# *Reflective Hard X-ray Optics: Recent Developments for Astrophysics and Free Electron Lasers*

Joint Instrumentation Seminar

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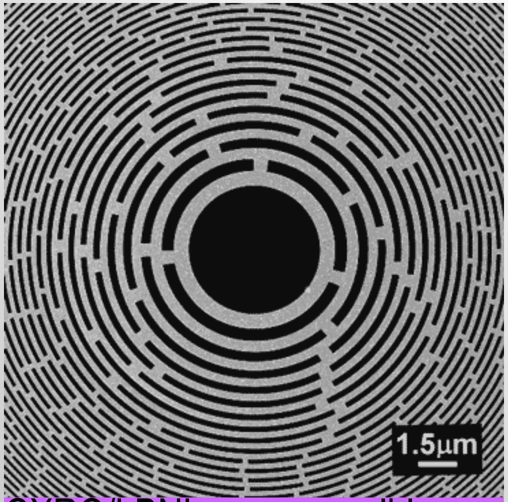
# X-RAY OPTICS PRIMER

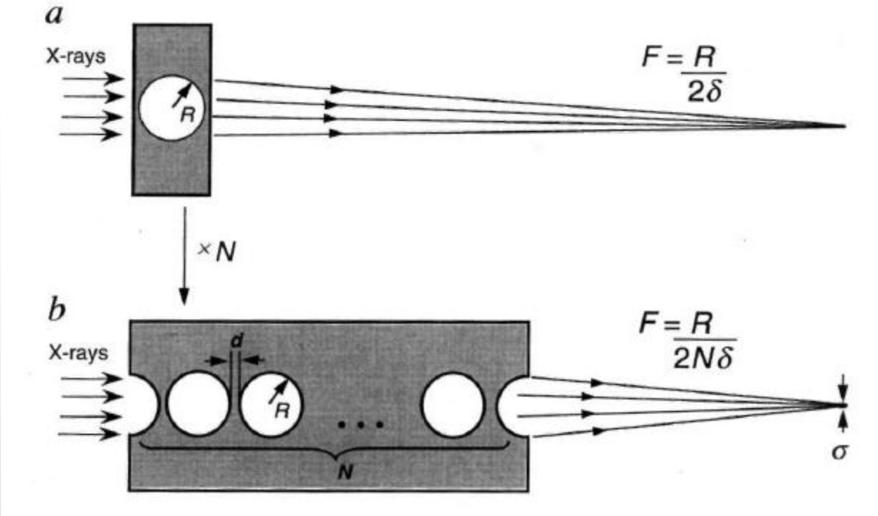
# X-ray optics can use a wide range of phenomena

## Diffraction

- Gratings
- Fresnel zone plates



CXRO/LBNL www.cxro.lbl.gov



A Snigirev et al. *Nature*, **384**, 49, (1996)

## Refraction

- Compound refractive lens

## Absorption

- Pinholes
- Anger cameras
- Coded apertures

KP Ziock et al. Proc IEEE NSS, (2003)

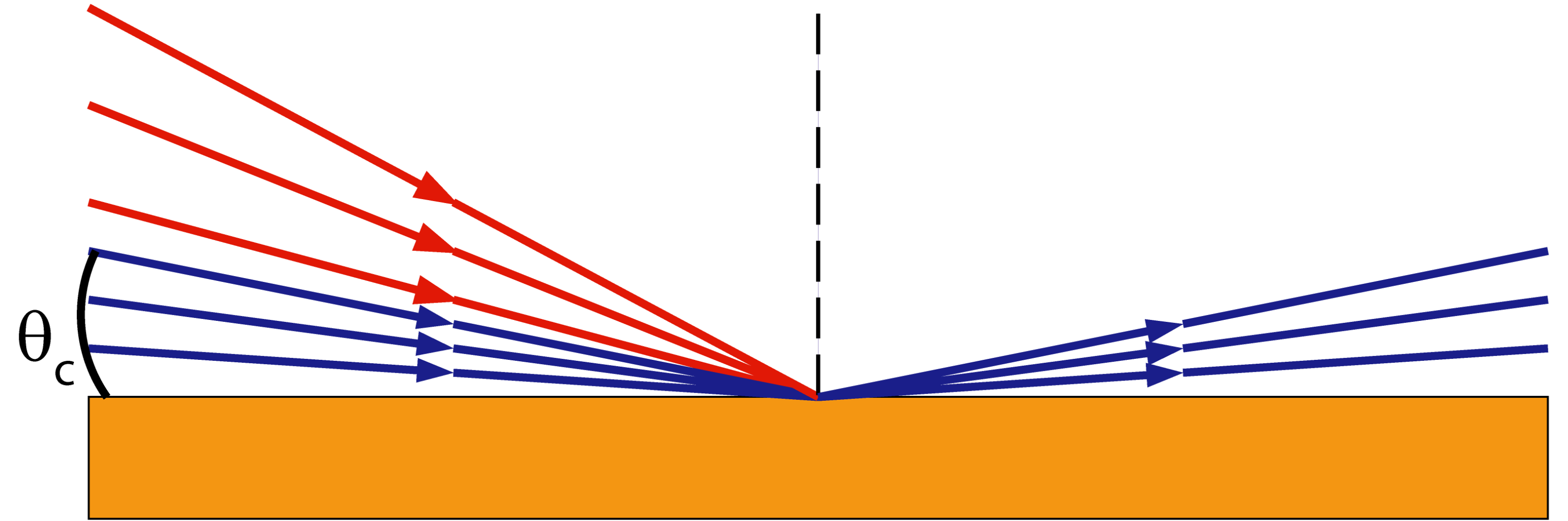
## Reflection

- Capillary optics
- Mirrors

Today's seminar

# Reflective x-ray optics

- Compton first discovered X-rays incident at small glancing angles are totally reflected
  - "The Total Reflexion of X-rays", *Philosophical Magazine*, **45**, 1121, (1923)
- Index of refraction for high energy photons $n = 1 - \delta - i\beta$
- Total external reflection of light occurs when the incident angle is less than the critical angle $\theta_C = \sqrt{2\delta}$.
- Critical angle drops rapidly with energy $\theta_c \sim E^{-1}$.



# Original reflective x-ray optic concepts

**"Formation of Optical Images by X-rays"**
**P Kirkpatrick, AV Baez**
***J Opt Soc Amer*, 38, 766, (1948)**

**"Spiegelsysteme streifenden Einfalls als abbildende Optiken für Röntgenstrahlen"**
**H Wolter, *Phys Ann* 10, 94, (1952)**

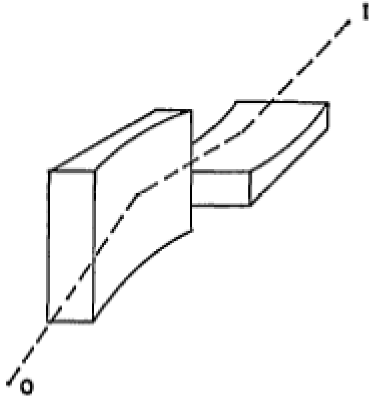


FIG. 11. Arrangement of concave mirrors to produce real images of extended objects with incidence at small grazing angles.

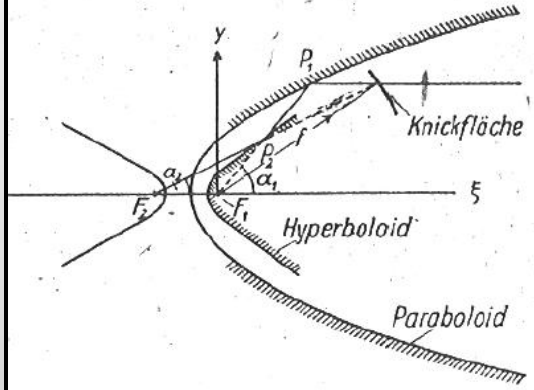


Abb. 15. Spiegelsystem 2. Art

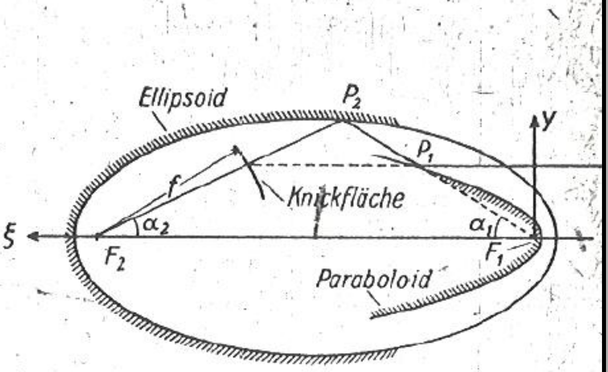


Abb. 16. Spiegelsystem 3. Art

- Two (or more) concave, spherical mirrors
- Does not meet the Abbe sine rule

- Even number of conic surfaces of revolutions (hyperbola+parabola, hyperbola+ellipse, etc.)
- Nearly satisfies Abbe sine rule
- Significant increase in solid angle (compared to KB)

# Wolter optics for x-ray astronomy

- Wolter originally proposed his designs for an x-ray microscope for biology
  - Not possible to fabricate
- Idea later adopted by Giacconi *et al.* for astronomy

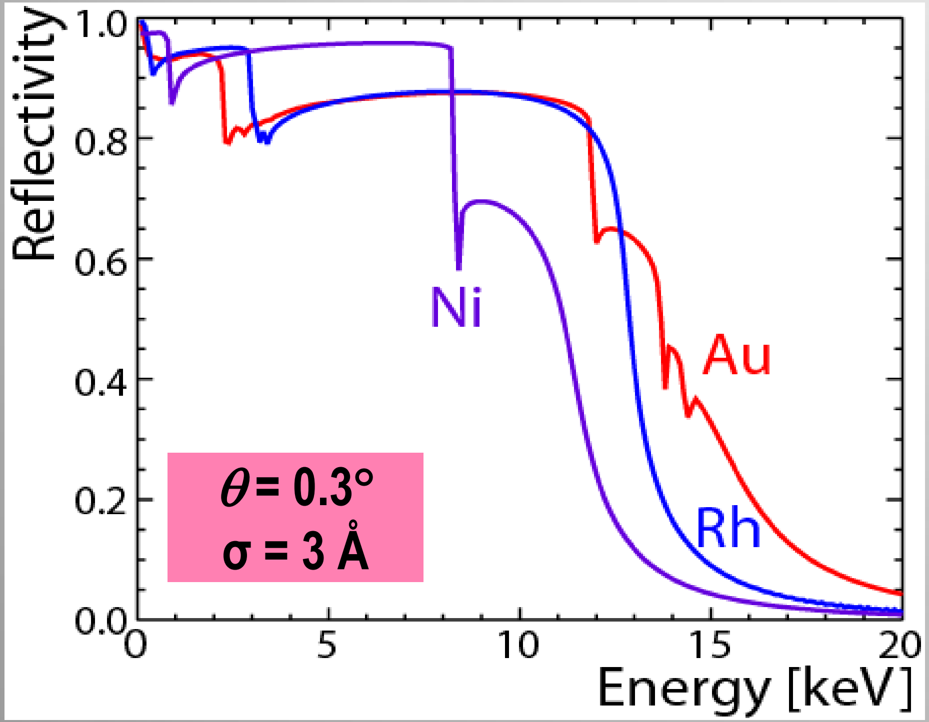
Credit: NASA

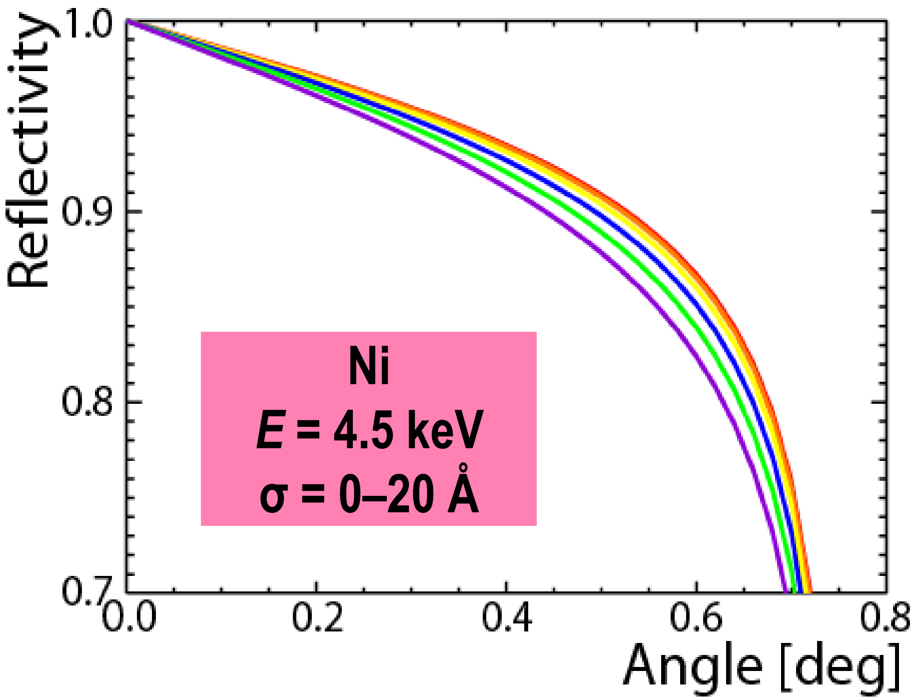
- Key innovation was the realization that mirrors could be nested inside one another to increase collecting area (solid angle)

# X-ray reflectivity

Limited to materials that:

- can be polished well or deposited smoothly (*e.g.*, Ni, Rh, Au, Ir)
- do not have absorption edges in operational band





