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**SPECTRAL AND PARAMETER ESTIMATION PROBLEMS ARISING IN
THE METROLOGY OF HIGH PERFORMANCE MIRROR SURFACES ***

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ABSTRACT

The accurate characterization of mirror surfaces requires the estimation of two-dimensional distribution functions and power spectra from trend-contaminated profile measurements. The rationale behind this, and our measurement and processing procedures, are described. The distinction between profile and area spectra is indicated, and since measurements often suggest inverse-power-law forms, a discussion of classical and fractal models of processes leading to these forms is included.

INTRODUCTION

This is an application paper concerned with the use of digital-signal-processing techniques in the metrology of mirror surfaces. Its purpose is to bring this area to the attention of the ASSP community and to outline the state of the art.

Interest in precision surface metrology has mushroomed in recent years because of the increasing number of applications which require accurate knowledge of surface topography, plus the increasing availability of precise digital measurement techniques. Areas of application include magnetic tapes and reading heads, audio, video and computer discs, laser and electronic components, precision-machined surfaces of all kinds, and conventional and unconventional optics.

Our particular interest is in optical elements for synchrotron-radiation research, which is perhaps the most demanding application of all [1]. These are glancing-incidence mirrors and reflection gratings which operate in high fluxes of very short-wavelength radiation: $\lambda = 0.1 - 100$ nm (1 nm = 10 Angstroms). Because of the small angles of incidence ($\theta = 0.1^\circ$ to 10°) they are frequently large and asymmetric; some a few cm wide and a metre long. Also, their surfaces are generally curved, often with steep and aspheric profiles. To top it off, their surfaces must be very smooth to minimize degradation of performance at the short radiation wavelengths at which they are used: Typically, surface roughnesses must be less than 10 to 20 Angstroms rms.

Good shape and good finish are not intrinsic to the exotic materials and methods used to generate these one-of-a-kind surfaces, so that the ability to make accurate and meaningful measurements of these quantities is essential for the specification, manufacture, acceptance and maintenance of these expensive components. This paper describes steps toward that goal.

TOPOGRAPHIC FUNCTIONS AND PARAMETERS

What should we measure? The important quantity is obviously the two-dimensional error function $Z(\vec{r})$; the difference between the actual and the design shapes of the surface under test. If we knew that we would know everything. But it is impossible to measure Z over the whole surface with the accuracy needed to predict precise mirror performance, and some sort of "statistical" approach is necessary. Just what, is determined by the finish-function relationship which, in optics, takes the form of diffraction theory.

This shows that the performance depends on Z through the Fourier transform of the phase error which it introduces into the reflected wavefront:

$$F(\vec{\xi}) = \int A(\vec{r}) e^{ik\vec{\xi}\cdot\vec{r}} e^{ikZ(\vec{r})} \sin \theta d\vec{r} \quad (1)$$

where A is the aperture function and $k = 2\pi/\lambda$.

It follows that the range of surface wavelengths of Z that are relevant is huge: from the minimum radiation wavelength (0.1 nm) to the maximum part length (1 m). However, the spectrum of Z is distinctly red; with strong low-frequency components and weak high-frequency ones. In optics these additive components are called "figure" and "finish" respectively; and we write $Z = Z_{fig} + Z_{fin}$. Eq. 1 may then be rewritten as a triple correlation of the corresponding transforms of the aperture function, the figure phase error, and the finish phase error. The last two are what interest us, and we examine them individually.

The evaluation of the figure and finish transforms are simplified by examining them in the "rough" and "smooth" limits respectively. These are defined by the conditions

EMA

$$\left(\frac{4\pi}{\lambda} \sin \theta\right)^2 \sigma_{fig}^2 \gg 1 \quad ; \quad \left(\frac{4\pi}{\lambda} \sin \theta\right)^2 \sigma_{fin}^2 \ll 1 \quad (2)$$

where the σ^2 's are the height variances obtained by integrating the power spectrum of Z over the appropriate ranges of surface frequencies. The dividing line between figure and finish is not well defined, but appears to lie at spacial wavelengths between 0.1 and 10 μ m for the surfaces we have examined.

