Revisiting PSD Analysis of Circularly Symmetric Surfaces

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Abstract: An extended PSD calculation is presented where 1D PSD's are calculated over diameters and then averaged together for circularly symmetric surfaces providing lower noise and a better estimate of the mid- and high- spatial frequency ranges of a single interferometric measurement. Results are compared to two other PSD calculation methods.
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1. Introduction

In the last two decades since the development and adoption of the new ISO10110 optical drawing standards [1], a larger number of optical surfaces are being specified with surface roughness as defined over a limited spatial frequency range. The advantage of this is that, in principal, it enables measurements by different instruments to provide comparable results. It also enables designers and fabricators the ability to target more than one spatial frequency range, or to ensure that artifacts from a particular fabrication process are minimized.

It seems relatively straight-forward to make surface measurements with one or more spatial frequency ranges, back out instrument transfer functions, calculate the combined PSD (Power Spectral Density) data, and then integrate over the specified spatial frequency range. However, there is no codified method for calculating the PSD, let alone for how to deal with instrument transfer functions and stitching. This work presents some findings related to methods of determining a scaled 1D PSD of circularly symmetric surfaces that is robust with hopefully minimal artifacts from the calculation. First, 3 different methods for determining PSD are outlined. Then results are compared. Results showing effects of criteria such as the choice of window function, amount of zero padding, and what terms to remove are also presented. This paper does not cover stitching methods or ways of accounting for instrument transfer functions. Those topics will be in future papers.

2. Determining PSD

In reviewing the literature, a number of different methods have been published to determine the PSD [2-8]. Lots of research has been presented looking at rectangular datasets, especially those obtained using interferometric microscopes (see, for example, refs. [2, 5]). Authors who have previously focused on circularly symmetric data include Walsh [4] and Novak [3]. During my research, I have previously presented results where six different methods were coded and compared [8].

The procedure to calculate PSD involves first preparing the dataset by: 1) read in phase map, 2) account for aspect ratio, 3) transform to square pixels, 4) specify clear aperture, 5) replace bad data points and outliers (>±5X rms) with interpolated nearest neighbor data or NaN (not a number), 6) fit and remove Zernike terms, and 7) make data zero mean. The next steps are 8) apply a window making sure the edge of the window corresponds with the edge of the data (Gaussian if circular, 2D Hann if rectangular, 1D Hann if linear), 9) zero-pad if desired, 10) calculate the PSD, 11) extract the final averaged 1D PSD, and 12) scale the final PSD using Parceval's theorem so that the total area under the curve equals the square of the rms (root mean square or Sq) of the data.

2.1 Calculating PSD

For this work, all calculations were done in Matlab. To determine a PSD, the steps listed above are followed. In step 10), the PSD of a *phase_map* is given by *PSD=abs(fftshift(fft2(ifftshift(phase_map)))).^2/PSD_area.* This calculation works either for 1D or 2D data. Most of the subtleties of these calculations are involved in preparing the data, and the order in which the preparation steps are performed. As an example we present a 150mm diameter mirror measured on a Fizeau interferometer as shown in Fig. 1. The left image shows the surface data after subtracting the 1st 8 "Fringe" Zernike terms [9]. Then we see a plot of a standard Gaussian window that goes to zero at the edge of the circular aperture. Next, we see the data after multiplication by the window function, and then after we double the array size with zeros. Zero-padding is performed to reduce ringing in the FFT function. The right image shows the scaled 2D PSD. Because we would like to ultimately get a band-limited rms, we could integrate an annular ring of the 2D PSD within the two spatial frequency limits. However, we traditionally look at 1D PSD plots, and extract data from them. They are much easier to compare side-by-side than the 2D PSD. In the future, it would be good to develop methods of determining band-limited rms and equivalent sorts of figures of merit directly from 2D data, but today we do not have agreed upon ways to do this. The rest of this work will look at 1D PSDs.