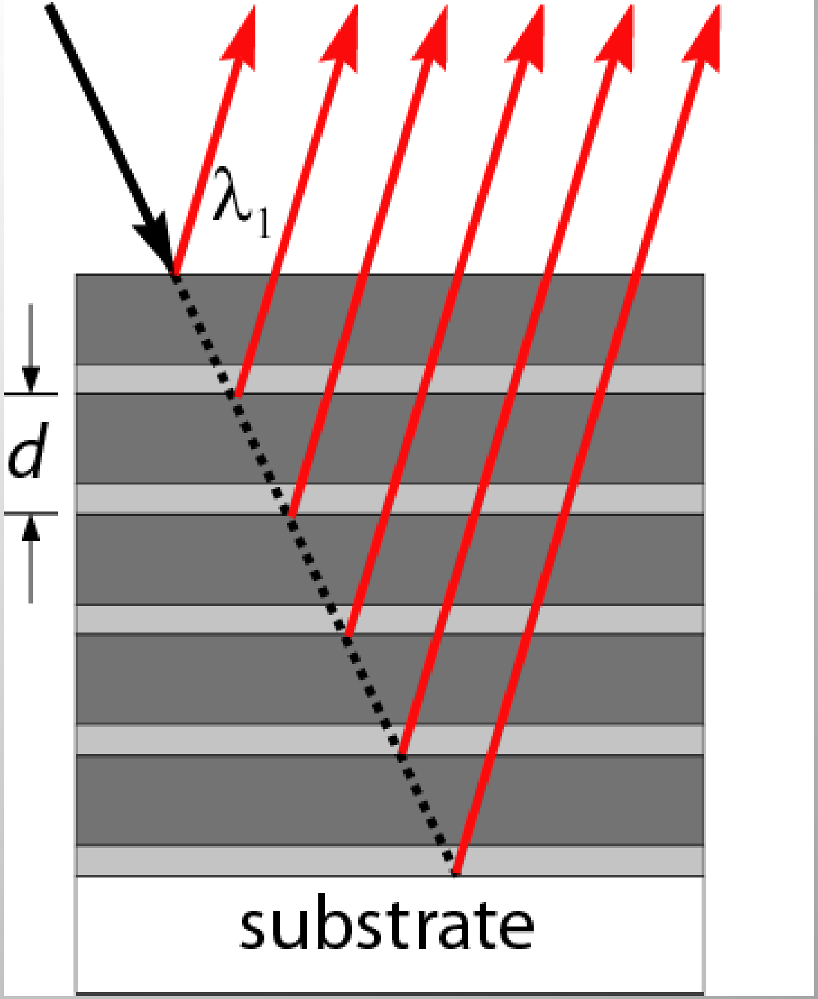
- Reflectivity depends not only on material, but also its high-spatial frequency roughness (*i.e.*, finish)

# X-ray multilayers

- At high energies, graze angles ($\theta_c$) become too shallow for efficient optics: switch to multilayers
- Alternating layers of high- and low-Z materials act as reflecting interfaces, following Bragg's law

$$m\lambda = 2d\sin\theta\sqrt{1-\frac{2\bar{\delta}}{\sin^2\theta}}.$$

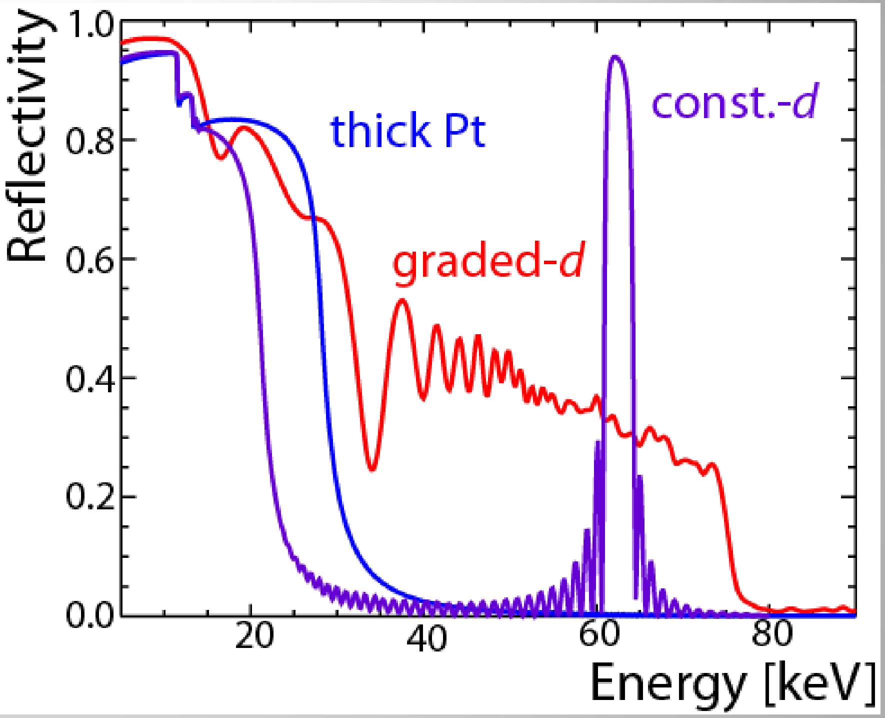
- Theory described in 1920s-1930s
- First proposed for X-ray applications in early 1970s by Spiller *et al.*
- Initially, constant-*d* designs used for high reflectivity for particular bands



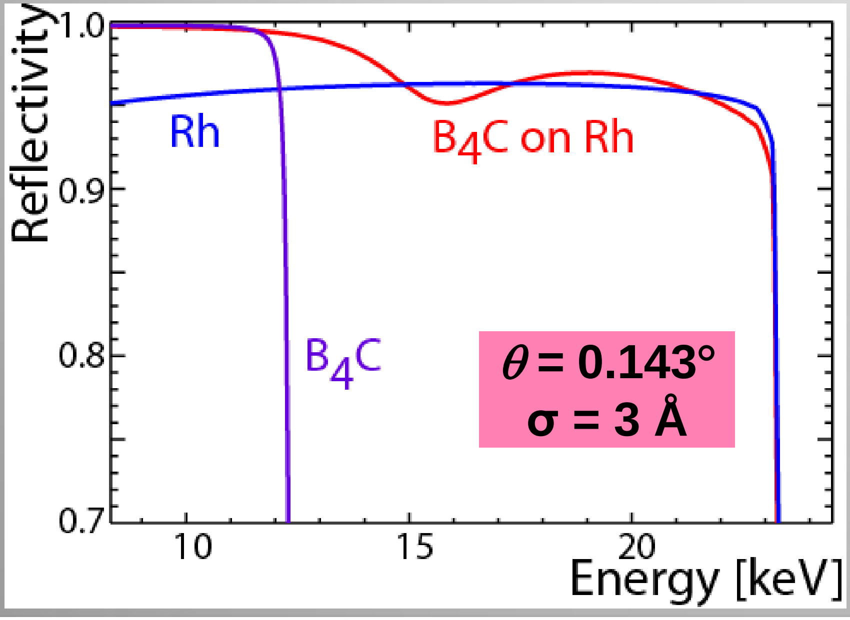
- Later, Christensen *et al.* proposed [*Proc SPIE*, **1736**, 229, (1992)] varying *d*, to satisfy the Bragg equation over a range of $\theta$ and $\lambda$ *(~1/E)* at high energies.

# Multilayer performance

- Recipes can be tuned for application; tremendous versatility
- Systems can consist of 1000's of bilayers to just a few layers ("overcoatings")
- Practically, limited by absorption, stress, absorption, material properties and other constraints (cost, time)

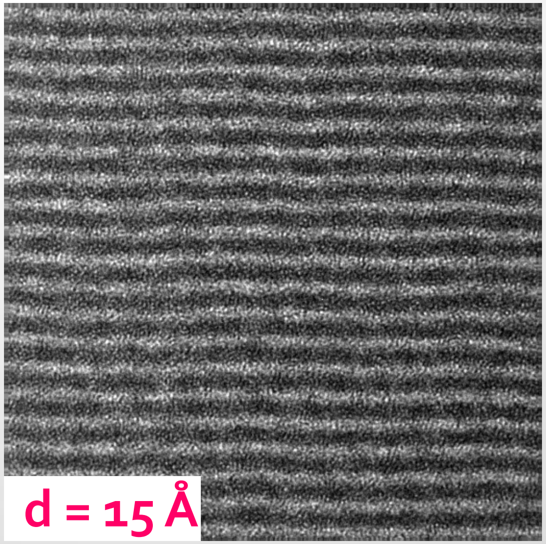


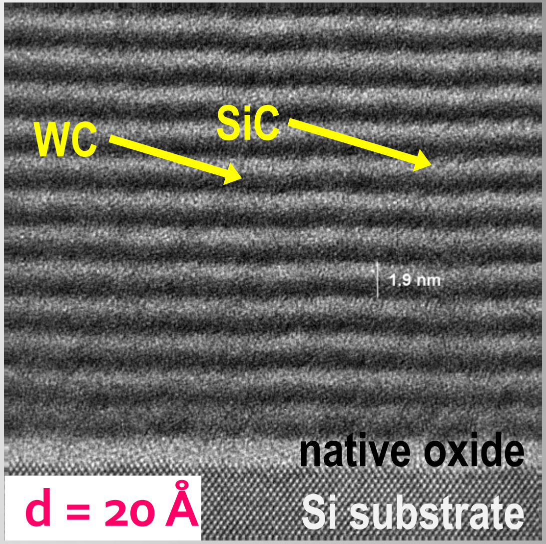
- Semi-infinite Pt coating with σ=3Å
- Constant-d: Pt/SiC, σ=3.0Å, N=90, d=35Å Γ=0.56
- Graded-d: Pt/SiC, σ=4.5 Å, N=566

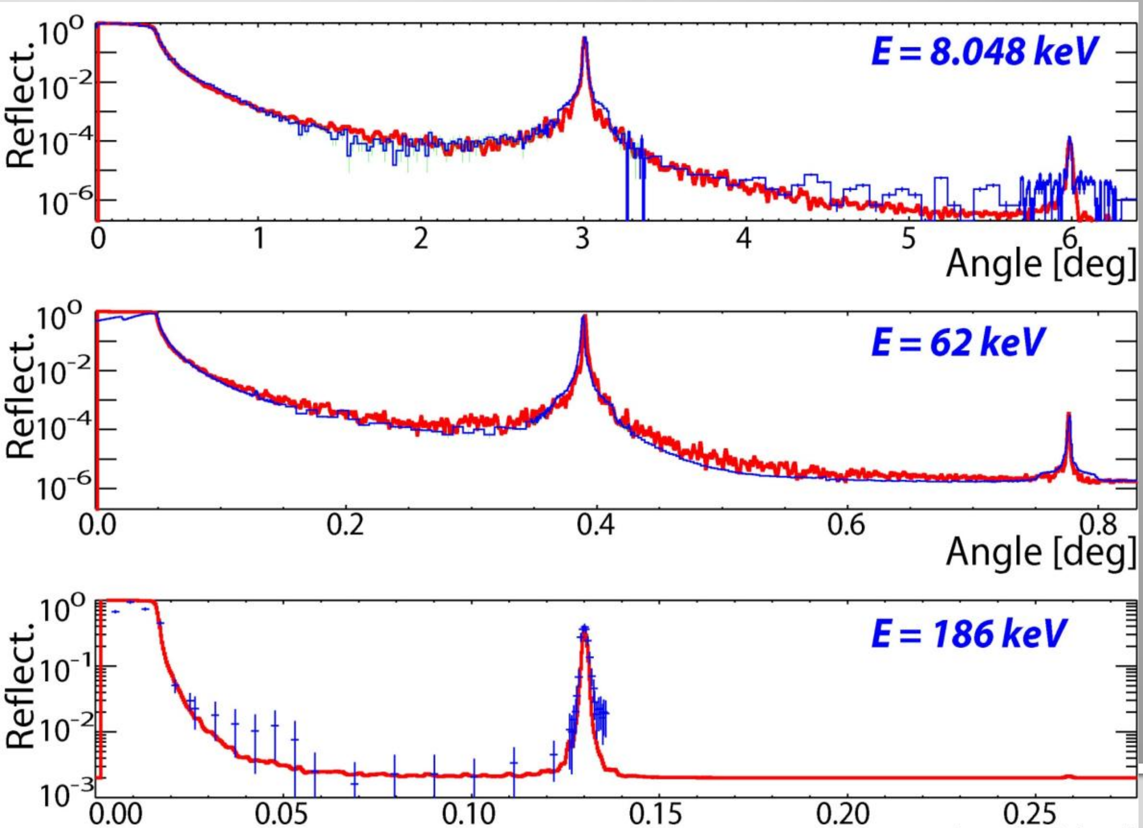


# How high can you go in energy?

- Several groups have published reflectance measurements from multilayers above 100 keV
    - Windt et al; Jensen et al;
    - High reflectivity reported; some discrepancies between measurements and theoretical values
- We have recently fabricated WC/SiC multilayers with periods of 10-20 Å and N = 300-500 and tested them at NSLS at 186 keV
    - Excellent agreement between model and data





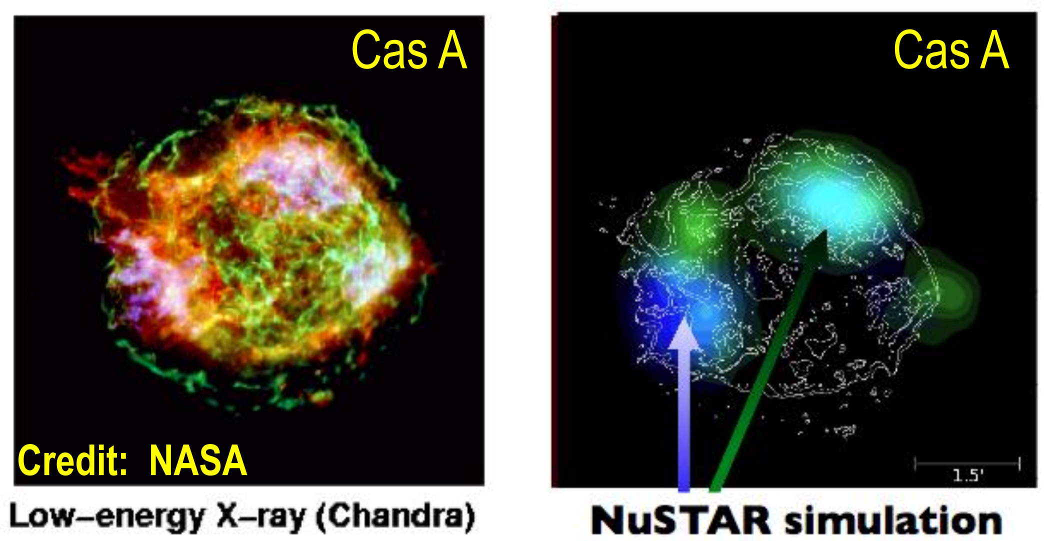


M Fernandez-Perea, MJ Pivovaroff *et al.*, in prep (2011)

