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Abstract. The design and evaluation of the expected performance of optical systems require sophisticated and reliable information about the surface topography for planned optical elements before they are fabricated. Modern x-ray source facilities are reliant upon the availability of optics with unprecedented quality (surface slope accuracy $<0.1 \mu\text{rad}$). The problem is especially complex in the case of x-ray optics, particularly for the X-ray Surveyor under development and other missions. The high angular resolution and throughput of future x-ray space observatories requires hundreds of square meters of high-quality optics. The uniqueness of the optics and limited number of proficient vendors makes the fabrication extremely time consuming and expensive, mostly due to the limitations in accuracy and measurement rate of metrology used in fabrication. We discuss improvements in metrology efficacy via comprehensive statistical analysis of a compact volume of metrology data. The data are considered stochastic, and a statistical model called invertible time-invariant linear filter (InTILF) is developed now for two-dimensional (2-D) surface profiles to provide compact description of the 2-D data in addition to one-dimensional data treated so far. The InTILF model captures stochastic patterns in the data and can be used as a quality metric and feedback to polishing processes, avoiding high-resolution metrology measurements over the entire optical surface. The modeling, implemented in our BeatMark™ software, allows simulating metrology data for optics made by the same vendor and technology. The data are vital for reliable specification for optical fabrication, to be exactly adequate for the required system performance. © 2019 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: 10.1117/1.OE.58.8.084101]

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1 Introduction

The design and evaluation of the expected performance of optical systems require sophisticated and reliable information about the surface topography for planned optical elements before they are fabricated. Modern x-ray source facilities are reliant upon the availability of x-ray optics of unprecedented quality, with surface slope accuracy better than $0.1 \mu\text{rad}$ and surface height error of less than 1 nm .^{1–5} The problem is especially severe in the case of x-ray optics for modern diffraction-limited-storage-ring and free-electron-laser x-ray source facilities, as well as x-ray astrophysics missions under development. The unprecedented high angular resolution and throughput of future x-ray space observatories, such as the X-Ray Surveyor mission,⁶ require high quality optics of hundreds square meters in total area. The uniqueness of the optics and limited number of proficient vendors make the fabrication extremely time consuming and expensive, mostly due to the limitations in accuracy and measurement rate of the available metrology.

Recently, a possibility to improve metrology efficiency via comprehensive statistical treatment of a compact volume of metrology data has been suggested (see Refs. 7–9 and references therein). It has been demonstrated^{8,9} that one-dimensional (1-D) surface slope metrology with super-polished x-ray mirrors can be treated as a result of a stochastic polishing process. In this case, autoregressive moving-average (ARMA) and an extension of ARMA to time-invariant linear filter (TILF) modeling^{10,11} allows a high degree of

confidence when fitting the metrology data with a limited number of parameters.

With the parameters of the determined model, the surface slope profiles of the prospective optics (before they are fabricated), made by the same vendor and technology, can be forecast. The forecast data are vital for reliable specification for optical fabrication, with evaluation from numerical simulation being necessary and sufficient for the required system performance, avoiding both over- and underspecification.^{12,13}

In this work, we continue investigations, started in Refs. 8–14; we consider surface slope metrology data stochastic and stationary and use a compact volume of metrology data to develop the TILF model¹⁵ and determine its parameters. We prove that the model thoroughly describes the surface topography over the entire spatial frequency range, important for the optical system performance. Otherwise, whole scale high-resolution measurements over the entire optical surface would be necessary. In addition to a significant time saving using the metrology data of a limited number of measurements, the model can be utilized to provide feedback to deterministic optical polishing.

This paper is organized as follows. First, we briefly review the mathematical fundamentals of 1-D ARMA modeling of topography of random rough surfaces (Sec. 2). In Sec. 3, we analyze a generalization of ARMA modeling with invertible time-invariant linear filters (InTILF). We have analytically shown that the suggested symmetric InTILF approximation has all advantages of one-sided AR and ARMA modeling, but it additionally has improved fitting

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accuracy. It is free of the causality problem, which can be thought of as a limitation of ARMA modeling of surface metrology data. We developed a new algorithm for identification of an optimal, symmetric InTILF model with a minimum number of parameters and smallest residual error for 1-D and 2-D data. As an extension to Ref. 14, where we verified the efficiency of the developed 1-D InTILF algorithm in application to modeling of a series of stochastic processes, which are generated with a known ARMA model, determined for surface slope data for a state-of-the-art x-ray mirror, in this paper, we discuss the generalization of the approach to 2-D InTILF modeling and the software that implements the method. The software allows the user to parametrize 1-D and 2-D stochastic data, to see stochastic patterns within it, and to generate statistically equivalent 1-D and 2-D data. To the best of our knowledge, the software is the first of its kind for 2-D stochastic surface metrology data. We verified the 2-D InTILF analysis via comparison with the analysis of the 1-D sections of the data. We discuss the results in Sec. 4. The paper concludes (Sec. 5) by summarizing the main concepts discussed throughout the paper and stating a plan for extending the suggested approach to using the suggested InTILF parametrization of surface metrology data to develop a surface quality indicator and use it to optimize surface polishing.

2 Brief Review of Statistical Modeling of 1-D Metrology Data

When a surface of a mirror is polished by a tool guided by its specific algorithm, the polishing process leaves a stochastic but unique pattern on the surface. The pattern is defined by the shape of the tools, and the character of its motion in the polishing process, which in turn is defined by the polishing algorithm and its parameters. The pattern is stochastic and cannot be reliably described using Fourier transform-based frequency analysis without giving consideration to statistical significance of the found spectrum. We used methods of statistical analysis suited for stochastic data to describe statistically significant characteristics of the stochastic pattern.