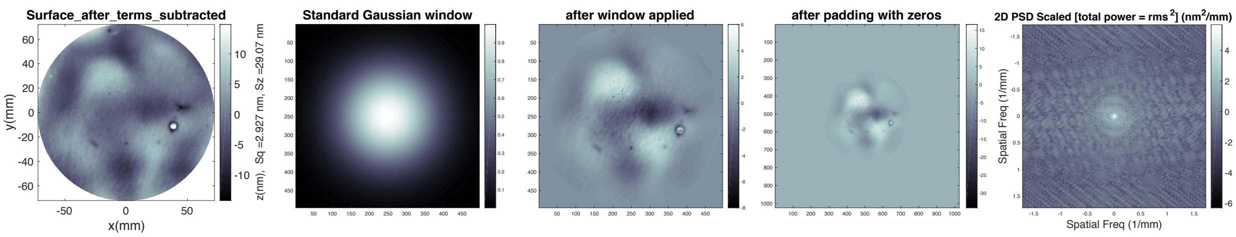

Fig. 1. (L to R) Surface data, standard Gaussian window, after window applied, after padding with zeros to double array size, and 2D PSD.

2.2 Averaging Rows (or Columns) of 2D PSD

For this technique, after the 2D PSD is calculated, all the rows (or all the columns) of the 2D PSD are averaged and folded over so you see the positive spatial frequencies. The scaling is such that the integral (sum) under the 1D PSD plot equals the rms^2 (or Sq). This technique has been in the Wyko/Veeco software for the last 3 decades and based in part on the work of Bennett [2]. This method was developed for looking at surface roughness with an interferometric optical profiler (microscope) assuming you have a rectangular array of data.

2.3 Radial Sum (Integral) of 2D PSD

This method utilizes an azimuthal integral sum around the center of the 2D PSD [10]. There are so few points at low spatial frequencies that this estimate is not good at low spatial frequencies. At mid- and high-spatial frequencies it is comparable to the other techniques and tends to be higher at the high-spatial frequencies.

2.4 Averaging 1D PSDs of Diameters

This is an extension of a method published by CSIRO for measurement of the LIGO optics [4]. For circularly symmetric optics measured on a Fizeau interferometer, the PSDs of several diameters of the data set were calculated and then averaged together. The noise of course is reduced as more diameters are calculated. Novak [3] suggested for the NIF optics that calculating the PSD for 4 diameters at 45° could provide enough information about the surface, but without averaging the PSDs, individual 1D PSD diameters are quite noisy. The method utilized here calculates the PSDs of a large number of diameters and averages them together. For this example, there are as many diameters as there are rows. First the data are remapped so that each diameter is on one row as shown in Fig. 2, and then a 1D Hann window is applied before zero-padding and calculating the 1D PSD of each diameter.

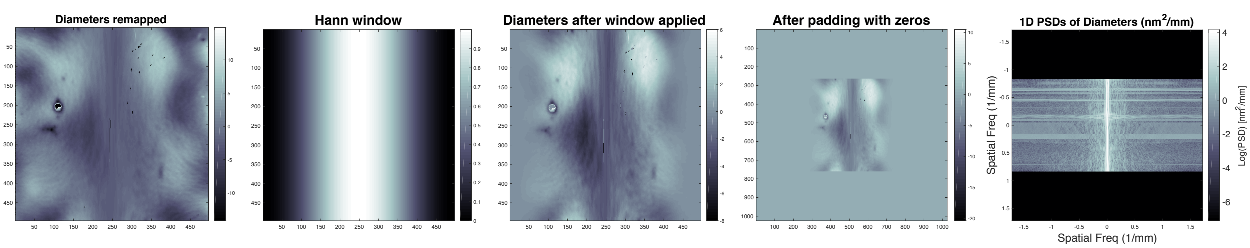

Fig. 2. (L to R) Surface data diameters remapped so that each diameter represents one row, Hann window, remapped diameters after window applied, after padded with zeros to double array size, and 1D PSDs of diameters.

Adding zero padding reduces ringing and helps reduce noise. Fig. 3 shows the average of 1D PSDs of diameters for different amounts of zero-padding for this 150mm mirror with the 1st 8 Zernike terms subtracted. No zero-padding indicates a 496x496 array. For zero-padding equal to 512, 1024, and 2048, the data are centered as more zeros are added. As the zero-padding is increased there is more frequency detail in the PSD which is offset by longer computation time.

Fig. 4 compares the 3 different PSD calculation methods outlined earlier with 3 different options for term removal. All of these calculations are zero-padded to 1024 and all are on the same scale. All curves have been scaled so that the area under each curve is equal to the rms squared of the appropriate data. As more terms are removed the overall rms value is reduced. With 36 Zernike terms removed (right), all methods yield similar results for mid- and high-spatial frequencies. However, at low spatial frequencies there are significant differences. The radial sum is affected substantially by the low number of points corresponding to low spatial frequencies. This implies that the estimate at low spatial frequencies isn't as robust as with the other PSD methods.

