Advancements in X-ray Wavefront Sensing and At-wavelength Metrology at the Advanced Photon Source

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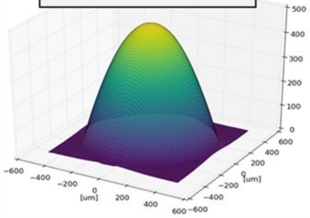
PhotonMEADOW23

Sep. 12-14, 2023

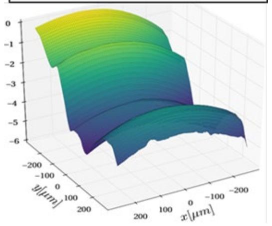
WAVEFRONT SENSING TECHNIQUES

Beamline X-ray optics characterization and diagnostics at the APS

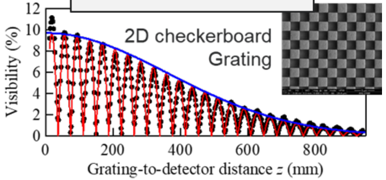
Thickness profile of a Be lens



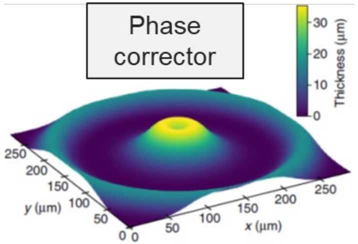
Distorted wavefront downstream of a mirror



Coherence function measurement



Phase corrector



X-ray wavefront sensing tools

- Grating interferometry
- Speckle tracking
- Coded-mask-based technique

Apply

Optics/beam characterization

- At-wavelength metrology
- Wavefront sensing
- Coherence measurements

Support **Extend**

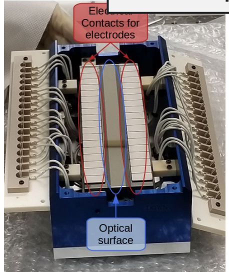
Optics development

- Wavefront-preserving optics
- Adaptive optics
- Phase corrector

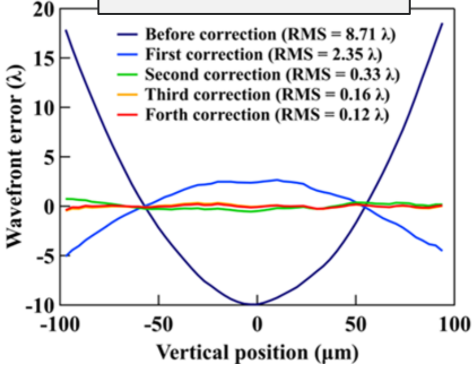
Beamline diagnostic

- Wavefront and coherence monitor
- Beamline control and optimization

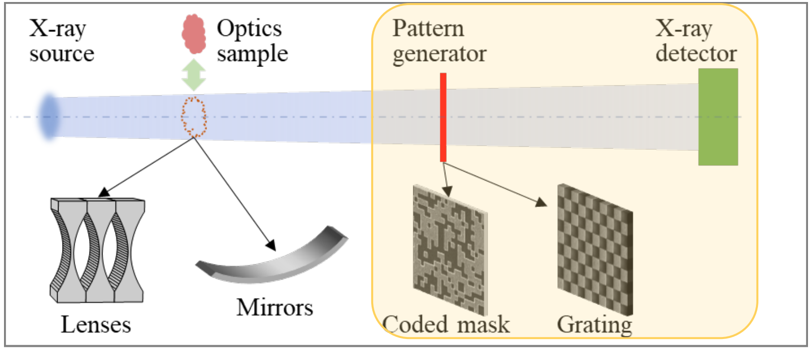
Adaptive optics



Wavefront correction

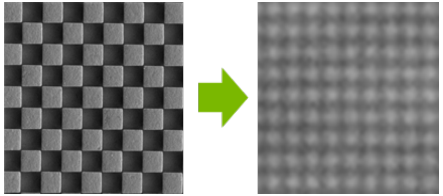


WAVEFRONT SENSING TECHNIQUES



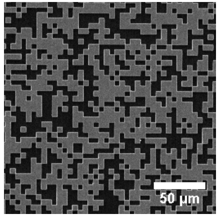
Grating interferometry

- Phase or absorption gratings with periodic pattern
- Fourier-based analysis for grating pattern shifts



Harold H. Wen et al. Opt Lett. 35, 1932 (2010)
W. Grizolli, et al. Proc. SPIE 10385, 1038502 (2017)
W. Grizolli, et al., AIP Conference Proceedings, 2054, 060017 (2019)

Coded-mask-based Wavefront Sensor

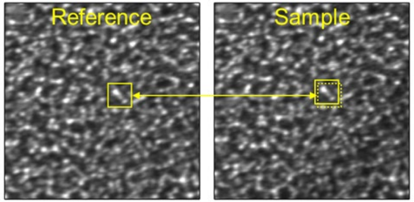


- Designed non-periodic pattern
- Ultra-high-contrast >30%
- Pre-knowledge of the pattern
- High spatial resolution
- High phase sensitivity
- Better noise robustness
- Flexible and easy to use

X. Shi, et al., US patent US20220265231 (2022).
Z. Qiao, et al., Appl. Phys Lett. 119, 011105 (2021).
Z. Qiao, et al., *Optica* 9, 391 (2022).
Z. Qiao, et al., Opt. Express 28, 33053 (2020).
Z. Qiao, et al., Proc. SPIE 11492, 114920O (2020).
Z. Qiao, et al., J. Imaging 7, 249 (2021).
X. Shi, et. al, Proc. SPIE 12240, 122400H (2022).

