Calculation of the power spectral density from surface profile data

J. Merle Elson and Jean M. Bennett

The power spectral density (PSD), in its two-dimensional form, has been designated as the preferred quantity for specifying surface roughness on a draft international drawing standard for surface texture. The correct calculation of the one-dimensional PSD from discrete surface profile data is given, and problems in using fast Fourier-transform routines that are given in some of the standard reference books are flagged. The method given here contains the correct normalizing factors. Two ways to reduce the variance of the PSD estimate are suggested. Examples are shown of the variance reduction possible in the PSD's.

Key words: Power spectral density, surface profiles, beryllium.

1. Introduction

Characterization of optical surfaces frequently involves the power spectral density function, often called the power spectral density (PSD). It can be calculated from measurements of the bidirectional reflectance distribution function (BRDF) or from surface profiles made by an optical or a mechanical profiler. The PSD, in its two-dimensional form, has been designated as the preferred quantity for specifying surface roughess.[1] Because different types of measuring instruments have different surface spatial bandwidth limits, the rms roughness that would be measured with a specific type of instrument can be determined by the integration of the two-dimensional PSD between the surface spatial frequency bandwidth limits that are appropriate for that particular instrument. As is shown in this paper, in order to be consistent with PSD values obtained from various types of instruments, the area under the two-sided PSD curve should equal δ^2, the square of the bandlimited rms roughness for the sample.

In principle, the method of obtaining the PSD from measured surface profile data is straightforward. One can take the square of the Fourier transform of the surface profile or take the Fourier transform of the autocovariance function that has been calculated from the surface profile, both of which should yield an identical estimate of the one-dimensional PSD.[2] There are well-documented ways of converting a one-dimensional PSD into the two-dimensional form.[3,4] The problem is in obtaining the correct one-dimensional PSD from one-dimensional surface profiles. Although the equations are explicit in integral form, actual surface data are discrete digitized data points, each of which is an average over the area covered by the probe of the profiler, and the profile is of a finite length.[5]

Generally speaking, to obtain a true PSD of a surface that has random roughness, we must take an ensemble average of PSD estimates calculated from profiles made at many different places on a surface. A PSD calculated from a single profile measurement is meaningless because the graph is exceedingly noisy and nonreproducible. PSD estimates from surface profiles taken on different parts of the same isotropic surface are inconsistent, and, for a given spatial frequency, they can differ by orders of magnitude.

To obtain an ensemble average PSD from surface profile data, there are two options. A large number of profiles can be taken at different places on the surface, the one-dimensional PSD estimate calculated from each profile, and the resulting graphs averaged together to obtain a smooth, noise-free curve. Realistically, to obtain an acceptably smooth PSD for surface profiles that contain 1000 to 5000 data points, this means averaging together at least 20 PSD estimates from profiles taken at different places

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on the sample. Taking this many profiles is exceedingly time consuming, so this option is not practical.

The second option is to smooth the PSD estimate of a single profile (or a small number of profiles) without introducing artifacts. When the profile length represents a much lower surface spatial frequency than is needed in the PSD, i.e., when the correlation length of the relevant surface features is much shorter than the total profile length, the profile can be broken into small pieces, the PSD estimate calculated from each subprofile, and the estimates averaged together. Of course, when this method is used, the low-frequency components in the original surface profile are lost. Both variance reduction methods, which are attempts to achieve the ideal ensemble average condition, are discussed in this paper. They both yield PSD curves that should represent the surface structure in the bandwidth region determined by the profile measurements.

Throughout the paper, we are assuming that the surface topography is random and isotropic. If there is periodicity or unidirectional surface structure, profiles need to be taken parallel and perpendicular to the structure direction, and the one-dimensional PSD calculations need to be handled separately. Conversion to the two-dimensional PSD has already been discussed for this case.[3,4]

A frequent problem and an area of confusion in calculating PSD's from surface profiles arise in obtaining the correct normalizing factor for the PSD. We realize that the general subject of normalization is well documented in the fast Fourier-transform (FFT) literature, but considerable areas of confusion can arise. For example, there are numerous books that describe methods of estimating power spectra, and these methods may involve questions of one sided versus two sided, sum-squared amplitude, mean-squared amplitude, or time-integral-squared amplitude. Thus it may not be totally obvious as to how surface roughness profile measurements can be related to the PSD and be compatible with BRDF measurements or theory. It is not necessarily straightforward to change from the time and frequency domain to the length and surface spatial wavelength domain, and there are numerous examples in the literature (which are not referenced here) in which authors have incorrect normalizing factors on their PSD's.