We postulate that irregular character of the surface topology of the polished mirror would be well represented by a stationary stochastic process of 1-D or 2-D depending on the data. The task then is to find a suitable mathematical model for the process. The model should be simple (with the smallest number of parameters), but it should describe the data with good precision. We measure the precision of the model by the difference between the computed autocovariance function (ACF) of the model and the actual sample ACF of the data.

We use linear models of stationary stochastic processes, namely autoregressive type models, moving-average models, and a combined ARMA model. In AR type models, the value of the measured surface height in a point of the discrete surface data is approximated using the values in the surrounding points.

As the result, the observed process X is modeled by the process Y

$$Y = (I - A) * X + \sigma * W, \quad (1)$$

where A is a linear operator, I is the identity operator, W is white noise random process, and σ^2 is the variance of the remaining error.

We also use the MA-type model Y (here B is a linear operator acting on white noise W)

$$Y = B * W, \quad (2)$$

especially for generation of similar processes and the combination of the two types of models:

$$Y = (I - A) * X + B * W. \quad (3)$$

Models of AR type turned out to be most suited for description of the surface slope data measured with high quality x-ray mirrors as surfaces under testing.⁸⁻¹⁴

In our previous work,^{10,11} we have described the construction of InTILF models of AR, MA, and ARMA types (symmetric ARMA models) and determination of its coefficients. We have shown that the optimal InTILF model of a given type (AR, MA, or ARMA) and given number of coefficients can be derived analytically using the ACF of the data. The best size of the filter is then determined with Akaike information criterion (AIC),^{16,17} which suggests at which size (number of coefficients) the extension of the model stops capturing more information.

In our previous work,^{10,11} we have shown that AR-type symmetric InTILF models precisely describe 1-D surface slope data obtained with high quality x-ray mirrors. We have demonstrated that InTILF models give

- good precision with the residual smaller than that of the ARMA models and
- good pattern capture qualified by a white noise residual, entirely devoid of pattern.

We have also shown that InTILF models with a small number of coefficients (5 to 12) are capable of successfully approximating surface metrology data. The criteria here is a small value (1% to 3% of the data variance) of the residual that is the difference between the original data and its representation via InTILF model.

3 Generalization InTILF Modeling to 2-D Case and BeatMark™ Software

In this section, we discuss generalization of stochastic modeling to analysis of 2-D surface metrology data. To the best of our knowledge, the extended InTILF suggested here is the first parsimonious descriptive model of 2-D invariant stochastic processes. We also first introduce an original software with the trademark name BeatMark,™ implementing the developed algorithms of InTILF modeling of 1-D and 2-D stochastic processes. The software has been developed in the course of our work on a related project supported by a NASA SBIR grant and now is available on the market.

3.1 Construction of 2-D InTILF

Autoregressive invertible time-invariant linear filter (AR InTILF) model Y of a given 2-D spatially invariant stochastic process X is determined by an operator A [similar to 1-D case given with Eq. (1) and considered in detail in Ref. 14]:

$$Y = (I - A) * X + \sigma * W, \quad (4)$$

where X and Y are 2-D processes as opposed to 1-D processes in Eq. (1) and W is a 2-D white noise random process.

A stochastic process is called spatially invariant if it is invariant under translations along the surface. The postulated spatial invariance of the stochastic data has an important corollary. We have shown (see Refs. 11 and 14) that just like in the case of time-invariant processes, the spatially invariant stochastic processes can be modeled with symmetrical optimal InTILF. This means that in the 1-D case, the array of the coefficients is symmetrical (even) about its center. Correspondingly, the 1-D filter A of size $(2N + 1)$ can be represented by a vector of $(2N + 1)$ coefficients. Because of the symmetry of the filter, the vector of coefficients is symmetrical about its center and thus the filter A of the size $(2N + 1)$ can be fully described by N nonzero coefficients (because the coefficients on the left side of the center are equal to the ones on the right and the central coefficient is zero).

In the 2-D case, the filter A is a matrix of coefficients and, as a matrix, it is axially symmetrical about both its central row and its central column.

We limit the 2-D model to a finite number of neighboring points within the finite masks, M is a rectangular area in the space of (k_1, k_2) coordinates, centered about the origin and limited by the absolute values of the coordinates by m_1 and m_2 correspondingly

$$M(m_1, m_2): |k_1|, |k_2| \leq (m_1, m_2). \quad (5)$$

The number of coefficients in the InTILF with the mask M is $(2m_1 + 1)(2m_2 + 1)$.

With accounting Eq. (5) in Eq. (4), the finite InTILF model Y can be expressed as

$$Y(t_1, t_2) = \sum_{(k_1, k_2) \in M} a(k_1, k_2) X(t_1 - k_1, t_2 - k_2). \quad (6)$$

The goal of the modeling is to find an optimal filter, determined by a set of coefficients

$A_{opt} = a(l_1, l_2)$, such that the model Y best fit the data X with minimum possible difference between X and its model Y :

$$A_{opt} = \arg \min(\|X - Y\|) = \arg \min(\|X - AX\|), \quad (7)$$

where $\arg \min[f(x)]$ is the value of x for which $f(x)$ attains its minimum. Here (l_1, l_2) refers to a coordinate point within the mask area M .

