REVISITING PSD ANALYSIS CONSIDERATIONS

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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 mimimized.

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, as I and others have discovered over the last two decades, there is no codified method for calculating the PSD, let alone for how to deal with instrument transfer functions and stitching.

I often get called on as a consultant to ensure that the customer is getting a surface that meets their specifications. It's not as easy as it seems to ensure that. Fabricators are not likely to give you the details about how they do their calculations. And interferometer makers don't want to give you the details of how their algorithms calculate a PSD. Plus, if you have to combine PSD's from multiple measurements or multiple instruments, it gets even more complex to get a satisfactory end result that all can agree upon.

My work on this topic began almost 30 years ago at Wyko when we were first developing PSD calculations. Over the years, I have had several clients ask for my advice in different calculations. What I present in this paper is the result of applying methods published in the literature as well as reverse-engineering curves I've received from different vendors. In the next section, I present procedures for calculating 6 different 1D PSD calculations. These methods will be illustrated using a simple example to compare results. The paper ends with a short discussion.

What this paper does not cover are stitching methods, and methods of measuring and accounting for instrument transfer functions. We'll save those for another day.

METHODS OF CALCULATING PSD

To calcuate the surface roughness (rms or Sq) of a surface over a specified spatial frequency range, we need to integrate the PSD between the limits of this range.

The 2D PSD

Rather than writing out this theory mathematically, the procedures will be outlined in pseudocode:

1. Read in the phase map
    a. Account for aspect ratio
    b. Transform to square pixels
    c. For simplicity arrays have even numbers of square pixels for these calculations
2. Replace bad data point with NaN (not a number)
3. Remove Zernike terms
    a. Make data zero mean
    b. Replace outliers >±5X rms with NaN
4. Specify the clear aperture
5. Window the data
    a. Gaussian window if circular
    b. 2D Hann window if rectangular
    c. Make sure edge of window coincides with edge of data aperture
6. Zeropad if desired
7. Calculate 2D PSD using

PSD_2D=abs(fftshift(fft2(ifftshift(map)))).^2/PSD_area

Where…

Spatial frequency interval = 1/ diam_PSD_array

Lowest spatial frequency = 1/ diam_PSD_array
Highest spatial frequency = 1/pixel_spacing

8. Scale the PSD
   a. Area under the PSD = rms^2
   b. Because of Parseval's theorem this becomes

*rms_PSD_2D = sqrt(sum(PSD(:)) * df^2 / (4 * pi^2))*

   c. The rms of the original data after terms removed and aperture applied is used accounting for bad pixels
   d. Each 1D or 2D PSD is scaled this way to integrate over spatial frequency and obtain the band-limited Sq (or rms)

Here is an example for a flat mirror measured in a Fizeau interferometer. All calculations performed in Matlab. FIGURE 1 shows the phase map as measured.

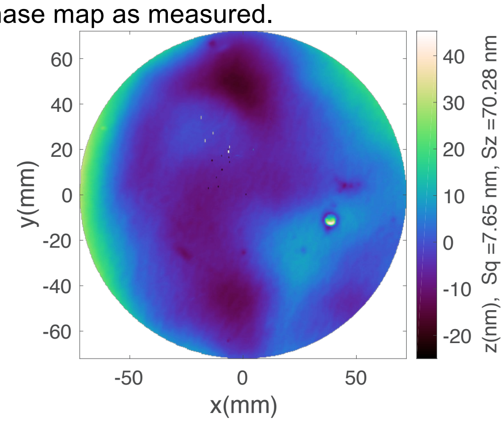

FIGURE 1. This phase map of a flat mirror has 496x496 pixels and was taken with a Fizeau interferometer. The artifact at 3 o'clock is a pit in the surface. The other missing data points (white dots at 11 o'clock) are from specs of dirt on the surface. These data get replaced by NaN (not a number).

After the Seidel Zernike terms (the first 8 "Fringe" terms plus the mean [2]) are removed, we are left with the residual phase map in FIGURE 2. FIGURE 3 shows the Gaussian damping window in the top plot, and the windowed phase data are shown in the bottom plot. NaN values have been replaced with zero (the mean value). Because of how the window-damping function works, the data are zero at the edges of the array. This will prevent ringing.

FIGURE 4 is a plot of the 2D PSD scaled so that the total power in the plot sums to the square of the rms of the data.