If we examine the diffraction integral in the rough-surface limit we find that figure errors lead to small-angle scattering, with an intensity distribution which is a mapping of the two-dimensional slope distribution function of $Z_{fig} : P(m)$. On the other hand, finish errors lead to large-angle scattering with an intensity distribution that maps the two-dimensional power spectrum of $Z_{fin} : S(f)$. These two two-dimensional functions are the most fundamental "statistics" of interest for the characterization of mirror topography.

Two rules of thumb follow from these results for imaging optics: First, the contribution of figure errors to the rms angular width of the image is twice the rms surface slope. Second, the integrated effect of finish scattering is to reduce the overall intensity of the figure-aberrated image by the factor

$$1 - \left(\frac{4\pi}{\lambda} \sin \theta\right)^2 \sigma_{fin}^2 \quad (3)$$

Because of the simplicity of these results surfaces are frequently characterized by the rms slope of their figure errors, and by the rms roughness of their finish errors, even though these numbers carry less information about the surface than the original functions P and S from which they are derived.

MEASUREMENT TECHNIQUES

Figure Measurements

Surface figure is traditionally measured by optical interferometry, which determines the difference between the shape of the surface under test and that of a real or virtual model of the design surface. Aside from laboratory curiosities this method is not readily adapted to the large, one-of-a-kind asymmetric, aspheric surfaces of interest here.

The best bet appears to be an optical stylus technique. Unfortunately though, there appear to be no commercially-available instruments which can measure the shape of our optics with the required precision over the desired range of surface wavelengths: a 0.5 microradian slope error for wavelengths between 1 μ m and 1 m.

However, several excellent companies are now considering the design and construction of such devices and we hope that a practical instrument will be available within the coming year.

Finish Measurements

For these we use the digital optical profilometer made by Wyko Corporation [2]. This is a non-contacting, visible-light method which measures the surface height with Angstrom precision at 1024 equally-spaced points along a linear surface profile.

It does this by imaging interference patterns formed between the surface and an internal reference onto a photodiode array in the focal plane of the microscope. The intensities of these patterns are measured, digitized, converted to optical phase differences, and then to surface-height values [3].

The range of surface wavelengths included in the measurements depends on which of three interchangeable microscope objectives is used. The minimum wavelength is determined by either the resolution of the objective or the Nyquist wavelength of the array (see later), and the maximum by the total trace length. Particular values are given below:

Objective	Resolution d_o (μ m)	Nyquist d_N (μ m)	Trace L (mm)
20 X	1.0	1.3	0.665
10 X	1.6	2.6	1.33
2.5 X	4.6	10.4	5.32

Such measurements cover a large and important part of the finish spectrum, although, naturally, they give no information for the large range of surface wavelengths below that of visible light.

DATA ANALYSIS

Figure Analysis

The processing of sampled slope data will be similar to that of the height data described below. Details await the availability of particular measuring instruments and real data.

Figure-Finish Filter

The raw profile data are modeled as

$$Z(I) = A + BI + CI^2 + Z_{fin}(I) \quad (4)$$

where the first three terms are the series expansion of the surface figure and Z_{fin} is the raw residual finish error, modeled here as an AR(1) process with an arbitrary correlation length. Values of A , B , and C and their associated errors are estimated for each profile by a generalized-least-squares procedure using, initially, a nominal value of the correlation length: $\sim 10 \mu$ m.

The values of A and B depend on the measurement conditions and are discarded, while C is a true surface parameter related to the local radius of curvature. So, even though the principal purpose of the filter is to detrend the measured data, it also gives an estimate of an interesting figure parameter.

The accuracy of the radii obtained in this way is not very high for large radii, but it still can be surprising: A radius of 50 m (164 feet) can be measured to 20% by examining a 1.33-mm profile of a surface with an rms roughness of 10 Angstroms.

We use radii obtained in this way to monitor the figure of surfaces provided to us by outside users and suppliers.