The optimal filter, represented as the set of coefficients $A_{opt} = a(l_1, l_2)$ can be related to the ACF of the data through a system of equations similar to the one we introduced and discussed in Ref. 14

$$q(k_1, k_2) = \sum_{(l_1, l_2) \in M} a(l_1, l_2) r_q(k_1, k_2, l_1, l_2). \quad (8)$$

In Eq. (8), q is the ACF of the data and r_q is a four-dimensional tensor defined through ACF.¹⁴

The system of equations Eq. (9) can be analytically solved to determine $A = a(l_1, l_2)$ using the approach applied in Ref. 14 to the case of 1-D InTILF modeling of the data of surface slope metrology with high quality x-ray mirrors.

Because ACF is symmetrical in x and y , it can be shown (similar to the consideration in Ref. 14) that an optimal 2-D InTILF is a matrix of size of M , its middle element $A(0,0)$ is equal to zero and

$$A(-l_1, -l_2) = A(-l_1, +l_2) = A(+l_1, -l_2) = A(+l_1, +l_2). \quad (9)$$

Such 2-D symmetrical filter of the size $(2m_1 + 1)$ by $(2m_2 + 1)$ is fully described by its $(m_1 + 1)(m_2 + 1) - 1$ coefficients.

The algorithm to determining the optimal InTILF model, outlined above, constitutes the computation method for evaluation of the coefficients A of the InTILF model of the given size. The algorithm was realized in MATLABTM code and tested on a few 2-D residual (after subtraction of the desired shape) surface height distributions measured with an interferometric microscope ZYGO NewViewTM-7300 available at the Advanced Light Source (ALS) X-Ray Optics Laboratory (XROL).^{18,19}

In Sec. 4, we present the results of the 2-D modeling and cross-check them with the 1-D data processing of the 1-D sections of the measured 2-D surface topography.

3.2 BeatMarkTM Software

The InTILF method developed for analyzing 1-D and 2-D stochastic processes was realized in BeatMarkTM software.²⁰ In particular, the software allows description of the stochastic properties of 1-D and 2-D surface topography with a small number of parameters. Based on the determined parameters (coefficients of the optimal InTILF), one can generate synthetic, statistically equivalent data needed, for example, for numerical simulation of optical system (beamline) performance and fabrication specification of x-ray optics before purchasing.^{12,13} The software is designed to process 1-D and 2-D data in formats of the main commercially offered surface profilometers and electron microscopes (Fig. 1). The demo version of the software as well as and sample processing are available upon request.

BeatMarkTM software has an intuitive, user-friendly GUI, allowing for a broad spectrum of functionalities including preprocessing of the data with detrending the profiles to remove the desired shape, trend, and periodical variation (cycling) of the residuals. The preprocessing step also allows the operator to exclude data points missed or corrupted in the metrology tests.

The major features of the developed InTILF modeling method and the dedicated BeatMarkTM software are as follows:

- representation of the 1-D and 2-D data with a small number of parameters that are the InTILF coefficients;
- generation of 2-D and 1-D data statistically equivalent to the original data;
- definition of Mirror Quality Metric through the InTILF analysis (implementation in BeatMarkTM software is in progress);
- operation with data from various metrology tools: interferometers, profilometers, long trace profilers, microscopes, such as, to list just a few, Ultra Surf, Zeiss CMM-Calypso, OptiTrace, Zygo Verifire,TM

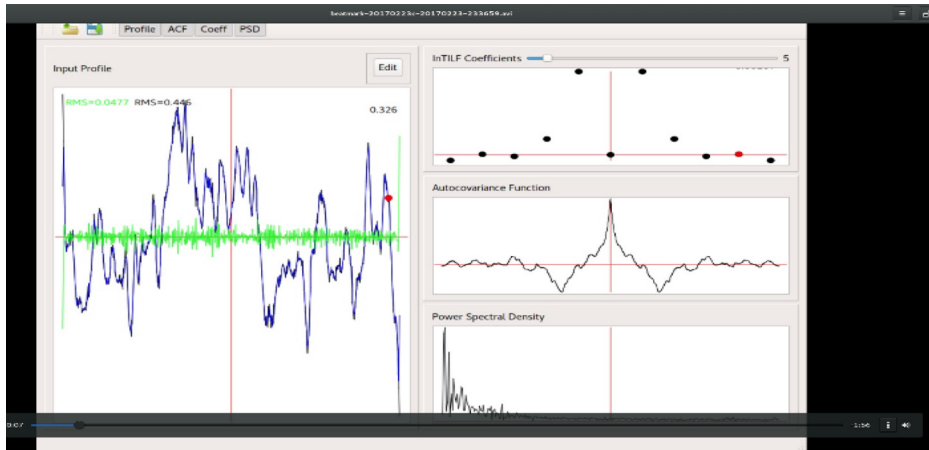


Fig. 1 BeatMark™ Software demonstration video (Video 1, AVI, 10396 KB [URL: <https://doi.org/10.1117/1.OE.58.8.084101.1>]).

DynaFiz,™ GPI,™ and ProTower interferometers, NewView™ series of interferometric microscopes, On Board Touch Probe, accepting a broad spectrum of data formats, such as csv, xyz, and Zygo’s dat for 1-D data, and xyz, tiff, giff, jpeg for 2-D data.

We also plan to use the analysis for feedback in polishing optimization.

