# Effect of broadband illumination on reconstruction error of phase retrieval in optical metrology

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## ABSTRACT

Phase retrieval is a promising method for optical system and surface metrology that makes use of intensity measurements of diffraction patterns. An iterative algorithm is used to solve the inverse problem to find the phase of the field producing the measured intensity distributions. For practical reasons, such as the reduction of coherent artifacts or to improve the signal-to-noise ratio of the measured data, it is often desirable to measure intensity distributions using broadband illumination. It is possible to perform phase retrieval with broadband data by incorporating a broadband model of the system into the phase retrieval algorithm. To do this, the system is modeled at several discrete wavelengths and the results from each are summed incoherently to produce a broadband result. This significantly increases the computational load. We show here that when aberrations are small, accurate estimates of the OPD distribution, on the level of $\lambda/1000$ RMS error, can be achieved using data with bandwidth up to about 10% as the input to a phase retrieval algorithm that assumes monochromatic data.

**Keywords:** Phase retrieval, broadband phase retrieval, phase measurement, optical metrology, Fourier optics, optical metrology, surface measurement, wavefront measurement.

## 1. INTRODUCTION

Phase Retrieval is a method of determining the phase of an optical field using simple measurements of the intensity pattern produced by the optical field in one or more planes [1]. Depending on the arrangement used, this phase information can be interpreted as the shape of an optical surface or as the aberration, optical path difference (OPD), produced by an optical system. In this way, the final results are much the same as produced by a phase-shifting interferometer, although these results are arrived at in very different ways.

In interferometry an optical instrument is used to produce intensity patterns in which the phase information is relatively simply encoded. Indeed, it is frequently possible for an experienced experimenter to interpret the shape of the OPD distribution from the interferogram with no further analysis required. If one adds more complexity to the arrangement, adding a phase shifter, the interferograms can be processed to obtain a quantitative result with simple computer processing. A schematic diagram of a typical phase-shifting Fizeau interferometer is shown in Fig. 1 [2].

Phase retrieval, in contrast, has a greatly simplified apparatus compared to interferometry. In its simplest embodiment, the arrangement may consist of only a detector array. An idealized schematic of this is shown in Fig. 2. The reduced complexity of the apparatus is replaced by more complex algorithms that interpret the intensity patterns and arrive at a quantitative result for the phase of the optical field. The simplicity of the arrangement reduces its cost and allows it to be very adaptable to different situations, so long as the particular situation can be modeled in the computer by the phase retrieval algorithm. In other words, when practical difficulties arise, they can usually be addressed by changes in software rather than changes to hardware.

In this work we examine a specific case of such a practical difficulty, an illumination source that has a finite spectral bandwidth rather than a single line of a laser. A finite-bandwidth source might be encountered in situations where no laser source can be conveniently included, and is particularly advantageous in situations where coherent artifacts are present when using perfectly coherent light. One might also choose to use a source with larger bandwidth over a filtered low-bandwidth source for reasons of signal-to-noise ratio.

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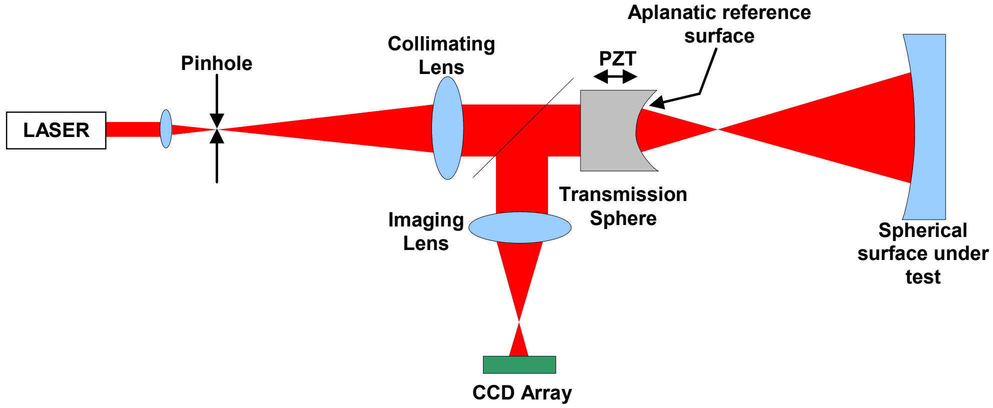


Fig. 1. Schematic diagram of a typical Fizeau phase shifting interferometer for testing a spherical surface.

