New Variance-Reducing Methods for the PSD Analysis of Large Optical Surfaces

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Edge data of a measured surface map of a circular optic result in large variance or "spectral leakage" behavior in the corresponding Power Spectral Density (PSD) data. In this paper we present two new, alternative methods for reducing such variance in the PSD data by replacing the zeros outside the circular area of a surface map by non-zero values either obtained from a PSD fit (method 1) or taken from the inside of the circular area (method 2).
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1. Introduction

Some space optical systems such as Terrestrial Planet Finder Coronagraph (TPF-C) require large optics with very high surface quality [1]. The developmental cycle of such optical systems includes, but is not limited to, the following two steps: (i) Deriving requirements or specs on the optical quality of individual optics before they are fabricated and (ii) evaluating the quality of those components against the pre-determined specs after they are fabricated. One of the preferred metrics used for specifying the quality of optical surfaces is the PSD [2-4]. It is computed from the Fourier spectrum amplitude of the surface height map of an optic obtained from measurements of the bidirectional reflectance distribution function, from surface profiles measured using an optical or mechanical profiler, or by using an interferometer. This paper is about calculating the PSD of an optic using its 2D surface map measured interferometrically.

Several different approaches have been reported on how to calculate PSD from surface height measurements [4-8]. The main problem one encounters when calculating the 2D-PSD of a circular surface is the scattering of the PSD data when they are plotted as a function of radial spatial frequency, or "spectral leakage". This is caused by the sharp circular edge of the measured surface map and introduces large variance relative to the pre-determined spec. Until now using windowing filters (such as Hann or Welch windows), zero-padding and averaging multiple sub-aperture PSDs have been the preferred methods used for reducing such variance in the calculated 2D-PSD data. In this paper, we introduce two new, alternative methods for reducing the edge effects of a surface map on the 2D-PSD data. The first method is applicable to the cases where the 1D-PSD obtained by radially averaging the corresponding 2D-PSD [8] can be roughly represented by an analytical PSD function, a function similar to the one used in the derivation of PSD specs. In this method the zeros outside the circular area of a surface map are replaced by the data obtained from a PSD fit. The second method is applicable to the cases where the shape of the optic does not cover the whole area of a square surface map. In this method the zeros corresponding to the outside area of the optical surface are replaced by the data taken from those corresponding to the inside area of the optic following an edge-symmetry rule to be described below.

2. Mathematical Description

The discrete PSD of a surface map $h_{\text{cir}}(x, y)$ of a circular optic is calculated from [8]

$$PSD_{\text{calc}}(u_m, v_n) = \frac{1}{A}\left|\Im\{h_{\text{cir}}(x_m, y_n)\}\Delta x \Delta y\right|^2 \quad , (1)$$

where the subscript "calc" means "calculated". The $[x, y]$ and $[u, v]$ pairs are the surface position and the spatial frequency variables in the horizontal and the vertical directions, respectively, and the $\Im$ symbol represents a 2D-FFT routine such as the fft2.m function in MATLAB. The $[\Delta x, \Delta y]$ pair are the width and the height ($\Delta x = \Delta y$ for a square pixel) of each pixel, and the A is the area of the whole $h_{\text{cir}}(x,y)$ map including all the zeros. Indices $m = 1,2,...,M$ and $n = 1,2,...,N$ ($M = N$ for a square surface map), respectively. We describe our new methods using an example of synthesized $h_{\text{cir}}(x, y)$ and its PSD data. The synthesized surface map, $h(x,y)$, is obtained from [8]

$$h(x_n, y_m) = \frac{1}{\Delta x \Delta y} \Im^{-1}\left\{ \mathbf{e}^{i\phi(u_n, v_m)} \sqrt{A \times PSD_{\text{true}}(u_n, v_m)} \right\} \ , \ PSD_{\text{true}}(u_m, v_n) = \frac{\sigma_0{}^2 A}{h_0} \frac{1}{1 + (\rho_{mn} / \rho_{HP})^p} \ , \quad (2)$$

where $h_0 = \sum_{m=1}^{M} \sum_{n=1}^{N} 1 / \left[1 + (\rho_{mn} / \rho_{HP})^p \right]$, $\rho_{mn} = \sqrt{u_m^2 + v_n^2}$ is the radial frequency, ρ_{HP} is the half-power frequency, p is the exponent of the inverse power-law, and σ_0 is the RMS value of $h(x,y)$. $\Im^{-1}$ represents an inverse-FFT algorithm, such as the ifft2.m function in MATLAB, and $\phi(u_m,v_n)$ is an anti-symmetric, randomly-valued phase map satisfying $-\pi \le \phi \le \pi$. Another important quantity used to compare different approaches in this paper is the "RMS Bias" defined as $\sigma_{\text{bias}}(u_m, v_n) = \sqrt{PSD_{\text{calc}}(u_m, v_n) / PSD_{\text{true}}(u_m, v_n)}$. It is a measure of the variance of the 2D-PSD$_{\text{calc}}$ relative to 1D-PSD$_{\text{true}}$ or 1D-PSD spec. In the ideal case, we have [Mean(σ_{bias}), STD(σ_{bias})] = [1.00, 0.00], where "STD" means Standard Deviation. We will use the latter to compare the performance of different PSD calculation approaches.