4 Two-Dimensional INTILF Analysis of Results of Interferometric Microscope Metrology with High Quality X-Ray Mirrors

In this section, we present the results of application of 2-D InTILF analysis to 2-D surface topographies of two different mirrors (named here “mirror A” and “mirror B”) fabricated for x-ray applications by different vendors using different polishing technologies. The 2-D InTILF models for the mirrors were analytically identified using the BeatMark™ software. We show that the modeling provides:

- high confidence of modeling that is the magnitude of the root-mean-square (rms) variation of the residual difference between the data and the model is small compared with the rms height variation of the modeled topographies and

- high accuracy pattern capture, meaning that the topography of the residual is white-noise-like without a noticeable contribution of the pattern of the original data.

We also compare the InTILF models for these mirrors with significantly different surface topography and show that InTILF analysis can provide a new metric of mirror surface quality, which can potentially be used as a feedback in mirror fabrication.

4.1 InTILF Modeling of Mirror A

The goal of the modeling is to minimize the residual:

$$\text{Residual} = \|\text{Original Data} - \text{Modelled Data}\|$$

in order to increase the accuracy of the model (aka filtered data) as much as possible, in terms of the data variance with the norm in terms of L_2 (or rms).

Figure 2 shows the surface height distribution of the mirror A measured with an interferometric microscope ZYGO NewView™-7300 equipped with 2.5× objective with ×2.0 zoom. The microscope is available at the ALS XROL.^{18,19} Figure 2(a) shows the rectangular surface area of 1.06 mm ×

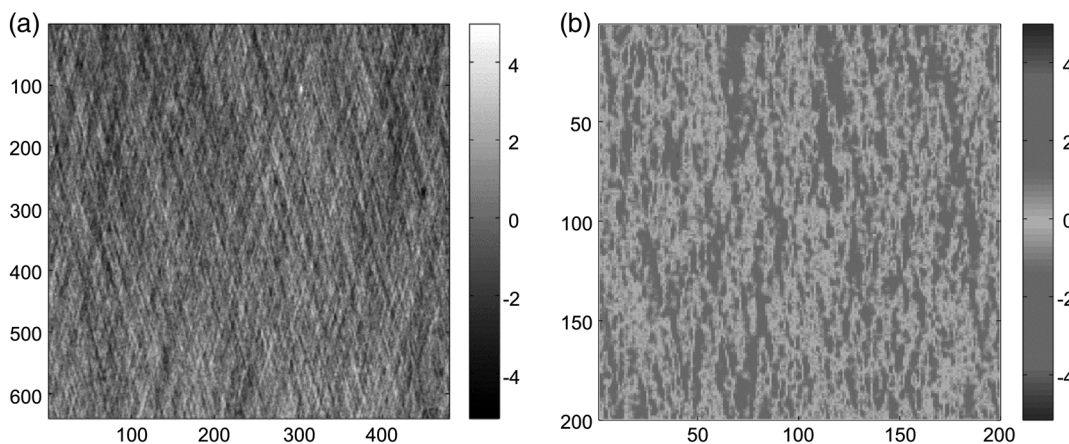


Fig. 2 (a) The measured 640 pixels × 480 pixels surface height distribution of mirror A with the rms variation of 6.75 Å and (b) its 200 × 200 pixels² subarea.

1.41 mm measured with the effective pixel size of $2.2 \mu\text{m}$ (the data set consists of 640×480 pixels²). The measured surface topography has a characteristic “diamond”-like pattern with rms variation of the surface height of 6.75 \AA . Figure 2(b) shows a subarea of 200×200 pixels² of the same height distribution.

Figure 3 shows the results of InTILF modeling of the $640 \text{ pixels} \times 480 \text{ pixels}$ height distribution of mirror A shown in Fig. 2(a). Figure 3(a) shows the topography reconstructed in the course of the 2-D InTILF modeling of the measured height distribution. Figure 3(b) shows the residual height distribution equal to the difference between the measured and the modeled data. The magnitude of the rms height variation of the residual is about 0.4 \AA , which is less than 6% of that of the measured topography. This result was obtained with the 2-D symmetrical InTILF of the size of 5×5 with only eight parameters.

During the optimization of the InTILF model, we varied the size of the filter and analyzed the change of the magnitude of the rms variation of the residual height distribution and its character aiming for the random, white noise-like one (see more detailed discussion in the Sec. 4.2, below). The similarity of the residual data [shown in Fig. 3(b)] to the white noise was shown by comparing its autocovariance with the flat and centrally peaked autocovariance of the white noise and using the independence criterium (the Diehard tests) for the residual data viewed as individual pixel-signals. The fact that the difference between the surface data and its InTILF model is devoid of pattern (the very definition of the white noise) is indicative of the model capturing all of the pattern present in the data. It also follows that the data lend itself to the description. Effectively this result (previously discussed for the 1-D InTILF models) shows the validity of the stochastic approach, and we consider it one of the central findings of this research. Further analysis (see Sec. 4.4) of the surface data coming from the different areas of the same mirror show the stability of the InTILF model throughout the surface, indicating that the model (and the process) is stationary.

In summary, the optimal 2-D symmetrical InTILF modeling of the mirror A topography has shown:

- the rms variation of the residual signal (the difference between the original data and the model) of less than 10% of that of the original data;

- very accurate and compact description of the stochastic properties of the 2-D surface topography with a model with only eight coefficients and white noise-like residual;
- the surface data can be viewed as stochastic because it is well described by the InTILF model as it captures the entire pattern of the signal, the difference between the model and the surface data being white noise, entirely devoid of pattern;
- the surface data can be viewed as invariant stochastic process because different areas of the same mirror are well described by the same InTILF model.