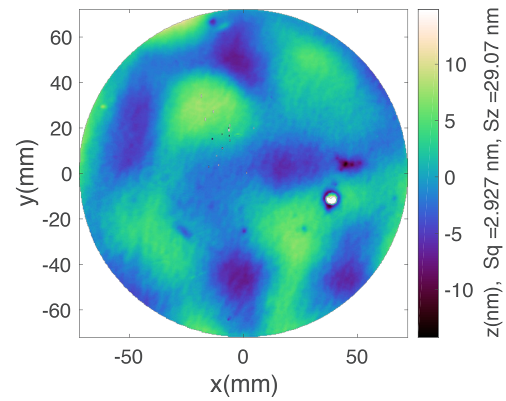

FIGURE 2. Residual phase map after the Seidel Zernike terms are removed.

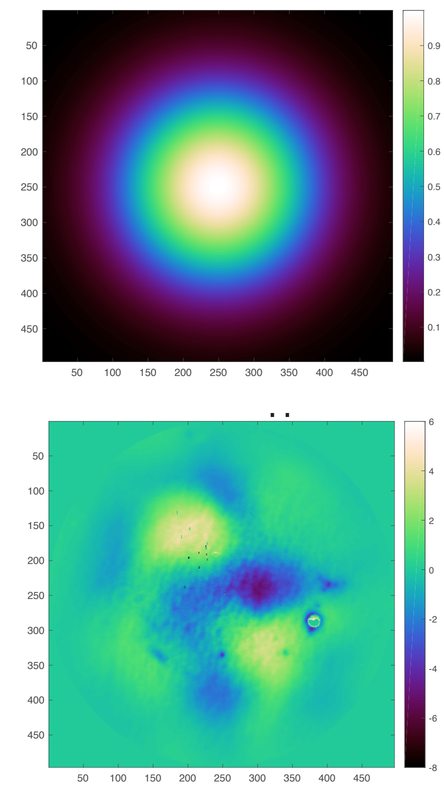

FIGURE 3. (Top) Circular Gaussian damping window function. (Bottom) Windowed residual phase data.

Methods of producing 1D PSD from 2D PSD

Now that we have a 2D PSD we can process this to find band-limited rms specifications. I want to point out that this is not something that's well-defined in practice. We could do this directly from the 2D PSD, but typically we look at 1D PSD plots. And therein is the crux. What's the best way to do this?

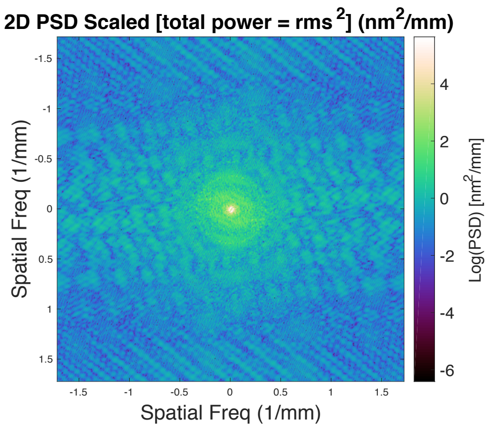

FIGURE 4. Two-dimensional PSD of windowed data in FIGURE 3. This has been scaled so that the total power = rms^2 of the residual data set in FIGURE 2.

After doing a literature search and talking to a lot of different vendors, I have found that there are as many different ways to do this [3-8]. I began to try the different published and stated methods on the same datasets, and found that they do not agree. No wonder we have difficulty comparing results. In this section, I will outline a number of different ways in which we can translate 2D PSD data into 1D PSD data.

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. This method was developed for looking at surface roughness with an interferometric optical profiler (microscope) assuming you have a rectangular array of data.

Averaging 1D PSDs of each row (or column)

This provides comparable data to taking the 1D PSD of each row (or column) of data in the original dataset and then averaging all the rows together. Elson and Bennett outline this method in their work [3].

It needs to be noted that when you have data with a circular aperture, this may not be the best approach. However, it is still widely used in many current commercial software packages.

FIGURE 5 shows a linear Hann window used to dampen data when taking the PSDs of individual rows (Top) and a plot of the 1D PSDs of each row in an array.

