}^{+L/2} dx\;\; Z(x) e^{i2\pi f_x x} \right|^2 \right\rangle, \quad f_x > 0$$

3.25.1.1 *Discussion*—The subscript "x" on "f_x" corresponds to the direction of the profile on the surface and can be omitted if no confusion is involved. In this definition the spatial frequency, f_x, is always positive and greater than zero. The value at $f_x = 0$ corresponds to the average value of the profile height, which is zero for detrended profiles. The factor of 2 accounts for the equal contribution from negative frequencies and ensures that the area under the positive-frequency profile spectrum equals the rms-squared (mean-square) profile height.

3.25.1.2 *Discussion*—A mathematical variant of the periodogram estimator is the correlation method. This is a two-step process that requires the estimation of an intermediate function, the autocovariance function, which is then Fourier transformed to obtain the periodogram estimate of the power spectrum. This method is not discussed in this practice since it is indirect, and when properly applied gives identically the same results as the direct transform method recommended in this practice.

3.25.1.3 *Discussion*—The signal-processing literature contains many different estimators of the power spectrum in addition to the periodogram. In general, they differ from the periodogram in that they incorporate different types and degrees of a-priori physical or mathematical information about the original data set. The periodogram, in contrast, includes the maximum number of degrees of freedom and is always used for first-cut evaluation and analysis. Details of the correlation and other spectral estimation methods are discussed in the literature found in "References" at the end of this practice.

(2) *area or two-dimensional PSD of the surface height, micrometers-fourth power*—This quantity has the dimensions of μm^4, and is a function of the spatial frequencies in both the x and y directions on the surface, f_x and f_y, in units of inverse micrometers, μm^{-1}. It is defined as follows:

$$S_2(f_x, f_y) = \underset{A \to \infty}{Lim} \left\langle \frac{1}{A} \left| \int\int_A dx\, dy\, e^{i2\pi(f_x x + f_y y)}\, Z(x, y) \right|^2 \right\rangle,$$
$$-\infty < f_x, f_y < +\infty$$

3.25.1.4 *Discussion*—The spatial frequency ranges included in this definition cover the entire frequency plane and are not limited to positive frequencies only as in the case of the profile spectrum. In the case of an isotropically-rough surface the area spectrum is a function only of the magnitude of the two-dimensional frequency vector: $f = \sqrt{(f_x^2 + f_y^2)}$. The profile spectrum can be derived from the area spectrum, but the area spectrum cannot, in general, be derived from the profile spectrum. Uniaxial and isotropically-rough surfaces are exceptions.

3.25.1.5 *Discussion of units*—The surface height fluctuations of optical surfaces are usually measured in units of nanometers (1 nm = 10^{-3} µm), or the non-SI units of Ångstroms (1 Å = 10^{-4} µm). Values of the *PSD*s estimated using height data in these units can be converted to the recommended units by multiplying by the following conversion factors:

(1) To convert S_1 in units of nm ^{2}µm to units of µm^3 multiply it by 10^{-6},

(2) To convert S_1 in units of Å ^{2}µm to units of µm^3 multiply it by 10^{-8},

(3) To convert S_2 in units of nm ^{2}µm ^{2} to units of µm^4 multiply it by 10^{-6}, and

(4) To convert S_2 in units of Å ^{2}µm^2 to units of µm^4 multiply it by 10^{-8}.

If the sample interval is given in millimeters instead of micrometers, the conversion factors for S_1 should be multiplied by an additional factor of 10^3, and those for S_2 should be multiplied by an additional factor of 10^6.

3.26 *radius of curvature, $\hat{R}_x$, units of choice—The radius of a circle fitted to the measured surface profile.*

3.26.1 *Discussion*—When the radius us large relative to the profile length its magnitude is most easily determined from the quadratic term in the detrending polynomial. If the average surface profile is written as $Z(x) = a + bx + cx^2$, the estimate of the radius of curvature in the x direction is $\hat{R}_x = 1/(2c)$. If Z and x are expressed in micrometers, $\hat{R}_x$ will be in micrometers. Since the radii of curvature of nominally flat surfaces can be quite large, other reporting units, such as meters or kilometers, may be more appropriate.

3.27 *random roughness, random surface profile*—A surface height profile that involves parameters that are distributed according to statistical distribution laws rather than having fixed or deterministic values.

3.27.1 *Discussion*—For example, the profile $Z(x) = A$ Cos $(2\pi f_x x + \phi)$ is deterministic if ϕ = const., but random if ϕ has a finite-width probability distribution function $P(\phi)$. Finish parameters and functions such as $Z(x)^2$, are then the values of those quantities averaged over $P(\phi)$.