The purpose of this paper is to help clarify some of these possible areas of confusion. We discuss the calculation of PSD's specifically with surface roughness in mind. We hope to clarify how the one-dimensional PSD can be calculated correctly and to flag problems in using FFT routines given in some of the standard reference books. Although the methods presented here may not be the only way to achieve correct normalized one-dimensional PSD's, they will at least alert the experimenter to problem areas and, it is hoped, will help make future-published PSD's accurately represent the surface statistics.

In this paper we discuss the basic theory we have used for obtaining the one-dimensional PSD from surface profile data, both in the integral form and in the digitized form. We show that the PSD obtained from digitized data has the correct normalizing factor by calculating the area under the two-sided PSD curve and showing that it is equal to δ^2, as measured by a surface profiler.

2. Power Spectral Density of Surface Roughness

2.A. Basic Theory

In the theory presented here, we restrict the discussion to the calculation of a one-dimensional PSD from surface profile data and show how this relates to a one dimensional BRDF, which describes scattering confined to a plane. For isotropic random surface roughness, the one-dimensional measured PSD can be modeled with an analytic function and then used to obtain an estimate for the corresponding two-dimensional PSD. This procedure is discussed elsewhere,[6] as is the two-dimensional BRDF.[6]

If $z(x)$ is the surface roughness height as a function of distance x, a finite-length Fourier transform may be written:

$$Z(k) = \int_0^L \mathrm{d}x\, z(x) \exp(-ikx), \tag{1}$$

where k is the wave number. Because surface profile measurements of $z(x)$ yield digitized data, we assume that the surface roughness data set consists of N values for $z(x)$ that are measured at equally spaced intervals Δx over a total length $L = N\Delta x$. If these discrete surface height data are adjusted to have a zero mean value, i.e., there are equal heights above and below a mean surface level, and are denoted by $z(n)$, $n = 0 \rightarrow N-1$, then the mean square of these N values, called the mean-square roughness δ^2, is given by

$$\delta_N^2 = \frac{1}{N} \sum_{n=0}^{N-1} z^2(n). \tag{2}$$

This value is bandwidth limited, as the magnitude of the highest surface spatial frequency resolved in the measurement process is $f_c = (2\Delta x)^{-1}$, which is the Nyquist frequency.

The digital analysis in this paper is based on standard FFT methods. The digital equivalent of Eq. (1) yields the Fourier transform $Z(m)$ as

$$Z(m) = \Delta x\, \hat{Z}(m), \qquad -N/2 \le m \le N/2, \tag{3}$$

where

$$\hat{Z}(m) = \sum_{n=0}^{N-1} z(n) \exp(-2\pi i m n/N), \qquad -N/2 \le m \le N/2. \tag{4}$$

Distance and wave number are now digitized with $x = n\Delta x$ and $k = 2\pi f_m$. The $f_m = m/(N\Delta x)$ are the spatial frequency components of the surface roughness. Note that typical FFT routines evaluate only the $\hat{Z}(m)$, as in Eq. (4), but to have the proper units and magnitude for the PSD, the coefficient must be included, as in Eq. (3).

When the rms roughness $\delta \ll \lambda$, a first-order perturbation theory calculation of the one-dimensional BRDF for scattering of a normally incident monochromatic plane wave of wavelength λ by random surface roughness yields

$$\mathrm{BRDF} = (2\pi/\lambda)^3 \cos\theta\, F(\theta, \lambda) \left\langle \frac{|Z(k)|^2}{L} \right\rangle, \tag{5}$$

where θ is the scattering angle, $F(\theta, \lambda)$ is an optical factor unrelated to surface roughness, and $\langle \cdots \rangle$ denotes ensemble average. The averaged PSD is given by

$$\mathrm{PSD} = \left\langle \frac{|Z(k)|^2}{L} \right\rangle, \tag{6}$$

where the wave-number argument for scattered light is $k = (2\pi/\lambda)\sin\theta$. Actually, k is a vector that, in this one-dimensional analysis, can be positive or negative. As shown in Fig. 1, positive and negative values of m correspond to scattering angles θ in the first and the second quadrants, respectively. Also, the argument of Eq. (6) can be $k > 2\pi/\lambda$, but this pertains to evanescent fields rather than scattered fields that propagate away from the surface.