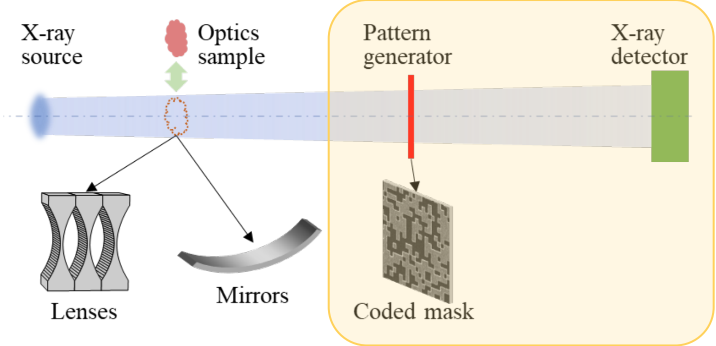
Speckle tracking

- Speckle generator (sandpaper, membrane filters) with completely random pattern
- Based on near-field speckle pattern shifting

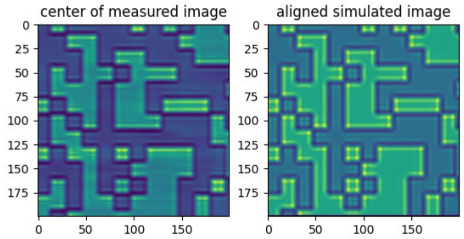


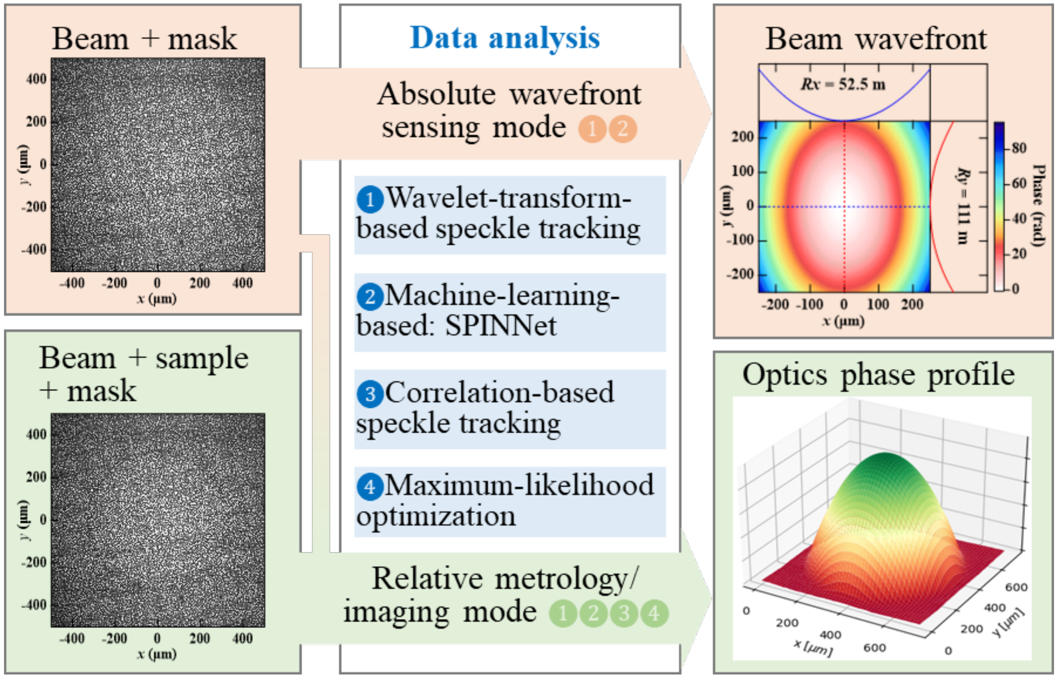
S. Berujon et al., J Synchrotron Radiat, 27, 284 (2020)
S. Berujon et al., J Synchrotron Radiat, 27, 293 (2020)

CODED-MASK-BASED WAVEFRONT SENSOR DESIGN



- **Two operation modes**
  - Relative metrology/imaging mode (two measured images)
  - Absolute wavefront sensing mode (simulated reference images)





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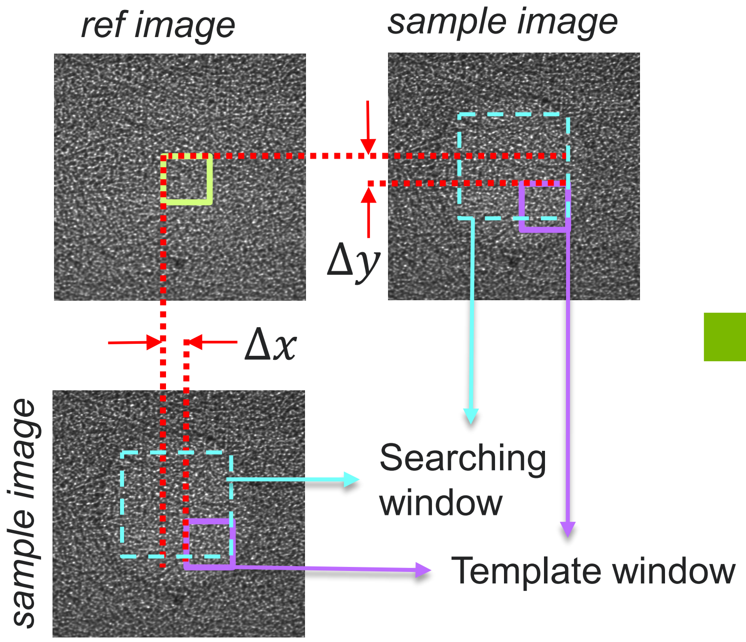
CODED-MASK-BASED WAVEFRONT SENSING

Single-shot measurements

- **Data analysis methods:**
  - Correlation-based speckle tracking



Pixel-by-pixel analysis

Find Δx and Δy to maximize c(x, y)

c(x, y) = cross-correlation(,)

CODED-MASK-BASED WAVEFRONT SENSING

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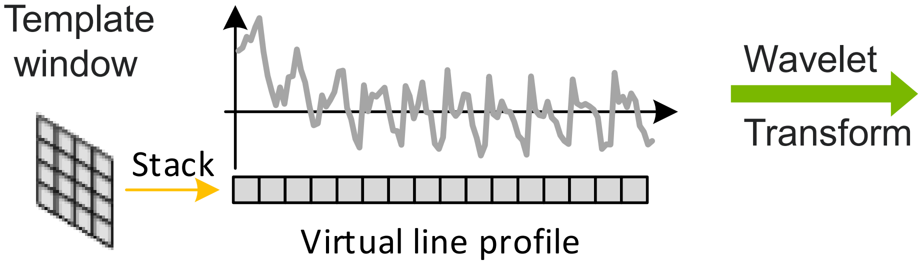
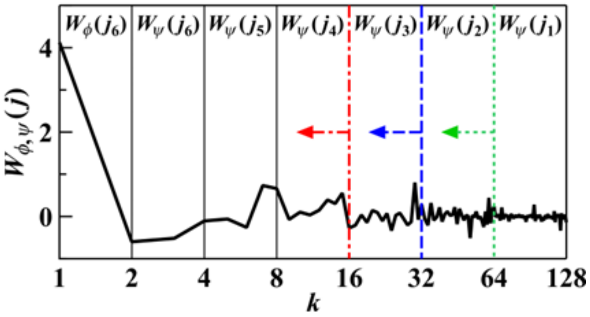
  - Correlation-based speckle tracking
  - **Wavelet-transform-based speckle tracking**