3.28 *restoration*—The signal-processing procedure in which measurements are compensated for a non-unit measurement transfer function by passing them through a digital filter that restores the effective measurement function to unity over its bandpass.

3.28.1 *Discussion*—The measured profile can be restored and the statistics of the restored profile can then be estimated. The most common spatial- and frequency-domain filters used for this purpose are "inverse" and "Wiener" filters. This practice does not discuss the details of such restoration processes, which may be found in standard signal-processing texts such as those given in "References" at the end of this practice.

3.29 *RMS profile roughness, Rq, nanometers*—The square root of the mean-square profile roughness.

3.30 *RMS profile slope, Δq, units of convenience*—The square root of the mean-square profile slope.

3.30.1 *Discussion*—The slope is dimensionless, although the fundamental unit is the radian. In practice it may be convenient to express the rms slope of highly polished surfaces in microradians.

3.31 *sample or sampling interval, D, micrometers*—The distance between adjacent measurements of the surface height along the x axis.

3.31.1 *Discussion*—The sample interval is usually chosen or recommended by the manufacturer of the profile instrument being used. The sample interval defines the Nyquist frequency and hence, the extreme *HFL* of the measurement. This practice does not address measurements with unequal sample intervals or those made along nonlinear traces over the surface.

3.32 *sampled profile, $Z(x_n)$, nanometers*—The surface height, $Z(x_n)$, measured at N equally-spaced points along the x axis.

3.32.1 *Discussion*—This practice uses the indexing convention for the position of the height samples,

$$x_n = (n-1)D, \qquad n = 1, 2 \cdots N$$

The distance between the first and last points in the profile trace is then $(N–1)D$.

3.33 *sampled slope, $m(x_n)$, units of convenience*—The surface slope, $m(x_n)$, measured at N equally-spaced points the x axis using the same indexing convention as for the sampled profile.

3.33.1 *Discussion*—Some instruments measure the surface slope directly, while others, in effect, measure the surface height at N+1 points and generate N slope values using the equation:

$$m(x_n) = \frac{1}{D}[Z(x_{n+1}) - Z(x_n)], \qquad n = 1, 2, \cdots N$$

3.34 *slope power spectrum, $S'(f_x)$, micrometers*—The statistical function that shows how the mean-square profile slope is distributed over surface spatial frequencies as follows:

$$S_1{}'(f_x) = \underset{L \to \infty}{Lim} \left\langle \frac{1}{L} \left| \int_{-L/2}^{+L/2} dx\, m(x) e^{i2\pi f_x x} \right|^2 \right\rangle = (2\pi f_x)^2 \cdot S_1(f_x)$$

The prime on S_1, on the left denotes that this is the *PSD* of the slope, while the unprimed S_1 on the far right is the *PSD* of the height.

3.34.1 *Discussion*—This simple connection between the slope and roughness power spectra permits one to be determined immediately in terms of the other.

3.35 *spatial frequency, fx, 1/micrometers*—The frequency parameter in the Fourier transform of the surface profile $Z(x)$.

3.35.1 *Discussion*—f_x is related to the spatial wavelength, d_x through $f_x = 1/d_x$. Similar quantities are defined for the y component, and the magnitude of the two-dimensional spatial-frequency vector, $f = \surd((f_x)^2 + (f_y)^2)$, that appears in the two-dimensional power spectral density of an isotropically-rough surface, $S_2(f)$.

3.36 *spatial wavelength, d_x, micrometers*—The reciprocal of the spatial frequency, f_x.

3.36.1 *Discussion*—The mechanical-engineering community frequently uses the symbol λ for the spatial wavelength, while the optical community reserves that symbol for the radiation wavelength.

3.37 *spectral models and spectral parameters*—A spectral model is an analytic expression for the power spectral density which contains a number of adjustable parameters called finish parameters. The values of these parameters are obtained by fitting estimates of the *PSD* of the surface height or slope fluctuations to the model.

3.37.1 *Discussion*—The fitting process performs a number of important functions: it averages out the fluctuations appearing in individual estimates of the power spectrum, it condenses the data into a few intrinsic surface parameters, and provides a mechanism for extrapolating the measured data outside the measurement bandwidth.

(*1*) *ABC spectral model*—The spectral model that has the following form for the profile *PSD*:

$$S_1(f_x) = \frac{A}{[1 + (Bf_x)^2]^{C/2}}$$

and

$$S_2(f) = \frac{A'}{[1 + (Bf)^2]^{(C+1)/2}}, \qquad A' = \frac{1}{2\sqrt{\pi}} \cdot \frac{\Gamma((C+1)/2)}{\Gamma(C/2)} \cdot AB$$

for the two-dimensional spectrum of an isotropically-rough surface.