2.B. Unaveraged Power Spectral Density

In this subsection, we consider one estimate of a PSD and realize that the true PSD is an ensemble average of many such estimates. We call the PSD estimate the unaveraged PSD. This is consistent with the software packages that accompany all commercial profilers that calculate an unaveraged PSD from a single profile. This usage is so widespread that researchers almost never take an ensemble average of PSD estimates when reporting measured PSD's.

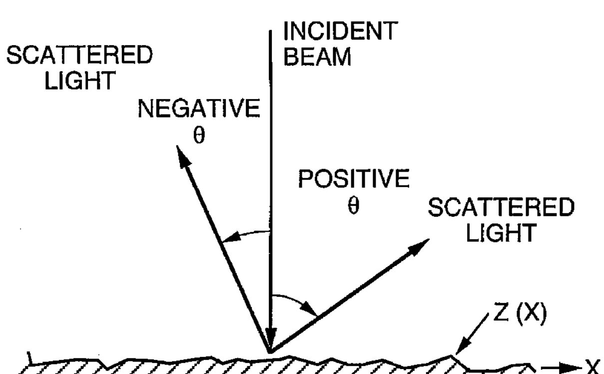

Fig. 1. Schematic diagram of a normally incident beam on a rough surface described by the random variable $z(x)$ and scattered light at positive and negative scattering angles θ.

We view the PSD as two-sided. Here we use the FFT periodogram method to estimate the PSD from surface profile measurements. With Eqs. (3) and (4), we convert Eq. (6) to the digital equivalent of an unaveraged PSD function as

$$\frac{|Z(2\pi f)|^2}{L} \rightarrow \frac{|Z(m)|^2}{N\Delta x} = \frac{\Delta x}{N} \left| \sum_{n=0}^{N-1} z(n) \exp(-2\pi i m n/N) \right|^2. \tag{7}$$

Note that the argument $k = 2\pi f \rightarrow 2\pi m/(N\Delta x)$. The only part of this digital conversion of k that changes is the index m. Thus we show the argument of Z as simply m. As in Eq. (1), the exponent of e in Eq. (7) is $-ikx \rightarrow -i[2\pi m/(N\Delta x)](n\Delta x)$. We now define the unaveraged PSD, $P_N(m)$, as

$$P_N(m) = \frac{\Delta x}{N} \left| \sum_{n=0}^{N-1} z(n) \exp(-2\pi i m n/N) \right|^2 = N\Delta x \hat{P}_N(m), \quad -\frac{N}{2} \le m \le \frac{N}{2}, \tag{8a}$$

where

$$\hat{P}_N(m) = \left[\frac{|\hat{Z}(m)|^2}{N^2} \right], \quad -\frac{N}{2} \le m \le \frac{N}{2}. \tag{8b}$$

We recall that standard FFT routines typically evaluate only the summation term $\hat{Z}(m)$ and that aliasing requires special treatment of the $m = \pm N/2$ terms. Also, as discussed below, many[7–9] PSD definitions are given in the form of Eq. (8b). However, to have the proper units and magnitude for $P_N(m)$, the coefficient $\Delta x/N$ must be included with the summation term in Eq. (8a). The $P_N(m)$ is a sample PSD estimate, which is based on a single surface profile that contains N points. As mentioned above, this estimate has a large variance about the true PSD that is shown in the numerical results. We know from PSD estimation theory using FFT methods[7,8] that, for a given f_m, the variance of $P_N(m)$ is independent of N and approximately proportional to the square of the true PSD. In other words, PSD's calculated from surface profile data measured in different places on the same surface will yield widely varying and inconsistent results for a given f_m. This problem can be partially overcome if K $P_M(m)$ functions are calculated from subsets of a single profile, each having M points, where $M < N$, with N being the number of points in the total profile. The K $\mathrm{PSD}_M(m)$ functions may then be averaged so that the variance in the PSD is reduced by $1/K$. This topic is discussed further in Subsection 2.C.

We may integrate the PSD over the Nyquist bandwidth limits of surface spatial frequency to obtain the area. Parseval's theorem says that the area under the PSD curve should equal the mean-square roughness. This provides the proper normalization for the

PSD. We obtain this result as follows:

$$\int_{-f_c}^{f_c} \mathrm{d}f \frac{|Z(2\pi f)|^2}{L} = \frac{1}{L}\int_{-f_c}^{f_c} \mathrm{d}f \left| \int_0^L \mathrm{d}x\, z(x) \exp(-2\pi i f x) \right|^2. \tag{9}$$