3. Numerical Examples

We compare the performance of our new methods with the direct PSD calculation and a Welch window (α=8) methods [8] using some numerical examples of synthesized $h_{\text{cir}}(x,y)$. The parameters used are: $M\Delta x = N\Delta y$=500mm, p=3, ρ_{HP}=2cyc/m, σ_0=100nm, and M=N=512, where "cyc" means "cycles".

Our first example is about a PSD directly calculated from a $h_{\text{cir}}(x,y) = h(x,y) \times cir(x,y)$, where $h(x,y)$ was obtained using Eq. (2) and is shown by the map inside the black circle in Fig. 1(a), and $cir(x,y)$ is a circular mask equaling to 1 inside the black circle and to 0 otherwise. In real applications, this $h_{\text{cir}}(x,y)$ is replaced by the measured surface map to be analyzed. The corresponding PSD data obtained using Eq. (1) are shown in Fig. 1(b) as a function of radial frequency, where the blue curve is the 1D-PSD obtained by radially averaging the corresponding 2D-PSD [8] and the green curve is the 1D-PSD obtained from the radial average of the original PSD function (or true PSD) defined in Eq. (2). In real applications, the green curve is equivalent to a PSD spec. In this case, the scattering of the 2D-PSD$_{\text{calc}}$ is caused by the sharp circular edge of the $h_{\text{cir}}(x,y)$.

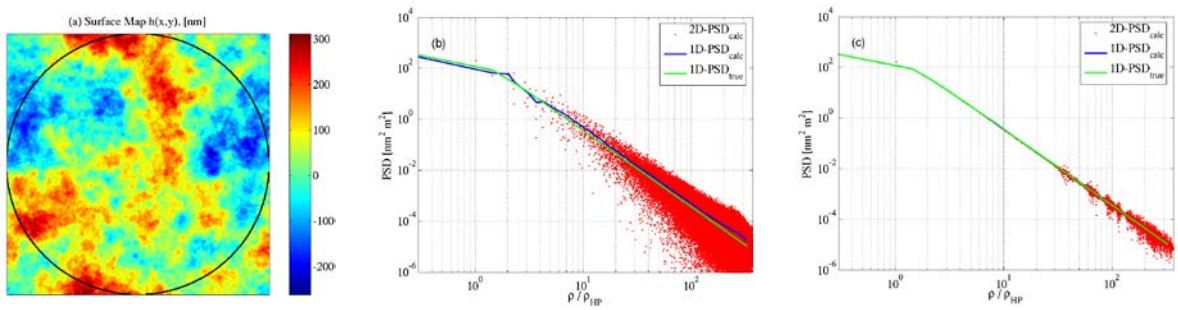

Fig. 1. (a) $h_{\text{cir}}(x,y)$ and $h(x,y)$. (b) 2D- and 1D-PSD's obtained from $h_{\text{cir}}(x,y)$ in part (a). (c) PSD's obtained from the h (x,y) in part (a).

Our first variance-reducing method works as follows. We fit to the 1D-PSD$_{\text{calc}}$ curve a PSD function using the following procedure: (1) Choose an analytical function for 1D-PSD$_{\text{calc}}$. (2) Calculate a surface height map, $h_{\text{calc}}(x,y)$, using the above PSD function and the spectral phase of the $h_{\text{cir}}(x,y)$. (3) Replace the values of $h_{\text{cir}}(x,y)$ outside the circular area with the values of $h_{\text{calc}}(x,y)$ to obtain a new surface map, $h^i(x,y) = h_{\text{cir}}(x,y) + [1 - cir(x,y)] \times h_{\text{calc}}{}^i(x,y)$, where the superscript "i" represents the PSD-fit iteration number. (4) Calculate the (1D-PSD)^i corresponding to the above $h^i(x,y)$. (5) Adjust the PSD parameter values in Eq. (2), and repeat Steps 1-4 for multiple iterations until the square-sum of the difference of 1D-PSD$_{\text{calc}}$ and (1D-PSD)^i can no longer be reduced, using the spectral phase of $h^i(x,y)$ after the first iteration. The surface map outside the circular area in Fig. 1(a) as well as the 2D-PSD$_{\text{calc}}$ and 1D-PSD$_{\text{calc}}$ results in Fig. 1(c) were obtained using this method after 100 PSD-fitting iterations. In both Fig.1(b) and Fig.1(c), the 2D-PSD$_{\text{calc}}$ data were re-scaled such that they have the same RMS value σ as that of the corresponding 2D-PSD$_{\text{true}}$, where $\sigma^2 = \sum_{m=1}^{M} \sum_{n=1}^{N} PSD(u_m, v_n) / A$. For the 2D-PSD$_{\text{calc}}$ in Fig. 1(b), the σ_{bias} parameters are [Mean(σ_{bias}), STD(σ_{bias})] = [1.13, 0.53], but for the 2D-PSD$_{\text{calc}}$ in Fig. 1(c) they are [1.01, 0.04], respectively. That is, if the 1D-PSD$_{\text{calc}}$ of a circular surface map can be fit by an analytical PSD function, then the variance of its 2D-PSD$_{\text{calc}}$ can be greatly reduced using the current method. In this paper, we refer to this method as "Fitting Method".