    Z. Qiao, et al., Proc. SPIE 11492, 114920O (2020).

$$I^{s/r}(t) = \frac{1}{\sqrt{n}} \sum_k W_\phi^{s/r}(j_m, k)\phi_{j_m,k}(t) + \frac{1}{\sqrt{n}} \sum_{j=j_1}^{j_m} \sum_k W_\psi^{s/r}(j, k)\psi_{j,k}(t)$$





Find Δx and Δy to minimize Euclidean distance square

$$r = \sum \left| W_{\phi,s} - W_{\phi,r} \right|^2$$

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CODED-MASK-BASED WAVEFRONT SENSING

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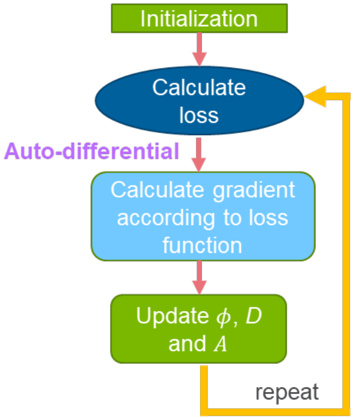
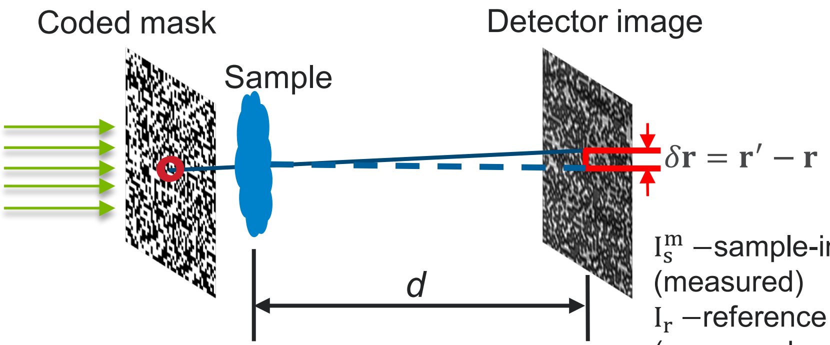
    Z. Qiao, et al., Proc. SPIE 11492, 114920O (2020).
  - **Maximum-likelihood optimization**

    Z. Qiao, et al., Appl. Phys Lett. 119, 011105 (2021).





$\mathrm{I_s^m}$ –sample-in image (measured)

$\mathrm{I_r}$ –reference image (measured or simulated)

$$I_s(\mathbf{r}') = \frac{A(\mathbf{r})}{C(\mathbf{r})}\{\bar{I}_r(\mathbf{r}) + D(\mathbf{r})[I_r(\mathbf{r}) - \bar{I}_r(\mathbf{r})]\}$$

Loss function minimization

$$\boxed{\sum[I_s - I_s^m \log(I_s)] + \alpha TV\left(||D||_2\right) + \alpha TV\left(||A||_2\right) + \beta TV(||\phi||_2)}$$

TV – total variation

Pixel wise optimization

Sample

Absorption: A

Phase: ϕ

Dark-field: D

CODED-MASK-BASED WAVEFRONT SENSING

Single-shot measurements

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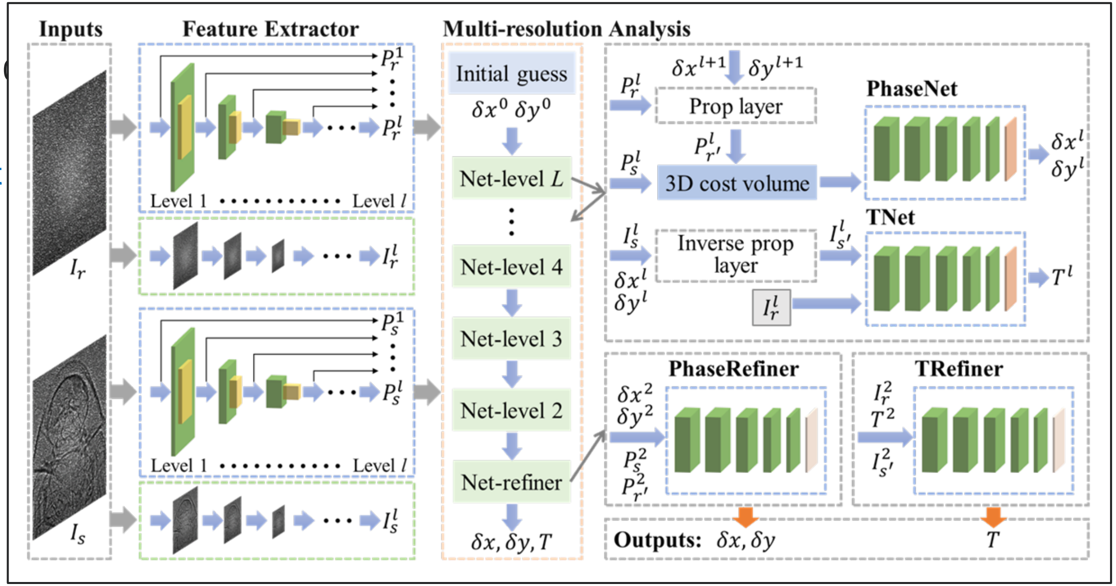
    Z. Qiao, et al., Proc. SPIE 11492, 114920O (2020).
  - Maximum-likelihood optimization

    Z. Qiao, et al., Appl. Phys Lett. 119, 0111(
  - **Machine-learning-based method:**

    SPINNet (Speckle-based Phase-contrast

    Imaging Neural Network)

    Z. Qiao, et al., Optica 9, 391 (2022).



CODED-MASK-BASED WAVEFRONT SENSING

Single-shot measurements

- **Data analysis methods:**
  - Correlation-based speckle tracking
  - Wavelet-transform-based speckle tracking

