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# Stochastic analysis of 1D and 2D surface topography of x-ray mirrors

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## ABSTRACT

The design and evaluation of the expected performance of new optical systems requires sophisticated and reliable information about the surface topography for planned optical elements before they are fabricated. The problem is especially complex in the case of x-ray optics, particularly for the X-ray Surveyor under development and other missions. Modern x-ray source facilities are reliant upon the availability of optics with unprecedented quality (surface slope accuracy  $< 0.1\mu\text{rad}$ ). 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 efficiency via comprehensive statistical analysis of a compact volume of metrology data. The data is considered stochastic and a new statistical model called Invertible Time Invariant Linear Filter (InTILF) is developed now for 2D surface profiles to provide compact description of the 2D data additionally to 1D data treated so far. The model captures faint patterns in the data and serves 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 forecast data is vital for reliable specification for optical fabrication, to be exactly adequate for the required system performance.

**Keywords:** surface metrology, time-invariant linear filter, TILF, autoregressive moving average, ARMA, power spectral density, PSD, fabrication tolerances, x-ray optics, surface slope profilometry topography

## 1. INTRODUCTION

The design and evaluation of the expected performance of new optical systems requires sophisticated and reliable information about the surface topography for planned optical elements before they are fabricated. The problem is especially severe in the case of x-ray optics for modern diffraction-limited-electron-ring and free-electron-laser x-ray source facilities, as well as x-ray astrophysics missions under development. The 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  $1\text{ nm}$ .<sup>1-5</sup> The unprecedented high angular resolution and throughput of future x-ray space observatories, such as the X-Ray Surveyor mission,<sup>6</sup> 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.<sup>7-9</sup> and references therein). It has been demonstrated<sup>8,9</sup> that one-dimensional (1D) 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<sup>10,11</sup> 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 (before fabrication) optics, made by the same vendor and technology, can be forecast. The forecast data is vital for reliable specification for optical fabrication, evaluated from numerical simulation to be necessary and sufficient for the required system performance, avoiding both over- and under-specification.<sup>12,13</sup>

In the present work, we continue investigations, started in Refs.<sup>8-14</sup> We consider surface slope metrology data stochastic and stationary and use a compact volume of metrology data to develop the model. The model can then be utilized to describe the entire volume of data and to provide feedback to deterministic optical polishing. We prove that the model developed based on a compact subset of metrology data describes the entire surface and a few smaller metrology experiments can substitute for time-consuming whole scale metrology measurements over the entire optical surface with the resolution required to cover the entire spatial frequency range, important for the optical system performance.

This paper is organized as follows. First, we briefly review the mathematical fundamentals of 1D 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 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 1D and 2D data. In Ref.,<sup>14</sup> we verified the efficiency of the developed 1D InTILF algorithm in application to modeling of a series of stochastic processes, which are generated with the known ARMA model, determined for surface slope data for a state-of-the-art x-ray mirror. In this paper (Sec.3), we discuss the generalization of the approach to 2D InTILF modelling and its implementation in original software BeatMark. The software allows the user to parametrize 1D and 2D stochastic data, to see stochastic patterns of it, and to generate statistically equivalent 1D and 2D data. To the best of our knowledge the software is the first of the kind for 2D stochastic data. In Sec.4, we present the results of successful application of 2D InTILF analysis to 2D surface topographies of two different mirrors fabricated for x-ray applications by different vendors using different polishing technologies. The 2D InTILF models for the mirrors were analytically identified using the BeatMark software. The paper concludes (Sec. 5) by summarizing the main concepts discussed throughout the paper and stating a plan for extending the developed 1D and 2D InTILF modeling and parametrization of surface topography data to optimization of surface polishing.

## 2. A BRIEF REVIEW OF STATISTICAL MODELING OF 1D METROLOGY DATA

When a surface of a mirror is treated by a polishing tool guided by its specific algorithm, the process leaves a unique pattern on the surface (or surface topography). The pattern is defined by the kind of the tools, the polishing algorithm and its parameters. In the case of state-of-the art x-ray mirrors, the pattern is very faint and cannot be reliably described using regular frequency analysis (such as Fourier transform) and may not be visible to the naked eye being still very important from the point of view of optical applications. We used methods of statistical analysis suited for stochastic data to find and describe the faint stochastic pattern.

Let us recall the statistical models developed for time series (statistical analysis of one dimensional stochastic data, developed primarily for prediction of financial markets), such as ARMA, which inspired the method. We would like to recall three useful models.<sup>15</sup> The models are designed to build the stochastic process  $Y$ , to best fit the original data  $X$ . Moving average model, MA, builds the stochastic process  $Y$  from white noise  $W$  by ‘bending’ it with a linear operator  $B$  in order to fit the original data  $X$ :

$$Y = B * W. \quad (1)$$

AR, auto regressive model, describes dependence (linear operator  $A$ ) between neighboring data points in the data  $X$

$$Y = A * (X - I), \quad (2)$$

where  $I$  is the identity operator).