# NUSTAR

# Hard x-ray astrophysics

- Want to make observations above ~10 keV where traditional x-ray mirrors (i.e. those coated with a simple metal reflective layer) lose effectiveness
- Why?
  - Nucleosynthesis: observe young supernova remnants like Cas A
  - Black hole surveys
  - Extragalactic science (e.g, blazars)
  - Compact objects (e.g., neutron stars)



Credit: NASA

Low–energy X–ray (Chandra)

NuSTAR simulation

Credit: NASA

Relativistic jets

# Moving from the soft x-ray band …

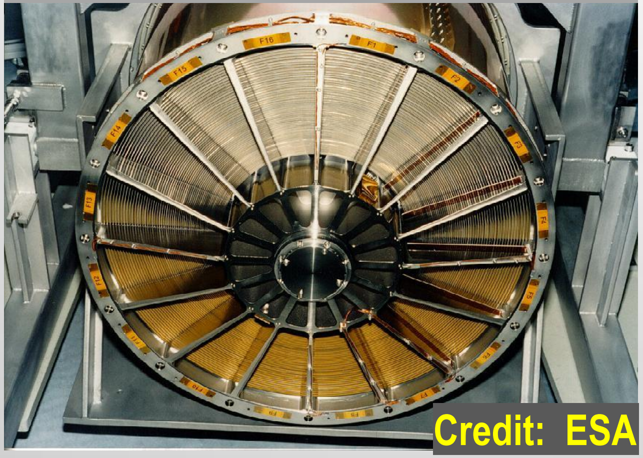
XMM-Newton; ESA

- 15″ HPD
- 3 telescopes,
  58 nested shells
- 120 m² surface area
- Mirrors: 200M DM ($120M US)
- Total: $700M US
- Replicated from precision mandrels

Chandra; NASA

- 0.5″ HPD
- 1 telescope,
  4 nested shells
- 10 m² surface area
- Mirrors: $700M US
- Total:$1600M US
- Polished monolithic blanks

***XMM* telescope**

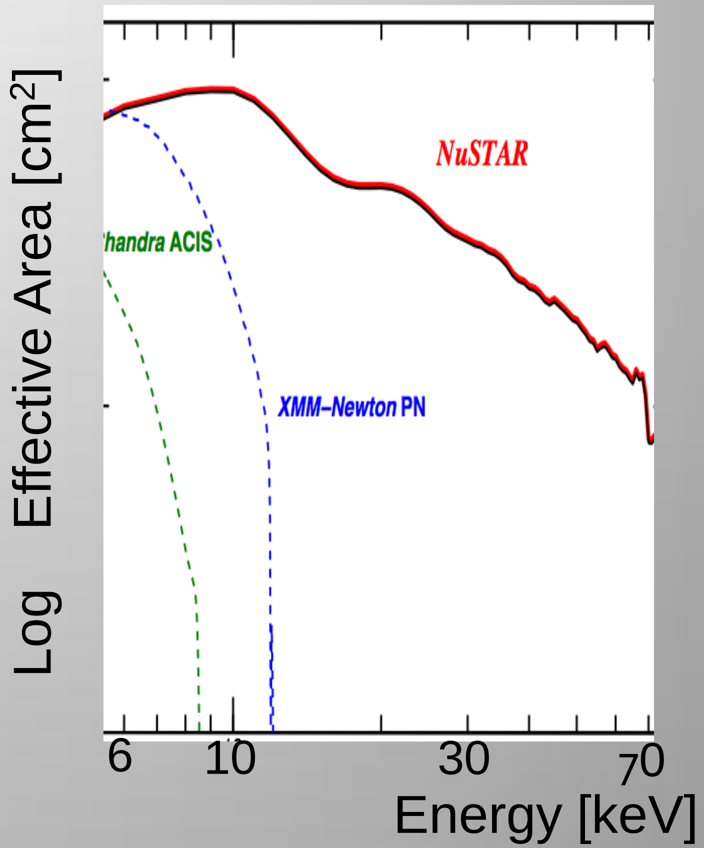


Credit: ESA

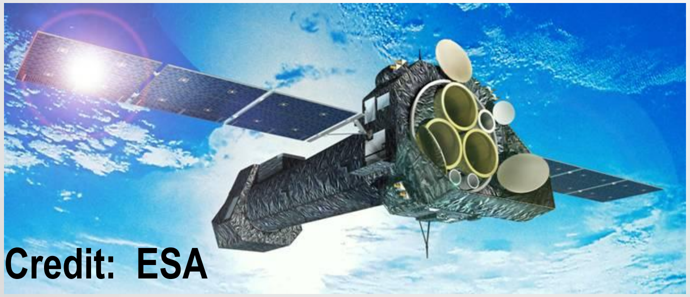
***Chandra* Zerodur substrate**

Credit: NASA

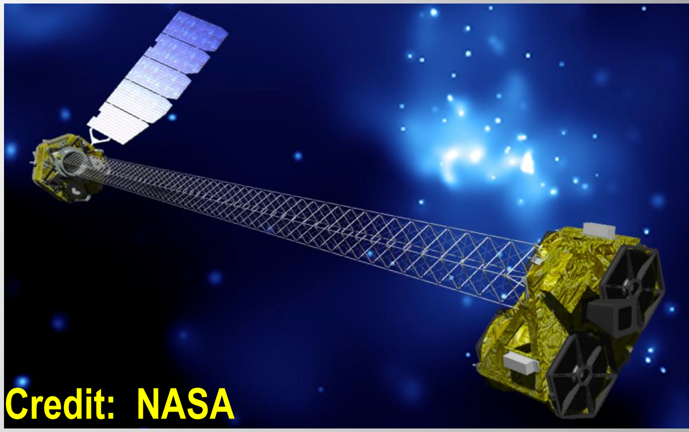
**NuSTAR requires large area above 10 keV**
**How do we do it within a SMEX program?**



# … into the hard x-ray band with NuSTAR



Credit: ESA



Credit: NASA

Credit: CXC

## XMM-Newton; ESA

- 15″ HPD
- 3 telescopes, 58 nested shells
- 120 m² surface area
- Mirrors: 200M DM ($120M US)
- Total: $700M US
- Replicated from precision mandrels

## Chandra; NASA

- 0.5″ HPD
- 1 telescope, 4 nested shells
- 10 m² surface area
- Mirrors: $700M US
- Total:$1600M US
- Polished monolithic blanks

## NuSTAR

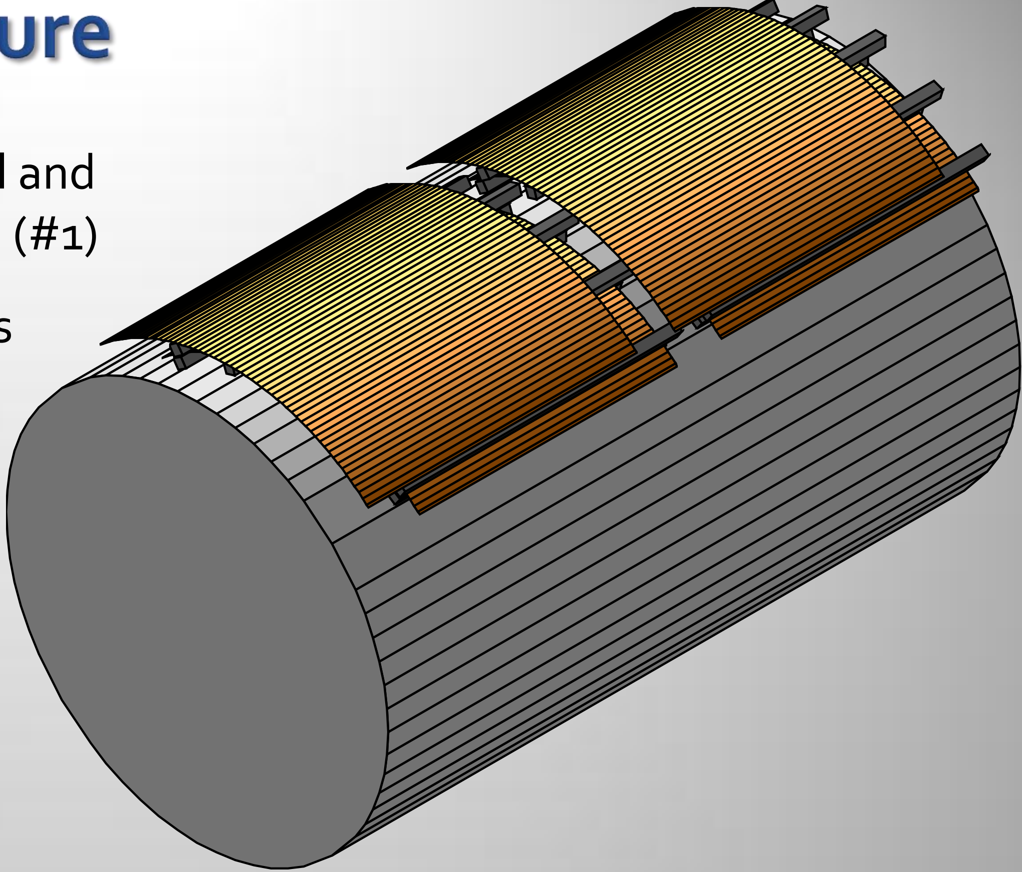
- 45″ HPD goal
- 2 telescopes, 130 nested shells
- 80 m² surface area
- Mirrors: $10–15M US
- Total: $100M US
- **Thermally-formed, multilayer-coated mirrors**

# Solution: glass substrates

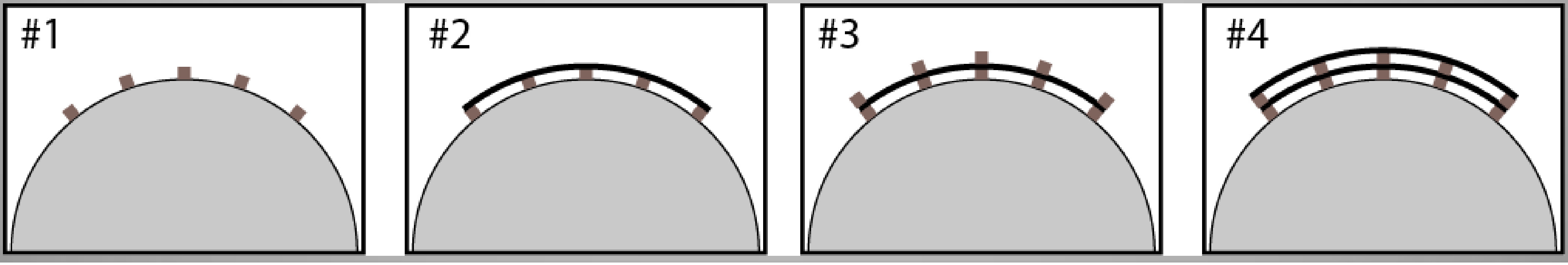
- Work dates back as far as 1988
  - Labov, *Applied Optics*, **27**, 1465, (1988).
- Columbia/DTU/LLNL starts in earnest in late 1990's for the High Energy Focusing Telescope (HEFT) balloon mission
- Start with flat panel float glass (Schott and Corning) which has nice thickness uniformity and excellent surface finish (roughness $\sigma$ = few Å)
- Thermally form ("slump") into near net shape
  - Take flat pieces of glass and turn into cylindrical shapes
- Coat with appropriate reflective coatings
- Assemble into an optic

# Optics assembly procedure

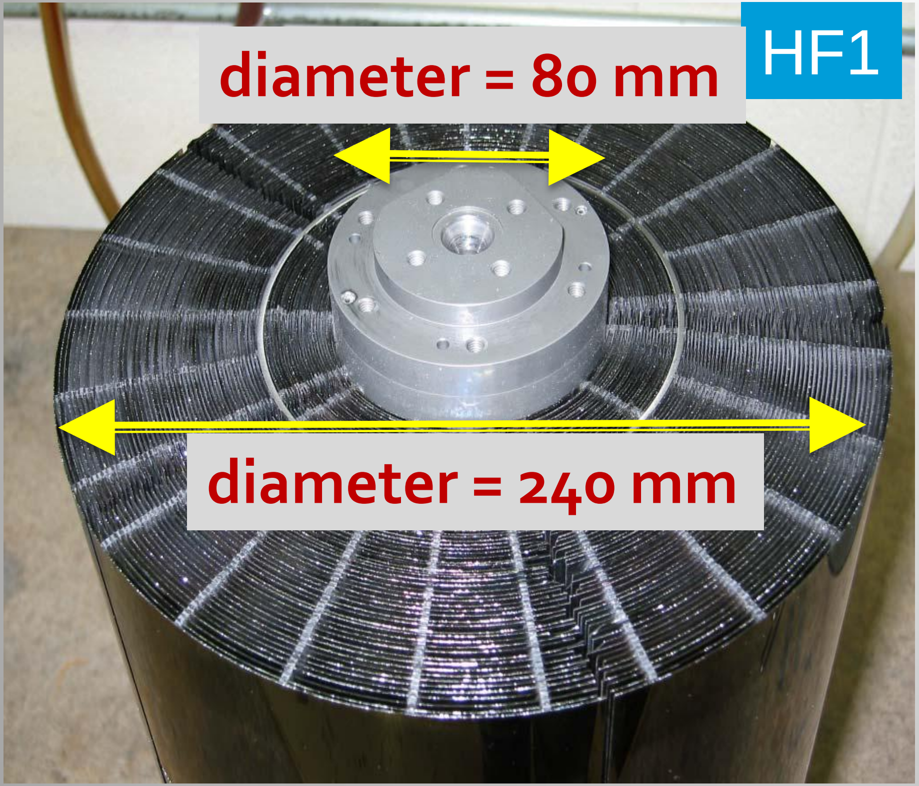
- Epoxy graphite spacers onto a mandrel and machined to the correct radius & angle (#1)
- Epoxy ML-coated substrates to spacers (#2)
- After epoxy cures, epoxy next layer of spacers to previous layer of glass (#3)
- Machine these spacers, epoxy another layer of glass into place (#4)
- Repeat until entire optic is assembled

