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Surface Specification in Terms of System Performance*

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Surface specification in terms of system performance

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ABSTRACT

This paper describes and illustrates simple expressions for evaluating the effects of conventional and fractal surface errors on image quality, and conversely, of specifying finish parameters in terms of system performance requirements.

1. INTRODUCTION

No manufacturing process is perfect, and the surfaces of all real optical elements contain residual shape errors. Those errors are undesirable since they introduce fluctuations in the reflected or transmitted wavefronts which degrade the performance of optical systems. The understanding of this finish-function relationship is critical in the fields of optical design, standards, and manufacturing.

Traditionally, shape errors are divided into two categories: long-spatial-wavelength or 'figure' errors, and short-wavelength or 'finish' errors. Figure errors are described deterministically and their effects are evaluated by geometrical optics (ray tracing). Finish errors, on the other hand, are described statistically and their effects are evaluated using rule-of-thumb diffraction results based on conventional finish models.

In the past, the dividing line between these two regimes has been determined largely by the bandwidths of the measuring instruments used. Now days, however, the availability of high-precision, broad-band measuring instruments, increased performance requirements, and novel manufacturing techniques have focussed interest on the need for a more comprehensive understanding of these issues.

This need is heightened by the fact that the figure and finish errors of highly-finished surfaces are frequently fractal-like; that is, their power spectral densities tend to diverge at long spatial wavelengths, rather than being flat as assumed in conventional finish models. This further blurs the distinction between figure and finish, and raises questions about the practical effects of these divergences.

In order to provide a unified view of the finish-function relationship we have examined a simple statistical diffraction theory of imaging,¹⁻⁴ Two general conclusions of these studies are that the distinction between 'figure' and 'finish' depends on the image property of interest and on the details of the imaging system involved, and that the effects of fractal errors are finite, despite the divergence of their power spectra at low frequencies.

The purpose of the present paper is to review these results, to present explicit expressions for simple cases, and to show how they can be used for the practical specification of optical surface quality.

2. GENERAL RESULTS

For simplicity we consider the on-axis imaging of a normal-incidence parabolic mirror, with shape errors characterized by the two-dimensional power spectral density $S_2(f')$, where f' is the surface spatial frequency. The two leading terms in the smooth-surface expansion of the image intensity distribution in the focal plane are then

$$I(\underline{\theta}) = I_0(\underline{\theta}) - (4\pi/\lambda)^2 \int d\underline{f}' K(\underline{f}, \underline{f}') S_2(\underline{f}') \quad (1)$$

where $\underline{\theta}$ is the observation angle relative to the optic axis, and $\underline{f} = \underline{\theta}/\lambda$.

The first term on the right, $I_0(\underline{\theta})$, is the image formed by a perfect mirror, and the second is the first-order correction for the shape errors, which is in the form of a weighted integral of the error power spectral density (PSD). The weighting factor or kernel, $K(\underline{f}, \underline{f}')$, tells how errors of frequency $\underline{f}'$ affect the image intensity at point $\underline{f}$ in the focal plane.

At large observation angles $I_0(\underline{\theta})$ vanishes and only the second term survives. In that limit K turns into a negative delta function and Eq.(1) reduces to

$$I(\underline{\theta}) = (16\pi^2 / \lambda^4) S_2(\underline{f}) \quad (2)$$

which is the small-angle form of the well-known scattering formula.

Our interest here, however, is in the effects of surface errors on the image core, where K has a more complicated form and plays a more important role. To do this we simplify matters by looking not at the detailed image shape, $I(\underline{\theta})$, but how three particular aspects of it are modified by surface effects. These are described next.

2.1 The on-axis Strehl factor

The on-axis Strehl or Debye-Waller factor is the factor by which the on-axis image intensity $I(0)$ is reduced by finish errors:

$$\text{On-axis Strehl factor} = I(0)/I_0(0) \quad (3)$$

This is a special case of the more-general ratio $I(\underline{\theta})/I_0(\underline{\theta})$ which is frequently, and incorrectly, taken to be independent of $\underline{\theta}$.