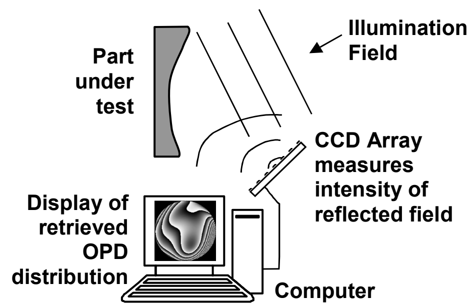


Fig. 2. An idealized representation of phase retrieval in optical metrology, where the only apparatus required to test the part is a known illumination field, a detector array and a computer.

The major question that this work was intended to answer was whether or not the extra code complexity and computation time associated with a broadband phase retrieval algorithm was necessary in order to retrieve the phase to the accuracies required by optical metrology. The strategy used to answer this question was to model in a computer the intensity patterns produced by broadband sources and then retrieve the phase using a phase retrieval algorithm making the monochromatic assumption. The true phase and the retrieved phase can be then compared and the error due to the monochromatic assumption can be computed.

## 2. PHASE RETRIEVAL BACKGROUND

Phase retrieval uses an iterative algorithm to solve for the phase of an optical field in a particular plane given only one or more measurements of intensity distributions. The planes where these intensity distributions are measured are usually chosen to be near-focus planes so that the light can be collected by a detector array of small dimensions. This is illustrated for the transmissive case in Fig. 3. Usually, the square-root of the intensities is taken to arrive at the field amplitudes.

There are two major classes of phase retrieval algorithm. One class is the Iterative Transform (or Gerchberg-Saxton) Algorithm [3]. Complex fields are propagated back and forth between planes where the amplitudes are known and are reinforced at each iteration. These algorithms are simple and often work well, but tend to stagnate in local minima. It is also difficult to account for non-ideal conditions with them.

The other class of algorithm, and the one used in this work, is a nonlinear optimization algorithm where a particular metric is maximized or minimized, usually using a gradient search approach, by varying parameters that describe the phase in the plane where the retrieval is performed. While not always the case, we generally refer to the plane where the phase is being determined as the pupil plane. In each iteration, the phase values are combined with an assumed amplitude distribution and propagated to each of the measurement planes. In this work we model the amplitude of the field in the pupil plane to be a uniform circle. If this is not the case, the amplitudes can be determined algorithmically

[4,5], or using a pupil camera. The phase can be parameterized in terms of a weighted sum of basis functions, such as the Zernike polynomials, or simply as an array of phase values at each pixel in the pupil plane. In this work, we have used the Zernike form.

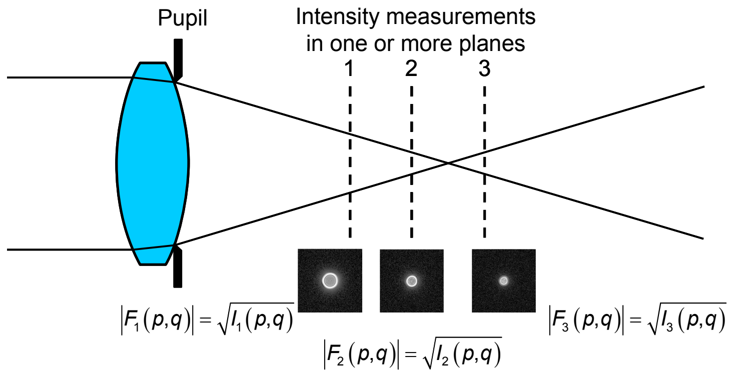


Fig. 3. Phase retrieval algorithms employ measurements of intensity distributions produced by an optical field in one or more near-focus planes to solve for the phase of the field in a remote plane, often a pupil plane. Here a situation where measurements are made in three planes is shown.