4.2 InTILF Modeling of Mirror B

Figure 4 shows the surface height distribution of the mirror B also measured with the ALS XROL interferometric microscope ZYGO NewView™-7300 equipped with $2.5\times$ objective with $\times 2.0$ zoom. Figure 4(a) shows the rectangular surface area of $1.06 \text{ mm} \times 1.41 \text{ mm}$ measured with the effective pixel size of $2.2 \mu\text{m}$ (the data set consists of $640 \text{ pixels} \times 480 \text{ pixels}$). In this case, the measured surface topography has a structure of horizontal “stripes” with the rms variation of the surface height of 1.74 \AA . Figure 4(b) shows a subarea of 100×100 pixels² of the same height distribution but with a better seen stripe pattern.

The optimal filter for this mirror was computed by BeatMark™ software and was found to be of the size of 3×15 . The modeled surface topography is shown in Fig. 5(a). In this experiment, the height data were preliminary normalized, and we show it in this form for better visualization. The rms variation of the residual signal (the difference between the original data and the model) shown in Fig. 5(b) is about 24% of that of the original data in Fig. 4(a). Note that the absolute value of the residual is much larger than the one found for mirror A. We find the difference instructive; it is discussed in Sec. 4.3.

4.3 Size of 2-D Filters

There is always a question of how to choose the best size for the filter. The answer depends on the stochastic properties of the data under treatment (in our case, the mirror surface height distribution). As mentioned above, our method allows

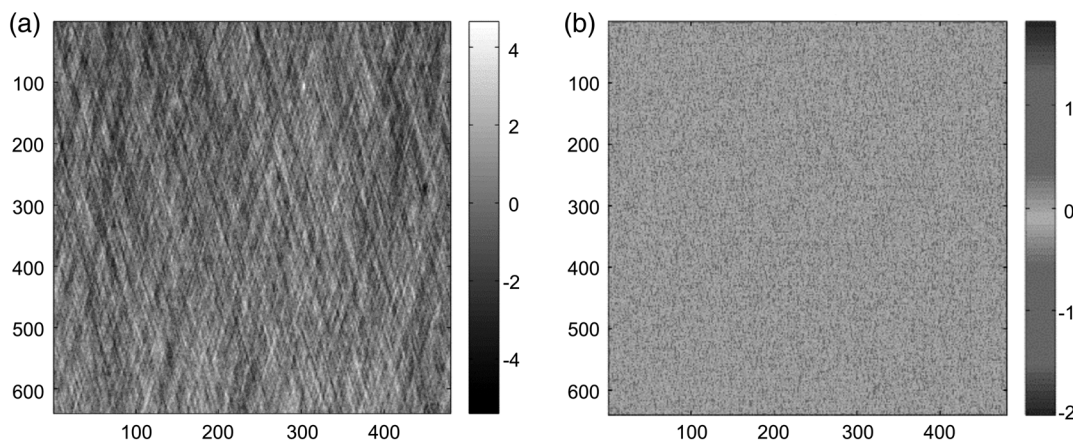


Fig. 3 (a) 2-D InTILF model of the mirror A surface height distribution (aka Y); (b) the 2-D residual X-Y.

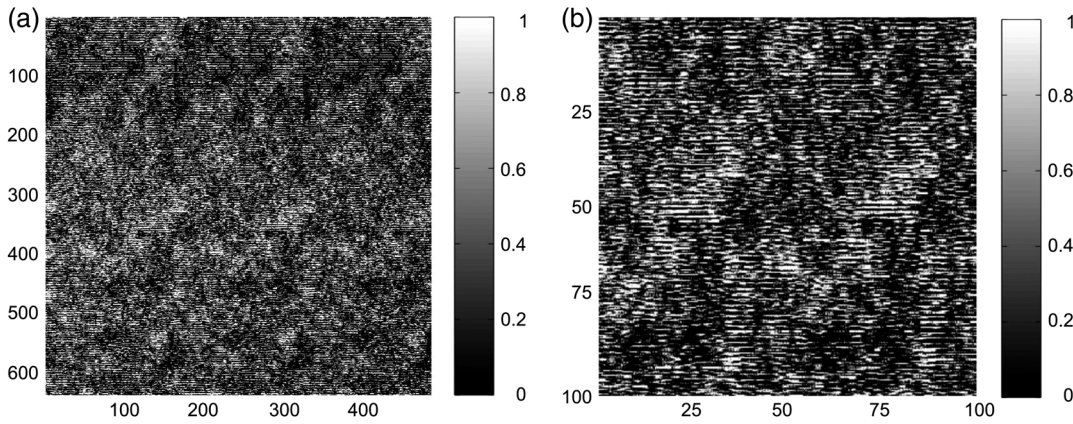


Fig. 4 (a) The measured 640 pixels \times 480 pixels surface height distribution of mirror B with rms variation of 1.74 Å and (b) its 100 \times 100 pixels² subarea.