2.2 The image-width factor

The image-width factor is the ratio of parabolic width of the image with errors to that without errors, where the parabolic width is the radius of the base of a parabola fitted to the image intensity distribution along the optic axis. That is,

$$\text{Image-width factor} = [I''(\theta)/I_0''(\theta)]_0^{-1/2} \quad (4)$$

where the double prime denotes the second derivative.

2.3 The Hopkins factor

The Hopkins factor is the ratio of the optical transfer function of the imaging system at a given image spatial frequency, g , with and without surface errors. The OTF is the Fourier transform (FT) of the image intensity distribution, normalized to unity at $g = 0$. That is,

$$\text{Hopkins factor} = \text{OTF}(g)/\text{OTF}_0(g) = \text{FT}_g\{I(\theta)\}/\text{FT}_g\{I_0(\theta)\} \quad (5)$$

The Hopkins factor describes how the surface errors attenuate different spatial frequencies in the image plane in addition to that of the system OTF itself.

3. COMMENTS

The weighting factor K in Eq.(1) has a particularly simple form for the on-axis Strehl factor, namely:

$$K(0, f') = 1 - I_0(f')/I_0(0) \quad (6)$$

This vanishes in the limit of zero spatial frequency, increases quadratically at low frequencies, and becomes one for spatial frequencies corresponding to diffraction outside the image core.

This result illustrates two important general features of the present diffraction calculation: how the low-frequency divergence of fractal spectra leads to finite effects in imaging, and how the geometrical-optics description evolves naturally in the limit of long surface spatial wavelengths.

The wiping out of the fractal divergence can be viewed in a number of ways: As due to the convolution of the divergence with the non-vanishing point-spread function of the imaging system, the fact that imaging is insensitive to spatial wavelengths longer than the illuminated area of the surface, or the fact that intensity measurements are insensitive to piston errors.

The geometrical-optics description of the effects of long spatial wavelengths comes from the fact that Eq.(6) is proportional to f'^2 at low frequencies, and the this times the height spectrum gives the slope (gradient) spectrum of the surface.

In other words, the diffraction calculation gives a unified first-order statistical view of imaging effects of the entire error spectrum, and does not require a distinction between 'figure' and 'finish' errors.

The answer to the question of what spatial wavelength separates the two regimes may or may not be meaningful, depending on the particular image feature of interest. But in the case of the on-axis Strehl factor, at least, it is approximately

$$W = \lambda [-I_0''(\theta)/2 I_0(\theta)]_0^{1/2} . \quad (7)$$

This length plays a special role in the discussion and we call it the coherence length of the system. It can vary from a fraction of a mm for system-limited optics up to the diameter of the mirror for diffraction-limited optics.

4. SYSTEM LIMITED OPTICS

In order to go further we must specify a form of the system response function I_0 . In this paper we consider the case of system-limited optics; that is, where the form of I_0 is determined by the finite source and detector sizes, as opposed to diffraction-limited optics, where I_0 is determined by the size of the illuminated area of the mirror. Here we take the system-limited form to be the Gaussian:

$$I_0(\theta) = [\pi \theta_0^2]^{-1} \exp[-(\theta/\theta_0)^2] , \quad (8)$$

where θ_0 is the rms width of the image. We choose this form since we are interested in the changes in shape due to surface errors rather than the details of the shape itself. The case of diffraction-limited optics, where I_0 is an Airy pattern, is discussed elsewhere^{4,5}.

Given the form of I_0 , all of the quantities mentioned above can be calculated. We quote two because of their particular interest. The coherence length of the system is

$$W = \lambda / \theta_0 , \quad (9)$$

and the optical transfer function of the system is

$$\text{OTF}_0(g) = \exp[-(g/g_0)^2] , \quad (10)$$

where

$$g_0 = 1/\pi \theta_0 F , \quad (11)$$

(and F is the focal distance. Here, g_0 is the system-imposed measure of the range of image spatial frequencies, analogous to $2 \text{ NA}/\lambda$ in diffraction-limited optics.