The propagation model we have used in this work is based on scalar diffraction theory [6]. Because we make measurements in multiple planes, we have chosen to use a two-step propagation algorithm. First, we use Fresnel propagation to propagate to the paraxial focal plane. Then we use angular spectrum propagation to propagate the small distance from the focal plane to each of the measurement planes. This has the desirable effect of keeping the sample spacing the same in each measurement plane [4].

To propagate broadband fields, we use the same model and propagate the field at a number of discrete wavelengths that adequately sample the spectrum. Since the spatial sample spacing in the planes to which we are propagating depends on wavelength, we must take care to ensure that the sample spacing of the propagated field is the same across wavelength. We do this by varying the size of the array used for the Fresnel transform, zero padding when necessary. For more details on this method, see Ref. [7].

In the monochromatic phase retrieval algorithm, the magnitude of the propagated pupil-plane field is compared with the measured field magnitudes using an error metric. In the broadband case, the propagated fields at the multiple wavelengths are summed incoherently before comparing with the measurements. In this work the comparison is done using a simple squared difference metric. An algorithm, such as the conjugate gradient algorithm [8], is used to minimize this metric. Analytic expressions for the gradient of the error metric with respect to the phase parameters greatly reduce the computation required in this optimization step [9]. The expressions for the gradient are different for the monochromatic and broadband cases [7]. In this work, however, we have employed only the less computationally intensive monochromatic phase retrieval algorithm.

## 3. NUMERICAL EXPERIMENT

### 3.1 Description of experiment

To determine the effect that broadband data has when used as the input to a monochromatic phase retrieval algorithm, we produced synthetic broadband data from known phase maps. The spectrum of the broadband data was chosen to be Gaussian, characterized by its full width $\Delta\lambda$ at $1/e$, truncated to the interval from $\lambda_o - 1.5\Delta\lambda$ to $\lambda_o + 1.5\Delta\lambda$, as shown in Fig. 4.

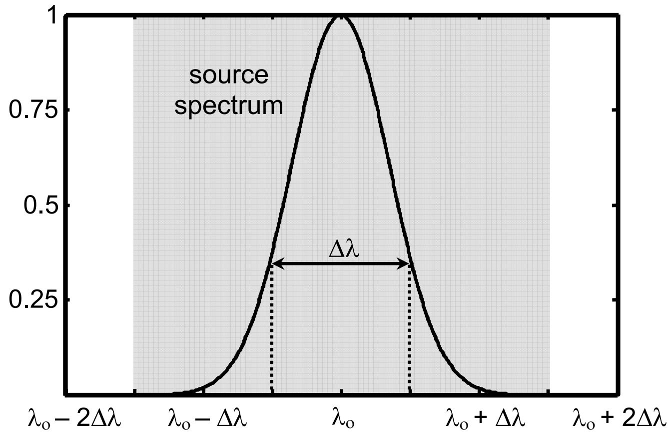


Fig. 4. The spectrum of diffraction patterns modeled was Gaussian with a $1/e$ width $\Delta\lambda$ and truncated to the range from $\lambda_o$ – $1.5\Delta\lambda$ to $\lambda_o + 1.5\Delta\lambda$.

OPD distributions were simulated from as many as 78 Zernike terms. The coefficients were Gaussian random variables, with variances chosen so that low order terms were weighted more heavily than higher order terms and so that rotationally invariant terms were weighted more heavily than asymmetric terms. This was meant to be consistent with the typical errors found in optical surfaces and systems. The standard deviations of the coefficients used are plotted in Fig. 5. This resulted in a set of OPD distributions with a mean RMS of $0.067\lambda_o$ with a standard deviation of $0.033\lambda_o$. We use either all 78 terms or the lower 36 terms in this work. Some example OPD distributions are shown in Fig. 6.