Letting $\mathrm{d}x \to \Delta x$, $\mathrm{d}f \to (N\Delta x)^{-1}$, $L = N\Delta x$, $x = n\Delta x$, and $f = m/(N\Delta x)$ in Eq. (9) yields the equivalent digital expression:

$$\begin{aligned}
&\left(\frac{1}{N\Delta x}\right)^2 \left[\tfrac{1}{2}|Z(-N/2)|^2 + \sum_{m=-(N/2)+1}^{(N/2)-1} |Z(m)|^2 + \tfrac{1}{2}|Z(N/2)|^2 \right] \\
&= \frac{1}{N^2} \sum_{n=0}^{N-1} \sum_{n'=0}^{N-1} z(n) z(n') \Bigg\{ \tfrac{1}{2}\exp[-\pi i(n-n')] \\
&\quad + \sum_{m=-(N/2)+1}^{(N/2)-1} \exp[2\pi i m(n-n')/N] \\
&\quad + \tfrac{1}{2}\exp[\pi i(n-n')] \Bigg\}.
\end{aligned} \tag{10}$$

The terms in parentheses on both sides of Eq. (10) contain the sums over the index m and reflect the aliasing inherent in discrete Fourier transforms, where the $m = \pm N/2$ terms have been written explicitly and weighted $1/2$ of the other terms in the sum. The right-hand side of Eq. (10) may be greatly simplified, as the term in the parentheses on the right-hand side reduces to $N\delta_{n,n'}$, where $\delta_{n,n'}$ is the Kronecker δ function. The Kronecker δ function and Eq. (2) permit the double sum on the right-hand side of Eq. (10) to be reduced to $N\delta_N^2$. Then Eq. (10) becomes

$$\left(\frac{1}{N\Delta x}\right)^2 \left[\tfrac{1}{2}|Z(-N/2)|^2 + \sum_{m=-(N/2)+1}^{(N/2)-1} |Z(m)|^2 + \tfrac{1}{2}|Z(N/2)|^2 \right] = \delta_N^2. \tag{11}$$

Equation (11) may be rewritten in terms of the PSD, as defined in Eq. (8a), as

$$\frac{1}{N\Delta x} \left[\tfrac{1}{2}P_N(-N/2) + \sum_{m=-(N/2)+1}^{(N/2)-1} P_N(m) + \tfrac{1}{2}P_N(N/2) \right] = \delta_N^2. \tag{12}$$

This result shows that the area under the two-sided PSD curve equals δ_N^2, the bandwidth-limited mean square of the surface roughness.

Many references (for example, Refs. 7–9) give alternative definitions for the PSD as a one-sided function defined only for $m = 0, 1, 2, \ldots, N/2$. Because Parseval's theorem must still be satisfied, the PSD must be scaled accordingly. Some one-sided definitions appear as

$$\hat{P}_N(m) = (1/N^2)|\hat{Z}(m)|^2, \qquad m = 0 \text{ or } N/2, \tag{13a}$$

$$\hat{P}_N(m) = (2/N^2)|\hat{Z}(m)|^2, \quad m = 1, 2, \ldots, (N/2) - 1, \tag{13b}$$

because $|Z(m)|$ is even for real data $z(n)$, or as

$$\hat{P}_N(m) = (1/N^2)|\hat{Z}(m)|^2, \qquad m = 0 \text{ or } N/2, \tag{14a}$$

$$\hat{P}_N(m) = (1/N^2)[|\hat{Z}(m)|^2 + |\hat{Z}(N-m)|^2], \quad m = 1, 2, \ldots, (N/2) - 1. \tag{14b}$$

Both definitions as given in Eqs. (13) and (14) automatically satisfy

$$\sum_{m=0}^{N/2} \hat{P}_N(m) = \delta_N^2. \tag{15}$$

Although Eqs. (13)–(15) are concise, they are unphysical for use as a PSD to relate roughness to the BRDF, as they are defined only for positive frequencies and are a factor of 2 too large. Many FFT-based commercial routines for calculating PSD's include smoothing algorithms and yield a one-sided PSD.[10] Modification to convert one-sided PSD software to yield two-sided PSD's should be straightforward. Nevertheless, in order for the PSD estimates to have the proper units and magnitudes to represent the spectra of surface roughness physically, the PSD should be two sided and have coefficients as shown in Eq. (8a).

2.C. Averaged Power Spectral Density

To calculate the scattering from an optical component such as the BRDF in Eq. (5), ideally we would like to have an ensemble average of PSD estimates, $|Z(k)|^2/L$, associated with the spatial components of surface roughness. One way to obtain such an average is to assume statistically ergodic and stationary surface statistics and to take multiple surface profiles of length N, calculate $P_N(m)$ results from each profile, and then form an averaged PSD. Although this process is time consuming, as it is necessary to take many independent profile measurements, it has been done here for one case, and the results are presented in Section 3.