Restoration Filter

The second output of the figure-finish filter is the set of raw finish residuals Z_{fin} . These are not the true profile values since they have suffered low-frequency attenuation in the figure-finish filter and high-frequency attenuation due to the anti-aliasing mechanisms in the measuring system.

The figure-finish filter is a rather sharp high-pass filter and its effects are generally ignored for frequencies greater than $2/L$, where L is the trace length [4]. High-frequency anti-aliasing effects are another story. These come from three sources: The microscope optics, the finite size of the pixel elements of the photodiode array, and an optional two-point moving-average filter built into the software provided with the instrument.

We model the cumulative transfer function of these mechanisms as

$$H(f) = [1 - f d_0] \left[\frac{\sin \pi f d_N}{\pi f d_N} \right] \quad (5)$$

where the first factor is due to the microscope optics and the second to the two-point averaging of boxcar pixels. (For unaveraged data the argument of the sinc function is halved.)

It is easy to see that $H(f)$ differs from unity over an extended range of frequencies within the instrument bandpass. To compensate for this we restore the raw finish data using an inverse filter with the transfer function $H(f)^{-1}$. How close to the first zero of $H(f)$ we can carry this depends on the SNR of the finish data. For the 20 X objective we cut off at a frequency of the order of $2f_N/3$ since the unrestored spectra of smooth surfaces tend to fall into noise above that point.

Spectral and Finish Parameter Estimation

The next step is to estimate the spectra of the detrended and restored profile data. Our first approach is to examine the periodogram of the individual data sets, using the full 1024 points to include the widest range of frequencies. We may also examine the smoothed periodogram, the average periodogram for segmented data sets, and parametric (MEM and MLM) estimates. The workhorse however, is the full-record periodogram.

To check the homogeneity (stationarity) of a given surface we take profiles at different locations (and orientations) on the surface and compare

their spectra. If they are similar enough we average them to get a more stable over-all estimate.

The rms surface-roughness values are obtained from the spectral estimates by integrating the profile spectra between particular frequency limits. The most useful results are obtained by running the system "wide open"; that is, including all frequencies between $f = 2/L$ and $2f_N/3$. However, for careful work, such as the examination of "lines" in the spectra of machined surfaces and grating structures, or the comparison of measurements made with different microscope objectives or with different measurement techniques, it is necessary to include restoration effects and to compare data only over common ranges of surface frequencies [5].

Examples will be included in the presentation.

PROFILE VS AREA STATISTICS

The profile, or one-dimensional spectra, S_1 , discussed above are different from the area, or two-dimensional spectra, S_2 , which determine the optical effects of surface finish. For an ideal profiling instrument the two are related by

$$S_1(f_x) = \int_{-\infty}^{+\infty} S_2(f_x, f_y) df_y \quad (6)$$

which cannot be inverted without additional information. For example, if we know that the profile was taken across the lay of a corrugated surface, such as a machined surface or a grating, we can write immediately that $S_2(f_x) = S_1(f_x) \delta(f_y)$.

On the other hand, if we know that the surface was isotropically rough, as might be expected for a flat polished surface, the above relationship becomes an Abel or half-integral transform:

$$S_1(f) = 2 \int_f^{\infty} \frac{f' df'}{(f'^2 - f^2)^{1/2}} S_2(f') \quad (7)$$

The inverse of this is the inverse-Abel or half-derivative transform:

$$S_2(f) = -\frac{1}{\pi} \int_f^{\infty} \frac{f' df'}{(f'^2 - f^2)^{1/2}} \frac{d}{df} S_1(f') \quad (8)$$

which may be written in a variety of mathematically equivalent forms. Unfortunately, this inversion can't be carried out for band-limited values of S_1 because the right-hand side requires knowledge of S_1 for all frequencies above f . We need additional information about the high-frequency tail of the spectrum.

An efficient way of incorporating such information into the analysis is to use models, such as parametric fits to real data or analytic forms as discussed below. However, in doing so one ought to distinguish between loaded models, which carry significant and reliable information, and empty models, whose principal effect, when all is said and done, is to have packaged our ignorance in a different form.