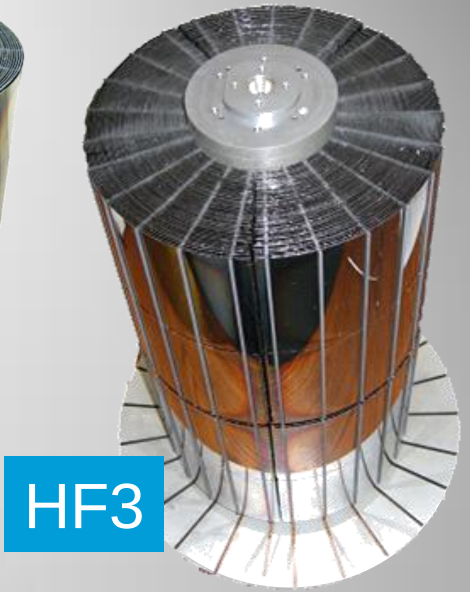


J.E. Koglin *et al.*, *Proc. SPIE,* **4851,** 607, (2003)



# HEFT optics





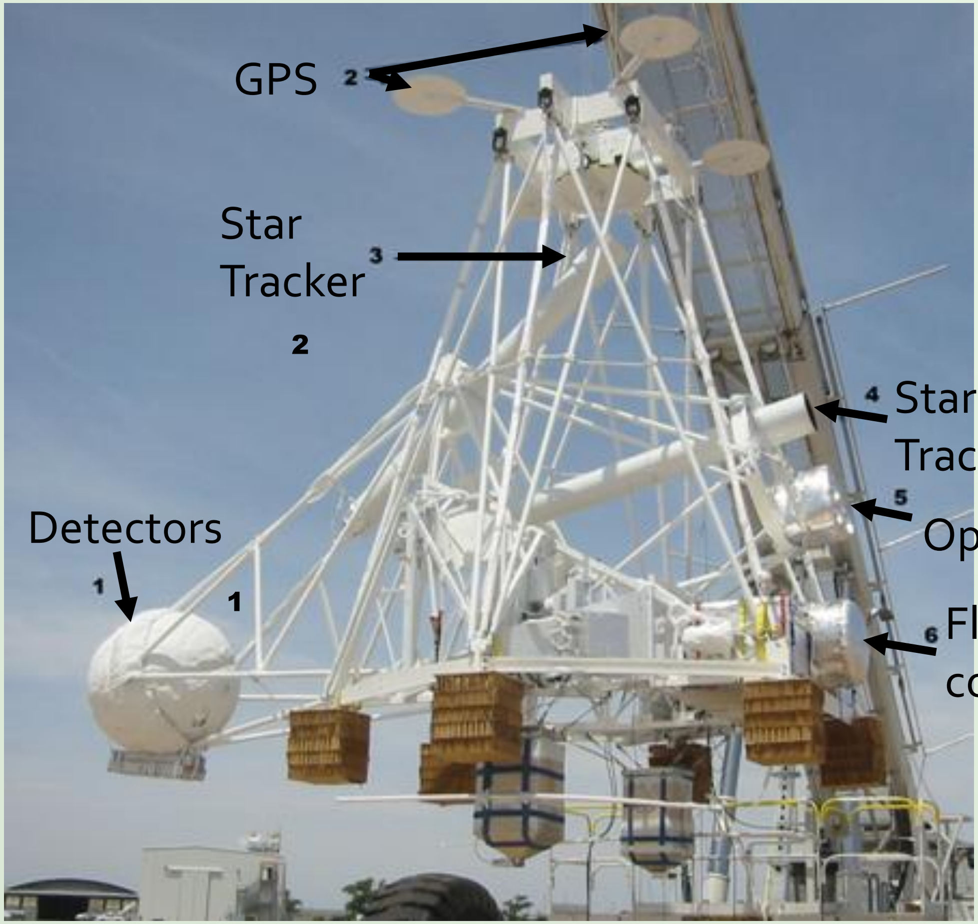
- Three optics built during ~2 year fabrication cycle (4400 mirror segments)

Caltech, Columbia, DSRI (DNSC) & LLNL

- In flight performance: 60–80″ HPD
- Prototype resolution: 43″ HPD
- *HEFT* flight module (72 layers)

J.E. Koglin *et al.*, *Proc SPIE*, **5168**, 100, (2004)
J.E. Koglin *et al.*, *Proceedings of The X-ray Universe 2005*, 955, (2006)

# HEFT ready for launch (summer 2005) New Mexico

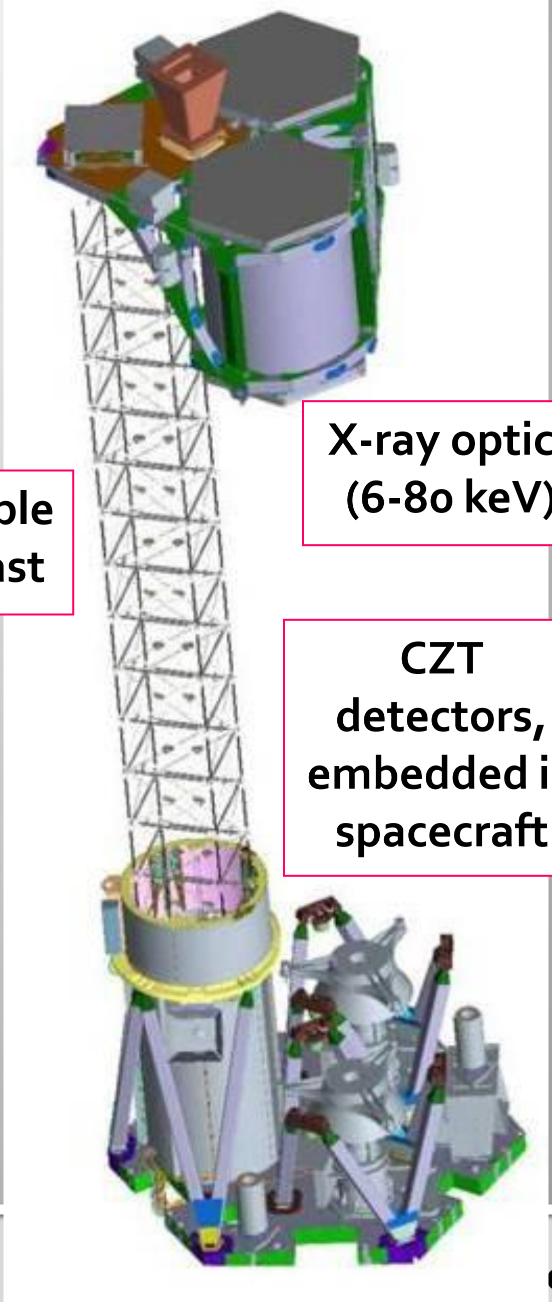


Flight Crew

F.A. Harrison *et al*., *Experimental Astronomy*, **20**, 131, (2005)

# NuSTAR (Nuclear Spectroscopic Telescope Array)

- NuSTAR starts in 2004 (PI Fiona Harrison, Caltech)
    - Leverages *HEFT* technology development
- NASA SMEX mission ($100M, not including launch); launch scheduled for 3 Feb 2012
- First focusing x-ray optics above 10 keV
    - order of magnitude more sensitivity than previous missions
    - CdZnTe focal plane array for extremely good spectroscopy (ΔE < 1 keV)



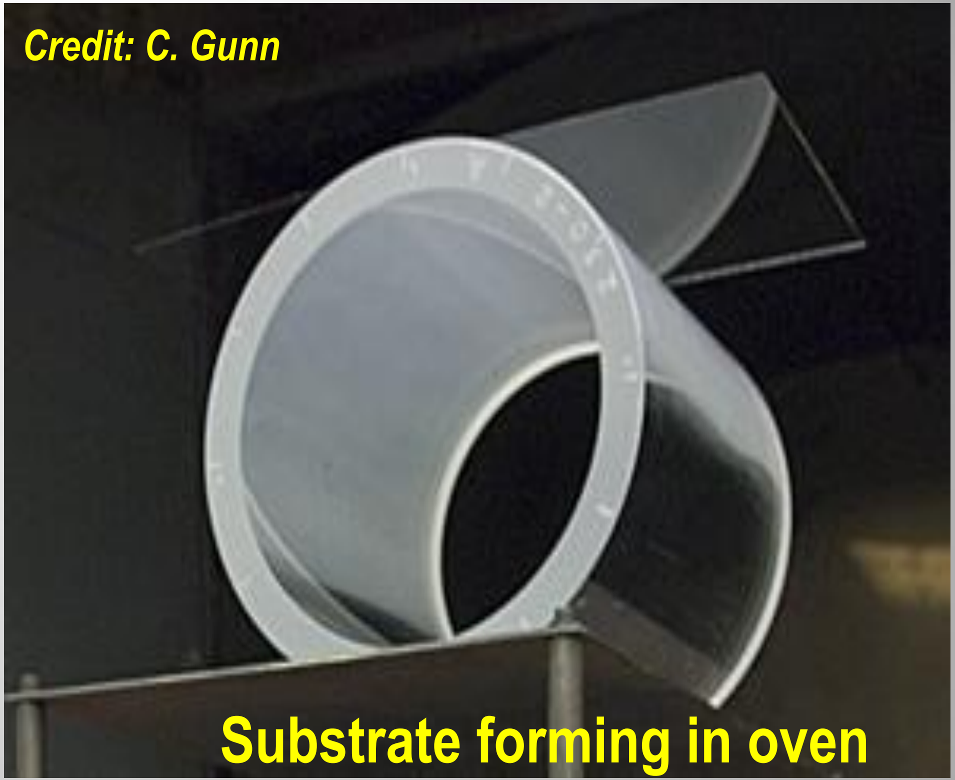
**Extendable 10-m mast**

**X-ray optics (6-80 keV)**

**CZT detectors, embedded in spacecraft**

# Optics start with thermally forming substrates

- Optics PI, Charles Hailey, Columbia University
- Team includes: Columbia U., DTU-Space, NASA GSFC, LLNL



Credit: C. Gunn

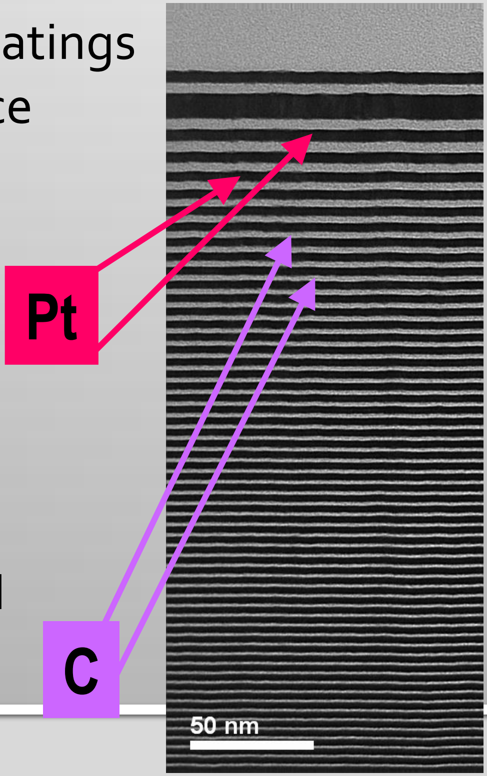
Substrate forming in oven

Credit: C. Gunn

- GSFC approach slumps glass directly onto highly polished mandrels
- Excellent figure (10–20″ HPD) has been demonstrated

# Depth-graded multilayer coatings provide broad band response

- Two material systems used, driven by need to detect Ti-44 lines at 68 & 78 keV
  - Pt/C provides highest response
  - W/Si less expensive and smoother
- 10 different multilayer recipes used
- X-ray testing to optimize coatings and understand performance
  - 8 keV (DTU)
  - 60 keV (NSLS)
  - 10-90 keV (RaMCaF)
- Extensive metrology to validate models
  - Surface roughness, TEM compositional studies

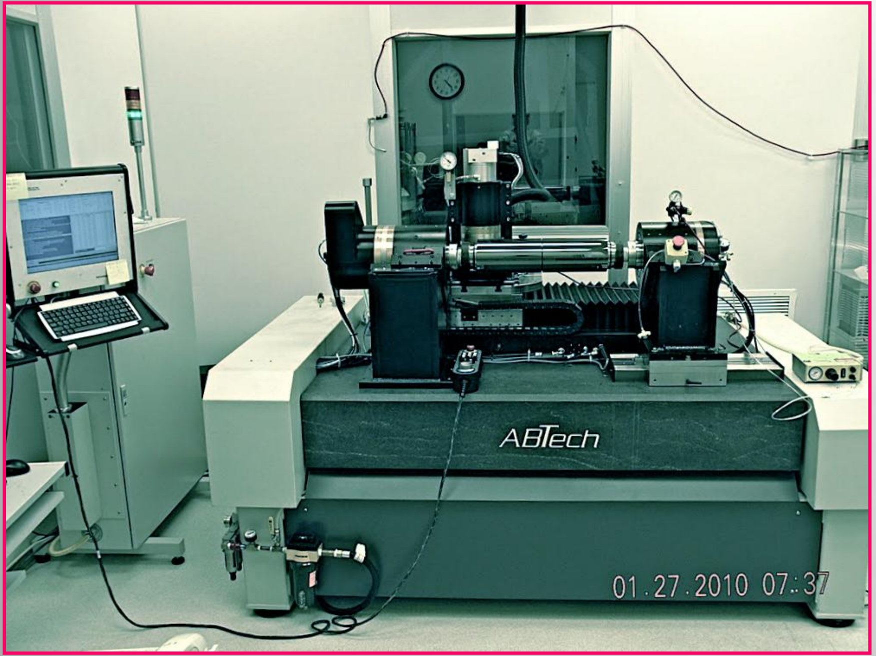



**High throughput magnetron sputtering chamber**

**Danish Technical University-Space Coating Facility**

F Christensen *et al.*, *Proc SPIE*, **8147**, (2011)