Another way to obtain an ensemble average of PSD estimates is to assume that the surface profile is many times longer than the correlation length of the surface roughness. We can then break this single profile into many shorter segments, each significantly longer than the correlation length, and can again form an average PSD as outlined below or from existing software.[7,8] In this case, the variance of the PSD estimate is significantly decreased at the expense of losing low spatial frequency information and having fewer spatial frequency values. We interpret this result as an ensemble average of the one-dimensional, two-sided PSD of the surface roughness.

From the second method, we can calculate average PSD estimates as follows. Assume that we have a surface profile of length L that contains N data points. We may subdivide this total length into K segments (which may overlap), each having M (a power of 2) values. We can calculate unaveraged PSD estimates, $P_M^{(k)}(m)$, for segments $k = 1 \rightarrow K$, where

$$P_M^{(k)}(m) = \frac{\Delta x}{M} \left| \sum_{n=0}^{M-1} z(n)\, w(n) \exp(2\pi i m n / M) \right|^2, \quad -\frac{M}{2} \leq m \leq \frac{M}{2}, \tag{16}$$

and where the right-hand side of this equation should be multiplied by $1/2$ when $m = \pm M/2$. We have introduced a window function $w(n)$ to reduce high-frequency leakage. The set of K PSD estimates may then be averaged to yield

$$P_A(m) = \frac{S}{K} \sum_{k=1}^{K} P_M^{(k)}(m), \tag{17}$$

where a scaling factor S has been introduced. We do this because the window function affects the $P_A(m)$ values so that Eq. (12) is no longer satisfied. We determine the scaling factor S by calculating the area under the $P_A(m)$ curve. Analogous to Eq. (12), we use Eq. (17) and calculate the area under $P_A(m)$, which yields

$$\frac{1}{M\Delta x}\left[\tfrac{1}{2} P_A(-M/2) + \sum_{m=(-M/2)+1}^{(M/2)-1} P_A(m) + \tfrac{1}{2} P_A(M/2) \right] = \frac{S}{K} \sum_{k=1}^{K} \delta_k^2 = S\bar{\delta}^2, \tag{18}$$

where δ_k^2 is the mean-square roughness of the windowed data associated with the area under the $P_M^{(k)}(m)$ curve. We choose S such that

$$S\bar{\delta}^2 = \delta_N^2. \tag{19}$$

This forces the area under the averaged $P_A(m)$ curve to be equal to δ_N^2. The number of segments K is determined by the integer part of $1 + (N - M)/M_s$, where M_s is the amount of segment overlapping, if any. Segments $k = 1 \rightarrow K$ contain data points $z[(k-1)M_s + 1] \rightarrow z[(k-1)M_s + M]$.

3. Numerical Results

The numerical results presented here depend primarily on FFT software that is commonly available. Commercial software[7,8] is also available to produce smoothed PSD estimates. The averaged and unaveraged PSD results shown in this section use the relations derived in Section 2. We show PSD estimates calculated from surface profiles taken on two different beryllium surfaces, samples 8 and 18, which have been studied previously.[6] Sample 8 was well-polished bulk beryllium with a minimum of oxide inclusions. It showed the typical grain structure of bulk beryllium when viewed under a Nomarski microscope. Sample 18 was sputtered beryllium on a smooth (<5-Å rms roughness) silicon carbide substrate. The sputtered beryllium was not polished. When viewed under a Nomarski microscope, the surface appeared to have a uniform distribution of tiny grains.

Surface profile data for samples 8 and 18 were taken with $\Delta x = 0.37$ μm (1000-μm profile length) and $\Delta x = 0.037$ μm (100-μm profile length). For the 1000-μm profile length, samples 8 and 18 had rms roughnesses of 6.4 and 26.7 Å, respectively. The rms roughnesses were 6.2 and 34.9 Å, respectively, for the 100-μm profile length. Note that the roughnesses for the polished beryllium (sample 8) were the same for the two profile lengths, indicating that there was no fine structure on the 100-μm profile that was being missed on the 1000-μm profile, and, conversely, that the long spatial wavelength surface structure had heights that were similar to the shorter spatial wavelength structure, suggesting a fractal surface. On the other hand, the 100-μm profile roughness was larger for the sputtered beryllium (sample 18), suggesting that the sputtered grains were being better defined with the shorter sampling distance. The autocovariance length of sample 8 was ~0.4 μm, which was somewhat longer than that of sample 18, with an autocovariance length of <0.2 μm.