ARMA is a combination model:

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

These models are inspired by needs for predictions, e.g., in econometrics based on observed 1D time series. We have modified these models to serve also for description of non-causal stochastic processes. The difference between predictive and descriptive models is in the physical relation between the data points treated by the model. The predictive models are mostly used for 1D time-series data and only the data points from the ‘past’ (or from one side) are used to predict with the model the next point. Descriptive models use all the neighboring points to describe the value at a given point. We call the descriptive (not predictive) models Invertible Time Invariant Linear Filters (InTILF).<sup>10,11,14</sup>

Let us consider the results of surface slope metrology of high quality x-ray optics as our original data,  $X$ . We use AR and ARMA type models to describe the data with a few parameters and MA type models for generation of statistically equivalent profiles. Note that AR models can be viewed as representation of the data as a linear combination of the data in the neighboring data points, or one way to describe a pattern in the data. MA type models are representations of the data as a linear transform of a white noise process (a stochastic process completely devoid of pattern). This ‘bending’ of the white noise can also be viewed as an alternative way to describe a pattern in the stochastic process.

In our previous work,<sup>10,11,14</sup> we have described the construction of InTILF models of AR, MA, and ARMA types (symmetric ARMA models) and determination of its coefficients. The optimal InTILF model of a given type (AR, MA, or ARMA) and given number of coefficient can be derived analytically using the auto covariance function (ACF) of the data. The best size of the filter can then be determined with Akaike information criterion (AIC),<sup>16,17</sup> which suggests at which size (number of coefficients) of the growth of the model in size does not capture more useful information.

We have also shown<sup>10,11,14</sup> that AR-type symmetric InTILF models precisely describe 1D metrology data obtained with high quality x-ray mirrors. We have demonstrated that InTILF models give

- good precision with the residual (that is the difference between the original data and its representation via InTILF model) smaller than that of the ARMA models, and
- good pattern capture that is the residual is a white noise, entirely devoid of pattern.

We have also shown that InTILF models with a small number of coefficients (5-12) are capable to successfully approximate the surface metrology data. The criteria here is a small (1- 3% of the data variance) value of the residual.

### 3. GENERALIZATION INTILF MODELING TO 2D CASE AND BEATMARK SOFTWARE

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

#### 3.1 2D InTILF construction

Auto Regressive Invertible Time Invariant Linear Filter (AR InTILF) model  $Y$  of a given two dimensional space invariant stochastic process  $X$  is determined by an operator  $A$  (compare with 1D case considered in Ref.<sup>14</sup>):

$$Y = A * X, \text{ where } A(\dots, \dots) = \{a(k_1, k_2), k_1, k_2 \in Z, a(0,0) = 0\} \quad (4)$$

A stochastic process is called space invariant if it is invariant under translations. The postulated spatial invariance of the stochastic data has an important corollary. We have shown that just like in case of time invariant processes, the space invariant stochastic processes can be modelled with symmetrical optimal InTILF. That means that in 1D case, the array of the coefficients is symmetrical about its center, and 1D symmetric filter  $A$  of the size  $(2N+1)$  is fully described by  $N$  non-zero coefficients because the coefficients on the left side of the filter are the same as the ones on the right.

Similarly, in 2D case the matrix of coefficients,  $A$ , is axially symmetrical about its central row and column with indexes  $x_0$  and  $y_0$ , respectively. The matrix has size  $(2x_0 - 1)(2y_0 - 1)$ , its middle element  $a(x_0, y_0)$  is equal to zero, and  $a(x_0 - k_1, y_0 - k_2) = a(x_0 - k_1, y_0 + k_2) = a(x_0 + k_1, y_0 - k_2) = a(x_0 + k_1, y_0 + k_2)$ . This 2D symmetrical filter  $A$  of the size  $(2x_0 - 1)(2y_0 - 1)$  is fully described by  $(x_0 y_0 - 1)$  coefficients. Physically, this means that we limit the model to a finite number of correlating neighboring points within the finite masks,  $M$ :

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

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

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

Where  $\arg \min(F(t))$  is the value of  $t$  for which  $F(t)$  attains its minimum.

The set of coefficients  $A_{opt} = a(l_1, l_2)$  can be related to the Auto Covariance Function of the data through a system of equations similar to the one we introduced and discussed in Ref.<sup>14</sup>:

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

In Eq. (8),  $q$  is the Auto Covariance Function (ACF) of the data and  $r_q$  is a four dimensional tensor defined through ACF.<sup>14</sup> The system of equations (8) can be analytically solved to find  $A_{opt} = a(l_1, l_2)$  using the approach applied in Ref.<sup>14</sup> to the case of 1D InTILF modeling of the data of surface slope metrology with high quality x-ray mirrors.