# NuSTAR telescopes assembled at the Nevis Laboratories, Columbia University



Glass is positioned and clamped for overnight cure of epoxy

Optic with more than 100 layers

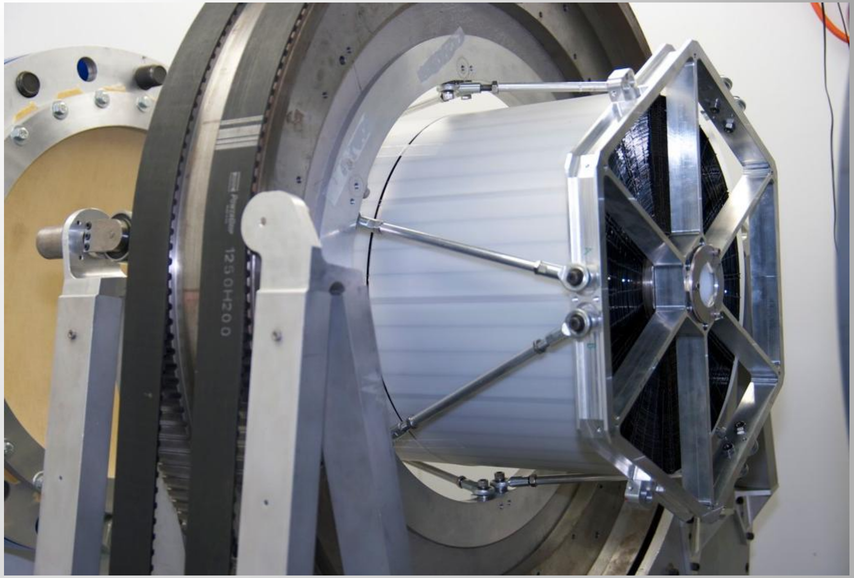
Two custom-built assembly machines are used to precisely mount the glass segments at Columbia's Nevis Laboratory

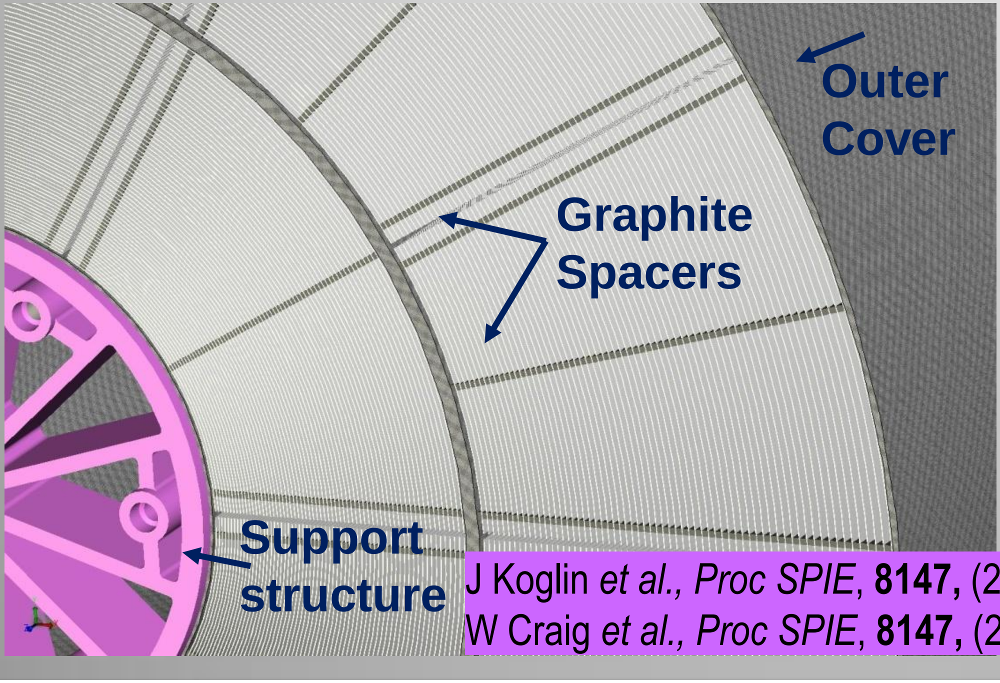
J Koglin *et al., Proc SPIE*, **8147,** (2011)
W Craig *et al., Proc SPIE*, **8147,** (2011)

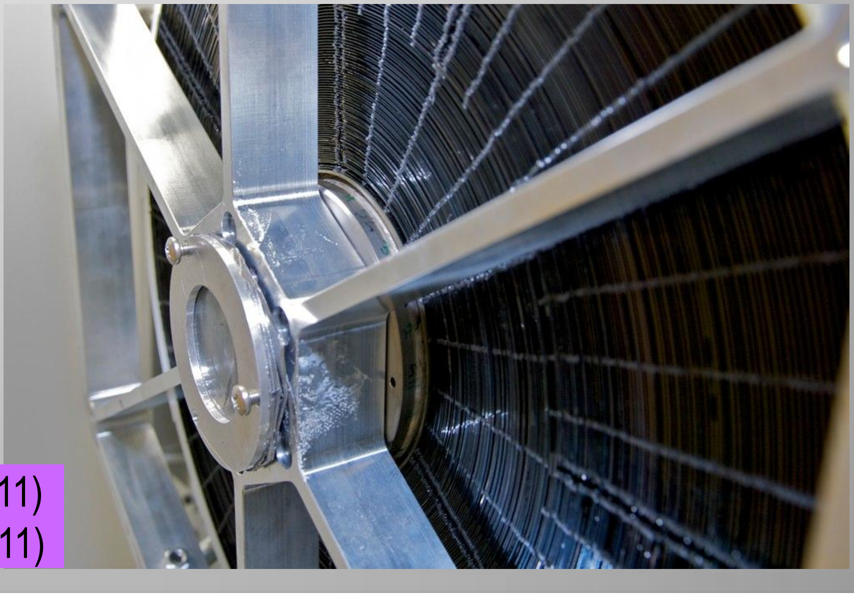
# NuSTAR telescope details

| | |
|---|---|
| Focal Length | 10.15 m |
| Shell Radii | 51–191 mm |
| Graze Angles | 0.074–0.224° |
| Shell Length | 225 mm |
| Mirror Thickness | 0.2 mm |
| Shells Per Module | 130 |
| Mirror Segments Per Module | 2340 |

C Hailey *et al. Proc SPIE* ,**7732**, (2010)



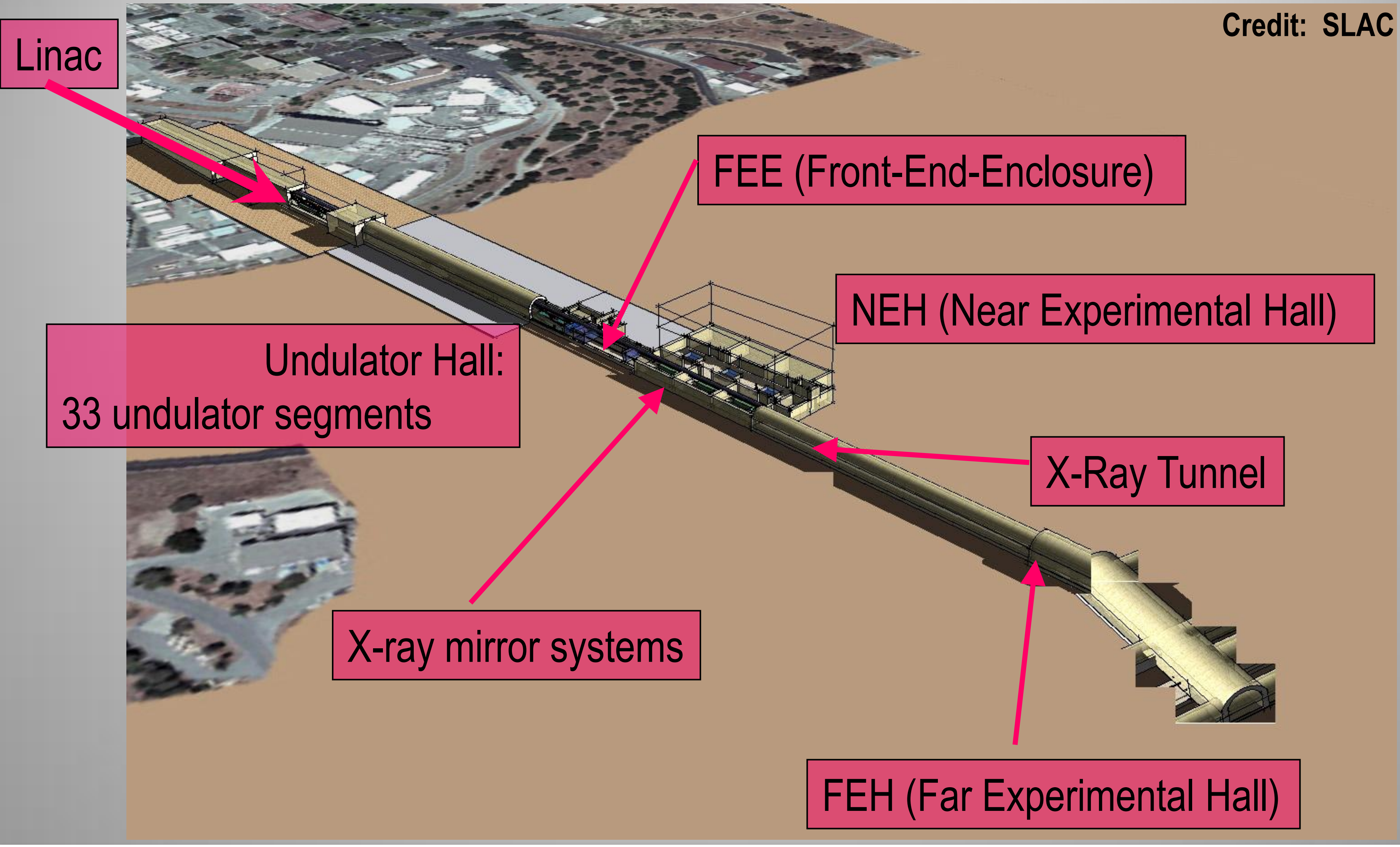




J Koglin *et al., Proc SPIE*, **8147,** (2011)
W Craig *et al., Proc SPIE*, **8147,** (2011)

# LCLS X-RAY OFFSET MIRRORS

# Linac Coherent Light Source (LCLS) at SLAC



# From the undulator hall to the users

- FEL (0.8-8 keV, 1st harmonic) comes with high-energy bremsstrahlung (spontaneous) emission that is both dangerous and contaminating
- To eliminate its presence, use a series of mirrors to filter out unwanted component, as well as deliver beam to different end stations

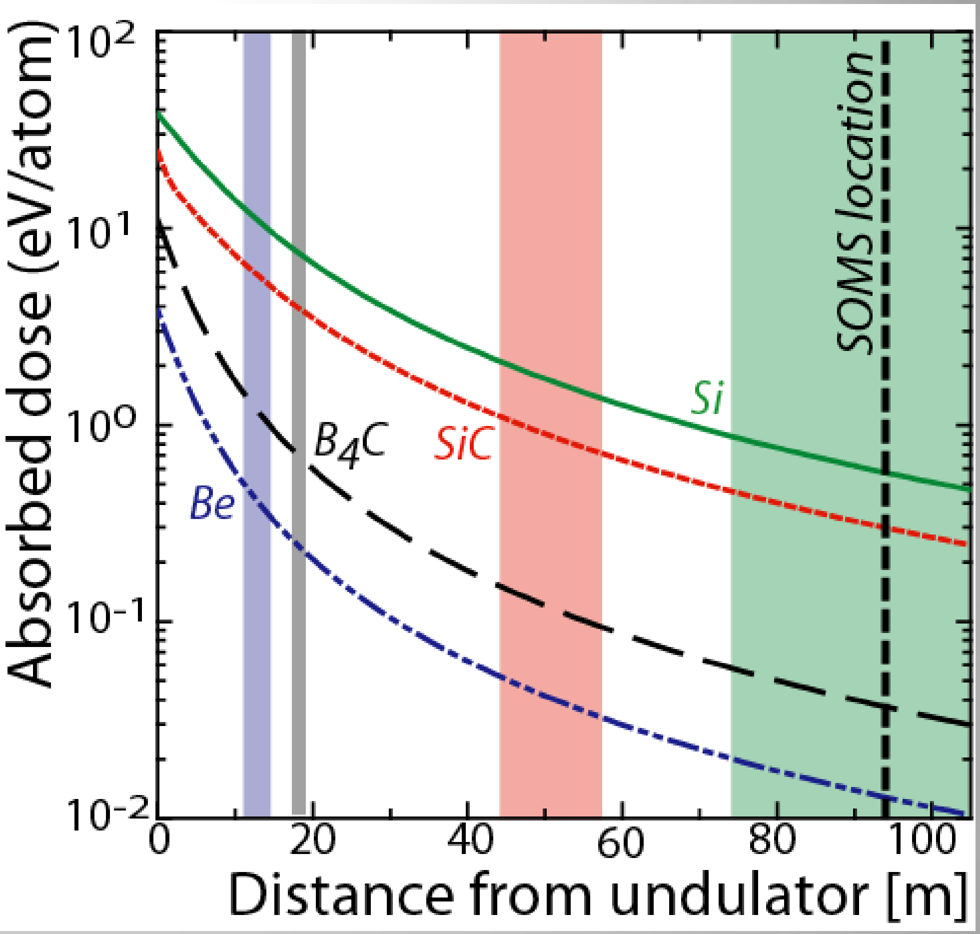
| Parameter | 0.827 keV | 8.27 keV |
|---|---|---|
| FEL pulse (rms) | 137 fs | 73 fs |
| FEL width (FWHM) | 81 μm | 60 μm |
| FEL divergence (FWHM) | 8.1 μrad | 1.1 μrad |
| FEL brightness [$\gamma$ $s^{-1}$ $mm^{-2}$ $mrad^{-2}$ $(0.1\%\ bw)^{-1}$] | $0.28\times10^{32}$ | $15\times10^{32}$ |
| Avg FEL power | 0.23 W | 0.23 W |
| Avg Spontaneous power | 0.24 W | 2.2 W |

**Science driver: safely transport beam to End Stations with minimal loss of coherence or intensity and no damage to optics**

**Solution: X-ray mirrors made by depositing thin films on very smooth, very flat precision-fabricated silicon substrates**

# Damage considerations

- Consider doses for:
  - thermal fatigue ($D_3$), reaching melt ($D_2$), melting ($D_1$)
  - $D_1 > D_2 > D_3$
- Experiments at FLASH show damage occurs for $D_1$-$D_2$
- Vertical bands indicate where materials will become damaged
  - Must place elements made from materials to the right of the bands to prevent damage



Plot courtesy of Stefan Hau-Riege (LLNL);
S Hau-Riege et al., *Opt Express*, **18**, 23933, (2010)

Very few materials will survive the fully saturated FEL!