3.37.1.1 *Discussion*—The finish parameters in this model are A, B and C, which have the dimensions of μm^3, μm ^{1}, and μm^0.

Discussion: This model is sometimes called the K-correlation model, and the quantity $B/(2\pi)$, the correlation length.

(*2*) *fractal spectral model*—The spectral model which has the following form for the profile PSD:

$$S_1(f_x) = \frac{K_n}{f_x^n}$$

and

$$S_2(f) = \frac{K_n'}{f^{n-1}}, \qquad K_n' = \frac{1}{2\sqrt{\pi}} \cdot \frac{\Gamma((C+1)/2)}{\Gamma(C/2)} \cdot K_n$$

for the two-dimensional spectrum of an isotropically-rough surface.

3.37.1.2 *Discussion*—The finish parameters in this model are K_n and n, which have the dimensions of μm$^{(3-n)}$ and μm^0. The dimensionless number n usually lies between 1 and 3 but need not be an integer. The quantity K_n is sometimes referred to as the spectral strength, and the parameter, n, the spectral index.

3.37.1.3 *Discussion*—The fractal model is the limiting case of the *ABC* model when the finish parameter B becomes very large. The value of the intrinsic mean-square profile and area roughness of the *ABC* model, obtained by integrating the *ABC* spectrum over all frequencies, is as follows:

$$R_q^2 = \int_0^\infty df_x\; S_1(f_x) = 2\pi \int_0^\infty f\, df\, S_2(f) = \frac{2\pi}{C-1} \frac{A'}{B^2}$$

which is finite for $C > 1$. The intrinsic value of the mean-square roughness of the fractal model is always infinite because of its divergence at low spatial frequencies. In contrast, the measured roughness values, obtained by integrating only over the measurement bandpass, are finite for the *ABC* for any value of C, and for the fractal model.

(*3*) *periodic spectral model*—The spectral model for a surface consisting of a periodic structure having the form:

$$S_1(f_x) = \frac{1}{2} \sum_{k=1}^{k=\infty} A_k{}^2 \cdot \delta(f_x - k/d_o)$$

and

$$S_2(f_x, f_y) = \frac{1}{4} \sum_{k=-\infty}^{k=+\infty} A_{|k|}{}^2 \cdot \delta(f_x - k/d_o) \cdot \delta(f_y)$$

for the two-dimensional spectrum. (All sums exclude the value $k = 0$.)

3.37.1.4 *Discussion*—The finish parameters of this model are the A_k's, the Fourier amplitudes of the periodic profile, and d_o, the fundamental spatial wavelength of the periodicity, both expressed in μm. $A_k{}^2/2$ is the mean-square roughness of the *k*-th harmonic of the profile ($k = 1$ is the fundamental), and

$\delta(F)$ is a unit-area function that is sharply peaked about the point $F = 0$. The value of the intrinsic mean-square profile and area roughness of the periodic model is as follows:

$$R_q^2 = \int_0^{\infty} df_x\ S_1(f_x) = \int_{-\infty}^{+\infty} df_x \int_{-\infty}^{+\infty} df_y\, S_2(f_x,f_y) = \frac{1}{2}\sum_{k=1}^{\infty} A_k^2$$

In contrast, the measured value is the right-hand side summed over those spectral lines that fall within the measurement bandpass.

(*4*) *composite spectral model*—A spectral model made up of a sum of terms involving different models or models with different parameters, or both.

3.38 *trace or profile length, L, micrometers*—The total length of the surface sampled by a linear profile measurement. In the indexing used in this practice

$$L = x_N = (N-1)D$$

where:

x_N = the position of the *N*-th or last point in the measurement, and

D = the same interval.

3.38.1 *Discussion*—The periodogram estimate is based on a Fourier representation of the surface profile. The basic periodicity of that expansion is *ND* rather than the literal profile length $L = (N–1)D$. Depending on the type of *FFT* used in the practical evaluation of the *PSD*, *N* may be required to be a power of 2, such as 1024, although in general, there is no restriction on *N* in the present practice.

3.39 *transfer function, measurement transfer function*—A function of spatial frequency having a magnitude between zero and one which describes the sensitivity of a linear measuring system to the amplitudes of different spatial-frequency components in the profile being measured.