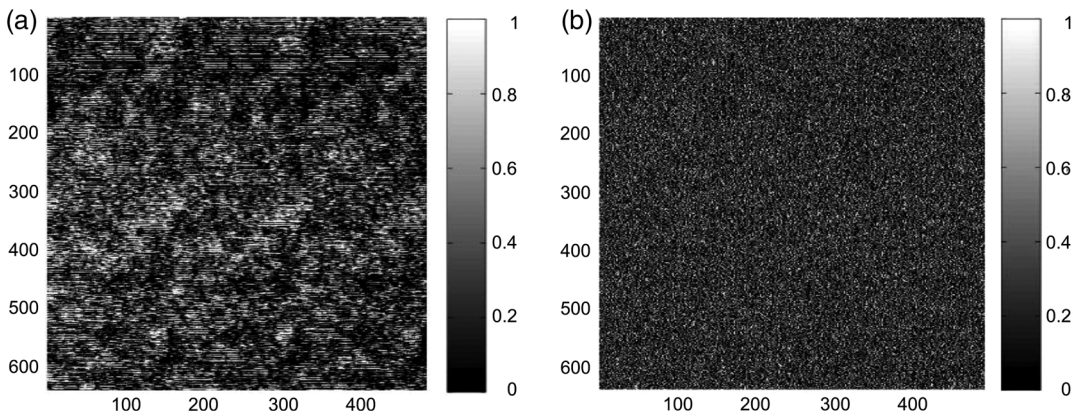


Fig. 5 (a) 2-D InTILF model of the mirror B surface height distribution (aka Y); (b) the 2-D residual X-Y.

analytic construction of an optimal filter for any given size and the larger the size, the better the approximation. However, in practice we see that the marginal improvements from an increase in filter size quickly diminish. AIC is used to determine the size of the optimal filter representing the best approximation accuracy return on its number of parameters as described in Refs. 16 and 17.

Below, we demonstrate that larger InTILF models are not materially different from those with the AIC determined optimal size.

Figure 6(a) shows the optimal 2-D filter for mirror B that corresponds to a matrix of coefficients with 15 columns and 3 rows. The optimal filter has strong “directionality,” meaning that the matrix of InTILF coefficients is longer along the horizontal direction. The directionality of the filter reflects the surface topography of mirror B with the pattern of horizontal strips.

One can ask what would happen to the residual (and the goodness of the fit with the model), if we do not stop increasing the size of the InTILF from 3 \times 15, but make the filter longer and/or wider. Figure 6(b) shows the middle row of coefficients of InTILFs of increasing horizontal length: 3 \times 15, 3 \times 17, and 3 \times 25. Note that, since the filter is symmetrical and the middle coefficient is zero, we only need 12 coefficients to define a middle row of the overall length of 25. When we find an InTILF of a prescribed size, we are not using the filter we found for the smaller size. The filters of

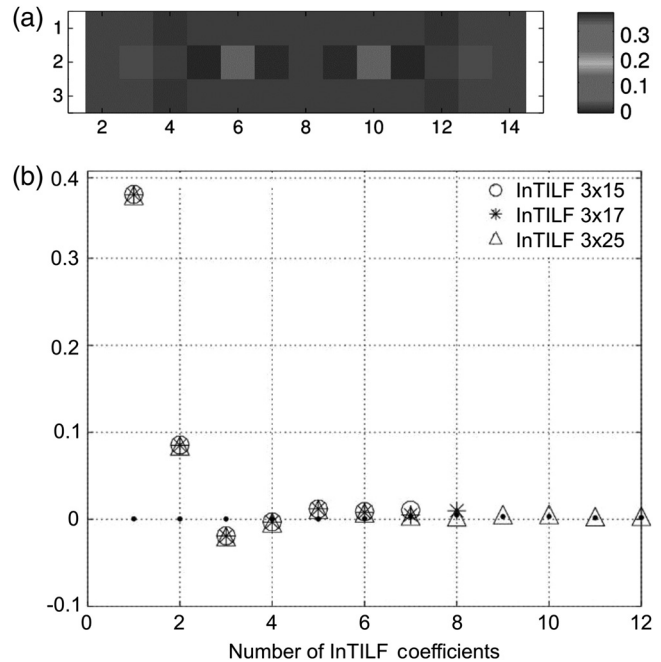


Fig. 6 (a) 2-D InTILF of 3 \times 15 elements optimal for mirror B; (b) middle row coefficients of InTILFs of 3 \times 15, 3 \times 17, and 3 \times 25 elements, evaluated for the mirror B topography. The coefficients along the right side of the filter’s mid-row are presented. The solid points show the standard deviation of the same coefficients of the three InTILFs.

different sizes are theoretically independent. In fact, if we increase the size of the filters from the minimal possible size of 3×3 to a given size $n \times m$, the coefficients of the InTILF fluctuate widely (over 50% difference in coefficients of the same number) while the filter's size increases from 3 to the optimal size. However, when the optimal size is reached, the material coefficients (the ones within the optimal size matrix) stabilize and no longer change with the increase of the filter size. The other coefficients outside of the optimal size matrix are smaller than some within the optimal size matrix.

In the case of mirror B, the mid-row coefficients are larger in value than the coefficients in other rows of the matrix [Fig. 6(a)]. We use the mid-row coefficients to illustrate the point, but the result is the same for any set of the InTILF coefficients.

Consider InTILFs A of different sizes $3 \times 15, 3 \times 17, \dots, 3 \times 25$. The middle (second) row of coefficients is a 1-D array of the size of 1×15 for the 3×15 case, 1×17 for the 3×17 case, and 1×25 for the 3×25 case. These coefficients are symmetrical about the middle of the row (because InTILF is symmetrical). Therefore, we may limit the comparison to the right half of the mid-row arrays and compare the arrays of $1 \times 7, 1 \times 8$, and 1×12 [Fig. 6(b)].

Figure 6 shows the behavior of these mid-row coefficients of InTILF for the three filters of which the first one is of the optimal size. Standard deviation for coefficients of the same number along the right side (the filter is symmetrical, so we are looking at the right side) of the mid-row of the InTILF matrix is also shown and it is found to be less than 0.1% of the value of the largest InTILF coefficient.