# Manufacturing approach for LCLS X-ray mirrors

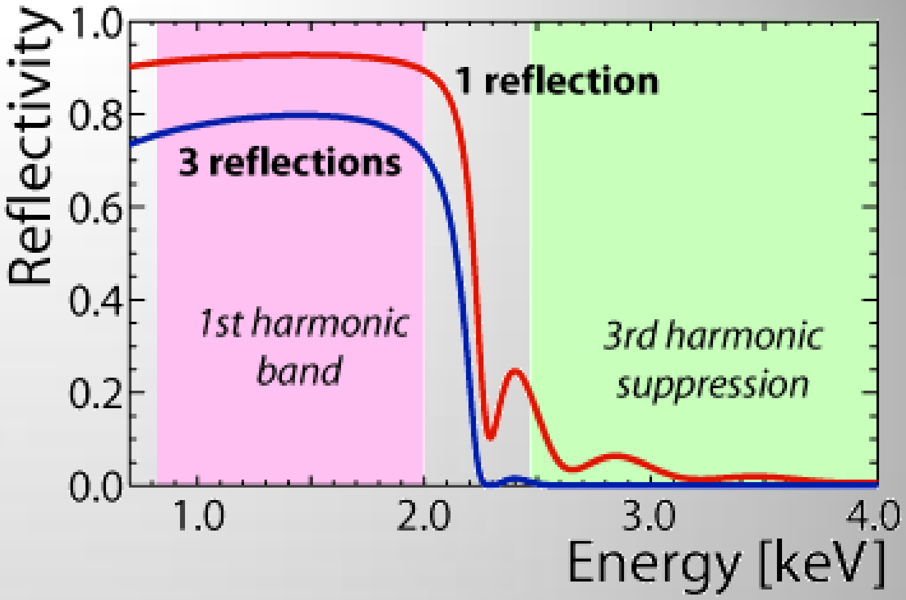
**For SOMS (0.8-2.0 keV): $B_4C$**

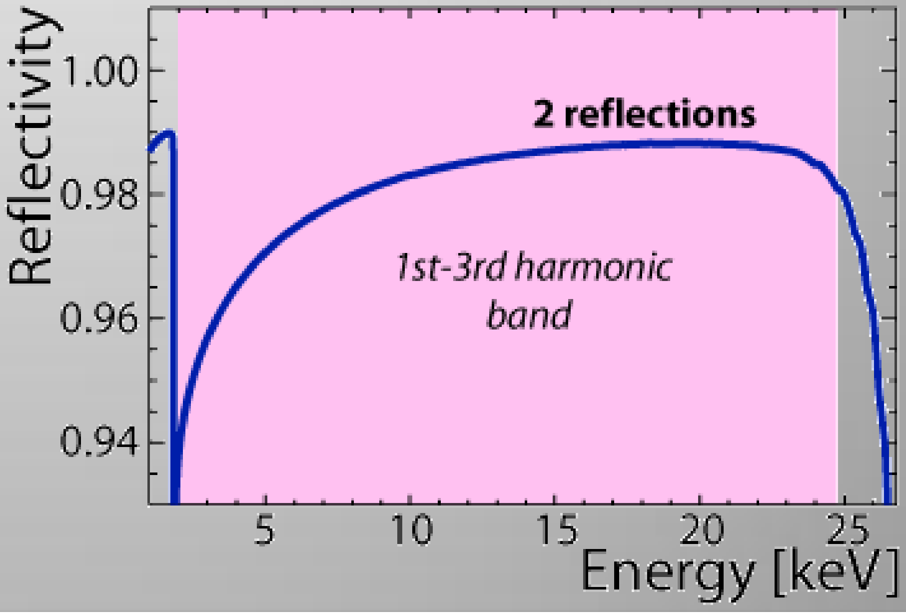
- Polish/figure $B_4C$ monolithic mirror: infeasible
- Procure Si substrate from commercial vendor, deposit 50-nm thick $B_4C$ reflective coating at LLNL

**For HOMS (2-25 keV): SiC**

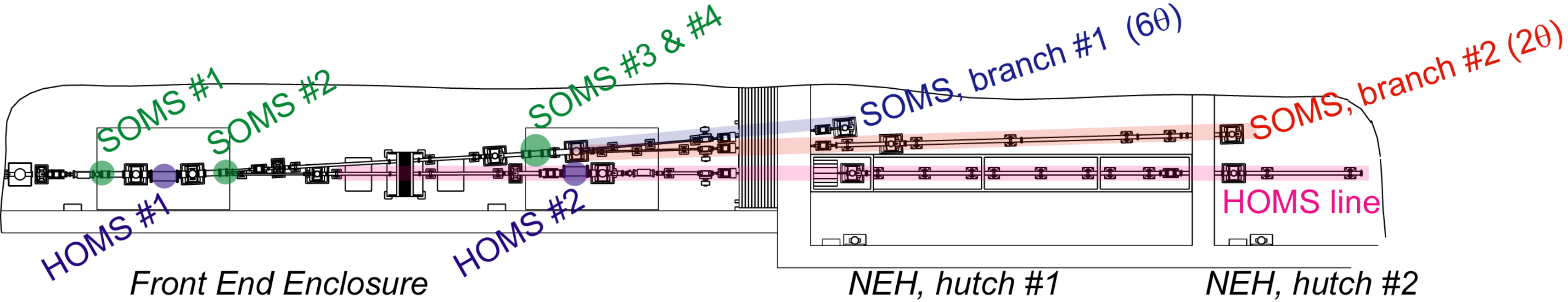
- Polish/figure SiC monolithic mirror: very challenging
- Procure Si substrate from commercial vendor, deposit 50-nm thick SiC reflective coating at LLNL

- For both systems, ensure coatings, mounting and pointing do not degrade substrate quality