3.39.1 *Discussion*—The ideal transfer function is unity within the measurement bandpass and zero for frequencies outside the bandpass. Real-world measurement transfer functions can deviate significantly from this. The transfer function is the Fourier transform of the impulse response function of the measuring apparatus.

3.40 *uniaxial or grating-like surface*—A surface whose roughness is confined to a particular direction or lay, so that it can be completely characterized by profile measurements perpendicular to the lay direction. Surfaces that display harmonic lines are frequently uniaxial.

3.40.1 *Discussion*—In contrast, an isotropic surface can also be completely characterized by profile measurements made in one direction, but there is no preferred direction as there is for uniaxial surfaces. Surfaces that are neither uniaxial nor isotropic can be characterized using the procedures described in this practice, although profile measurements taken on many directions across the surface may be needed to generate a complete statistical description of the surface under test.

3.41 *window function, data window, $W(x_n)$*—A bell-shaped or smooth-edged function which multiplies the detrended profile data set before it is inserted into the periodogram estimation routine.

3.41.1 *Discussion*—The window function "smoothes out" possible discontinuities at the ends of the measured, finite-length data set in order to eliminate the spurious oscillations which those discontinuities would otherwise generate in the spectral estimate. As long as the window function performs its function of reducing the contributions from the ends of the data record and has the proper normalization, its shape is of secondary importance.

3.42 *zero padding*—The procedure of adding zero values to a data set to bring the total number of data points, *N*, to a power of two to facilitate the evaluation of the *FFT* appearing in the periodogram spectral estimate.

3.42.1 *Discussion*—The window functions should be applied to the data set before zero padding. Zero padding is less important with the ready availability of arbitrary- *N FFT* computing packages.

4. Significance and Use

4.1 There is currently some confusion in the roughness-measurement community concerning the use of estimators and the calculation of power spectral densities (*PSD*s) from discrete data sets. Use of the present practice will eliminate these differences and result in the use of consistent units for the *PSD* and related parameters. It also provides a uniform reporting procedure for digital roughness data that will facilitate communication between different workers and different laboratories.

5. Procedure

5.1 The estimators defined in this section are based on the analysis of a data set $\{Z(n)\}$ consisting of *N* discrete values of the surface profile $Z(x_n = (n–1)D)$ measured at equally-spaced locations along a straight line of length *L*, where $n = 1$ to *N*. If $Z(n)$ is the measured profile, the detrended profile is given by:

$$Zd(n) = Z(n) - [a + b \cdot n + c \cdot n^2] \tag{1}$$

where the quantity in the square bracket is the quadratic detrending polynomial. The estimated values of the polynomial coefficients *a*, *b*, *c*, denoted by $\hat{a}$, $\hat{b}$, and $\hat{c}$, are determined by least-squares fitting of the polynomial to the measured profile data as now described. The degree of the detrending polynomial is chosen by the following considerations: Removing piston only (zeroth-order polynomial, *a*) is useful for instructional purposes but is inadequate in practice. It affects only the zero-frequency or "dc" term in the power spectral density. Removing piston and tilt (first-order polynomial, $a + b \cdot n$) is sufficient for the removing uncertainties in the rigid-body positioning of a nominally flat sample in the measurement apparatus. Removing piston, tilt and curvature (second-order polynomial, $a+b \cdot n+c \cdot n^2$) removes an additional quadratic term in the profile that may result from instrumental (extrinsic) effects or true (intrinsic) curvature in the surface being measured. See "detrending" for additional discussion.

5.1.1 Piston detrending is as follows:

$$\hat{Z}d(n) = Z(n) - [\hat{a}] \tag{2}$$

and

$$\hat{a} = +M_0 \tag{3}$$

where M_o is evaluated using the general moment expression,

$$M_P = \frac{1}{N} \sum_{n=1}^{n=N} n^P \cdot Z(n) \tag{4}$$

which appears here and the other detrending polynomials discussed in 5.1.2.

5.1.2 Piston and tilt detrending is as follows:

$$\hat{Z}d(n) = Z(n) - [\hat{a} + \hat{b} \cdot n] \tag{5}$$

where:

$n = 1, 2 \cdots N$

and

$$\hat{a} = + \frac{2}{N-1} \cdot [(2N+1) \cdot M_0 - 3 M_1] \tag{6}$$

$$\hat{b} = - \frac{6}{N-1} \cdot \left[M_0 - \frac{2}{N+1} \cdot M_1 \right]$$

5.1.3 Piston, tilt, and curvature detrending is as follows:

$$\hat{Z}d(n) = Z(n) - [\hat{a} + \hat{b} \cdot n + \hat{c} \cdot n^2], \tag{7}$$

where:

$n = 1, 2, \cdots N$

and

$$\hat{a} = + \frac{3}{(N-1)(N-2)} \cdot [(3N^2 + 3N + 2) \cdot M_0 - 6(2N+1) \cdot M_1 + 10 \cdot M_2]$$

$$\hat{b} = - \frac{6}{(N^2-1)(N^2-4)} \cdot [3)N + 1)(N+2)(2N+1) \cdot M_0 - 2(2N+1)(8N + 11) \cdot M_1 + 30(N+1) \cdot M_2] \tag{8}$$

$$\hat{c} = + \frac{30}{(N^2-1)(N^2-4)} \cdot [(N+1)(N+2) \cdot M_0 - 6(N+1) \cdot M_1 + 6 \cdot M_2]$$

NOTE 1—The estimated values of the coefficients depend on the degree of the polynomial being detrended. For example, the value of the coefficient â for piston and piston-plus-tilt detrending derived from the same data set are generally different.

NOTE 2—Despite these apparent differences, the mean values of each of the detrended profiles given by

$$M\text{ean value} = \frac{1}{N} \sum_{n=1}^{N} Zd(n) = 0 \tag{9}$$

vanishes in all cases. This means that the "dc" value of the estimated power spectrum of the detrended profile is zero, which offers a convenient numerical check on the numerical processing routines used.

NOTE 3—Least-squares fitting routines are available in many computer packages. Analytic results are given above for reference and checking.

5.2 *RMS Roughness:*

5.2.1 There are two different estimators for the rms roughness, R_q— one expressed in configuration space, and the other in frequency space, as follows:

$$\hat{R}_q^2(\,Config) = \frac{1}{N} \sum_{n=1}^{n=N} \hat{Z}d(n)^2 \tag{10}$$

and

$$\hat{R}_q^2(Freq) = \frac{1}{ND} \sum_{m=1}^{m=1+N/2} \hat{S}_1(m) \tag{11}$$

where $\hat{S}_1(m)$ is the periodogram estimate of the *PSD* based on $\hat{Z}d(n)$ discussed in 5.4.

NOTE 4—These two estimates of R_q^2 are mathematically identical if the periodogram is evaluated using a unit data window, $W(n) = 1$. Although a unit window function is not recommended for general use, the numerical identity of the Eq 10 and Eq 11 in that case offers a convenient check on the programming of the periodogram estimator.

NOTE 5—If a non-unit data window is used in the calculation of the *PSD* the two estimates of the rms roughness given will not, in general, be numerically identical for a particular profile measurement. On the other hand, the two estimates are identical for an ensemble average over a large number of profile measurements. In other words, the two estimates of R_q^2 are statistically the same.

NOTE 6—The first estimator has the advantage of familiarity and simplicity since it is expressed directly in terms of the detrended values of the measured profile data. Its disadvantage is that it involves, perforce, the transfer function of the measuring apparatus, and in a nonobvious way. In contrast, the frequency-space form may be more complicated to evaluate but has the advantage that it permits the bandwidth to be included in the rms value to be varied by selecting the range of *m* values included in the frequency sum. In addition, it permits the effects of a non-unit instrumental transfer function within that bandpass to be examined directly, and to be divided out by restoration processes, if its form is known independently.

NOTE 7—The spectra of real surfaces frequently tend to diverge at low spatial frequencies so that the values of the rms roughness obtained using either estimator may depend significantly on the value of the *LFL* of the measurement process, or chosen as a reference value. In some cases, the presence of a non-vanishing *LWL* can give a finite value of the profile roughness when its intrinsic value is infinite or undefined.

5.3 *RMS Slope:*

5.3.1 There are two different estimators for the rms slope, Δ_q— one expressed in configuration space, and the other in frequency space, as follows:

$$\hat{\Delta}_q^2(\,Con\,fig) = \frac{1}{N \cdot D^2} \sum_{n=1}^{n=N-1} [\hat{Z}d(n+1) - \hat{Z}d(n)]^2 \tag{12}$$

and

$$\widehat{\Delta}_q^2(Freq) = \frac{1}{ND} \sum_{m=1}^{m=1+N/2} \hat{S}_1(m) \cdot [2\pi(m-1)/ND]^2 \tag{13}$$

NOTE 8—The magnitudes of these two estimates are generally different since the first treats the profile as a collection of straight-line segments connecting the measurement points, while the second connects them with a bandwidth-limited interpolation curve and involves a smaller bias error.