    Z. Qiao, et al., Proc. SPIE 11492, 114920O (2020).
  - Maximum-likelihood optimization

    Z. Qiao, et al., Appl. Phys Lett. 119, 011105 (2021).
  - **Machine-learning-based method:**

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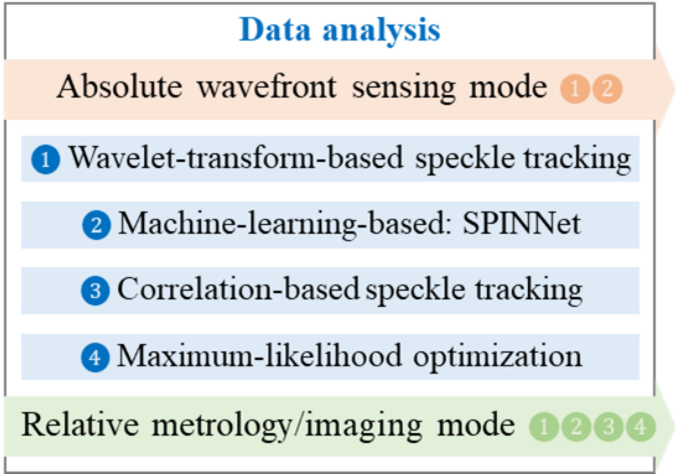
    Z. Qiao, et al., Optica 9, 391 (2022).

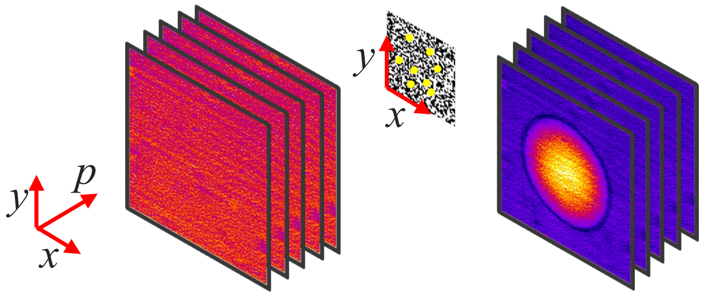


CODED-MASK-BASED WAVEFRONT SENSING

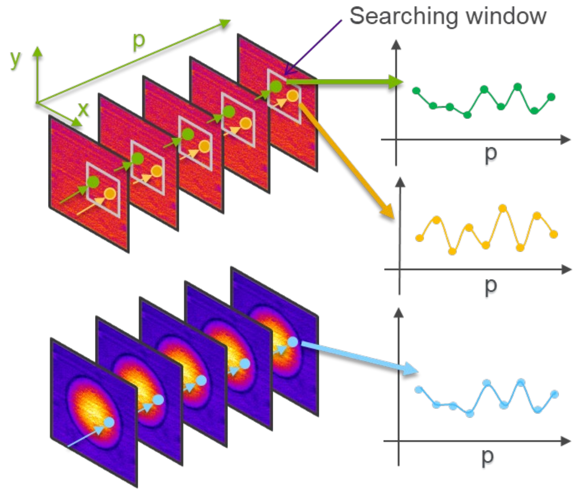
Scanning mode measurements for improved resolution and sensitivity

- **Relative metrology/imaging mode**

Reference image stacks Sample image stacks



2D/1D scan of the mask in transverse plane



- **Data analysis methods:**
  - Correlation-based speckle vector tracking
  - Wavelet-transform-based speckle **vector** tracking
    Z. Qiao, et al., Opt. Express 28, 33053 (2020).
  - Maximum-likelihood optimization
    Z. Qiao, et al., J. Imaging 7, 249 (2021).

Maximize 1D cross-correlation

Minimize Euclidean distance square of Wavelet coefficients

Minimize loss function summing over all images

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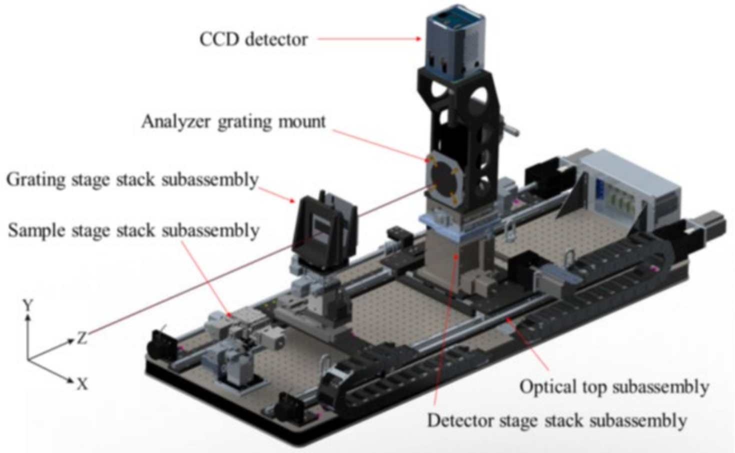
WAVEFRONT SENSING INSTRUMENTS



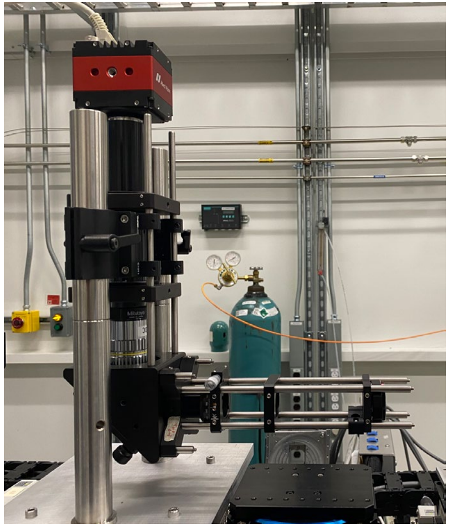
L. Assoufid et al., Rev. Sci. Instrum. 87, 052004 (2016).

Portable WF sensor

APS beamlines

- X-ray optics and detector testing beamline (1-BM)
- Instrumentation Development, Evaluation, & Analysis (IDEA) beamline (28-ID-B) (Oct. 2021 — Apr. 2023)