The algorithm to determining the optimal InTILF model, outlined above constitutes the computation method to find the coefficients  $A$  of the InTILF model of the given size. The algorithm was realized in Matlab code and tested on a few 2D residual (after subtraction of the desired shape) surface height distributions measured with an interferometric microscope ZYGO NewView<sup>TM</sup>-7300 available at the Advanced Light Source (ALS) X-Ray Optics Laboratory (XROL).<sup>18,19</sup>

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

### 3.2 BeatMark Software

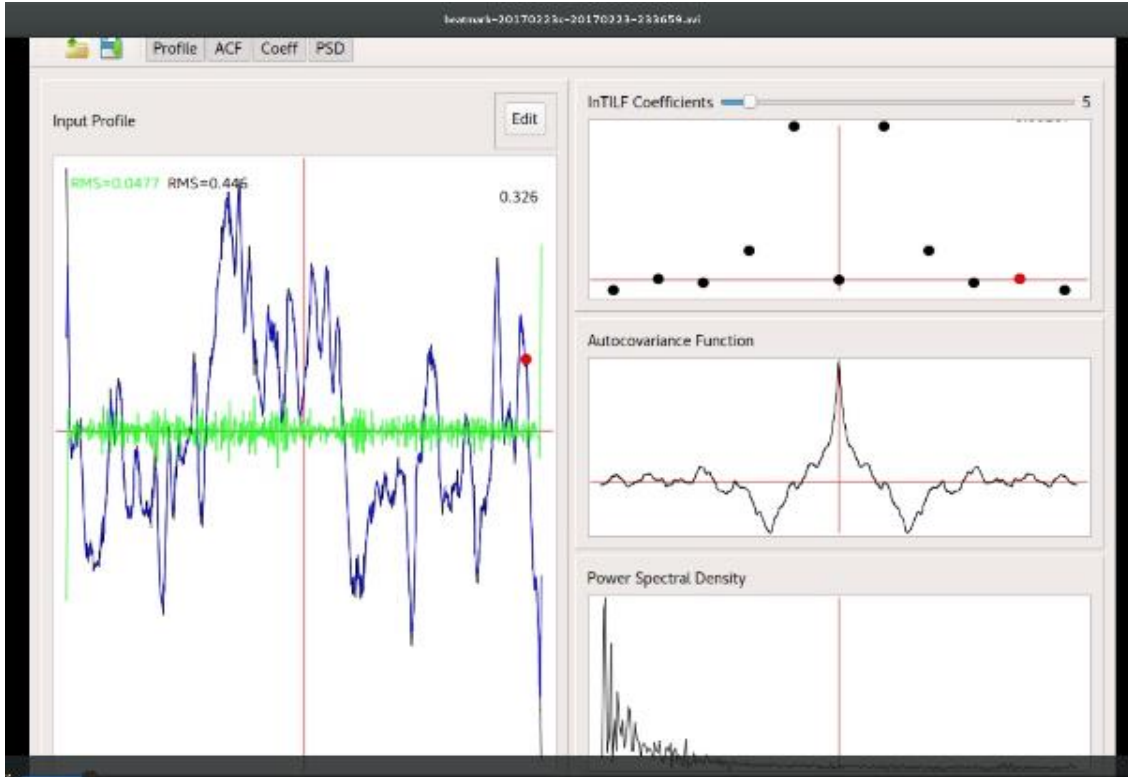
The developed InTILF method for analyzing 1D and 2D stochastic processes was realized in BeatMark software. In particular, the Software allows describing the statistical properties of 1D and 2D surface topography with a few parameters. Based on the determined parameters (coefficients of the optimal InTILF),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

BeatMark Software is going to be demonstrated in our presentation and we include a demo video in Video 1.

BeatMark software has an intuitive, user-friendly GUI, allowing for 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, removing corrupted and missed data points.

In summary, let us list the major features of the developed InTILF modeling method and the desiccated BeatMark software:

- representation of the 1D and 2D data with a small number of parameters that are the InTILF coefficients;
- generation of 2D and 1D data statistically equivalent to the original data;
- definition of Mirror Quality Metric through the InTILF analysis (implementation in BeatMark software is in progress);
- operation with data from various metrology tools: interferometers, profilometers, long trail profilers, microscopes, such as, to list just a few, Ultra Surf, Zeiss CMM-Calypso, OptiTrace, Zygo Ferifire, 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, zygo, and dat for 1D data, and tiff, giff, jpeg for 2D data;
- potentially, optimization of parameters of polishing processes (the work in this direction is in progress).