NOTE 9—The notes for the rms roughness estimators just made generally apply to slope estimates as well. One difference is that the significant bandwidth effects on the slope occur principally at the *HFL* rather than the *LFL* as is the case for rms roughness measurements.

5.4 *Periodogram Estimators of the Profile Power Spectral Density:*

5.4.1 Form for height-measuring profilometers is as follows:

$$\hat{S}_1(m) = \frac{2D}{N} \cdot |FFT(m)|^2 \cdot K(m) \tag{14}$$

where the spatial frequency is evaluated at the discrete values, and

$$f_x = \frac{m-1}{ND} \tag{15}$$

where:

$m = 1, 2, \cdots (1 + N/2)$

5.4.2 The symbol *FFT* stands for discrete Fourier transform, which is always evaluated using some version of the fast Fourier transform as follows:

$$FFT\,(m) = \sum_{n=1}^{n=N} e^{i2\pi(n-1)(m-1)/N} W\,(n) \cdot \hat{Z}d(n) \tag{16}$$

where:

$W(n)$ = data window discussed in the following subsection, and

$K(m)$ = book-keeping factor:

thus:

$$K\,(m) = \begin{cases} 1/2 & \text{for } m = 1 \text{ or } 1 + N/2 \\ 1 & \text{otherwise} \end{cases} \tag{17}$$

NOTE 10—Eq 16 and Eq 17 apply for the conventional case of even *N*. Different forms apply for odd *N*.

NOTE 11—The case $m = 1$ corresponds to the zero-frequency or dc component of the detrended surface profile and $m = 2$ corresponds to the spatial frequency $1/ND$, which is essentially the reciprocal of the trace length, $(N–1)D$. On the opposite extreme, the frequency corresponding to $m = 1 + N/2$ is the Nyquist frequency, $1/2D$. The extreme range of surface wavelengths included in the measurement is therefore $1/ND < f < 1/2D$. In other words, the extreme $LFL = 1/ND$, the extreme $HFL = 1/2D$, and the dynamic range of the measurement is $N/2$.

NOTE 12—A convenient and readable reference to the *FFT* and its evaluation is Chapter 12 in *Numerical Recipes* by Flannery, Teukolsky and Vetterling **(1)**.[2]

NOTE 13—*The Brookhaven National Laboratory Report* **(2)** contains further background information on these procedures along with a computer program and numerical examples. (The BASIC routines used there involve different forms for the quantities M_p appearing in the expressions for the detrending polynomials than those discussed in this practice, although the numerical values of the detrending polynomials are identical in both cases.)

NOTE 14—The periodogram estimator just given is not the only method of estimating the power spectral density from a set of profile data, but it is the most direct and common method. It is sufficient for general use, and is a necessary first step to be taken before adding embellishments such as post-processing or considering more complicated estimators. This practice does not exclude the use of post-processing or alternative methods of analysis, but does require that the basic periodogram estimates just described be included in the discussion for comparative purposes.

5.4.3 Form for slope-measuring profilometers is as follows:

$$\hat{S}_1(m) = \left(2\pi \cdot \frac{m-1}{ND} \right)^{-2} \cdot \frac{2D}{N} |FFT\,(m)|^2 \cdot K\,(m) \tag{18}$$

where:

$$FFT'(m) = \sum_{n=1}^{n=N} e^{\,i2\pi(n-1)(m-1)/N}\, W\,(n) \cdot \hat{M}d(n) \tag{19}$$

and $\hat{M}$d(n) is the value of the profile slope measurements detrended using either the least-squares piston or the piston-plus-tilt expressions given in 5.1.

NOTE 15—This estimate of the profile power spectrum is the power spectrum of the profile slope divided by $(2\pi\, f_m)^2$. The prime on the *FFT* on the left denotes that it involves slope rather than height data.

NOTE 16—The case $m = 1$ corresponds to zero spatial frequency and must be excluded in the use of the above expressions.

5.5 *Periodogram Estimators of the Rms Profile Roughness and Slope:*

5.5.1 The periodogram estimator of the rms profile height, $\hat{R}_q$, is as follows:

$$\hat{R}_q = \sqrt{\frac{1}{ND} \sum_{m=2}^{1+N/2} \hat{S}_1(m)} \tag{20}$$

5.5.1.1 This quantity has the same dimension as the original height measurements and is independent of the magnitude and dimensions of the sampling interval, *D*.