Zoomable WF sensor



Compact WF sensor

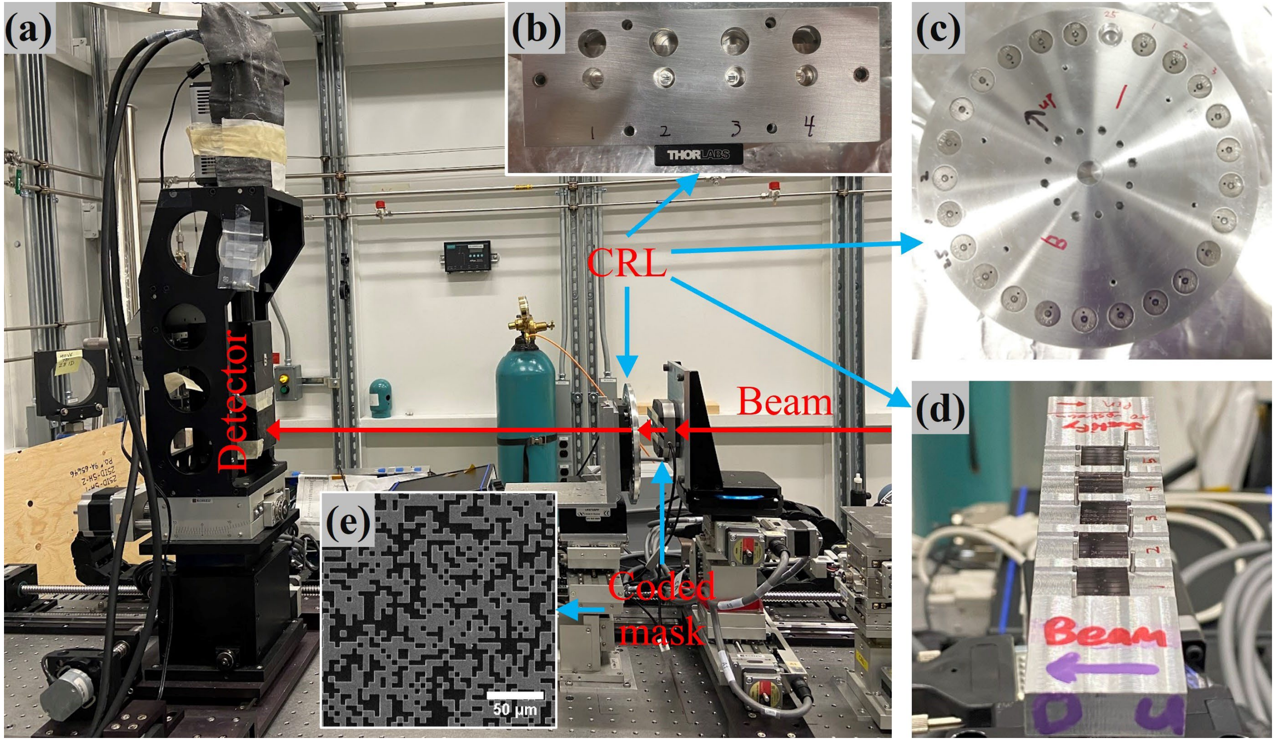
A standard diagnostic tool optimized for each APS-U beamline.

M. Frith, et al., Rev. Sci. Instrum. (2023) submitted.

AT-WAVELENGTH METROLOGY APPLICATION

AT-WAVELENGTH METROLOGY APPLICATION

CRL measurements at APS 28-ID-B and 1-BM beamline



- APS and APS-U beamlines:

  >600 Be lenses, >100 Al and diamond lenses
- Other facilities:

  Australian Synchrotron: 159 Al and Be lenses
- Many R&D lenses from ESRF, Euclid, JJ X-ray, Materion, KIT, RXoptics, PALM-scientific, APS-LDRDs

X. Shi, et al., Proc. SPIE 12695 (2023) submitted.

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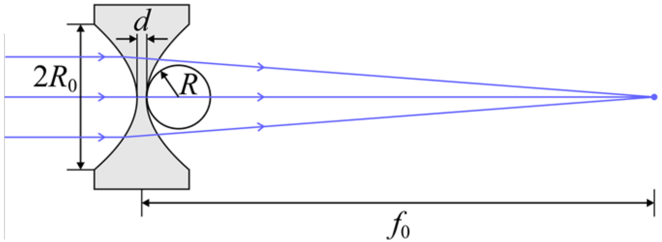
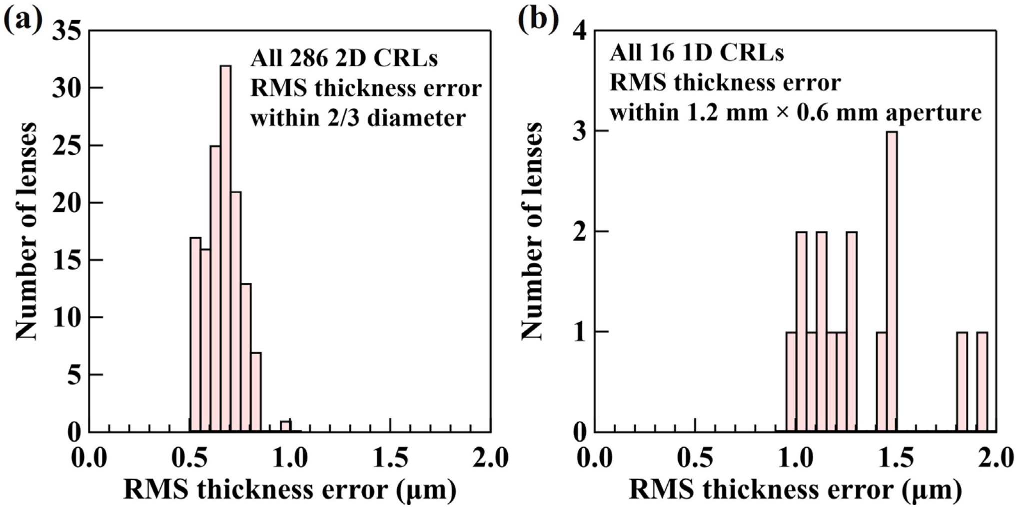
AT-WAVELENGTH METROLOGY APPLICATION

CRL measurements at APS 28-ID-B and 1-BM beamline



- **Radius of curvature *R*:** radius values standard deviation <1%, all within ±2.5% of the mean value
- **Thickness error**: RMS thickness error after removing best-fit parabola over the central two-third of the lens diameter < 1.0 μm
- **Defects and cracks:** <5% lenses were detected with defects >10 μm PV thickness error, replacement lenses within specs.