The unaveraged PSD results that follow were obtained from Eq. (8). The averaged PSD results were obtained with Eqs. (16)–(19), and the window function

$$w(n) = 1 - \frac{2}{M-1}\left| n - \frac{M-1}{2} \right|. \tag{20}$$

Figure 2 shows unaveraged and averaged PSD's for sputtered beryllium, sample 18, on a log–log plot versus spatial frequency, with $\Delta x = 0.37$ μm. The averaged PSD curve has been displaced an order of magnitude higher for clarity. The PSD is in units of angstroms squared times micrometers, and the spa-

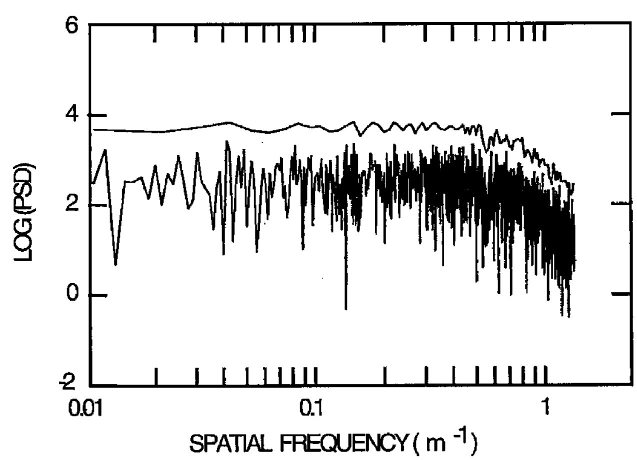

Fig. 2. Graph of log(PSD) versus spatial frequency for sample 18 calculated from surface profile data. The digitization interval Δx = 0.37 μm, and the profile length is 1000 μm. The averaged and the unaveraged PSD's are shown where the averaged curve is intentionally displaced 1 order of magnitude above the unaveraged curve.

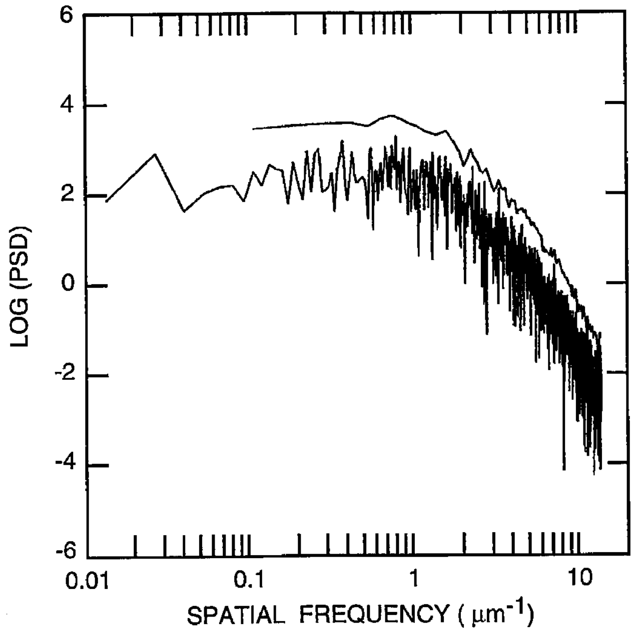

Fig. 3. Same as Fig. 2, except $\Delta x = 0.037$ μm, and the profile length is 100 μm.

tial frequency is in units of inverse micrometers. The total number of data points $N = 2661$, $M = 256$, and $M_s = 128$, which yields $K = 19$ profile segments. The smoothing calculation is considerably easier than taking 19 independent profiles on different parts of the surface and then averaging the PSD's. Figure 3 shows comparable PSD curves for the same sputtered beryllium surface with $\Delta x = 0.037$ μm. Figures 2 and 3 are combined in Fig. 4, which shows the averaged PSD's plotted together on the same log–log graph, where the ○ and △ symbols are for $\Delta x = 0.37$ and 0.037 μm, respectively. Because this sample has an autocovariance length of <0.2 μm, the shorter sampling interval data, $\Delta x = 0.037$ μm, should provide the most accurate results at the higher spatial frequencies (the △ curve). On the other hand, the longer sampling interval ○ curve should be more reliable at the low spatial frequency end. Thus we interpret the falloff of the ○ data to be caused by lack of resolution, and the two curves of Fig. 4 appear to be consistent.