5. SURFACE ERRORS AND MODELS

The errors that affect imaging are the spatial fluctuations in the phase of the wavefront reflected from the mirror, $\varphi(\underline{x})$. In the case of a single-surface mirror these are related to the height fluctuations, $Z(\underline{x})$, according to

$$Z(\underline{x}) = (\lambda/4\pi) \varphi(\underline{x}) \quad (12)$$

In the case of multilayer mirrors the phase fluctuations are a complicated function of the topography of the substrate and the multilayer geometry and composition. In that case $Z(\underline{x})$ derived from Eq. (12) is an effective value which may not be simply related to particular surface features. The detailed connection between the effective roughness and multilayer structure is the subject of much lively investigation⁶. Here, however, we focus on the separate problem of understanding how the effective surface roughness, whatever its source, affects imaging.

For simplicity we take Z to be statistically isotropic, in which case the results considered above can be expressed uniquely in terms of the profile spectrum, $S_1(f)$ instead of the more general area spectrum, $S_2(\underline{f})$, appearing in Eqs. (1,2).

Equation 1 relates image properties to a weighted integrals of the surface PSD, and constitutes a non-parametric solution to the prediction-specification problem in the smooth-surface limit.

In practice, though, it is convenient to express these results parametrically -- that is, to model the PSDs in terms of simple analytic expressions involving a few adjustable parameters and to express the results of Eq. (1) in terms of them. These 'finish' parameters are taken to be intrinsic properties of the surface, although they may or may not correspond directly to more familiar surface descriptors such as the roughness or slope.

6. CONVENTIONAL VS FRACTAL SURFACE MODELS

Conventional and fractal finish models are two forms that appear frequently in the literature and are convenient for illustrating the use of the present results. They represent the extreme forms of the more general ABC model which could also be used for this purpose⁷. Real surfaces, of course, can involve composite models, but here, for simplicity, we consider only two elemental forms.

The PSDs of conventional finish models are expressed in terms of two intrinsic parameters -- the rms roughness σ_o and the correlation length ℓ_o . The features that identify this class of models are that their PSDs are flat up to frequencies determined by the reciprocal correlation length, after which they fall towards zero, and that the area (or volume) that they define in frequency space, the mean-square surface roughness,

$$\sigma_o^2 = \int d\underline{f}' S_2(\underline{f}') = \int_0^\infty df' S_1(f') \quad (13)$$

is finite. The PSDs of fractal finish models, on the other hand, are characterized

by two different intrinsic finish parameters -- the spectral strength K_n and the spectral index n , where

$$S_1(f) = K_n / f^n, \quad (14)$$

and n lies between 1 and 3. The identifying features of this class of models are that their rms roughness diverges at the low-frequency limits of integration in Eq. (13), and their PSDs are structureless functions of frequency; that is, they show no characteristic length scale or correlation length.

7. EXAMPLES OF PROFILE POWER SPECTRA

Figure 1 shows the PSDs of the top surfaces of three multilayer x-ray mirrors made by David Windt et al. at AT&T Bell Laboratories. Data are shown over the spatial wavelength range from 10 nm to 1/2 mm. Two types of instruments were used to cover this range -- atomic force microscopy for the high frequencies and visible-light microscopy for the low frequencies.

Fig. 1. Measured PSDs of three multilayer x-ray mirrors.

Two remarkable features of these results are that the spectra of these two very different kinds of measurements generally agree, and that their composite shapes appear to be fractal-like -- since they are approximately linear in this log-log plot. For the purposes of later comparison we characterize these results as

$$S_1(f) = 10^{-9} / f^{5/3} \cdot \mu\text{m}^3. \quad (15)$$

Figure 2 shows the PSD of a silicon synchrotron x-ray mirror measured at Brookhaven. In this case the spatial wavelength range is 10 μm to almost 1 meter. Again, two instruments were used to cover this range -- a Wyko profiling microscope for the short wavelengths and the Brookhaven LTP for the long ones.