Video 1. BeatMark 1D Demo.<sup>20</sup>

#### 4. 2D INTILF ANALYSIS OF RESULTS OF MICROSCOPE METROLOGY WITH HIGH QUALITY X-RAY MIRRORS

In this section, we present the results of application of 2D InTILF analysis to 2D 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 2D InTILF models for the mirrors were analytically identified using the BeatMark software. We show that the modeling provides:

- high efficacy 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 to 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 1 presents 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.<sup>18,19</sup> The left-hand plot in Fig. 1 shows the rectangular surface area of 1.06 mm × 1.41 mm measured with the effective pixel

size of  $2.2 \mu\text{m}$  (the data set consists of  $640 \times 480 \text{ pixels}^2$ ). The measured surface topography has a characteristic ‘diamond’ like pattern with rms variation of the surface height of  $6.75 \text{ \AA}$ . The right-hand plot in Fig. 1 presents a sub-area of  $200 \times 200 \text{ pixels}^2$  of the same height distribution.

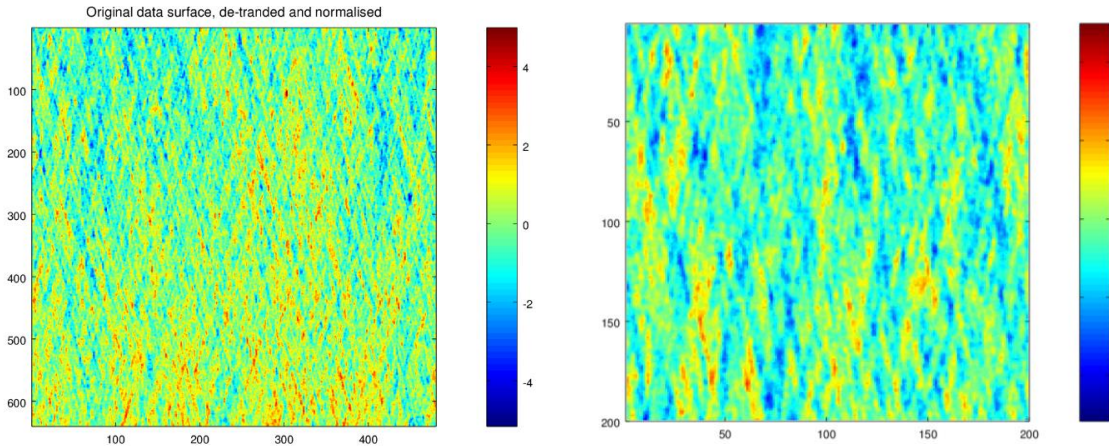


Figure 1:  $640 \text{ pixels} \times 480 \text{ pixels}$  surface height distribution of mirror A (the left-hand plot) with rms variation of  $6.75 \text{ \AA}$  and its  $200 \times 200 \text{ pixels}^2$  subarea (the right-hand plot).

Figure 2 depicts the results of InTILF modeling of the  $640 \text{ pixels} \times 480 \text{ pixels}$  height distribution of mirror A shown in Fig. 1, the left-hand plot. The left-hand plot in Fig. 2 presents the topography reconstructed in the course of the 2D InTILF modeling of the measured height distribution. The right-hand plot in Fig. 2 shows the residual height distribution equal to the difference between the measured and the filtered data. The magnitude of rms height variation of the residual is about  $0.4 \text{ \AA}$  that is less than 6% of that of the measured topography. This result was obtained with the 2D symmetrical InTILF of the size of  $5 \times 5$  with only 8 parameters.