Statistics of all APS-U Be lenses
(after replacements)



X. Shi, et al., Proc. SPIE 12695 (2023) submitted.

AT-WAVELENGTH METROLOGY APPLICATION

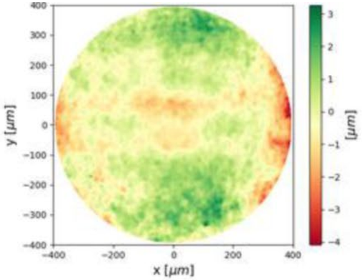
CRL measurements at APS 28-ID-B and 1-BM beamline

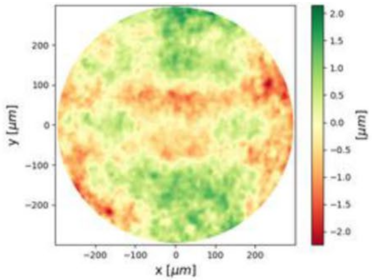
Example good lens

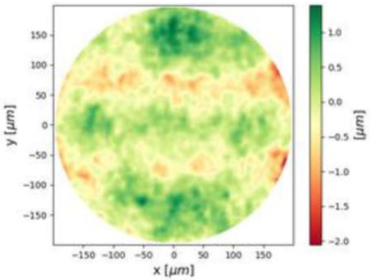
Radius: 193.3 µm;
800 µm fitting diameter
RMS: 0.99 µm
PV: 7.17 µm

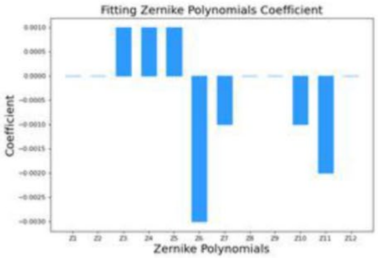
600 µm fitting diameter
RMS: 0.64 µm
PV: 4.36 µm

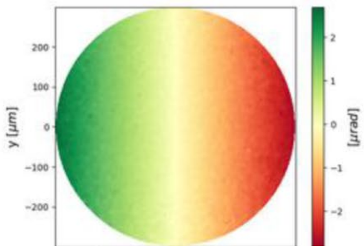
400 µm fitting diameter
RMS: 0.41 µm
PV: 2.84 µm

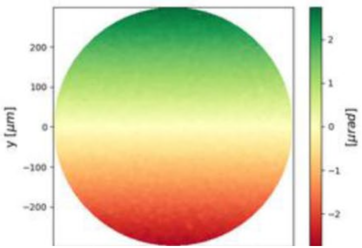


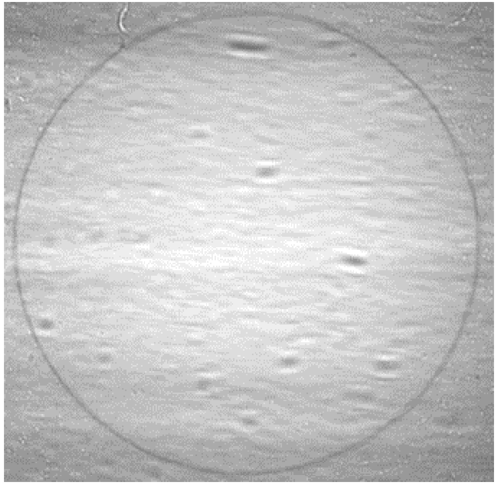












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AT-WAVELENGTH METROLOGY APPLICATION

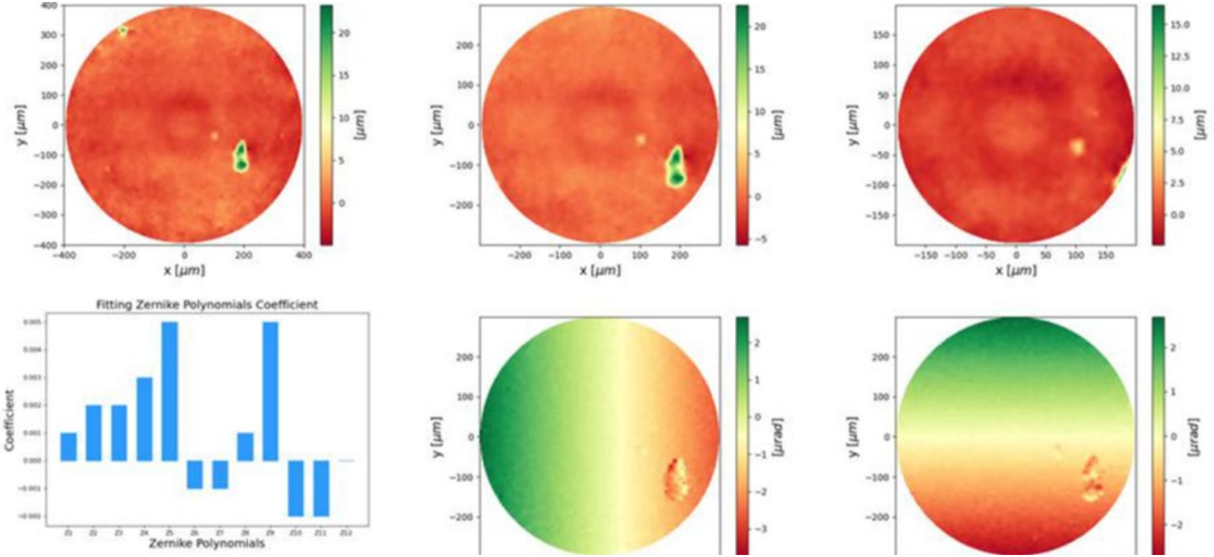
CRL measurements at APS 28-ID-B and 1-BM beamline

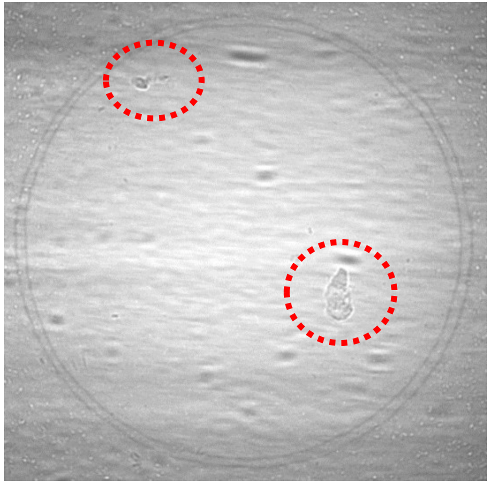
Example rejected lens

Radius: 196.9 μm;
800 μm fitting diameter
RMS: 1.70 μm
PV: 28.15 μm

600 μm fitting diameter
RMS: 1.88 μm
PV: 28.04 μm

400 μm fitting diameter
RMS: 0.79 μm
PV: 18.49 μm





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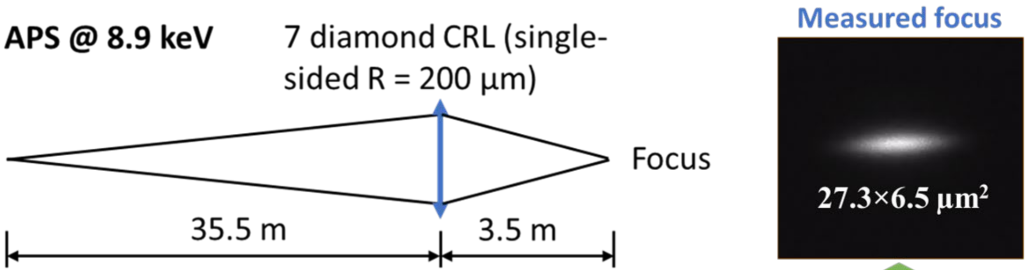
AT-WAVELENGTH METROLOGY APPLICATION