Fig. 2 Measured PSD of a synchrotron-radiation x-ray mirror.

Once again the results of the two different measurement techniques are in good agreement, and aside from isolated low-frequency artifacts, the composite PSD is again fractal-like. We characterize these results as

$$S_1(f) = 3 \times 10^{-8} / f^{4/3} \quad \mu\text{m}^3 \quad (16)$$

Figure 3 shows the PSD of an AXAF mirror provided by Paul Reid at Hughes-Danbury, based on measurements made with a special interferometer they have developed for this purpose. The spatial-wavelength range covered in this figure is from a few mm to over 1 m. The turn-up at the high-frequency end is due to instrumental noise, but the linear trend in the data has been shown to continue at higher frequencies using other instruments.

Figure 3. Measured PSD of an AXAF hyperbola.

Again, the curve is fractal-like, and we characterize it as

$$S_1(f) = 10^{-12} / f^{7/3} \quad \mu\text{m}^3 \quad (17)$$

These three figures show that the PSDs of many practical surfaces are fractal-like, out to very long spatial wavelengths, and justifies examining the effect of this type of wavefront error on image quality.

8. IMAGE EFFECTS OF CONVENTIONAL SURFACES

When the surface correlation length is much smaller than the system coherence length, W , the corrections to the three image properties discussed above have the well-known forms:

$$\text{On-axis Strehl factor} = 1 - (4\pi/\lambda)^2 \sigma_o^2 \quad (18)$$

$$\text{Image-width factor} = 1 \quad (19)$$

$$\text{Hopkins factor} = 1 - (4\pi/\lambda)^2 \sigma_o^2 \quad (20)$$

This last is valid in the practically-important region $g \gg \ell_o/\lambda F$.

The fact that the Hopkins factor is essentially independent of the image spatial wavelength means that the generalized Strehl factor, $I(\theta)/I_o(\theta)$, is independent of θ and equal to the value in Eq.(18). In other words, the effect of conventional surface finish is to reduce the overall image-core intensity without changing its shape. The blip in the OTF at very small values of g that makes $\text{OTF}(0) = 1$ corresponds to a broad, weak scattering continuum that is added to this scaled-down core distribution. Together, they satisfy the conservation of energy.

These results are easily converted to conditions on the rms surface roughness by requiring that the correction factors in Eqs.(18-20) be less than some reasonable number, say, 0.2. In that case

$$\sigma_o \leq \sqrt{0.2} \lambda / 4\pi \quad (21)$$

This well-known result gives, for example, $\sigma_o \leq 0.5 \text{ nm}$ for $\lambda = 14 \text{ nm}$, and $\sigma_o \leq 22.5 \text{ nm}$ for $\lambda = 0.6328 \mu\text{m}$.

9. IMAGE EFFECTS OF FRACTAL SURFACES

The expressions for the three image correction factors can also be evaluated in closed form for the fractal PSD in Eq. (14):

$$\text{On-axis Strehl factor} = 1 - (4\pi/\lambda)^2 \cdot$$

$$\cdot K_m W^{m-1} \cdot \frac{\sqrt{\pi}}{2} \cdot \frac{\Gamma((3-m)/2) \Gamma((m-1)/2)}{\Gamma(m/2)} \quad (22)$$

$$\text{Width factor} = 1 + (4\pi/\lambda)^2 \cdot$$

$$\cdot K_m W^{m-1} \cdot \frac{\sqrt{\pi}/8}{m-1} \cdot \frac{\Gamma((3-m)/2) \Gamma((m-1)/2)}{\Gamma(m/2)} \quad (23)$$

$$\text{Hopkins factor} = 1 - (4\pi/\lambda)^2 \cdot$$

$$\cdot K_m W^{m-1} \cdot \frac{\pi^{(3/2)-m}}{m-1} \cdot \frac{\Gamma((3-m)/2)}{\Gamma(m/2)} \cdot \left(\frac{g}{g_0}\right)^{m-1} \quad (24)$$

where again, the coherence length is given by $W = \lambda/\theta_0$.

