BeatMark Software to reduce the cost of x-ray mirrors
(Stochastic Analysis of Surface Metrology data)

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Second Star Algonumerix: http://www.secondstaralgonumerix.com
Overview

1. Our team and collaborators
2. Challenges in X-Ray mirror fabrication for Lynx X-Ray surveyor
3. What does the method solve?
4. Stochastic processes and InTILF analysis method
5. BeatMark software
6. 2D analysis method and 2D profile generation
7. Application to Polishing Optimization
8. Conclusions
Our Team has over 160 years combined experience in developing new mathematical methods into software

Research and Math

Anastasia Tyurina
CEO and CTO

Prof. Yury Tyurin
head of math development

Software team

Dr. Sergey Panov (Lead/physics)

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(licensing) (IP)

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Jacob Panov (NHS)

SECOND STAR SBIR-II NNX16CM09C
Second Star works with amazing collaborators

Polishing and metrology tools manufacturer

Dave Mohring (SBIR) Mike Bechtold (CEO)

Ed Fess (R&D head)

The best Metrology Lab in US

Dr Valeriy Yashchuk

Our collaborators think that if our technology works it will bring a revolution in polishing
Misha Gubarev
The project would not be where it is now without his expertize and support

https://www.gofundme.com/mikhail-v-gubarevs-memorial
The X-ray Surveyor requires X-ray mirrors to achieve large throughput with high angular resolution (0.5 arcsec) in order to avoid X-ray source confusion and background contamination. High angular resolution is critical for providing unique identifications of faint X-ray sources.

**Lynx - X-ray Surveyor Mission Concept*  

- 292-segmented shells nested into 42 individual mirror modules with overall size of 3 m outer diam.;
- ~ 0.2 arcsec root-mean-square (rms) slope error;
- $600$-$1000$ M estimated total cost of the mirrors

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What can our InTILF method do for X-ray mirror fabrication?

Decrease Fabrication Cost
- Faster and easier fabrication through simplified and standardized quality control
- Polishing optimization
- Enable medium size mirror manufacturers to join the X-ray mirror market

Increase Fabrication Speed
- Less metrology
- Less re-polishing

Increase Fabrication Predictability
- Metrics of quality and comparison of mirrors
- Generation of statistically equivalent metrology data
- Simulation of the X-ray mirror behavior within an X-ray optical system

see Opt Eng 54(2) 025108, Specification of x-ray mirrors in terms of system performance (Yashchuk, Samoylova, Kozhevnikov)
BeatMark software package is developed to improve the iterative polishing and metrology process

Step 1: InTILF analysis
BeatMark concept step 2: Optimization of polishing and metrology process

Polishing with parameters $P = (q_1, q_2, \ldots)$

Optimized Polishing

InTILF Quality Metric

Future: improved metrology

InTILF Parametrization

Data (multiple resolutions)

BeatMark

P1  P2  P3

P1  P2  P3

Metrology
Patterns left on the mirror by polishing process are bad for imaging

Yashchuk, Samoylova, and Kozhevnikov: Specification of x-ray mirrors in terms of system performance (0pt Eng. 54-2-025108-2015)

Simulated x-ray mirror profiles of the same surface height error rms

Simulated x-ray mirror imaging of a single point source (left) and its cross sections (right)

X-ray Mirror performance simulation

It is not just rms!
Logic of the project

• Periodic process – spectral characteristics (aka correlations) are surmised by Fourier transform

• Stochastic process – spectral characteristics (aka correlations) are surmised with statistical tools

• We think we can optimize the polishing and metrology process because we learned to characterize stochastic surface data with
  Invertible Time Invariant Linear Filters (InTILF)
InTILF method provides characterization of the surface based on small metrology samples.
BeatMark prototype software

UseCase1: 1d data to parameters (InTILF coefficient)

1-d profile data may be long ~ 1000 points

A small number of parameters (seen up to 12 coefficients)