4.4 Stability of 2-D InTILF Analysis of Surface Height Topography of Uncorrelated Surface Areas

In order to verify the stability (uniqueness) of the InTILF modeling surface topography of a mirror with overall surface area much larger than the measured areas, we compare the models for uncorrelated (separated by much more distance than the linear size of the measured area) areas of the same

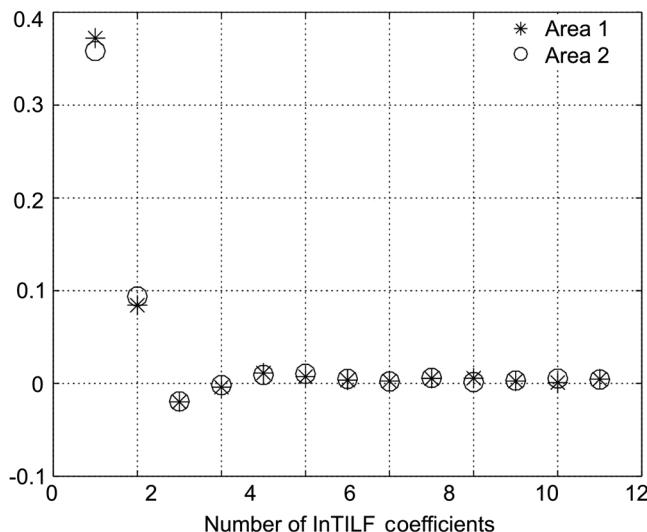


Fig. 7 Coefficients of the InTILF of 3×23 elements evaluated for the surface topography of two uncorrelated areas of mirror B. The coefficients along the right side of the filter's mid-row are shown.

mirror measured in the same manner. Such data were obtained in the interferometric microscope measurements with mirror B in a manner and experimental arrangement the same as described above in Sec. 4.2. Note that the stability of 1-D TILF modeling of surface slope distributions has been proved in Ref. 14.

Figure 7 shows the results of 2-D symmetrical InTILF modeling of metrology data corresponding to two uncorrelated surface areas of mirror B. For these data sets, the difference between the coefficients of the InTILF with the size of 3×23 is less than 4% of the numerical value of the average of coefficients themselves.

5 Discussion and Conclusion

In this work, we have continued the investigation started in Refs. 8–11, and 14 that will potentially allow us to analytically model 2-D surface topography of high-quality x-ray optics and characterize/parameterize the polishing capabilities of different vendors for x-ray optics. In the modeling, the treated data are considered to be stochastic and the statistical model called InTILF is used to best fit the data with a limited number of parameters. The classical work by Church and Berry²⁰ provides a comprehensive analysis of the problems and the limitations of reliable spectral estimations of measured surface profile data. The work also introduces treatment of the metrology surface as a stochastic random process described by an autoregressive (AR) model. The ideas are developed in Refs. 21 and 22. The surface description based on the AR model or the extended ARMA model provides a way to replace the spectral estimation problem by that of parameter estimation. We have suggested and demonstrated a generalization of 1-D InTILF approach^{10,11,14} to a symmetric 2-D InTILF approximation and have analytically shown that all the advantages of 1-D InTILF modeling are realized in the 2-D case, including the improved accuracy and efficiency of the fitting. In this context, the model is called accurate if it captures all of the pattern in the data, that is if the difference between the data and the model (residual) is white noise (devoid of pattern). This finding, namely, that InTILF models capture all of the pattern in the metrology data also definitively confirms the ultimate adequacy of the InTILF modeling and more generally the entire approach to surface data from ultraprecisions mirrors as stochastic.

We have developed a new analytical algorithm for identification of an optimal symmetric InTILF with a minimum number of parameters and the smallest residual error, which is applicable to 1-D and 2-D data arrays. The algorithm has been implemented in original BeatMarkTM software.²⁰ To characterize BeatMark in comparison with the existing applications providing statistical analysis of the 1-D data, we looked at the industry standard for 1-D stochastic analysis—EViews software. It is based on ARMA models. The 1-D InTILF model discussed in Ref. 10 is a development of the technique, gives better accuracy with fewer coefficients for the same data. We were not able to find any software generalizing the technique to 2-D data analysis. Neither do we know of ARMA-like theoretical analysis for 2-D stochastic data.

In this paper, we demonstrated the capabilities of BeatMark software in application to surface topography of two x-ray mirrors fabricated by different vendors using

different polishing technologies. The modeling has accurately described the stochastic patterns in the 2-D surface height distributions of these significantly different mirrors measured with an interferometric microscope.

We have also verified the uniqueness of the 2-D TILF parametrizations for the case of multiple 2-D surface height distributions measured over uncorrelated surface areas of the same mirror.

Based on the parametrization with the symmetrical 1-D and 2-D InTILF models, the expected surface profiles (in the slope and height domain) of prospective (before fabrication) x-ray optics can be reliably simulated (forecast) prior to purchasing. The simulated 1-D surface slope and 2-D height distributions of prospective optics can be used for estimations of the expected performance of new x-ray optical systems (beamlines, x-ray telescopes, etc.) as discussed in Refs. 12 and 13.

We should mention here one interesting observation that is waiting for a thorough explanation. In the examples of the metrology data treated in this paper, we have found that 2-D InTILF analysis appears to provide better accuracy as compared with 1-D processing of the same data. This result was not anticipated and needs to be confirmed by further analysis of 1-D and 2-D data from additional different mirrors; it is outside the scope of this paper and will be discussed in more detail elsewhere.