Note that each of these results appears in the form of the conventional results, except that the quantities replacing the mean-square roughness in Eqs. (18-20) are no longer intrinsic surface quantities, but depend on system parameters through the coherence length, W . Their square roots, the effective values of σ , would still be in nanometers, but they would not correspond to any physical dimension of the surface.

Since W is finite for all real systems, so too are the magnitudes of the fractal corrections. It is interesting to note that most of the calculations of surface-scattering in the literature assume an infinite, coherently-illuminated surface at the outset -- i.e. infinite W -- which automatically limits them to the use of conventional finish models. To put it another way, Nature loves fractals, but it needs a length scale to keep their effects finite. In the case of conventional surfaces this is the surface correlation length, ℓ_0 , and in the case of fractal surfaces, the system coherence length, W .

10. NUMERICAL EXAMPLES OF FRACTAL EFFECTS

If we require that the magnitudes of the correction terms in Eqs. (20-24) be less than 0.2, we can translate them into requirements on the two fractal parameters K_h and n . Results are illustrated in Figs. 4 and 5.

In these examples we use the values $\theta_0 = 100$ nanoradians and $\lambda = 14$ nanometers, which corresponds to a coherence length $W = 0.14$ mm on the mirror surface. This is, of course, much smaller than normal mirror diameters. In contrast, W is essentially the mirror diameter in the case of diffraction-limited optics^{4,5}.

Fig. 4. K-n plot showing lines for 20% effects on the on-axis Strehl (solid) and width factors (dotted).

Fig. 5. K-n plot showing lines for 20% effects on the on-axis Strehl (solid) and Hopkins factors (dotted).

Figure 4 shows the results derived from the Strehl and width corrections as solid and dotted lines, and Figure 5 shows the Strehl and Hopkins results, again as solid and dotted lines. The three Hopkins lines -- from top to bottom -- correspond to the image spatial frequencies $(g/g_0)^2 = 1/2, 1$ and 2 . In all cases K_n is in units of μm^{3-n} .

Real fractal surfaces correspond to points in this K-n space. Points falling above a given line are BAD since they correspond to a correction of more than 20% in the indicated quantity, while those falling below the lines are GOOD since they correspond to corrections of less than 20%. It follows that of the three image features considered here, the on-axis Strehl factor is the most restrictive.

The three black circles correspond to Eqs. (15-17) -- from left to right, the BNL, AT&T and HDOS surfaces. For this application, then, the first would fail while the others would pass. Of course, this says nothing about the intrinsic quality of these the surfaces -- whatever that means -- but does show how K-n plots can be used for evaluating, specifying and qualifying surfaces for particular applications.

11. STATISTICAL CONSIDERATIONS

The present paper uses physical optics to translate measurements of the effective roughness of a given surface into predictions of its imaging properties. We do this by using the measurements of a particular surface to "estimate" the PSD of an ensemble of statistically-equivalent surfaces, calculating the ensemble-average imaging effects in terms of that PSD, and taking those ensemble results as predictions of the properties of the original mirror.

This enables us to make full use of a-priori physical information contained in finish models, to compensate for bandwidth and positional limitations in the original measurements, and to present the results in terms of a few simple parameters.

The price paid for these advantages and simplifications are the statistical errors associated with these predictions, which define the limits of any statistical approach. General reasoning, however, argues that these errors should be negligible for conventional surfaces and/or system-limited imaging because of the large number of degrees of freedom involved in individual measurements. That is, the large number of correlation lengths or coherence lengths contained in the mirror diameter. A more detailed analysis of these effects is now under way.

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