InTILF Analysis

Use case 2

Characteristic Parameters

InTILF data generation

Generated 1-d profile data

UseCase3: 2D data to parameter Matrix

2D surface data may be large ~ 2000 X 2000 points

A small Matrix of parameters allow for 25 X 25

InTILF Analysis

UseCase4: generation of 2D data

2D data generation

Generated Data is statistically equivalent to the original data
BeatMark prototype demo
BeatMark software is the first to provide:

- statistical analysis of 2D metrology profiles (surface)
- generates 2D profiles statistically equivalent to a given 2D profile
Projects status

1) Software development
   • 1D application – commercial prototype is ready
   • 2D application developed for finding InTILF models
   • 2D surfaces generation
   • Format readers, a few developed, ongoing

2) Application to polishing
   • OptiPro completed two polishing data collections
   • LBNL received re-measured one set of samples is re-measuring the other
   • Second Star is analyzed the first data collection the results will be presented
   • The team is discussing the analysis of the second data collect
BeatMark-2D analysis

BeatMark assessment of Mirror A:
InTILF 5x5 matrix
Residual < 1 %

BeatMark assessment of Mirror B:
InTILF = 3 x15 matrix
Residual = 23%
2D InTILF analysis of Mirror B

Original data (mirror B)  Filtered data = InTILF Model  Residual is White noise like
2D InTILF analysis is stable along the mirror

Good agreement of InTILF coefficients along the mid-row of InTILF matrices computed for metrology data from Site 1 and Site 2. The difference is < 3.5% value
Generation of 2D InTILF model (use case 4)

Original data

Generated data

Non-isotropic 2D field

ACF of the data

Simulations demonstrate high spectral fidelity

Simulations demonstrate high spectral fidelity
Data Collection 1:

10 Samples Polished with different polishing parameters

Two polishing parameters:
• speed (in rpm) and
• pressure (in mm)
were varied around perceived optimal values of
• 600 rpm
• 2 mm.

Application of BeatMark to Polishing Optimization (BeatMark step 2, slide 9)
Samples were measured with different instruments

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Measured by</th>
<th>Dimension – 1D or 2D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interferometer</td>
<td>OptiPro</td>
<td>2</td>
</tr>
<tr>
<td>UltraSurf</td>
<td>OptiPro</td>
<td>2</td>
</tr>
<tr>
<td>Profilometer</td>
<td>OptiPro</td>
<td>1</td>
</tr>
<tr>
<td>New View</td>
<td>OptiPro</td>
<td>2 (at higher resolution)</td>
</tr>
<tr>
<td>Interferometer</td>
<td>LBNL</td>
<td>2</td>
</tr>
</tbody>
</table>
Samples measured by different Instruments

For the rough analysis that we did in this first experiment we saw no material differences in analysis results. This will have to be monitored when we progress toward finer experiments.
1D profiles for all instruments

OptiPro Interferometer

OptiPro UltraSurf
All Sections as measured by LBNL

These are sections of the mirror samples (we checked that they are uniform about the angle)

Pixels 1 - 600

Mirror Height
Two methods of mirror quality comparison

- Shape analysis (large effects)
- Stochastic analysis (finer effects)
Method 1: Sape analysis. “Basic” vectors (aka Characteristic vectors)

Express all other differences deltas as “vectors” in the space of functions as a linear combination of “vectors” V1 and V2:
Method 1: Vector decomposition with basic vectors

Method 1 shows good potential in optimizing for polishing parameter ‘pressure’. The dependence of a sample shape on pressure appears “linear” in its magnitude. Not so for the rotation speed.

\[ \delta(k) = a(k) \times V1 + b(k) \times V2 \]

Matrices \( A = \{a(k)\} \) and \( B = \{b(k)\} \)

Pressure in mm
Method 2: InTILF-Quality indicator computed for OptiPro and LBNL data

Quality Indicator, based on InTILF was computed for samples using good quality central segments.