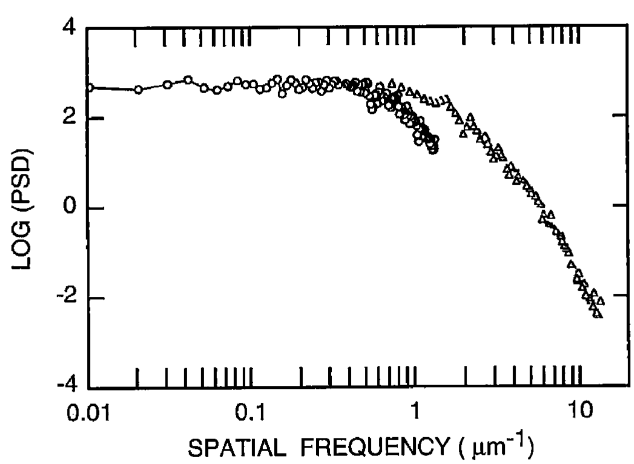

Fig. 4. Graph of log(PSD) versus spatial frequency for sample 18, with the averaged curves in Figs. 2 and 3 combined. The calculated values marked by ○ and △ are for $\Delta x = 0.37$ and 0.037 μm, respectively.

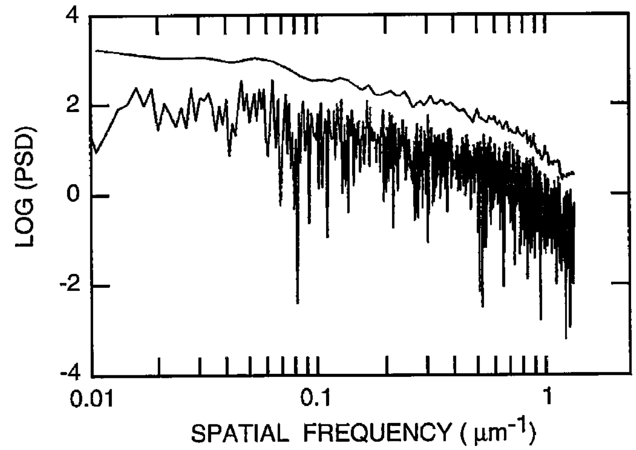

Fig. 5. Graph of log(PSD) versus spatial frequency for sample 8 calculated from surface profile data. The digitization interval $\Delta x = 0.37$ μm, and the profile length is 1000 μm. The averaged and unaveraged PSD's are shown where the averaged curve is intentionally displaced 1 order of magnitude above the unaveraged curve.

Comparable results for polished beryllium, sample 8, are shown in Figs. 5–7, which correspond to Figs. 2–4 for sputtered beryllium, sample 18. Because polished beryllium has a distribution of grain sizes, the PSD curve has a negative slope from spatial frequencies of 0.01–~2 μm^{-1} and then drops precipitously at higher frequencies, where little grain structure is present. On the other hand, sputtered beryllium, sample 18, contains large numbers of grains that have sizes in the 0.1–1-μm^{-1} range. For lower spatial frequencies, the substrate flatness dominates.

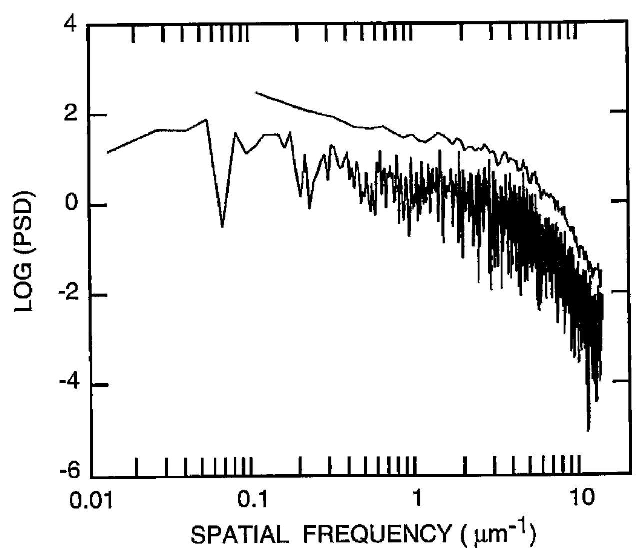

Fig. 6. Same as Fig. 5, except $\Delta x = 0.037$ μm, and the profile length is 100 μm.