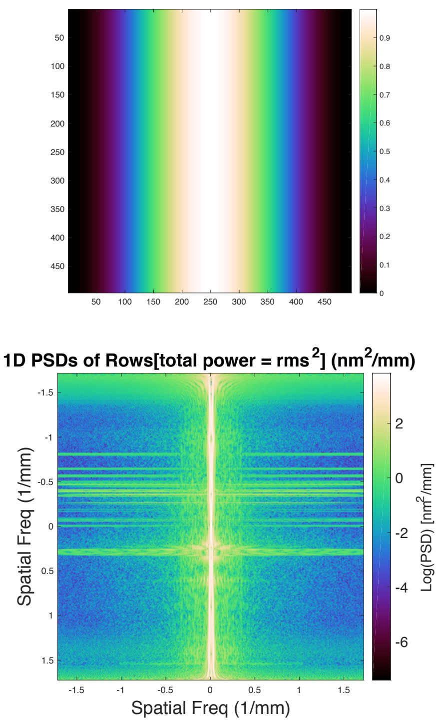

FIGURE 5. (Top) Linear Hann damping window function. (Bottom) 1D PSDs of each row of data in FIGURE 2.

FIGURE 6 shows 6 different types of 1D PSD plots, two of which I have described so far.

Fat rows of 2D PSD

Because of the inconsistency of the previous 2 techniques with circular apertures, Zygo in their MetroPro software [9] have been using "fat" rows for a 1D PSD estimate. Single rows of the 2D PSD are too noisy to provide good data, but average a few rows (or columns) near the center together and you get a better estimate of the PSD.

The example shown in FIGURE 6 averages 2.5% of the rows near the center (for a 496x496 array that's about 24 rows). This technique is more consistent between data sets that have circular or rectangular apertures. However, this estimate can end up missing some features depending upon orientation unless radial slices at different orientations are considered. It tends to be quite a bit noisier and provides a lower estimate than other techniques.

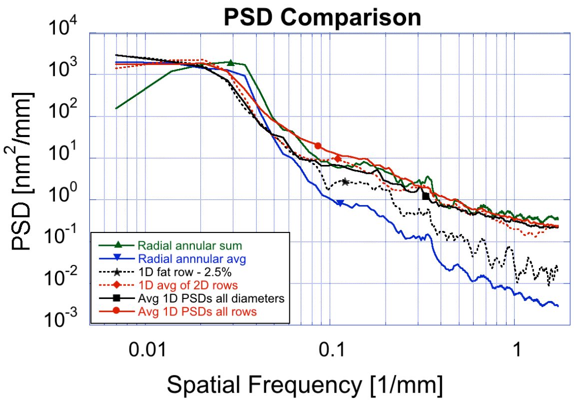

FIGURE 6. One-dimensional PSD plots of FIGURE 2 data set. This has been scaled so that the total power = rms^2 for each curve.

Radial integral of 2D PSD

This method appears in work from JPL [7]. They take a radial slice from the center to the edge of the 2D PSD and rotate it around the center to create an average of the values for each radius. This provides a much less noisy version of a slice out of the 2D PSD. It will average features that change with the azimuth, but it's good for circularly symmetric optics. In FIGURE 6 you can see that this estimate is much lower than the other techniques for higher spatial frequencies.

Radial sum of 2D PSD

Because of the issues with having a low estimate (and thereby likely underestimating the actual values) in the method above, this method using a sum rather than an average was developed [8]. It is another technique that is used for circularly symmetric optics with circular apertures. However, because there are so few points at low spatial frequencies, this estimate is not good at low spatial frequencies. At mid- and high-spatial frequencies it comparable to the other techniques and tends to be higher at the high-spatial frequencies (see FIGURE 6).

Chordal PSD (1D PSDs of all Diameters)

This is an extension of a method published by CSIRO for measurement of the LIGO optics [5]. For circularly symmetric optics measured on a Fizeau interferometer, the PSDs of several chord diameters of the data set were calculated and then averaged together. The noise of course is reduced as more chords are calculated. Novak [4] suggested for the NIF optics that calculating the PSD for 4 chords at 45° could provide enough information about the surface, but without averaging the PSDs of individual chords are noisy.

I propose extending this and calculating the PSDs of a large number of chordal diameters and then averaging them together. For this example, there are as many chords as there are rows. First the data are remapped so that each chord is on one row as shown in FIGURE 7 for the dataset in FIGURE 2. FIGURE 8 shows the PSDs of each chordal diameter in a row.