Our second variance-reducing method is explained in Fig. 2(a). In this method, the zero-value of $h_{\text{cir}}(x,y)$ at data point P' is replaced by its value at data point P. In this figure, C is the center of the circular surface map, the

points P, B and P' all lie on the line connecting C to P', B is on the circular boundary, and PB=BP'. In this paper, we refer to this method as "Filling Method". Note that some of the data points "filled" using this method repeat themselves. For the current case of $M = N = 512$, we found 19.3% data points repeat once, and 2.7% data points repeat twice when picking the "nearest" points to replace the zeros outside the circular surface map area.

The circular surface map $h_{cir}(x,y)$ in Fig.2(b) is the same as Fig. 1(a), but the data outside its circular boundary were obtained using this second method. Figure 2(c) shows the statistical results of 2D-σ_{bias} obtained from 100 realizations of $h_{cir}(x,y)$ using Eq. (2). Each realization is obtained from a unique set of random spectral phase map $\phi(u_m,v_n)$. In this figure, the case of "As is" corresponds to the 2D-σ_{bias} obtained from $h_{cir}(x,y)$ directly, keeping its zero values outside the circular area unchanged. The curve "Welch" corresponds to the case where a Welch window

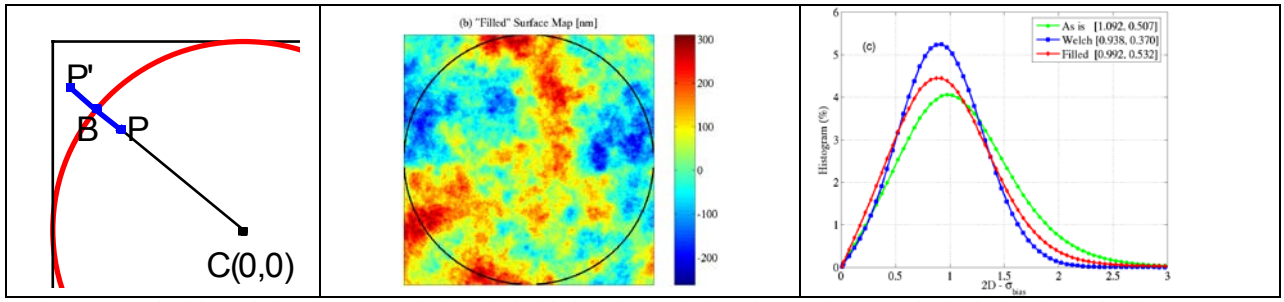

Fig. 2. (a) Method for replacing the zero at pixel P' pixel with the value at pixel P. (b) A surface map obtained using the method in part (a). (c) Histogram of 2D-σ_{bias} obtained in 100 $h_{cir}(x,y)$ realizations using three different methods.

with α=8 is applied to each $h_{cir}(x,y)$ map. The Welch window is defined as $w(r) = 1 - | r / r_0 |^{\alpha}$, where $r = (x^2 + y^2)^{1/2}$ and r_0 is the radius of the circular area shown by a black circle in Fig. 2(b). A Welch window index of α=8 was found to represent a good compromise between smearing and leakage [7], so we used that value in our simulations.

The curve named "Filled" in Fig. 2(c) was obtained using the second method explained in Fig. 2(a). Shown in the figure legends are [Mean(σ_{bias}), STD(σ_{bias})] values resulted by the corresponding PSD calculation approaches. As we can see from STD(σ_{bias})=0.532 of the "Filled" case, the "Filling Method" does not improve the scattering characteristics of the resulted 2D-PSD$_{calc}$ data, but it greatly improves the Mean(σ_{bias}) value. The "As is" approach yields Mean(σ_{bias}) > 1, and the "Welch" gives Mean(σ_{bias}) < 1, deviating from 1 by +9.2% and -6.2%, respectively. Therefore, if one chooses to use the Mean(σ_{bias}) as a metric to compare the measured PSD data with its spec, then the current "Filling Method" is the best method as compared to the other two approaches.

The "Filling Method" can also be used to an optical surface having an annular shape, that is, whose non-zero surface map values have an annular shape defined by $r_{out} \geq r \geq r_{in}$, where r_{out} and r_{in} are the radii of the outer and inner circular boundaries, respectively. The only condition for this to work is $r_{out} - r_{in} \geq r_{in}$, which is the case in most real situations.

4. Summary

We have proposed two new, alternative methods, "fitting method" and "filling method", to reduce the variance of the 2D-PSD data calculated from the measured surface height map of a circular optic. We have compared the performance of these methods with the usual "as is" approach and a Welch window method using some examples of synthesized surface maps. Trying all four approaches simultaneously to obtain both the 2D- and the 1D-PSD data when one has the resources and the need is desirable, and will allow one to gain a fairly good picture about the PSD error of a measured optical surface. The information provided in this paper will enable one to do such calculation fairly easily.

5. References

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