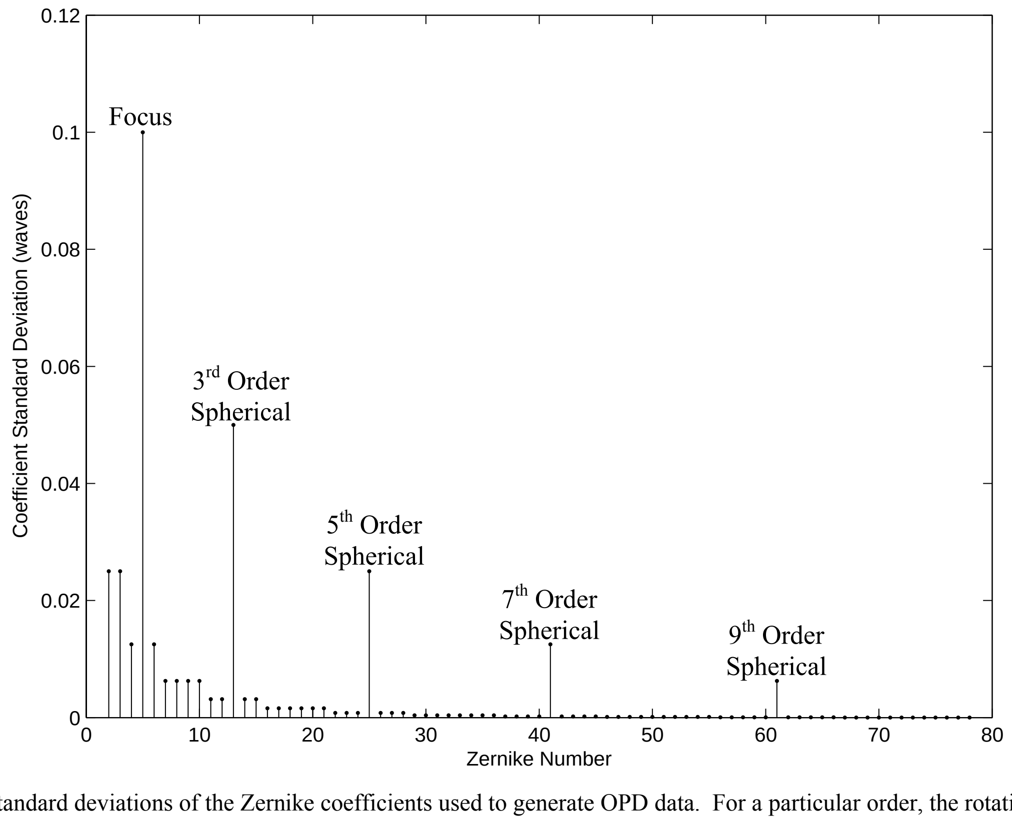


Fig. 5. Standard deviations of the Zernike coefficients used to generate OPD data. For a particular order, the rotationally invariant terms are weighted more heavily than the asymmetric terms. The ordering used here is the single index scheme from Ref. [2].

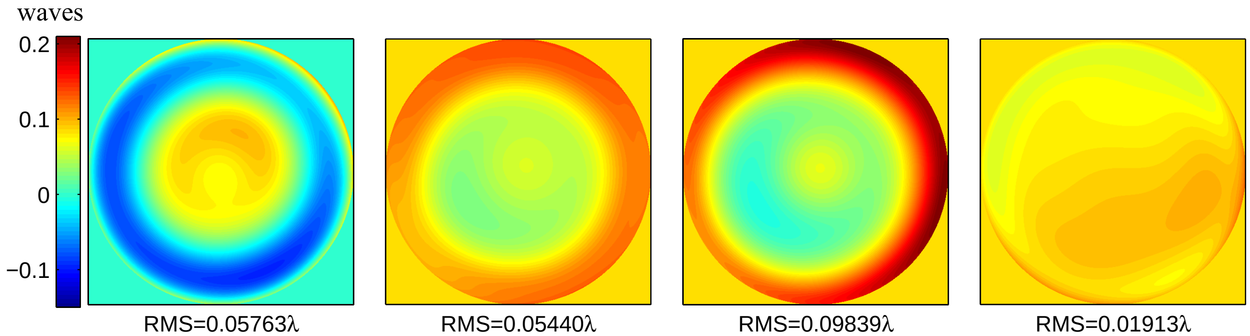


Fig. 6. Examples of OPD distributions used to generate simulated intensity data input to phase retrieval algorithm. The waves quoted here are at 404.65 nm.