# Layout of mirror systems

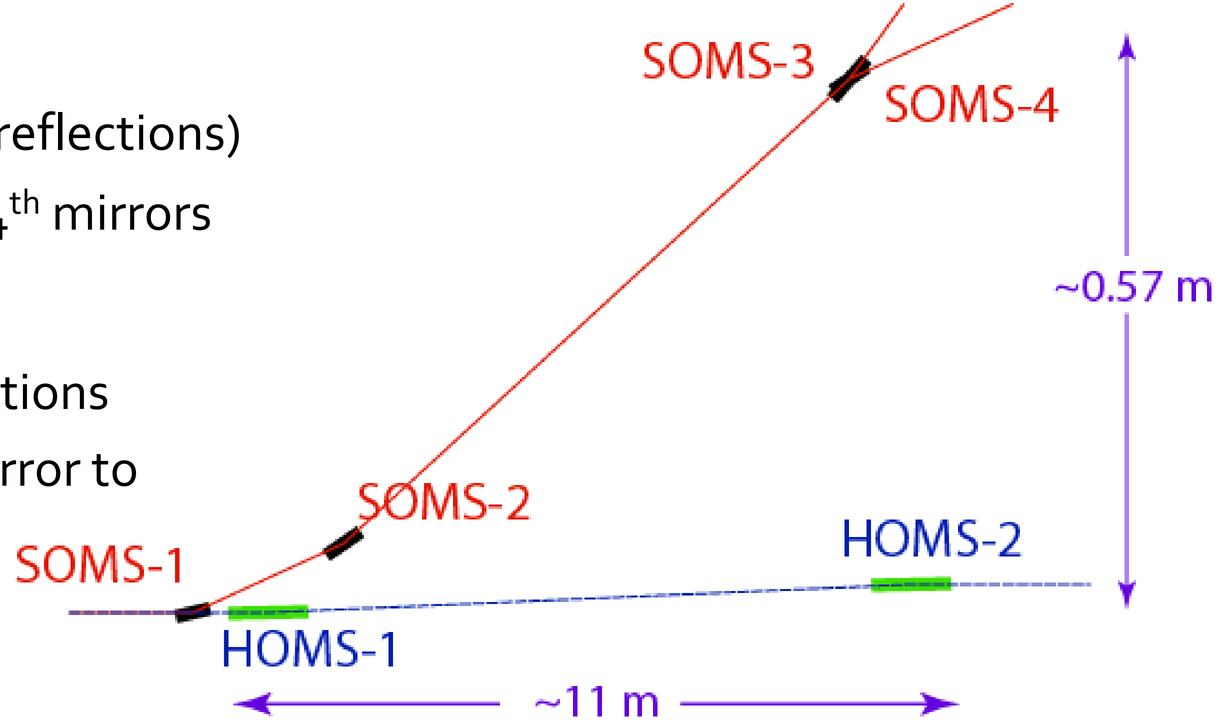


## SOMS: $0.8 < E < 2$ keV

- Total of four mirrors (3 reflections)
- Choose between 3rd & 4th mirrors

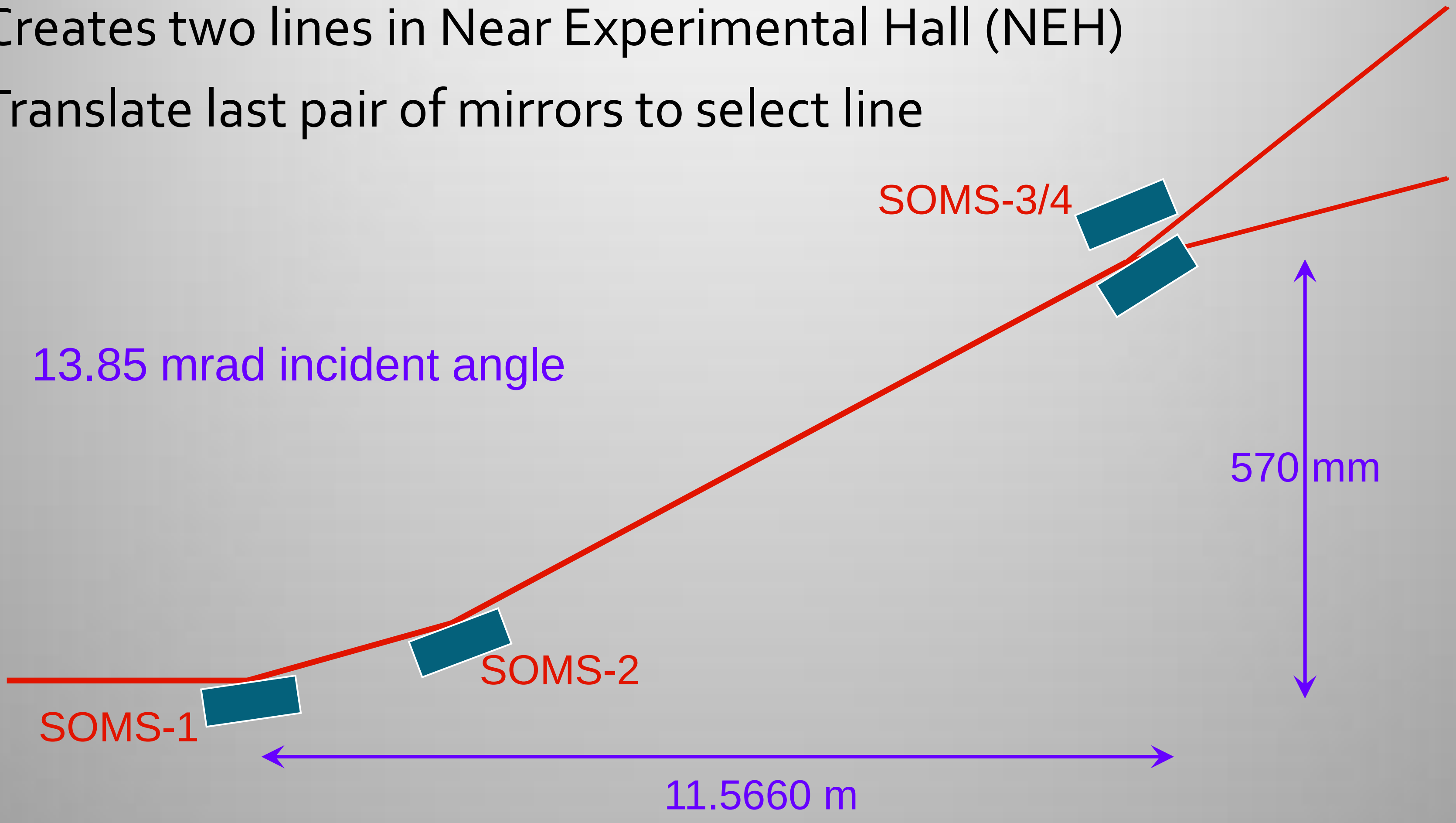
## HOMS: $2 < E < 24.8$ keV

- Two mirrors/two reflections
- Withdraw 1st SOMS mirror to access beamline



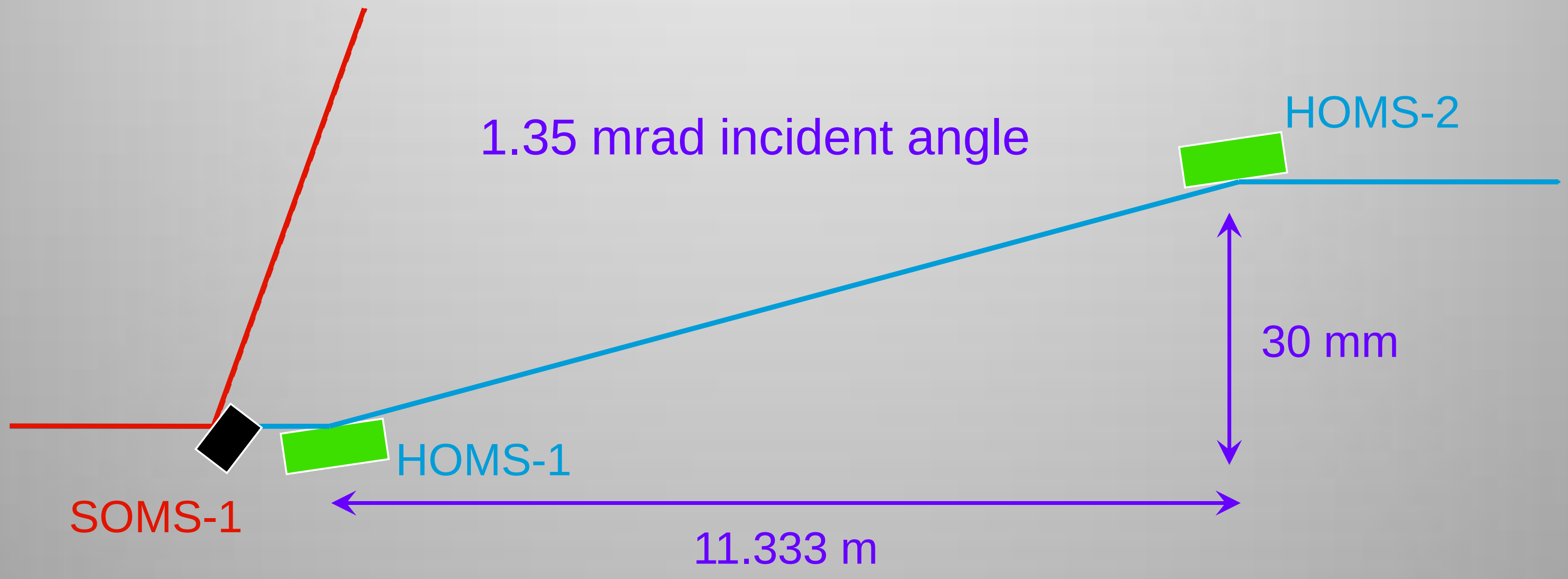
# SOMS: Soft X-ray offset mirror system

- Three reflection design to maximize horizontal deflections
- Creates two lines in Near Experimental Hall (NEH)
- Translate last pair of mirrors to select line



# HOMS: Hard X-ray offset mirror system

- Periscope design, 30 mm horizontal offset
- Withdraw first SOMS mirror to send hard beam to Fall Experimental Hall (FEH)



# Summary of LCLS x-ray mirror specifications

## Guiding design philosophy

- Maximize throughput (high reflectivity, sufficiently long mirrors)
- Limit increase in beam size
- Minimize wave-front distortions
- Balance against state of the art vendor capabilities
- Start with metrology data from recent mirrors delivered to SSRL; iterate with potential vendors to explore possibility for improvements
- Use formalism developed by Church & Takacs (and others)

**Balance requirements against manufacturability**

| Error Category | | Specification | Spatial Wavelength |
|---|---|---|---|
| Figure | Height Error | ≤ 2.0 nm rms‡ | 1 mm to Clear Aperture† |
| | Slope Error | ≤ 0.25 μrad rms‡ | |
| Mid-Spatial Roughness | | ≤ 0.25 nm rms | 2 μm to 1 mm |
| High-Spatial Roughness | | ≤ 0.4 nm rms | 20 nm to 2 μm |

† SOMS mirrors: Flat, planar, $250\times30\times50$ mm$^3$, Clear Aperture = $175\times10$ mm$^2$

† HOMS mirrors: Pseudo-planar**, $450\times30\times50$ mm$^3$, Clear Aperture = $385\times15$ mm$^2$

**Substrate ground curved, and then bent flat

‡limited by manufacturers' capabilities

M. Pivovaroff *et al., Proc SPIE*, **6705**, (2007)

# Reflective coating requirements for LCLS X-ray mirrors

- Figure: Coating should preserve the substrate figure specification of 0.25 μrad rms & 2 nm rms $\sigma_{total}^2 = \sigma_{sub}^2 + \sigma_{film}^2$

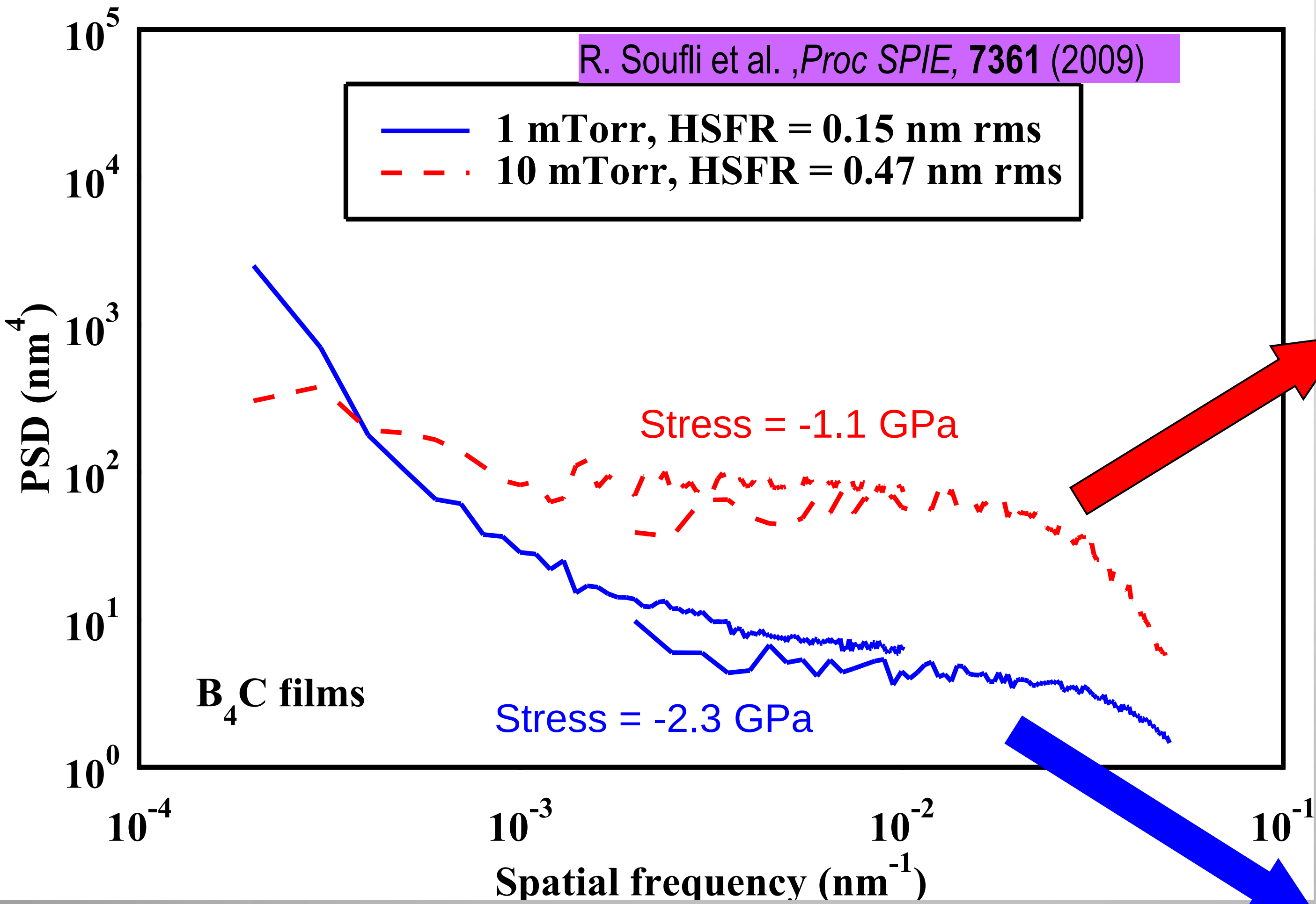
➔Coating is allowed to contribute < 1 nm rms figure error across clear aperture (175×10 mm$^2$ for SOMS, 385×5 mm$^2$ for HOMS)

- Roughness: Coating should have low HSFR (will inherently replicate MSFR)
- Stress: Coating should have low stress (< 1GPa for ~50 nm coating thickness), to prevent figure deformation or delamination from Si substrate
- Lifetime stability: Coating should be stable over time in ambient conditions, and under the operating conditions of LCLS X-ray mirror system

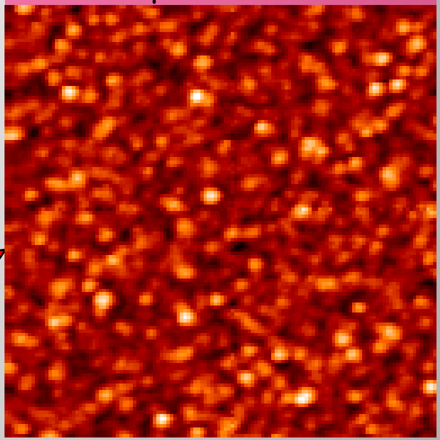
**"Mag 4" magnetron sputtering tool can accommodate 450 mm long substrates**

**Underneath view of LLNL chamber lid with 5 sputtering targets**

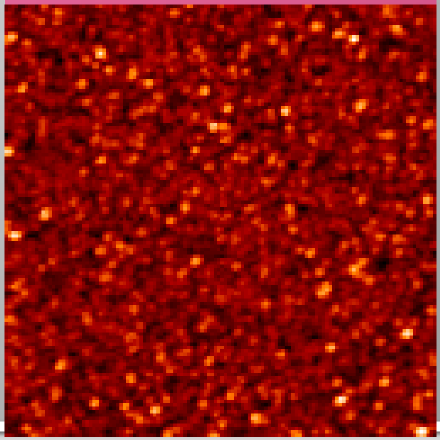
# Boron carbide thin film development for LCLS SOMS mirrors


R. Soufli et al. ,*Proc SPIE*, **7361** (2009)

500×500 nm$^2$ detail from 2x2 µm$^2$ AFM scan



500×500 nm$^2$ detail from 2x2 µm$^2$ AFM scan

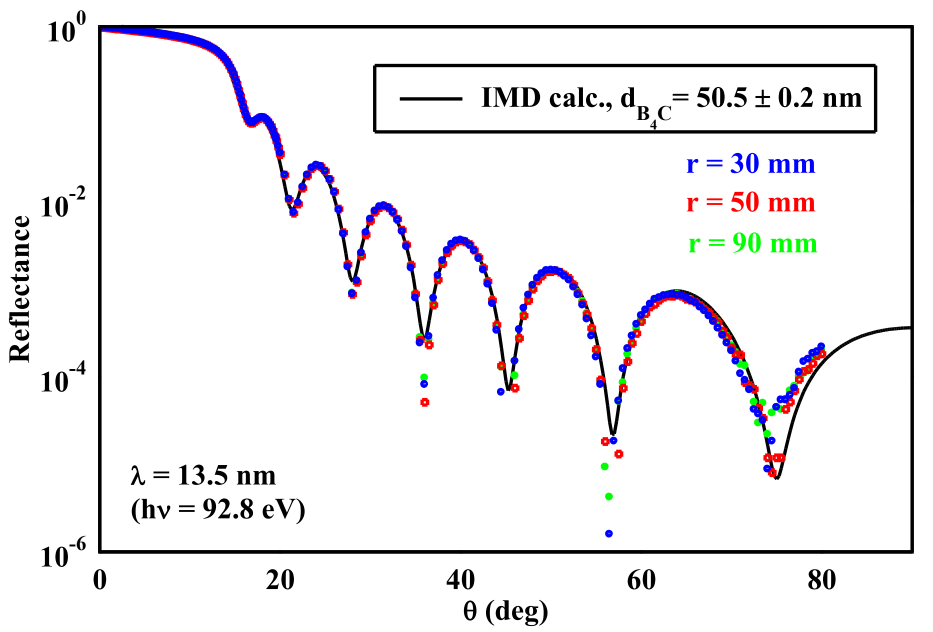


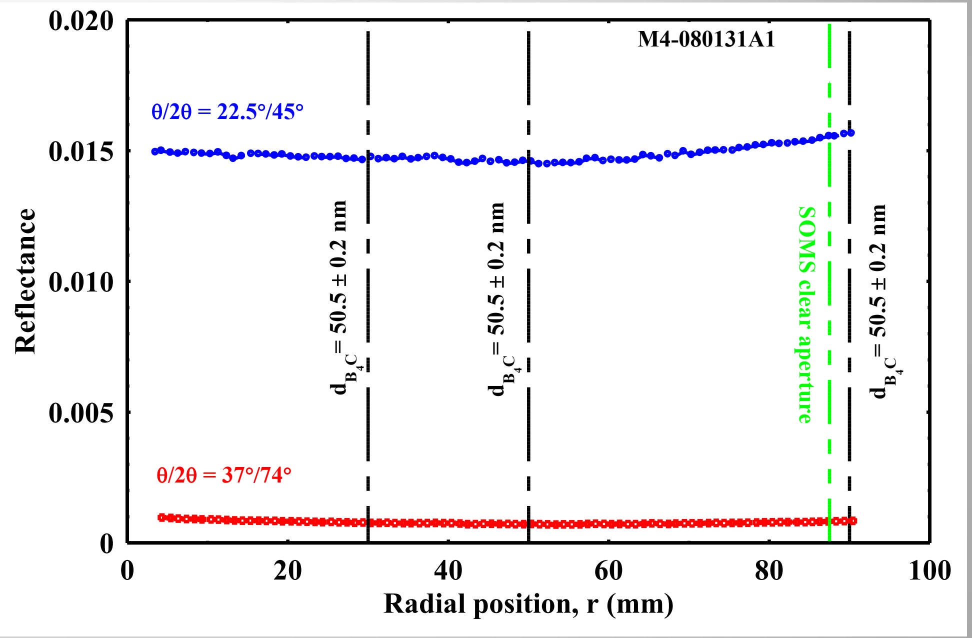
$$\sigma^2 = 2\pi\int_{f_1}^{f_2} f\, S(f)\, df$$

where S(f) ≡ PSD (nm$^4$), $f_1$= 5×10$^{-4}$nm$^{-1}$ $f_2$ = 5×10$^{-2}$ nm$^{-1}$