When only tilt is removed all the methods are relatively close at low spatial frequencies, but diverge substantially at high spatial frequencies. Here the average of 1D PSDs of diameters provides the most conservative (highest) values at high frequencies. When only the 1st 8 Zernike terms (Seidels) are removed, the methods are the closest (see Fig. 4).

The bottom plot in Fig. 3 compares different term removals for the average of 1D PSDs of diameters scaled so that the PSD curve area equals the square of each curve's rms . There is an obvious difference in the data removing tilt as compared to removing higher-order terms. As higher-order terms are removed, the PSD estimates become more consistent at high spatial frequencies implying they are likely getting near the instrument noise level at the highest spatial frequencies.

The average of 1D PSDs of diameters provides a consistent PSD estimate for circularly symmetric optics that does not fall off as much at low spatial frequencies than the radial integral. It will average out any azimuthal structure just as the radial integral technique will, but this method is more consistent across both low- and high-spatial frequency techniques when compared to the other 2 techniques, and therefore shows promise.

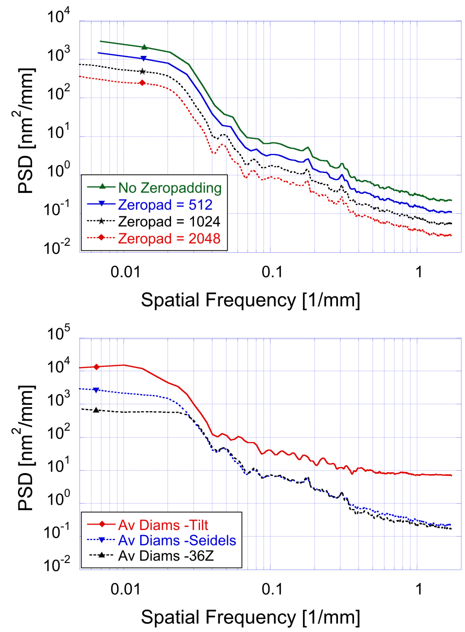

Fig. 3. Average of 1D PSDs of diameters: (Top) Effects of different amounts of zero-padding. Plots shifted to not overlap. (Bottom) Effects of term removal.

Ultimately, we want a quality measurement that is stable, robust, and sampled enough over all spatial frequency ranges. The door is still open to develop even better measures of quality that can help us produce higher precision and more consistent optical surfaces.

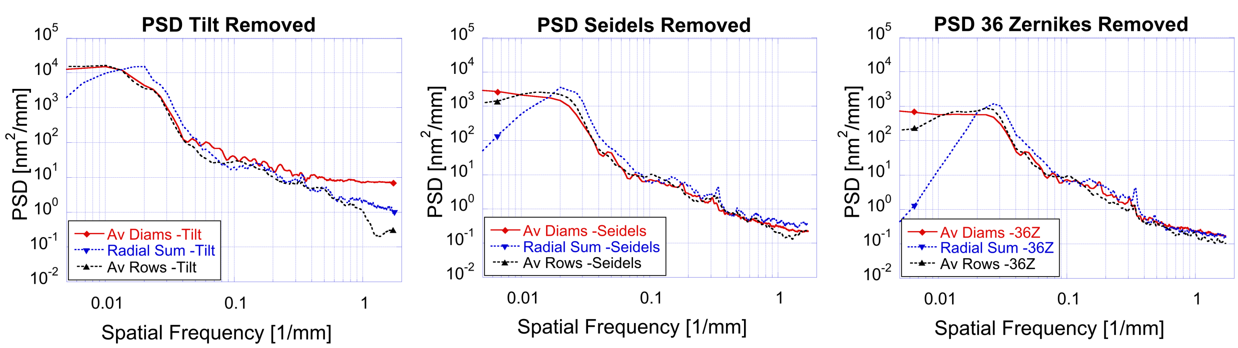

Fig. 4. Comparison of 3 different PSD calculation methods: Average of 1D PSDs of diameters, Radial integral (sum) of 2D PSD, and Average of rows of 2D PSD. (L) Tilt removed, (C) Seidels removed (1st 8 "Fringe" Zernikes), (R) 36 "Fringe" Zernikes removed.

4. References

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