Broadband measurements were simulated for 50 different realizations of the OPD for 26 different spectral bandwidths $\Delta\lambda$, and phase retrieval was performed for each of these 1300 cases. In each trial, two intensity patterns were computed: one 25 mm inside and the other 30 mm outside the focal plane of a 5000 mm focal-length lens with an NA of 0.1. These computed patterns are the input for the phase retrieval algorithm. The bandwidths, $\Delta\lambda$, were in the range from 0 to 100 nm with a center wavelength $\lambda_o$ of 404.65 nm. This corresponds to percentage bandwidths $\Delta\lambda/\lambda$ of 0 to 24.7%. The resulting simulated data size was 256 × 256, but the arrays holding the field information were padded additionally to give each different wavelength the same sampling in the measurement planes. Five spectral samples across the modeled region were used for the narrowest non-monochromatic bandwidth examined, sufficient sampling for this smooth spectrum. 152 samples were used for the widest bandwidth. Realistic noise was also added to the data. Poisson noise was added assuming that the brightest pixel had a full-well capacity of 24,000 photoelectrons, as well as Gaussian-distributed, signal-independent read noise with a standard deviation of 16 photoelectrons. The data was also quantized to 12 bits. Example computed intensity patterns and the corresponding spectra are shown in Fig. 7. It is clear that broadband light blurs high-frequency detail in the patterns and reduces the contrast of the lower-frequency features.

We also examined the effect of spatial frequency content on the reconstruction error of the OPD. Reconstructions were performed in the case where the algorithm used a set of Zernikes the same size as was used to generate the data, a set of Zernikes with fewer terms that used to generate the data, and a set with more terms than used to generate the data.

We also simulated smaller sets of data with larger aberrations to examine how aberration strength might effect the retrieval results.

### 3.2 Results

Fig. 7 (c), (f), and (i), show some example retrieved intensity patterns from our monochromatic phase retrieval algorithm. In the case shown, the RMS OPD was $0.058\lambda$ at the center wavelength of 404.65 nm, and was formed using 36 Zernikes distributed as described above. The reconstructed intensity in the monochromatic case, (c), is indistinguishable from the measurement input to the algorithm. In the 12% bandwidth case, (f), there are substantial differences from the input measurement, particularly in the high-frequency detail. The general shape of the intensity pattern is very similar. In the 25% bandwidth case, the agreement is even worse, but again the general shape of the pattern has some correspondence to the measurement.

If we examine examples of the OPD distributions generated by the phase retrieval algorithm shown in Fig. 8, we see that there is excellent agreement between the true OPD distribution (a) and the retrieved OPD distributions in the monochromatic (b), and 12% bandwidth (c) cases, both differing from the true OPD distribution by less than $\lambda/1000$ RMS. There is some agreement in the 25% bandwidth case, but it is much poorer, being in error by $0.018\lambda$ RMS.

We have also performed retrieval over a much larger ensemble of OPDs and bandwidths and these results are summarized in Fig. 9. The mean RMS error, over a set of fifty OPDs at each bandwidth examined, is plotted as a function of bandwidth. Nonconverging results (those with a particularly large error metric) have been removed.