FINISH MODELS

Models have obvious uses: As above, to extrapolate data outside the range of the original measurements, and as below, to parameterize data for ease of discussion and to gain insight into the nature of the finishing process which may provide a basis for improvements.

Classical Models

These are expressed in terms of signal power and a finite number of length scales. ARMA models are one class of models which may be used to fit data. An interesting single-scale model is that having a correlation function of the form $t^{\nu} K_{\nu}(2\pi a t)$, where t is the magnitude of the lag, K_{ν} is a modified Bessel function, and $1/a$ is the characteristic length. The corresponding 1- and 2-dimensional "K-correlation spectra" are:

$$S_m(\xi) = \frac{\pi^{-m/2}}{2} \left(\frac{a}{\pi}\right)^{\nu} \frac{\Gamma(\nu+m/2)}{(a^2+\xi^2)^{\nu+m/2}} \quad (9)$$

where $n = 1$ and 2 , respectively. These forms have the nice features of reducing to an AR(1) process for $\nu = \frac{1}{2}$, and leading to power-law spectra at high frequencies, $f \gg a$.

This last is relevant since we frequently see profile spectra that fall off as f^{-q} , where $q \sim 1$ for the smoothest surfaces, $q \sim 2$ for good surfaces, and $q \sim 3$ for rougher ones [6].

Similar power-law spectra appear in related contexts: $1/f$ profile spectra are predicted for the thermodynamic roughening of solid surfaces and capillary-waves on liquid surfaces. $1/f^2$ spectra correspond to a magnification-invariant profile, and one that has sharp vertical edges (eg a telegrapher's signal). An $1/f$ profile spectrum is expected for what the oceanographers call the fully-aroused sea.

Fractal Models

Fractal surfaces, which contain all length scales, also give rise to power-law spectra [7]. At low frequencies this simple behavior may break down because of the presence of a finite outer-length scale, analogous to the length $1/a$ in the case discussed above.

Fractals are characterized by two parameters: the Hausdorff-Besicovitch dimension D , and a length parameter called the topothese. D is related to ν and q according to

ν	$q = 2\nu + 1$	$D = (5 - q)/2$
0	1	2
0.5	2	1.5
1	3	1

Equation (9) is valid for any value of q , integral or not. But the fractal dimension D must lie between 1 and 2. Again, there is no restriction to integral or half-integral values.

For example, Mandelbrot et al. describe studies of the surfaces of steel specimens which show power-law profile spectra with $D = 1.118$ ($q = 2.764$), for surface wavelengths between $0.1 \mu\text{m}$ and 1 mm [8].

Rules of Thumb

Profiles appear to prefer power-law spectra. In that case their 1- and 2-dimensional forms must be related according to

$$S_1(\xi) = \frac{1}{\xi} \quad S_2(\xi) = \frac{\Gamma((q+1)/2)}{\Gamma(1/2)\Gamma(q/2)} \cdot \frac{1}{\xi^{q+1}} \quad (10)$$

If we integrate these over equal bandwidths (a circular annulus in two dimensions) we get the following for the ratio of the variances

$$\frac{\sigma_2^2}{\sigma_1^2} = \frac{\Gamma(1/2)\Gamma((q+1)/2)}{\Gamma(q/2)} \quad (11)$$

For $q = 1, 2, 3$ this has the values of 1^2 , $(1.25)^2$ and $(1.41)^2$ respectively.

Two rules of thumb follow from this analysis: First, two-dimensional spectra fall off one power of f faster than their profile spectra (this also follows from simple dimensional analysis), and the variance of the area roughness lies between 1 and 2 times its corresponding profile values.

APPLICATIONS

The figure-finish measurement scheme described above is used routinely for monitoring and measuring the properties of optical surfaces at the National Synchrotron Light Source at Brookhaven.

It has also been used for a survey of precision-machined surfaces [9], a direct comparison of mechanical and optical measurements [5], and a preliminary comparison between measured x-ray scattering and that predicted from profile measurements [1].

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