We are also working on an application of the developed methods and analytical algorithms to the optimization of machining parameters of polishing tools. For this application, we aim to construct a reliable surface quality indicator based on the BeatMark™ analysis that will be used as an optimization criterion in the feedback to polishing parameters optimization. In the field of ultraprecision surface polishing (and the polishing in general as far as we know about it), there is a large list of polishing parameters, such as

- shape of a polishing tool,
- path of the polishing process,
- rotation speed,
- pressure of the polishing tool on the workpiece,
- and a long list of other variable parameters.

The consensus in the field is that rotation speed and pressure are the most impactful among the easily changeable parameters of the polishing process. In our further work in progress, we are attempting to optimize the polishing process for the two parameters of rotation speed and pressure. The polishing parameter optimization work is not yet complete and is not covered in the publication. If successful, this could be a revolutionary impact in the polishing industry, increasing the efficacy of the processes and reducing both the metrology cycle (avoiding high-resolution metrology measurements over the entire optical surface) and fabrication cost of state-of-the-art x-ray mirrors.

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References

1. L. Assoufid et al., "Future metrology needs for synchrotron radiation grazing-incidence optics," *Nucl. Instrum. Methods A* **467–468**, 267–270 (2001).
2. K. Yamauchi et al., "Wave-optical analysis of sub-micron focusing of hard x-ray beams by reflective optics," *Proc. SPIE* **4782**, 271–276 (2002).
3. L. Samoylova et al., "Requirements on hard x-ray grazing incidence optics for European XFEL: analysis and simulation of wavefront transformations," *Proc. SPIE* **7360**, 73600E (2009).
4. S. Moeller et al., "Photon beamlines and diagnostics at LCLS," *Nucl. Instrum. Methods A* **635**(1-1S), S6–S11 (2011).
5. M. Idir and V. V. Yashchuk, "Optical and x-ray metrology," in: *X-ray Optics for BES Light Source Facilities, Report of the Basic Energy Sciences Workshop on X-ray Optics for BES Light Source Facilities*, D. Mills and H. Padmore, Co-Chairs, U.S. Department of Energy, Office of Science, Potomac, MD, pp. 44–55 (2013) http://science.energy.gov/~media/bes/pdf/reports/files/BES_XRay_Optics_rpt.pdf (accessed 10 February 2015).
6. J. A. Gaskin et al., "The x-ray surveyor mission: a concept study," *Proc. SPIE* **9601**, 96010J (2015).
7. V. V. Yashchuk et al., "Correlation analysis of surface slope metrology measurements of high-quality x-ray optics," *Proc. SPIE* **8848**, 88480I (2013).
8. Y. V. Yashchuk and V. V. Yashchuk, "Reliable before-fabrication forecasting of expected surface slope distributions for x-ray optics," *Opt. Eng.* **51**(4), 046501 (2012).
9. Y. V. Yashchuk and V. V. Yashchuk, "Reliable before-fabrication forecasting of expected surface slope distributions for x-ray optics," *Proc. SPIE* **8141**, 81410N (2011).
10. V. V. Yashchuk, Y. N. Tyurin, and A. N. Tyurina, "Application of the time-invariant linear filter approximation to parametrization of surface metrology with high-quality x-ray optics," *Opt. Eng.* **53**(8), 084102 (2014).
11. V. V. Yashchuk, Y. N. Tyurin, and A. N. Tyurina, "Application of time-invariant linear filter approximation to parameterization of one- and two-dimensional surface metrology with high quality x-ray optics," *Proc. SPIE* **8848**, 88480H (2013).
12. V. V. Yashchuk, L. Samoylova, and I. V. Kozhevnikov, "Specification of x-ray mirrors in terms of system performance: new twist to an old plot," *Opt. Eng.*, **54**(2), 025108 (2015).
13. V. V. Yashchuk, L. Samoylova, and I. V. Kozhevnikov, "Specification of x-ray mirrors in terms of system performance: a new twist to an old plot," *Proc. SPIE* **9209**, 92090F (2014).
14. V. V. Yashchuk, Y. N. Tyurin, and A. Y. Tyurina, "Modeling of surface metrology of state-of-the-art x-ray mirrors as a result of stochastic polishing process," *Opt. Eng.* **55**(7), 074106 (2016).
15. P. J. Brockwell and R. A. Davis, *Time Series: Theory and Methods*, 2nd ed., Springer, New York (2006).
16. H. Akaike, "A new look at the statistical model identification," *IEEE Trans. Autom. Control* **19**(6), 716–723 (1974).
17. V. V. Yashchuk et al., "A new x-ray optics laboratory (XROL) at the ALS: mission, arrangement, metrology capabilities, performance, and future plans," *Proc. SPIE* **9206**, 92060I (2014).

18. V. V. Yashchuk et al., "Advanced environmental control as a key component in the development of ultra-high accuracy ex situ metrology for x-ray optics," *Opt. Eng.* **54**(10), 104104 (2015).
19. A. Tyurina and P. S. Panov, "BeatMark demonstration and manual," 2018, <http://www.secondstaralgonumerix.com/presentations/2017/01/beatmark-20170423.webm>.
20. E. L. Church and H. C. Berry, "Spectral analysis of the finish of polished optical surfaces," *Wear* **83**, 189–201 (1982)
21. S. M. Kay, *Modern Spectral Estimation: Theory and Application*, Prentice Hall, Englewood Cliffs (1988).
22. V. V. Yashchuk et al., "Air convection noise of pencil-beam interferometer for long-trace profiler," *Proc. SPIE* **6317**, 63170D (2006).

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