

SEMI MF1811-1116 (Reapproved 1121) GUIDE FOR ESTIMATING THE POWER SPECTRAL DENSITY FUNCTION AND RELATED FINISH PARAMETERS FROM SURFACE PROFILE DATA

This Standard was technically approved by the Silicon Wafer Global Technical Committee. This edition was approved for publication by the global Audits and Reviews Subcommittee on August 12, 2021. Available at www.semiviews.org and www.semi.org in November 2021; originally published by ASTM International as ASTM F1811-97; previously published November 2016.

NOTICE: Paragraphs entitled ‘NOTE:’ are not an official part of this Standard or Safety Guideline and are not intended to modify or supersede the official Standard or Safety Guideline. These have been supplied by the global technical committee to enhance the usage of the Standard or Safety Guideline.

NOTICE: The section symbol (§) is used to reference a numbered section, paragraph, or header and all subordinate paragraphs, headers, and embedded material (i.e., EXCEPTIONs, lists) therein. The paragraph symbol (¶) is used to reference a particular numbered paragraph and embedded material therein. When duplicated (i.e., §§ and ¶¶) the symbols are used to reference more than one section or paragraph, respectively.

1 Purpose

1.1 There is some confusion in the roughness-measurement community concerning the use of estimators and the calculation of power spectral densities (PSDs) from discrete data sets. Use of this Guide can 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 can facilitate communication between different workers and different laboratories.

2 Scope

2.1 This Guide 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.

2.2 This Guide 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.

2.3 The data analysis procedures described in this Guide 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 this Guide through various parameters and functions that are defined in §§ 4 and 5, such as their sampling intervals, bandwidths, and measurement transfer functions.

2.4 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 Guide may have a different physical significance than those derived from random or periodic surfaces.

2.5 The statistical parameters and functions that are discussed in this Guide 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 Guide 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 Guide these numerical procedures are called ‘estimators’ and the results that they produce are called ‘estimates.’

2.6 This Guide 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.

2.7 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 Guide 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 Guide. Details of these and related subjects can be found in the references listed in § 7.

2.8 Raw measured profile data generally contain trending components that are independent of the microtopography of the surface being measured. These components should 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 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.

2.9 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:

$$A_{meas}(f_x) = A_{true}(f_x)T(f_x) \quad (1)$$

where:

A = the Fourier amplitudes.

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

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.

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

2.10.1 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.

2.10.2 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 bandpass ratio of the measurement.

2.10.3 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.

2.11 If the measurement transfer function is known to deviate significantly from unity within the measurement bandpass, the measured 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 Guide places no requirements on its use.

2.12 This Guide 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.

2.13 In order to make a quantitative comparison between profile data obtained from different measurement techniques, the statistical parameters and functions of interest should be compared over the same or comparable spatial-frequency regions. The most common quantities used to compare surfaces are their 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 PSDs to extrapolate the PSDs outside their measurement bandwidth.

2.14 Examples of specific bandwidth 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 $1.48 \mu\text{m}^{-1}$; that is, a bandpass ratio 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 bandpass ratio of $512/1$ or more. In the latter case the sub-range of 0.0125 to $1 \mu\text{m}^{-1}$ 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.

2.15 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 Figure 1. This is called a 'top-hat' or binary filter function. Before the ready availability of digital frequency-domain processing as employed in this Guide, 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 Guide recommends the determination of rms roughness and slope values using top-hat windowing of the measured PSD in the frequency domain.

2.16 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.

2.16.1 The rms roughness does not carry any information about the transverse scale of the surface roughness. That is, it is 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.

2.16.2 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. ANSI/ASME B46.1 discusses additional surface statistics, terms, and measurement methods applicable to machined surfaces.

2.17 The units used in this Guide are a self-consistent set of SI units that are appropriate for many measurements in the semiconductor and optics industry. This Guide 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.

NOTICE: SEMI Standards and Safety Guidelines do not purport to address all safety issues associated with their use. It is the responsibility of the users of the Documents to establish appropriate safety and health practices, and determine the applicability of regulatory or other limitations prior to use.

3 Referenced Standards and Documents

3.1 SEMI Standards and Safety Guidelines

SEMI M59 — Terminology for Silicon Technology

SEMI ME1392 — Guide for Angle Resolved Optical Scatter Measurements on Specular or Diffuse Surfaces

3.2 ANSI Standards¹

ANSI/ASME B46.1 — Surface Texture (Surface Roughness, Waviness and Lay)

3.3 ASTM Standards²

ASTM E284 — Standard Terminology of Appearance

NOTICE: Unless otherwise indicated, all documents cited shall be the latest published versions.

4 Terminology

4.1 *Introduction* — This section provides the definitions of special terms used in this Guide, 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 § 5. Definitions of terms not included here can be found in SEMI M59, SEMI ME1392, ASTM E284, or ANSI/ASME B46.1.

4.2 Definitions

4.2.1 *averaging, aperture or local* — smoothing of an estimate of the power spectral density (PSD) function by replacing its value at a given spatial frequency by its average over a local frequency range using a particular weighting function.

4.2.1.1 *Discussion* — The averaged quantities should include the same range of surface spatial frequencies.