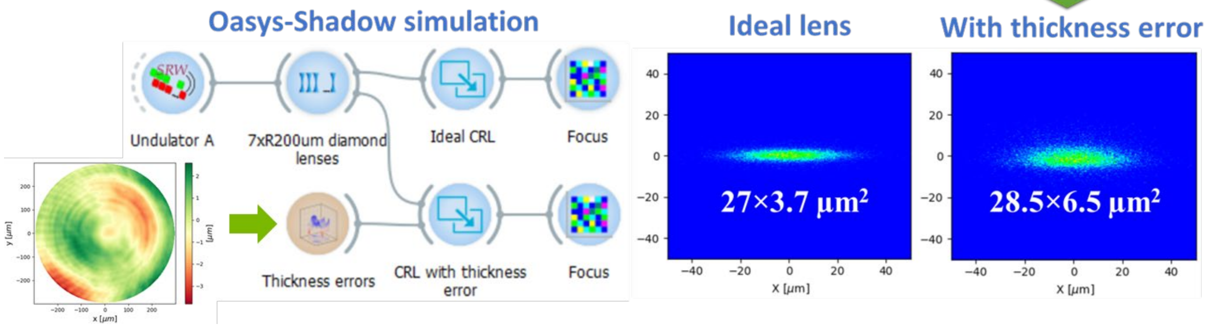
CRL thickness error database

- **Transfocator arrangement**

Cassette	1	2	3	4	5	6	7	8
Type	2D	2D	2D	2D	2D	2D	2D	2D
N	1	1	1	2	4	8	8	16
R, µm	1000	500	200	200	200	200	100	100
	H74	F1	T296	D104	C135	C138	D180	D290
				D137	C137	C142	D183	D292
					C149	C143	D185	D293
					D126	C147	D189	D296
						C151	D193	D297
						C154	D195	D301
						D101	D199	D305
						D102	D205	D306
								D307
								D309
								D681
								D682
								D685
								D686
								D687
								D688

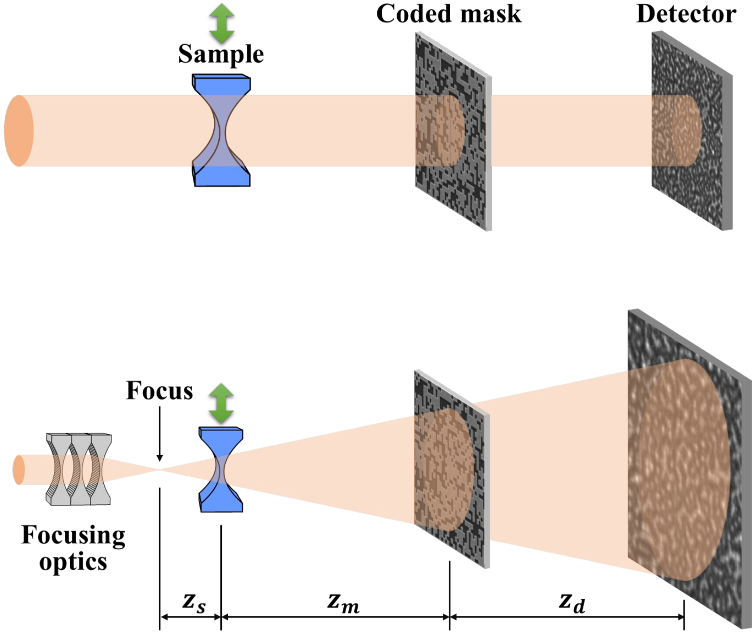
- **Performance simulation and beamline design**