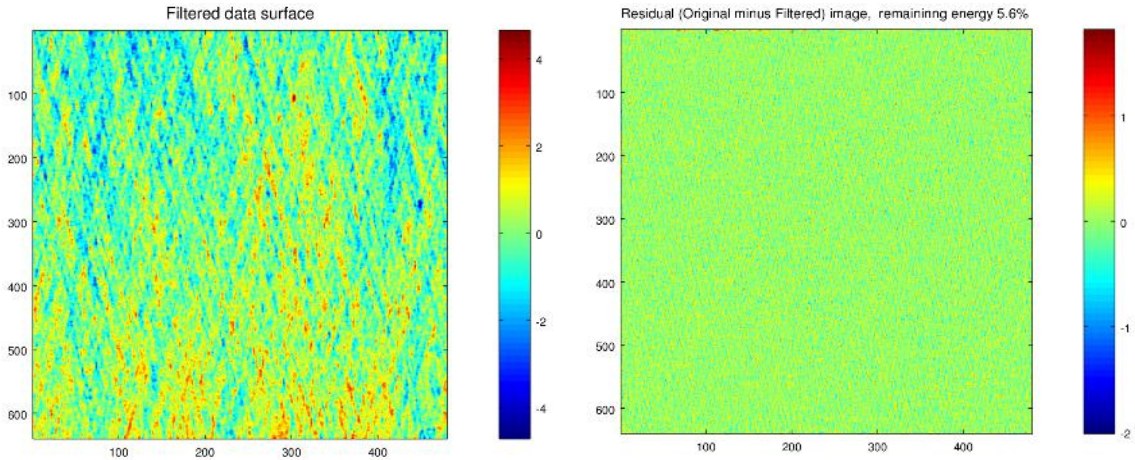


Figure 2: 2D InTILF model of the mirror A surface height distribution,  $Y$  (the left-hand plot) and the 2D residual  $X-Y$  (the left-hand plot).

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).

In summary, the optimal 2D symmetrical InTILF modeling has resulted in:

- 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 2D surface topography with a model with only 8 coefficients and white noise like residual.

#### 4.2 InTILF modeling of mirror B

Figure 3 presents the surface height distribution of the mirror B also measured with the ALS XROL interferometric microscope ZYGO NewView™-7300 equipped with 2.5× objective with ×2.0 zoom. Similar to Fig.2, the left-hand plot in Fig. 3 shows the rectangular surface area of 1.06 mm × 1.41 mm measured with the effective pixel size of 2.2 μm (the data set consists of 640 pixels × 480 pixels). In this case, the measured surface topography has a structure of horizontal ‘strips’ with rms variation of the surface height of 1.74 Å. The right-hand plot in Fig. 3 presents a sub-area of 200 × 200 pixels<sup>2</sup> of the same height distribution but with better seen strip pattern.

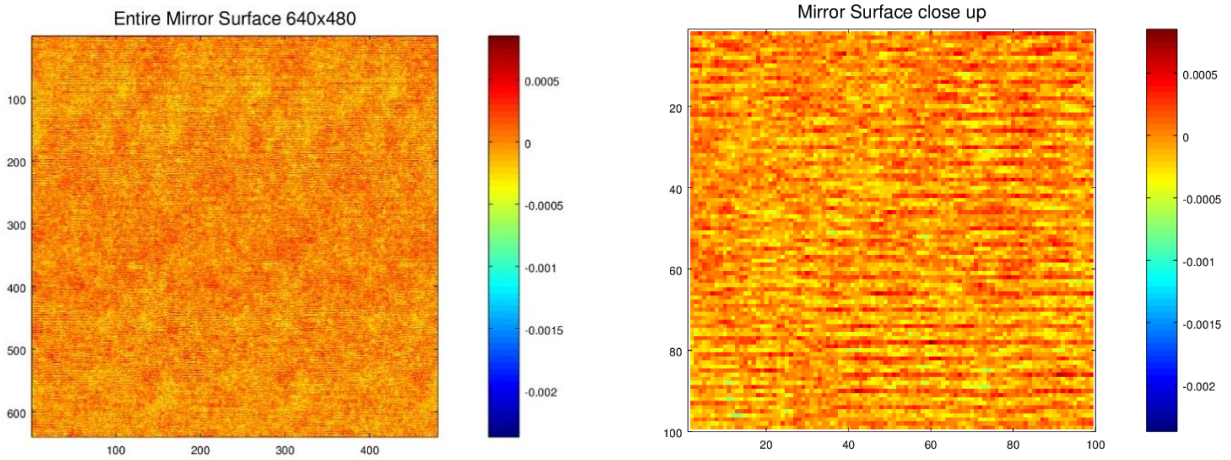


Figure 3: 640 pixels × 480 pixels surface height distribution of mirror B (the left-hand plot) with rms variation of 1.74 Å and its 100 x 100 pixels<sup>2</sup> subarea (the right-hand plot).

The optimal filter for this mirror was computed by BeatMark software and was found to be of the size 3 x 15. The filtered data is shown in Fig.4 (center). For comparison the original data is shown on the left. All three plots are shown in black and white to keep a simple scale (shown on the right) for visual comparison. In this experiment the data was first normalized and we show it in this form also for easier visual observation. The residual of the model was measured at 24%. Please note, that the value of the residual is much larger than the one found for mirror A. We find the difference instructive, it is discussed in Sect. 4.3.