4.2.2 *averaging, data* — numerical averaging of statistical estimates of the PSD, the mean-square roughness or the mean-square slope derived from different measurements, in order to obtain a single, composite result.

4.2.2.1 *Discussion* — 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. Again, the averaged quantities should include the same range of surface spatial frequencies.

4.2.3 *bandpass ratio* — ratio of the high- to low-frequency limits of the bandwidth of a given measurement technique.

4.2.3.1 *Discussion* — The ratio HFL/LFL is a useful single-number characteristic of a measuring apparatus. It completely describes the measurement effects on surfaces with power-law power spectra.

4.2.4 *bandwidth, bandwidth limits* — range of surface spatial frequencies included in a measurement or specification.

4.2.4.1 *Discussion* — Bandwidth is specified by a high-frequency limit (HFL) and a low-frequency limit (LFL). The bandwidth and the measurement transfer function over the bandwidth should 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.

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

NOTE 1: The term, bias, is defined similarly in SEMI M59 with respect to a test measurement as “the difference between the population mean of the test results from a measurement process and the true (accepted reference) value of the property being measured.” To maintain the difference between the deviation of an estimator and a measurement result, the term, *bias error*, is used in this Guide.

4.2.5.1 *Discussion* — The periodogram estimator of the power spectral density (PSD) given in this Guide 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.

¹ American National Standards Institute, 25 West 43rd Street, New York, NY 10036, USA; Telephone: +1.212.642.4900, Fax: +1.212.398.0023, <http://www.ansi.org>

² ASTM International, 100 Barr Harbor Drive, West Conshohocken, PA 19428-2959, USA; Telephone: +1.610.832.9585, Fax: +1.610.832.9555, <http://www.astm.org>

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

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

4.2.7 *detrended profile, $Z_d(x)$* — the raw or measured profile after removing instrumental and surface trends. The detrended profile is the input for the statistical estimation routines described in § 5.

4.2.7.1 *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 Guide 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.

4.2.8 *ensemble* — infinitely large collection (infinite ensemble) of quantities, the properties of which are governed by some statistical distribution law.

4.2.8.1 *Discussion* — For example, ensembles include surface profiles, and rms roughness values.

4.2.9 *ensemble average value* — value of a particular surface parameter or function averaged over the appropriate distribution functions.

4.2.9.1 *Discussion* — The ensemble average value of the quantity A is denoted by $\langle A \rangle$. 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.

4.2.10 *estimate* — ensemble-average value of a roughness statistic from a finite set of measured profile data.

4.2.10.1 *Discussion* — In this Guide, a circumflex is used to distinguish estimates from the corresponding ensemble-average quantities (see also ¶ 2.6).

4.2.11 *estimator* — algorithm or mathematical procedure for calculating an ‘estimate.’

4.2.12 *fast Fourier transform (FFT)* — algorithm for calculating the Fourier transform (discrete Fourier transform or *DFT*) of a set of numerical data.

4.2.12.1 *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. It is now ubiquitous and can be found in any computer data analysis package (see ¶ 5.4.2 for details).

4.2.13 *finish parameters and functions* — numbers or functions that characterize surface height fluctuations.

4.2.13.1 *Discussion* — The values and forms of finish parameters and functions 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. 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 Guide is concerned exclusively with the properties of surface profiles.

4.2.14 *fluctuation error* — general term denoting the deviation of a quantity from its mean, average or detrended value.

4.2.14.1 *Discussion* — Fluctuation errors are usually measured in terms of their mean-square or rms values. For example, R_q is the rms fluctuation error in the surface height and Δ_q is the rms fluctuation error in the 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 Guide.

4.2.15 *high-frequency limit (HFL) [1/μm]* — highest spatial frequency contained in a profile data set or specification.

4.2.15.1 *Discussion* — The HFL of a measurement is determined by the details of the measurement process, and its value in specifications is determined by the user. If the sampling interval in the measurement process is D , the extreme value of the HFL is given by the Nyquist criterion, $HFL = 1/(2D)$. 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.

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

4.2.16.1 *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 PSDs 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 (band-width limited) finish parameters is not always made in the literature.

4.2.17 *impulse response, of a profile measuring system* — measured shape of an impulse or infinitely-sharp ridge lying perpendicularly to the profile direction.

4.2.17.1 *Discussion* — In the case of a linear measuring system the impulse response is the Fourier transform of the system transfer function. 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.

4.2.18 *isotropic surface* — surface whose intrinsic finish parameters and functions are independent of the rotational position of the surface about its surface normal. Also known as *statistically-isotropic surface*.

4.2.18.1 *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 ¶ 4.2.41.

4.2.19 *linear systems, linear measurement system* — a signal-processing concept more precisely described as a linear, shift-invariant system.

4.2.19.1 *Discussion* — 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 ¶ 2.9. All practical measurement systems are taken to be linear over their operating ranges.

4.2.20 *low-frequency limit (LFL) [1/μm]* — lowest spatial frequency contained in a profile data set or specification.

4.2.20.1 *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.

4.2.21 *mean-square roughness, R_q^2 [nm²]* — ensemble-average value of the square of the height of the detrended profile.

4.2.21.1 *Discussion* — This value is given by the following relationship:

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

where:

$Z_d(x)$ = detrended surface profile, and