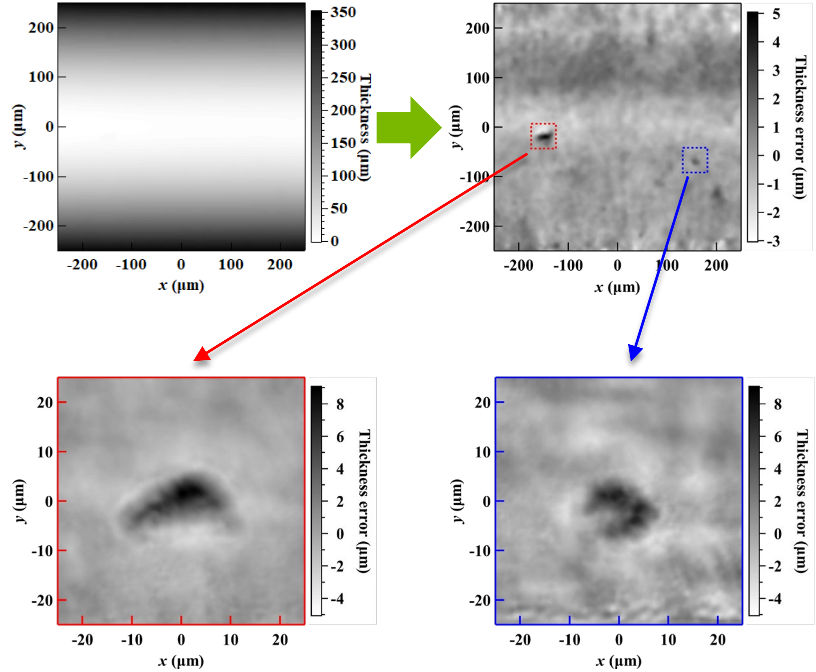
AT-WAVELENGTH METROLOGY APPLICATION

Variable-resolution metrology of CRL



Effective pixel size 0.65 µm

Effective pixel size 0.068 µm



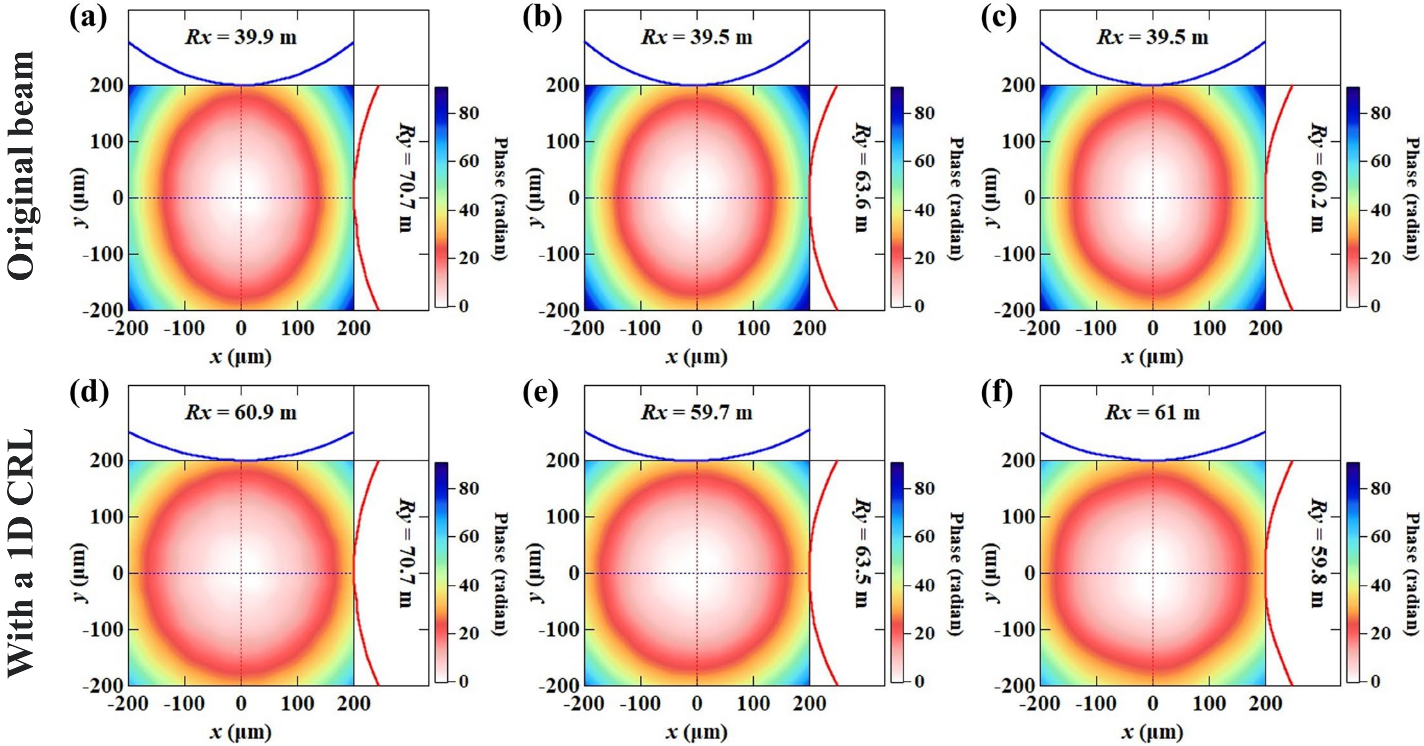
Magnification: $\frac{z_s + z_m + z_d}{z_s} = 9.5$

X. Shi, et al., Proc. SPIE 12240, 122400H (2022).

WAVEFRONT SENSING APPLICATIONS

WF SENSOR PROTOTYPE TESTING

Absolute wavefront measurements at APS 28-ID-B



M. Frith, et al., Rev. Sci. Instrum. (2023) submitted.

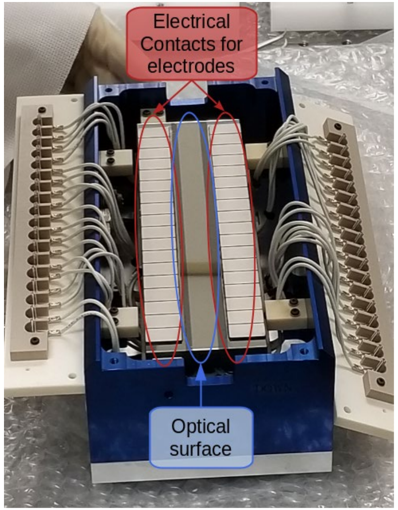
WAVEFRONT SENSING APPLICATION

Adaptive mirrors: dynamic focusing and wavefront shaping

APS mechanical bender mirrors

J. Anton, et al., Proc. SPIE 11100, 111000B (2019).

JTEC bimorph mirrors



X. Shi, et al., Proc. SPIE 11491, 1149110 (2020).

WAVEFRONT SENSING APPLICATION

Advanced beamline optics automatic control system

- Real-time machine-learning-driven control system of a deformable mirror for achieving aberration-free X-ray wavefronts
  L. Rebuffi, et al., Opt. Express **31**(13), 21264 (2023).

- AutoFocus: AI-driven alignment of nanofocusing X-ray mirror systems
  L. Rebuffi, et al., Opt. Express (2023) submitted.
  Optica Open. Preprint. doi: 10.1364/opticaopen.23934903.v3

An optics automation system combining adaptive optics, wavefront sensing, and ML/AI control algorithm for beamline auto-alignment/focusing and wavefront control.

12:30 – 13.00 AI-driven real-time optics control system to achieve aberration-free coherent wavefronts at 4th-generation synchrotron radiation and free electron laser beamlines
Luca Rebuffi

SUMMARY

- The APS established a full bank of techniques and tools for advanced X-ray metrology and wavefront sensing
- Evaluated quality and performance of various optical components at the IDEA Beamline and 1-BM beamline
- Complete design and fabrication of dedicated WF sensors for the commission and operation of APS-U beamlines
- Future work:
  - WF sensing technique
    - Develop calibration procedure and analysis for nanofocusing beam WF sensing
    - Improve SPINNet (training with targeted beamline conditions)
    - User friendly data collection and analysis code development
  - Continue developing ML-based control and AI-based auto-alignment system

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Lahsen Assoufid
Yudong Yao
Mathew Cherukara

Kazuto Yamauchi (OSAKA Uni.)
Takato Inoue (Nagoya Uni.)
Yoshio Ichii (JTEC Corporation)

Gautam Gunjala (UC Berkeley & ALS-LBNL)
Antoine Wojdyla (ALS-LBNL)
Kenneth Goldberg (ALS-LBNL)
Laura Waller (UC Berkeley)

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THANK YOU!

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