The data is numerically different (for sample measurement errors related issues), but qualitatively points to the same optimal sample 1.
Method 2: InTILF-Quality indicator computed for OptiPro and LBNL data

Quality Indicator, based on InTILF was computed for samples using good quality central segments.

The data is numerically different (for sample size related normalization issues), but qualitatively points to the same optimal sample 1.
Design of data collection 2

Recall experiment 1: Samples Polished with different polishing parameters

Two parameters: speed (in rpm) and pressure (in mm) were varied around perceived optimal values of 600 rpm and 2 mm.

10 samples

Test 2 samples polishing parameters and sample numbers

30 samples
To study non-linear dependence on speed
Conclusions:

BeatMark software package – the prototype implementation of InTILF

• characterizes mirror surfaces with a small number of parameters
• needs only modest amount of metrology data to characterize the entire surface
• generates simulated ‘metrology’ profiles statistically equivalent to the original profile (1D or 2D)

We are working on using the BeatMark (and InTILF) to:

• provide the surface quality assessment through a quality metric
• look to work on validation of q-metrics with XFEL
• lead to significant improvements in polishing

Possible development of InTILF method may lead to comprehensive analysis of metrology data taken by instruments with different Modulation Transfer Function.
Acknowledgments

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Thank you for your attention!

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Appendix
InTILF analysis of mirror B

Height distribution of the mirror B measured with the ALS XROL interferometric microscope ZYGO NewView™-7300 equipped with 2.5× objective with ×2.0 zoom.

Surface area 1.06 mm × 1.41 mm
effective pixel size of 2.2 μm (640 pixels × 480 pixels)

Measured surface topography has a structure of horizontal ‘strips’ with rms variation of the surface height of 1.74 Å.
BeatMark-2D assessment of two mirrors

BeatMark assessment of Mirror A:
InTILF 5x5 matrix
Residual < 1 %

BeatMark assessment of Mirror B:
InTILF = 3 x15 matrix
Residual = 23 %

How many parameters do fully describe a mirror?
A: 25  B: 45
Construction of 2D InTILF model, mirror A

1. Start with 2D data
2. Compute Auto Covariance Function
3. Compute InTILF (2D matrix)
2D InTILF analysis of Mirror A

**Mirror A data:** height distribution 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. 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 µm (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 6.75Å.

25 parameters fully describe the mirror A

**2D InTILF model accuracy:** residual rms ~1%
Stationary Random Process (SRP) and its Auto-covariance function (ACF) in 2D

Natural extension to 2D:

\[
SPR: \ x(t_1, t_2): Z^2 \rightarrow R^2 \ & \ E(X(t_1 + h_1, t_2 + h_2) * X(t_1, t_2)) = E(x(h_1, h_2)X(0)), \ \forall h = (h_1, h_2) \Rightarrow introduce ACF \ Q_x(h) = Q_x(h_1, h_2) = E\{x(t_1 + h_1, t_2 + h_2)x(t_1, t_2)\}.
\]

In 2D b) means that for any natural number \( m \), any \( m \) integers \( h_1, \ldots, h_m \) and any real numbers \( z_1, \ldots, z_m \)

\[
\sum_{i=1}^{m} q(h_i - h_j)z_iz_j \geq 0
\]

ACF \( Q(.,.) \) of a stationary random process on a lattice \( Z^2 \) can be represented as:

\[
q(h_1, h_2) = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{ih_1 x_1 + ih_2 x_2} \mu(dx_1, dx_2), (h_1, h_2) \in Z^2
\]
Polishing optimization idea

• Ideal mirror surface deviates from its form very slightly and in an absolutely random manner – white noise random

• White noise is an absolutely random process completely devoid of pattern

• A polishing tool might leave a pattern (correlations) on a mirror. If it is detected and characterized, the mirror can be improved by optimizing polishing parameters.

• Our task is to detect and characterize the pattern

We are in search of the stochastic pattern