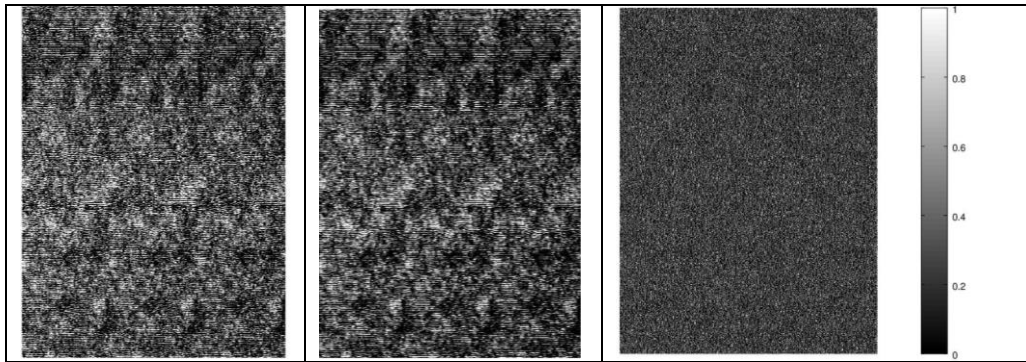


Figure 4: 2D InTILF model of the mirror B(X, left-hand plot) surface height distribution, Y (the central plot) and the 2D residual X-Y (the right-hand plot).

#### 4.3 Size of 2D 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 to analytically construct 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 diminishes. Akaike



information criterion 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.<sup>16,17</sup>

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

Figure 5 shows the optimal filter for mirror B. In this case, the optimal filter has strong ‘directionality,’ meaning that the matrix of InTILF coefficients is longer along the horizontal direction. The filter constitutes a matrix of coefficients with 15 columns and three rows. 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 at 3 x 15, but make the filter longer and/or wider. Figure 5 shows the middle row of coefficients of InTILFs of increasing horizontal length: 3x15, 3x17 and 3x25. 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 different sizes are theoretically independent. In fact, if we grow the size of the filters from the minimal possible size of 3 x 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 filters size grows 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 do no longer change with the growth 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. We will use the mid-row coefficients to illustrate the point. Consider InTILFs  $A$  of different sizes 3x15, 3x17, ..., 3x25. The middle (second) row of coefficients is a 1D array of the size of 1x15 for the 3x15 case, 1x17 for the 3x17 case, and 1x25 for the 3x25 case. These coefficients are symmetrical about the middle of the row (because InTILF is symmetrical). Therefore, we may limit the comparison to the right-hand half of the mid-row arrays and compare the arrays of 1x7, 1x8 and 1x12.

The right-hand plot in Fig. 5 illustrates the behavior of these mid-row coefficients of InTILF for the three filters of which the first one is of the optimal size. We chose the mid-row because in the case of this particular mirror all filters have largest coefficients concentrating in the mid-row, but we could have considered any set of InTILF coefficients. Standard deviation for coefficients of the same number along the right hand 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.

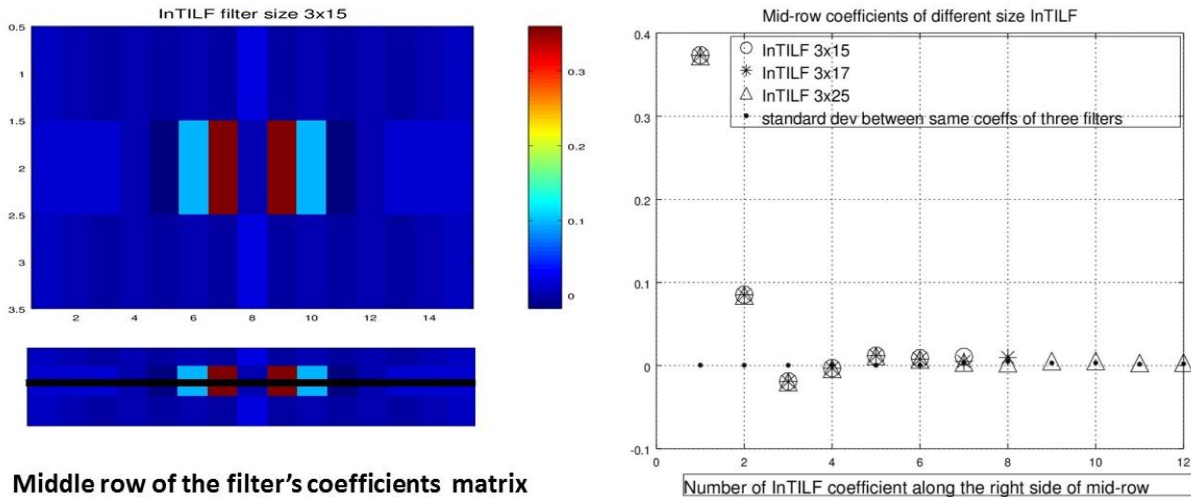


Figure 5: Optimal 2D InTILF for mirror B (left) with mid-row marked and the coefficients of mid-row of InTILFs of varying sizes (right).