5.5.2 The corresponding estimator for the rms profile slope, Δq, is as follows:

$$\hat{\Delta}q = \sqrt{\frac{1}{ND} \sum_{m=2}^{1+N/2} \hat{S}_1{}'\,(m)} = 2\,\pi \sqrt{\frac{1}{(ND)^3} \sum_{m=2}^{1+N/2} (m-1)^2 \cdot \hat{S}_1(m)} \tag{21}$$

5.5.2.1 In evaluating these quantities the height measurements, *Z*, and the sampling interval, *D*, must be expressed in the same length units. Although $\hat{\Delta}_q$ is in the dimensionless units of radians, its magnitude scales as 1/ *D*.

5.6 *Window Functions:*

5.6.1 Window functions appear in a wide variety of signal-processing applications, with different shapes and normalizations. Although this practice recommends the use of the Hann or Blackman data window, other forms are included for comparison. All are normalized so that:

$$\frac{1}{N} \sum_{n=1}^{n=N} W\,(n)^2 = 1 \tag{22}$$

in order to preserve the magnitudes of average values of the mean-square profile statistics.

5.6.2 Particular forms are:

(*1*) Rectangular or Daniell window:

$$W\,(n) = 1 \tag{23}$$

(*2*) Hann, or raised Cosine window:

$$W\,(n) = \sqrt{\frac{2}{1728}} \cdot [24 - 24\,Cos\{2\pi(n-1)/N\}] \tag{24}$$

(*3*) Hamming window:

$$W\,(n) = \sqrt{\frac{2}{1987}} \cdot [27 - 23\,Cos\{2\,\pi(n-1)/N\}] \tag{25}$$

(*4*) Blackman window:

$$W\,(n) = \sqrt{\frac{2}{1523}} \cdot [21 - 25\,Cos\{2\,\pi(n-1)/N\} + 4\,Cos\{4\pi(n-1)/N\}] \tag{26}$$

NOTE 17—The choice of window functions is of minor importance for randomly-rough surfaces as long as it smoothes the data at the ends of the data record. The rectangular or Daniell window does not do this, but is useful for numerical checking.

NOTE 18—In the case of profiles with a smooth *PSD*, the principal effect the window shape is to change the fine-scale fluctuations in the periodogram estimate without changing its ensemble-average value, except, perhaps, near the *LFL*.

NOTE 19—In the case of profiles involving periodicities, the window shape can change the shape of the sharp lines in the *PSD*, albeit without changing their areas. The choice of the window shape then involves a trade-off between line width and smoothness. The raised Hann or Blackman windows are recommended for general use.

NOTE 20—If the estimation routines are applied to deterministic profiles, such as individual steps, pits, or bumps, a data window must still be used to minimize effects of the finite data record, but the object should be placed in the center of the profile where the window function is relatively flat.

5.7 *Zero Padding:*

5.7.1 The fastest *FFT* routines require the total number of data points to be a power of two, such as $N = 2^{10} = 1024$. If the number of measured points, *N*, is not a power of two but lies between 2^a and 2^b, the power-of-two routines can be used by dropping $N - 2^a$ points from one end of the original data set, or by adding $2^b - N$ zeros and replacing N in the routines everywhere by 2^b.

5.7.2 The first method is wasteful of data, while the second uses the full set of measured data but requires that the estimated *PSD* be renormalized by multiplying it by the factor $2^b/N$.

5.8 *Averaging of Statistical Quantities:*

5.8.1 Power spectral density functions, the mean-square roughness, and slope values estimated from a number of individual profiles that have the same statistical properties can each be averaged together to obtain composite results. In the case of homogeneously- and isotropically-rough surfaces the profiles can lie in any position and direction on the surface under test. In the case of homogeneously- but anisotropically-rough surfaces they can lie anywhere on the surface but must lie parallel with each other, preferably perpendicular to the surface axis. Averaging data lowers the errors associated with individual measurements.

6. Numerical Test Sequences

6.1 Table 1 presents a set of numerical data for testing the execution of the users' implementations of algorithms discussed in Section 5.

6.2 Although these simulated profile data are in standard notation, they have been generated by a random number generator corresponding to a constant *PSD* and are not the results of an actual measurement. In addition, the number of data points has been limited to $N = 32$ and the profile heights have been rounded to digits with magnitudes less than 100 to simplify their manual input into the users' programs.

6.3 Actual measured data sets would generally involve many more data points with height values involving a larger number of significant digits, and with different orders of magnitude than those used in this test sequence.

6.4 In order to provide a means for checking the proper inclusion of the sampling distance, *D*, in the spectral-estimation routines, the value $D = 0.1$ has been used.

6.5 Table 2 and Table 3 give the values of the periodogram estimates of the profile power spectral density, $\hat{S}_1(m)$, of the data in Table 1 for the three different types of detrending described in 5.1. The values of these estimates depend on the data window used. Table 2 uses a rectangular window and Table 3 uses the Blackman window.