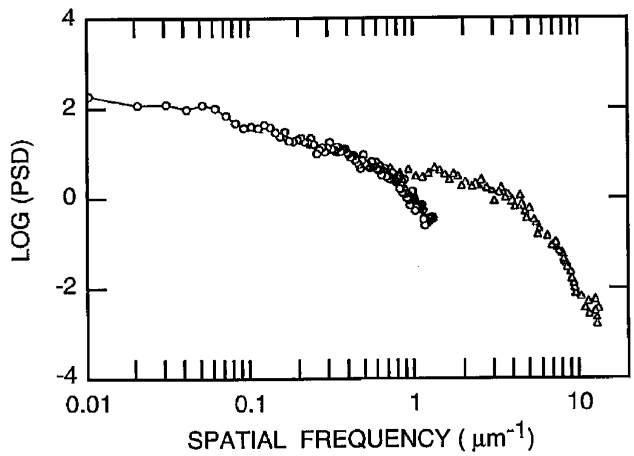

Fig. 7. Graph of log(PSD) versus spatial frequency for sample 8, combining the averaged curves in Figs. 5 and 6. The calculated values marked by ○ and △ are for $\Delta x = 0.37$ and 0.037 μm, respectively.

Because sputtered beryllium, sample 18, has mostly high spatial frequency structure with a minimum of low spatial frequency components, we used it to verify statements made above concerning variance reduction by taking multiple profiles at different places on the surface and forming averages of the PSD's. For these tests, we used $\Delta x = 0.037$ μm. We took 20 160-μm-long profiles (4232 points/profile) at different places on the surface. Figure 8 shows unaveraged and averaged PSD's calculated for the first 4096 data points in the profiles; again the averaged PSD curve has been displaced an order of magnitude higher for clarity. The data in Fig. 8 have been plotted as log(PSD) versus a linear spatial frequency scale. Although there are 2048 data points in these PSD curves instead of the 128 points in the PSD curves in Fig. 3, the variance reduction appears to be comparable. When the PSD's from 10 profiles were averaged together, the variance was approximately twice that of the average of 20 PSD's shown in Fig. 8. In addition, PSD's were calculated from single profiles containing 8192, 4096, and 2048 points. The variances of these curves were similar, also in agreement with theory, which states that the variance of a PSD estimate is independent of the number of points in the profile.

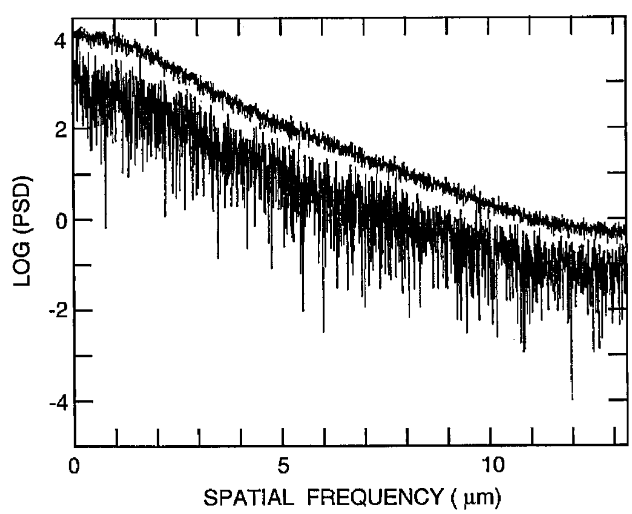

Fig. 8. Graph of log(PSD) versus spatial frequency on a linear scale for sample 18 calculated from surface profile data. The digitization interval $\Delta x = 0.037$ μm, and the profile length is 160 μm. The unaveraged PSD was calculated from a single profile. PSD's calculated from 20 profiles measured at different places on the same surface were averaged to give the upper curve, which is intentionally displaced 1 order of magnitude above the unaveraged curve.

4. Conclusions

We have shown how to calculate a one-dimensional PSD from digitized surface profile data using the correct normalizing factor, so that the PSD is consistent with one-dimensional PSD's obtained from scattering measurements. Because the PSD estimates from digitized surface profile data inherently have large variances relative to the true PSD, two smoothing methods have been suggested. One method is to take K profiles on different parts of the surface, calculate the PSD from each profile, and then form an averaged PSD. However, this method is time consuming, because it is necessary to take as many as 10–20 profiles to reduce the variance sufficiently. Another method is to break a profile into K subprofiles that need to be independent, i.e., the correlation length between surface features must be much less than the total profile length, then calculate PSD's from all the subprofiles and average them. Both approaches have been demonstrated to work effectively for data taken on two different beryllium surfaces.

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References and Notes

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