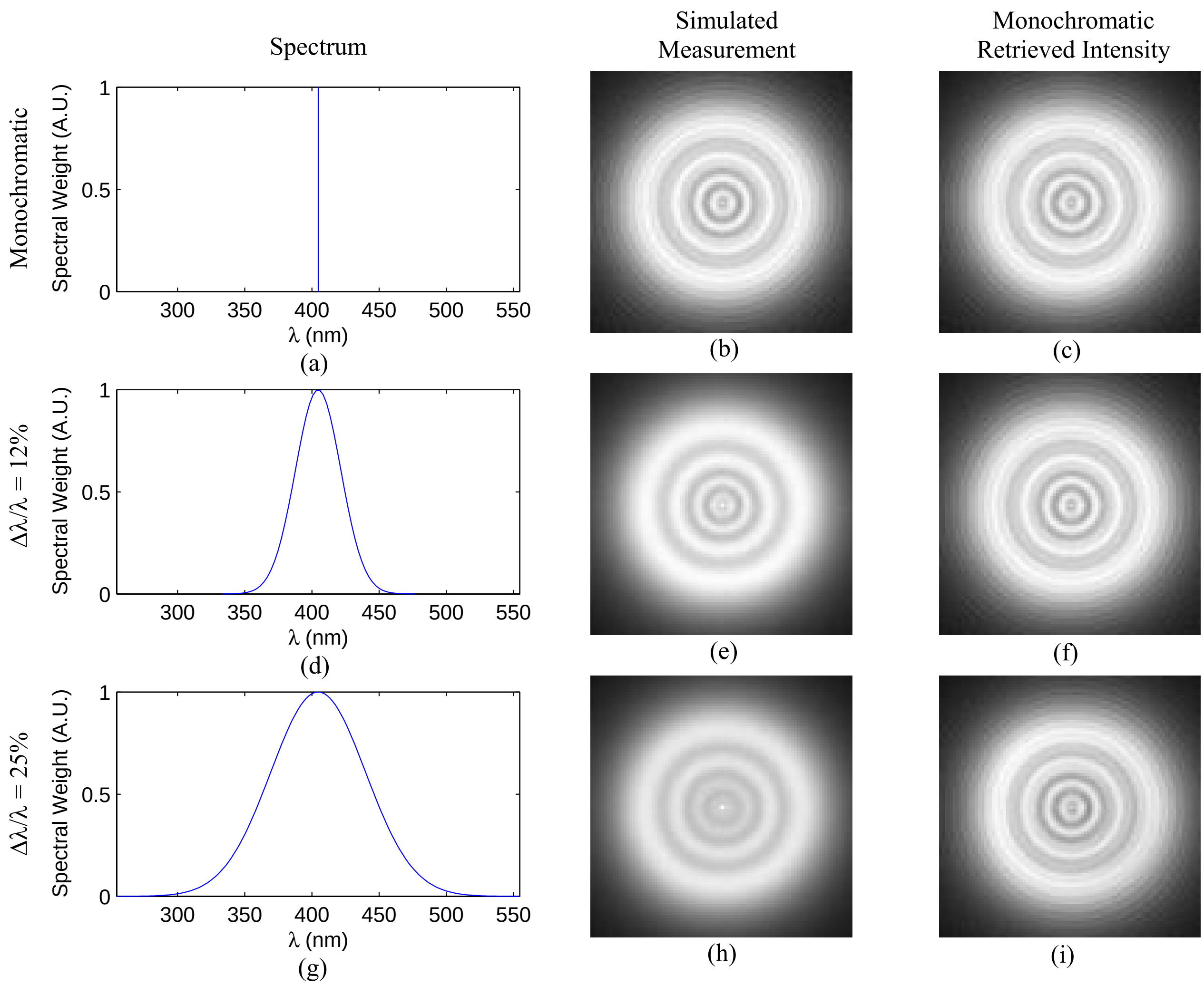


Fig. 7. The spectra (a), (d), (g) used to simulate phase retrieval data intensity data (b), (e), (h), are monochromatic, and have 12% and 25% bandwidth, respectively. The resulting retrieved intensity data using a monochromatic phase retrieval algorithm are shown in (c), (f), and (i).