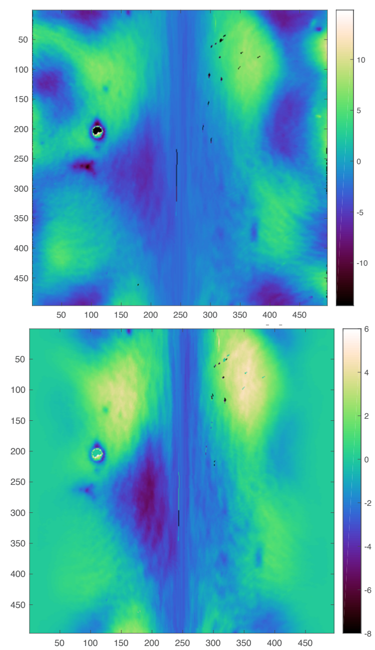

FIGURE 7. (Top) Each row is a chord at a different angle of the data set in FIGURE 2. There are as many chords as there are rows. (Bottom) After applying a linear Hann window.

In my opinion this method provides a more consistent PSD estimate for circularly symmetric optics than any of the other methods. It will average out any azimuthal structure just as the radial average and radial sum techniques will, but this method is more consistent across both low- and high-spatial frequency techniques when compared to those other 2 techniques, and therefore shows promise.

Zero Padding

Zero padding is another consideration when calculating PSDs. Adding more zero padding does reduce ringing and helps to reduce noise. FIGURE 9 shows the average of 1D chordal diameter PSDs for different amounts of zero padding. The FFT function in Matlab doesn't care whether the array is a power of 2 or not.

For these plots, no zeropadding indicates a 496x496 array. For zeropad = 512, the data are centered in a 512x512 array of zeros. For zeropad = 1024, and 2048, more zeros are added. It is noticeable that as you increase the zero padding you get more detail in the 1D PSD estimate. Of course there is a tradeoff with calculation time.

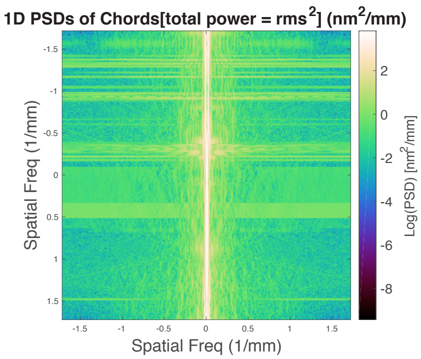

FIGURE 8. 1D PSDs of each row of data in FIGURE 7. Each row corresponds to a different chordal diameter of FIGURE 2.

DISCUSSION

It is obvious from the work presented that the choice in method used to calculate the 1D PSD makes a difference in the result and ultimately will change the outcome of a bandlimited surface rms (Sq) estimate.

There are many factors that need to be taken into account. Several of them have been presented here. The most obvious is choosing a method depending upon whether the data are circularly symmetric or have a circular aperture versus having a square or rectangular data. I have also shown how PSD estimates can change with zero padding. This study in not exhaustive in that I haven't presented other variables such as binning, terms removed, and filtering that can affects PSDs. There is still a lot of work to do in this area in order to help codify the best methods to use for these calculations. Choose carefully.

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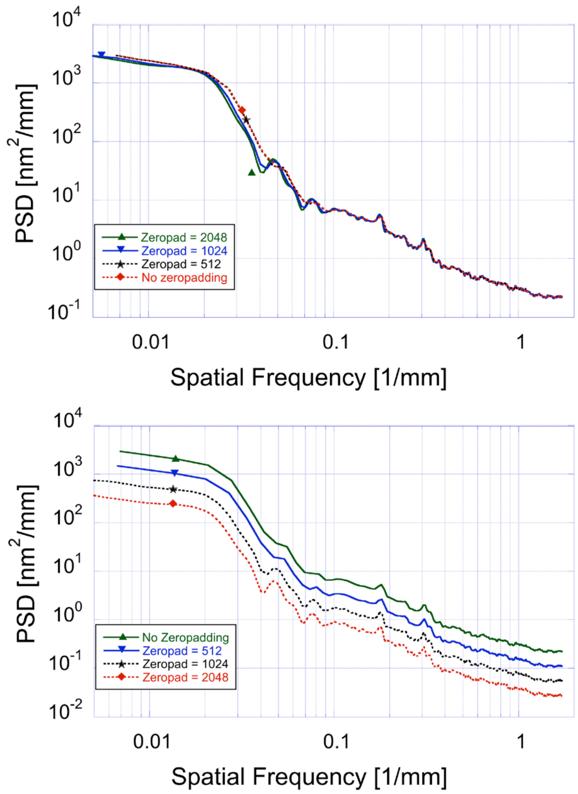

FIGURE 9. (Top) Average of 1D PSDs of all chordal diameters for different amounts of zero padding of windowed data from FIGURE 7. (Bottom) Same curves as top plots, but separated and no longer scaled correctly.

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