#### 4.4 Stability of 2D 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 mirror measured in the same manner. Such data were obtained in the interferometric microscope measurements with mirror B in the manner and experimental arrangement the same as described above in Sec. 4.2. Note that stability of 1D TILF modeling of surface slope distributions has been proved in Ref.<sup>14</sup>

Figure 6 depicts the results of 2D symmetrical modeling of metrology data coming from two uncorrelated areas of mirror B. For these data sets, the difference between the InTILF coefficients is less than 4% of the numerical value of the average of coefficients themselves.

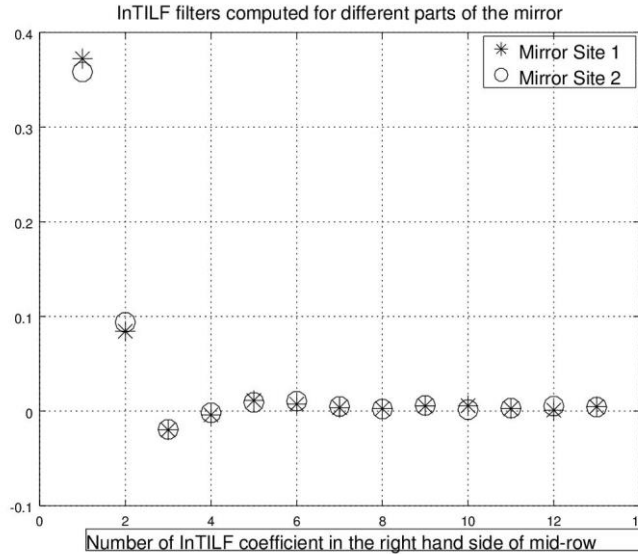


Figure 6: Mid-row of InTILF coefficients for two uncorrelated areas of mirror B.

## 5. DISCUSSION AND CONCLUSION

In this work, we have continued the investigation, started in Refs.<sup>8-11,14</sup> that will potentially allow us to analytically model 2D 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 is considered to be a result of a stochastic process and statistical model called Invertible Time Invariant Linear Filter is used to best fit the data with a limited number of parameters.

We have suggested and demonstrated a generalization of 1D InTILF approach<sup>10,11,14</sup> to a symmetric 2D InTILF approximation and have analytically shown that all the advantages of 1D InTILF modeling are realized in the 2D case, including the improved accuracy and efficiency of the fitting.

We have developed a new analytical algorithm for identification of an optimal symmetric InTILF with minimum number of parameters and smallest residual error and applicable to 1D and 2D data arrays. The algorithm has been implemented in original Beatmark<sup>TM</sup> software. In this paper, we have firstly introduced the software and demonstrated its capability and high efficiency on the examples of fitting 2D surface height distributions of two x-ray mirrors measured with an interferometric microscope ZYGO NewView<sup>TM</sup>-7300. The modeling has captured faint patterns in the metrology data and can serve as a quality metric and feedback to polishing processes, avoiding high resolution metrology measurements over the entire optical surface. We have also verified the uniqueness of the 2D TILF parametrizations for the case of multiple 2D surface height distributions measured over uncorrelated surface areas of the same mirror.

Based on the parametrization with the symmetrical 1D and 2D InTILF models, the expected surface profiles (in the slope and height domain) of prospective x-ray optics can be reliably simulated (forecast) prior to purchasing. The simulated 1D surface slope and 2D height distributions of prospective optics (before they are fabricated) can be used for

estimations of the expected performance of new x-ray optical systems (beamlines, x-ray telescopes, etc.) as discussed in Refs.<sup>12,13</sup>

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

We are also working on application of the developed methods and analytical algorithms to optimization of machining parameters of polishing tools. For this application, we 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. This work is in progress. If successful, this will revolutionary impact the polishing industry increasing the efficacy of the processes and reducing metrology cycle and fabrication cost of state-of-the-art x-ray mirrors.