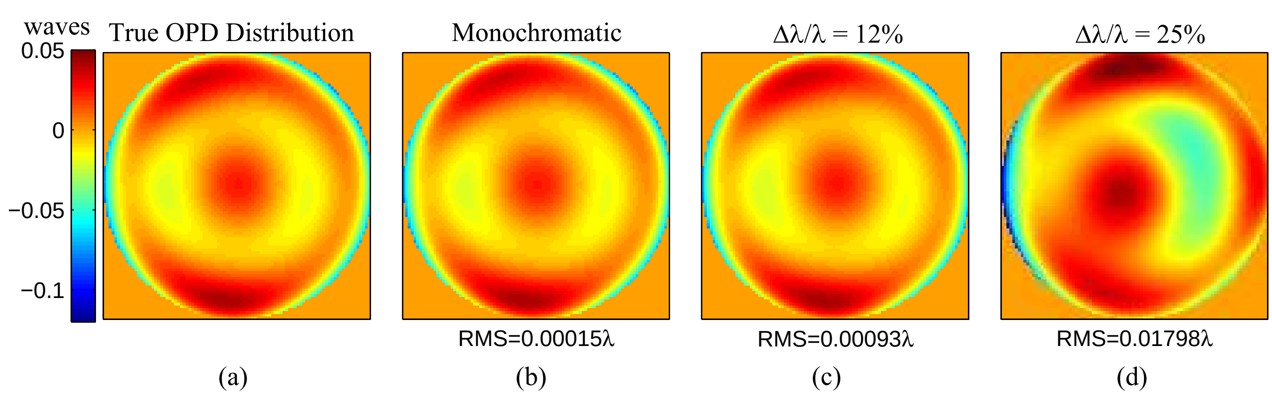


Fig. 8. True OPD distribution (a), and retrieved OPD distributions where the simulated data was computed using (b) monochromatic light and broadband light with (c) 12% and (d) 25% bandwidth. Tip, tilt and focus are removed and the number of waves are quoted at the center wavelength of 404.65 nm.

The solid line in Fig. 9 indicates the case where the simulated OPD distribtion and the retrieval were both constrained to have 36 Zernike coefficients. This performed well for surprisingly large bandwidths, achieving average errors of $\lambda/1000$ for bandwidths as high as 10%.

We also examined the situation where the simulated OPD distribution had more higher-order terms, 78 Zernikes, than assumed by the phase retrieval algorithm, with only 36 Zernikes. This performed poorly by comparison for all bandwidths, including monochromatic, shown as the dotted line in Fig. 9. If we compare only the first 36 Zernikes of the true OPD distribution to the 36 Zernikes retrieved (dashed line), we see that the agreement is better, but is still worse than if we used the correct number of terms. When we used more Zernikes in the phase retrieval algorithm than were present in the true OPD distribution (dot-dashed line close to the solid line) we see that there is very good correspondence between that and the case where we used the correct number of terms, up to about 20% bandwidth. Above 20%, the agreement rapidly gets worse. We hypothesize that the higher order terms are manipulated by the algorithm in such a way to reduce the contrast to agree with the broadband data. From these results we see that for low to moderate spectral bandwidths it is better to try to fit too many phase terms than too few.