6.6 The dimensions of the power spectral densities in these tables is length-cubed = (units of Z)^2· (units of *D*), and its magnitude at a given spatial frequency scales as the sampling interval, *D*.

TABLE 2 Periodogram Estimates $\hat{S}_1(m)$ for Different Types of Data Detrending

	Rectangular data window			
m	None	Piston	Piston+Tilt	Full Quadratic
1	120.0500	0	0	0
2	205.9506	205.9506	182.5409	14.81781
3	142.1861	142.1861	137.3580	204.3631
4	56.98463	56.98463	44.47469	53.08546
5	147.9039	147.9039	139.6268	126.5831
6	58.60630	58.60630	55.67305	50.13899
7	248.4120	248.4120	264.7417	266.1277
8	152.8321	152.8321	158.6038	154.5160
9	185.1250	185.1250	192.8103	190.0105
10	28.81090	28.81090	26.22179	25.40131
11	28.61438	28.61438	27.90264	28.74841
12	153.1641	153.1641	145.7812	145.2367
13	356.5711	356.5711	366.4113	365.4717
14	199.1965	199.1965	202.6268	203.4514
15	41.53757	41.53757	40.26207	40.50671
16	163.6550	163.6550	168.8428	169.0258
17	16.20000	16.20000	17.87214	17.87215

TABLE 3 Periodogram Estimates $\hat{S}_1(m)$ for Different Types of Data Detrending

	Blackman data window			
m	None	Piston	Piston+Tilt	Full Quadratic
1	312.4632	87.20874	90.11245	9.832211
2	536.6033	268.4217	260.2453	76.63136
3	195.1412	166.9871	162.0176	93.70938
4	1.046170	1.046172	1.041742	1.303189
5	30.14155	30.14156	30.16028	30.25176
6	54.87353	54.87350	54.91950	54.94658
7	188.9816	188.9818	188.8795	188.8293
8	74.45938	74.45934	74.50156	74.51955
9	45.28967	45.28967	45.27541	45.29324
10	59.40473	59.40471	59.41950	59.41210
11	94.24771	94.24768	94.23248	94.23342
12	202.7328	202.7328	202.7405	202.7253
13	289.7414	289.7414	289.7450	289.7637
14	130.1287	130.1287	130.1230	130.1162
15	76.22277	76.22275	76.22527	76.22248
16	62.42836	62.42840	62.42742	62.43071
17	5.585947	5.585948	5.585947	5.584926

6.7 The spatial frequency is given as follows:

$$f_m = (m - 1)/\, ND \tag{27}$$

where:

m = 1 corresponds to the dc or piston part of the profile, and
m = $1 + N/2 = 17$ is the Nyquist frequency in (units of D^{-1}).

6.7.1 Note that since the window function has been applied

TABLE 1 Simulated Height Data[A]

n	Z(n)	n	Z(n)	n	Z(n)	n	Z(n)
1	–38	9	–40	17	3	25	–35
2	15	10	45	18	6	26	23
3	36	11	20	19	17	27	4
4	22	12	3	20	20	28	–8
5	29	13	47	21	24	29	–45
6	–43	14	–18	22	16	30	26
7	–1	15	45	23	–5	31	1
8	–5	16	43	24	–17	32	6

[A] A total of N = 32 data points.

after the detrending process, the dc terms do not necessarily vanish for a non-rectangular window functions.

6.8 Table 4 gives values of $\hat{R}_q$ derived from the spectra in Table 2 and Table 3 using the expression given in Table 4.

6.8.1 As mentioned, the unit of $\hat{R}_q$ is the same as that of the height measurement since the magnitude and dimensions of the sampling interval, D, cancels out in the evaluation of R_q.

6.9 The data in Table 2 through Table 4 are adequate for checking the users' implementation of the estimators described in Section 5, and further test data are not included in this practice.

TABLE 4 Values of the Estimates $\hat{R}_q$ for Different Types of Detrending Followed by Different Types of Data Windowing

Data Window	Type of Data Detrending			
	None	Piston	Piston+Tilt	Full Quadratic
Rectangular	26.13517	26.13517	26.05133	25.34362
Hann	25.49031	24.02299	23.91725	22.31003
Hamming	25.53997	24.26072	24.15406	22.58759
Blackman	25.29220	23.38999	23.30221	21.54917

7. Keywords

7.1 estimates; estimators; power spectral density; rms values; root mean square; roughness; slope; surface roughness; surface slope; surface statistics

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