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## REFERENCES

- [1] Assoufid, L., Hignette, O., Howells, M., Irick, S., Lammert, H., and Takacs, P., "Future metrology needs for synchrotron radiation grazing-incidence optics," *Nucl. Instrum. Methods A* 467-468, 267-70 (2001).
- [2] Yamauchi, K., Yumamura, K., Mimura, H., Sano, Y., Saito, A., Kanaoka, M., Endo, K., Souvorov, A., Yabashi, M., Tamasaku, K., Ishikawa, Y., and Mori, Y., "Wave-optical analysis of sub-micron focusing of hard x-ray beams by reflective optics," *Proc. SPIE* 4782, 271-276 (2002).
- [3] Samoylova, L., Sinn, H., Siewert, F., Mimura, H., Yamauchi, K., and Tschentscher, T., "Requirements on Hard X-ray Grazing Incidence Optics for European XFEL: Analysis and Simulation of Wavefront Transformations," *Proc. SPIE* 7360, 73600E-1-9 (2009).
- [4] Moeller, S., Arthur, J., Brachmann, A., Coffee, R., Decker, F.-J., Ding, Y., Dowell, D., Edstrom, S., Emma, P., Feng, Y., Fisher, A., Frisch, J., Galayda, J., Gilevich, S., Hastings, J., Hays, G., Hering, P., Huang, Z., Iverson, R., Krzywinski, J., Lewis, S., Loos, H., Messerschmidt, M., Miahnahri, A., Nuhn, H.-D., Ratner, D., Rzepiela, J., Schultz, D., Smith, T., Stefan, P., Tompkins, H., Turner, J., Welch, J., White, B., Wu, J., Yocky, G., Bionta, R., Ables, E., Abraham, B., Gardener, C., Fong, K., Friedrich, S., Hau-Riege, S., Kishiyama, K., McCarville, T., McMahon, D., McKernan, M., Ott, L., Pivovarov, M., Robinson, J., Ryutov, D., Shen, S., Soufli, R., and Pile, G., "Photon beamlines and diagnostics at LCLS," *Nucl. Instrum. and Methods A* 635(1-1S), S6-S11 (2011).
- [5] Idir, M., and Yashchuk, V. V., Co-Chairs, "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, pp. 44-55, U.S. Department of Energy, Office of Science, Potomac, MD (March 27-29, 2013); <[http://science.energy.gov/~media/bes/pdf/reports/files/BES\\_XRay\\_Optics\\_rpt.pdf](http://science.energy.gov/~media/bes/pdf/reports/files/BES_XRay_Optics_rpt.pdf)> accessed: February 10, 2015.
- [6] Gaskin, J. A., Weisskopf, M. C., Vikhlinin, A., et al., "The X-Ray Surveyor mission: A concept study," *Proc. SPIE* 9601, 96010J -1-14 (2015) [doi:10.1117/12.2190837].

- [7] Yashchuk, V. V., Artemiev, N. A., Lacey, I., and Merthe, D. J., "Correlation analysis of surface slope metrology measurements of high quality x-ray optics," Proc. SPIE 8848, 88480I-1-15 (2013) [doi: 10.1117/12.2024694].
- [8] Yashchuk, Y. V. and Yashchuk, V. V., "Reliable before-fabrication forecasting of expected surface slope distributions for x-ray optics," Opt. Eng. 51(4), 046501-1-15 (2012).
- [9] Yashchuk, Y. V. and Yashchuk, V. V., "Reliable before-fabrication forecasting of expected surface slope distributions for x-ray optics," Proc. SPIE 8141, 81410N-1-15 (2011).
- [10] Yashchuk, V. V., Tyurin, Y. N., and Tyurina, A. Y., "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] Yashchuk, V. V., Tyurin, Y. N., and Tyurina, A. Y., "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-1-13 (2013).
- [12] Yashchuk, V. V., Samoylova, L., and Kozhevnikov, I. V., "Specification of x-ray mirrors in terms of system performance: new twist to an old plot," Opt. Eng., 54(2), 025108 (2015).
- [13] Yashchuk, V. V., Samoylova, L., and Kozhevnikov, I. V., "Specification of x-ray mirrors in terms of system performance: A new twist to an old plot," Proc. SPIE 9209, 92090F/1-19 (2014).
- [14] V. V. Yashchuk, Y. N. Tyurin, 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 (Jul 15, 2016); doi:10.1117/1.OE.55.7.074106.
- [15] Brockwell, P. J. and Davis, R. A., [Time Series: Theory and Methods], Second Ed., Springer, New York (2006).
- [16] Akaike, H. (1973), "Information theory and an extension of the maximum likelihood principle", in Petrov, B.N.; Csáki, F., 2nd International Symposium on Information Theory, Tsahkadsor, Armenia, USSR, September 2-8, 1971, Budapest: Akadémiai Kiadó, pp. 267–281.
- [17] Akaike, H., "A new look at the statistical model identification", IEEE Transactions on Automatic Control, 19(6): 716–723 (1974), MR 0423716; doi:10.1109/TAC.1974.1100705.
- [18] Yashchuk, V. V., Artemiev, N. A., Lacey, I., McKinney, W. R., and Padmore, H. A., "A new x-ray optics laboratory (XROL) at the ALS: Mission, arrangement, metrology capabilities, performance, and future plans," Proc. SPIE 9206, 92060I -1-19 (2014) [doi:10.1117/12.2062042].
- [19] Yashchuk, V. V., Artemiev, N. A., Lacey, I., McKinney, W. R., and Padmore, H. A., "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), 104104/1-14 (2015); doi: 10.1117/1.OE.54.10.104104.
- [20] <http://www.secondstaralgonumerix.com/presentations/2017/01/beatmark-20170423.webm>