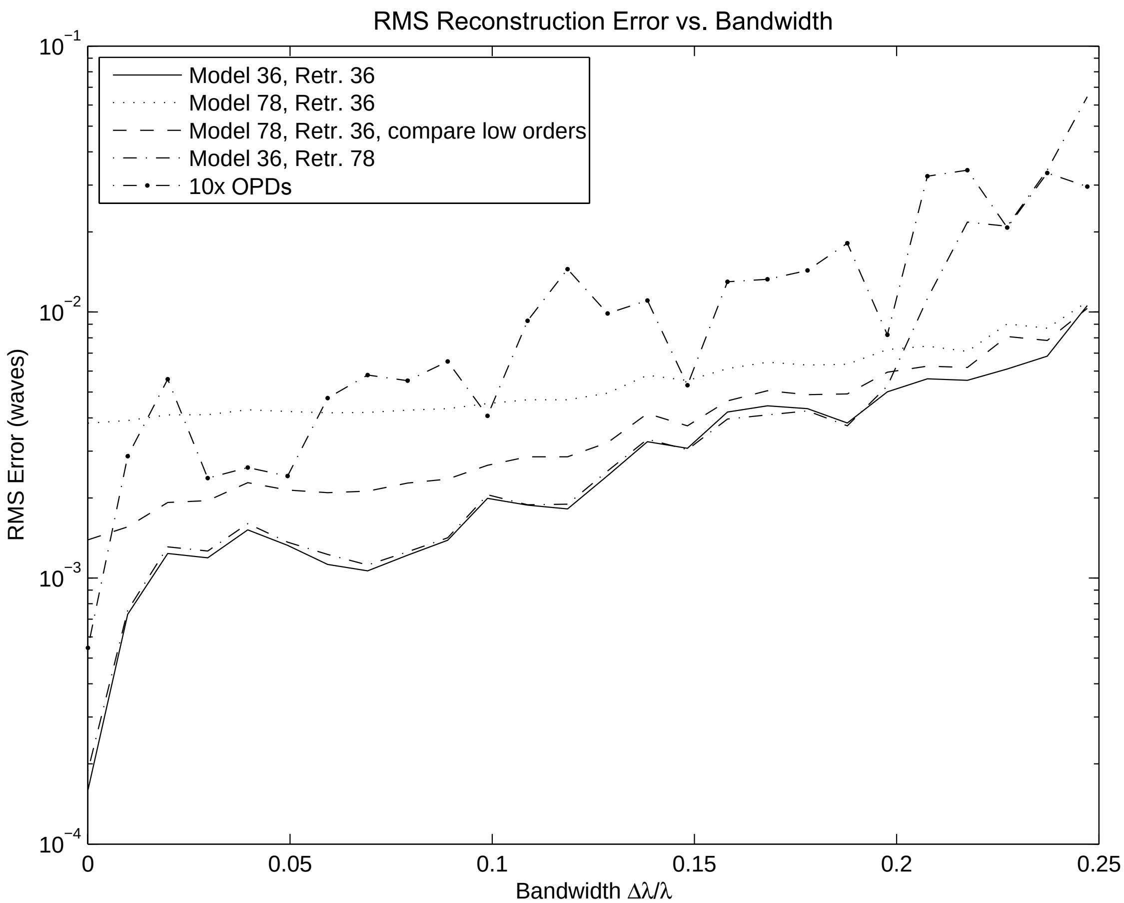


Fig. 9. Mean retrieval errors versus bandwidth for 50 OPD realizations, for a monochromatic phase retrieval algorithm, where the modeled measurement data and phase retrieval algorithm used the same number of terms (solid line), where the modeled data had more terms (dotted line), and where the modeled data had fewer terms (dot-dashed line near the solid line.) We also compare only the common lower order terms when the algorithm used fewer terms than the modeled data (dashed line). The dash-dot line with the circular markers shows the case when OPD distributions with ten times greater aberrations were modeled and retrieved using the same number of coefficients in the retrieval and the modeled data.

We also investigated the case of greater aberrations present in the OPD distribution. We simulated a smaller set of data (thirty OPD realizations per bandwidth) with ten times more aberration than was present in the first data. We then simulated intensity measurements and performed retrievals with 36 coefficients used in both. The resulting reconstruction errors, shown by the dash-dot line with circles in Fig. 9, are several times worse than that for the smaller errors considered, but is still quite good (a fraction of $\lambda/100$) for moderate bandwidths.

## 4. SUMMARY

We have described a monochromatic phase retrieval algorithm that can be applied to optical metrology problems. We apply this algorithm to situations where the measurement data may not be monochromatic. We discussed a method for simulating broadband intensity measurements, and how it can be included in a phase retrieval algorithm. The inclusion increases the complexity and computation time of the phase retrieval algorithm. We instead examined the errors introduced by using a monochromatic algorithm on broadband data. We have shown that errors on the order of $\lambda/1000$ can be achieved for bandwidths as large as 10%, a surprisingly large value, in cases where the OPD is relatively small. We also demonstrated that this error worsens when larger aberrations are present. We also showed that it is important to include enough high-order terms in the phase retrieval algorithm to capture the OPD distribution accurately, as even the low-order terms can be in error when the high-order terms are not included in the forward model. We found that it is better to err on the side of using a larger number of terms in the phase retrieval algorithm than present in the OPD distribution than using too few, although at larger bandwidths errors can worsen. Future work should examine more fully the relationship between the RMS of the OPD and accuracy of monochromatic phase retrieval and whether using even more higher orders causes the onset of this worse error regime at smaller bandwidths, including the case of a point-by-point phase retrieval.

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