# SOMS and HOMS coating thickness uniformity is well within 1 nm rms specification

**Measurements obtained at ALS beamline 6.3.2. (LBNL)**





R. Soufli *et al.*, *Proc SPIE*, **7077**, (2008)

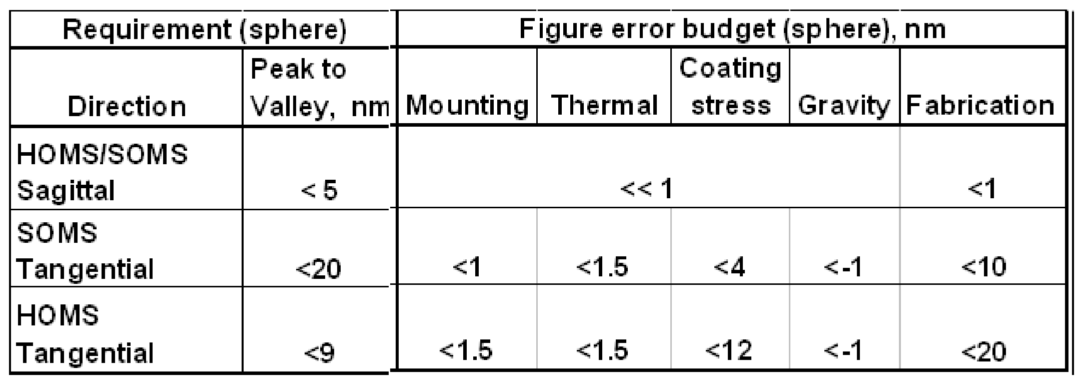
- $B_4C$ measured thickness variation: < 0.4 nm P-V, < 0.14 nm rms (< 0.28% rms) across the 175-mm SOMS clear aperture
- SiC measured thickness variation: < 1 nm P-V, < 0.34 nm rms (< 0.7 % rms) across the 385-mm HOMS clear aperture

# HOMS and SOMS engineering challenges

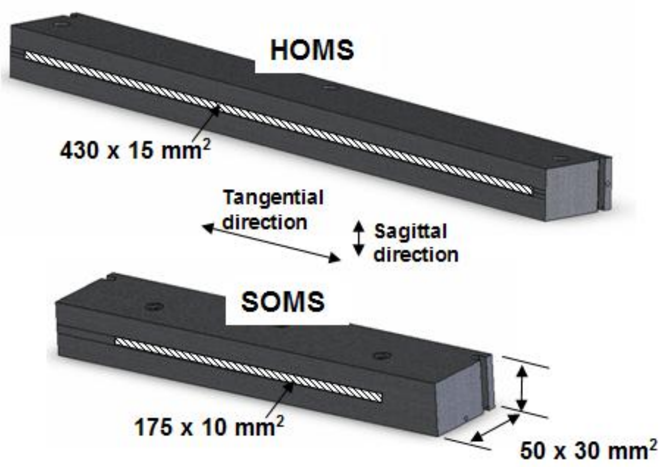
- Pointing
  - Facility requirement of less than 10% increase in spot size
    - SOMS < 900 nrad
    - HOMS < 90 nrad
- Flatness requirements
  - Ideally, better than 1 nm rms height errors for coherence preservation
  - High-stress coatings will impart spherical curvature—manufacturer with concave bend to compensate
  - Ensure bending can remove spherical curvature induced by coatings
  - Design a mounting system that imparts minimal change to mirror
- Design for thermal and vibrational stability

# The mirror & mount are designed to meet figure-error budget

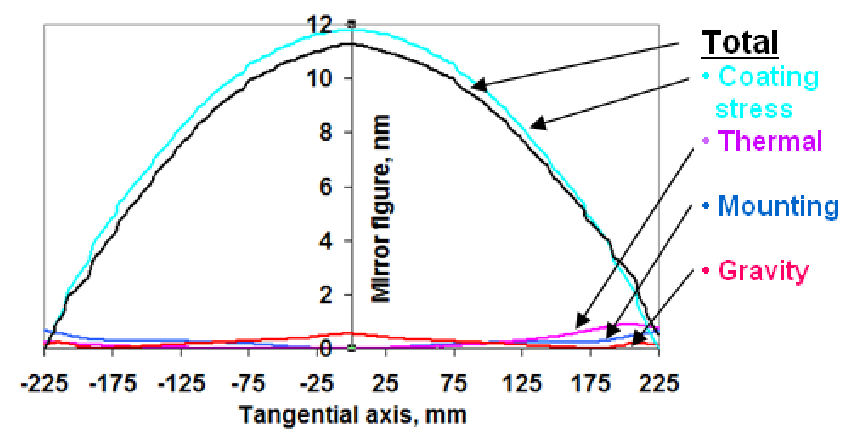
To limit intensity ellipticity to 10%



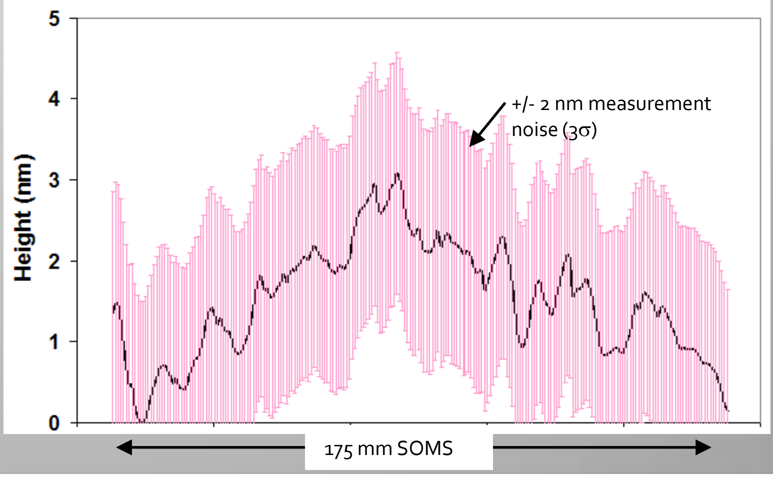
| Requirement (sphere) | | Figure error budget (sphere), nm | | | | |
|---|---|---|---|---|---|---|
| Direction | Peak to Valley, nm | Mounting | Thermal | Coating stress | Gravity | Fabrication |
| HOMS/SOMS Sagittal | < 5 | << 1 | | | | <1 |
| SOMS Tangential | <20 | <1 | <1.5 | <4 | <-1 | <10 |
| HOMS Tangential | <9 | <1.5 | <1.5 | <12 | <-1 | <20 |



Finite element analysis guided optimization of the mirror and mount design (HOMS case is plotted);
Analysis was benchmarked to measurements

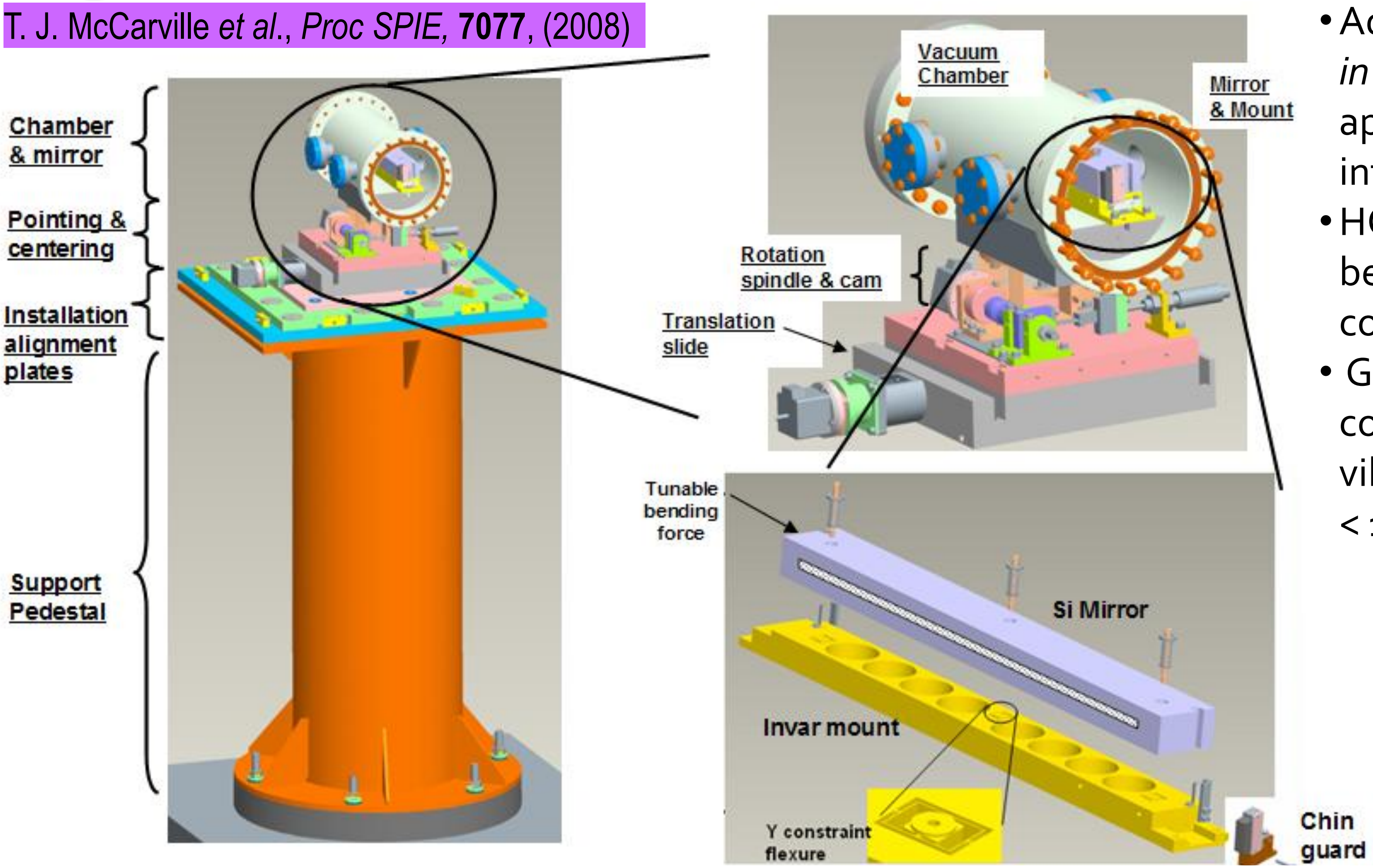


Coated SOMS measured every 2 min for 48 hr
12"-aperture interferometer calibrated with 3-flat test



# HOMS and SOMS installation and alignment at LCLS

T. J. McCarville *et al*., *Proc SPIE,* **7077**, (2008)



- Mounting employs flexures
- Adjust, based on *in situ* full-aperture interferometry
- HOMS figure can be remotely controlled
- Good design controls vibrational jitter < 10 nrad

- Thermal stability for rotation/translation is 70/300 nrad/0.1° C
- T-controlled enclosure demonstrates ±0.01 °C temperature and ±30 nrad HOMS stability

# HOMS #1 figure coated and installed on mount

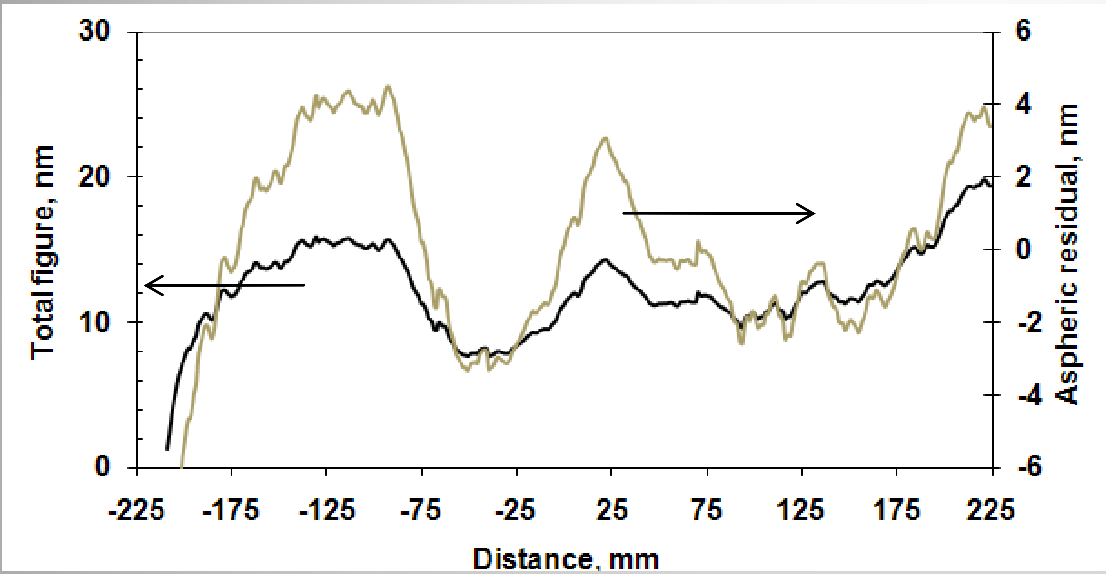
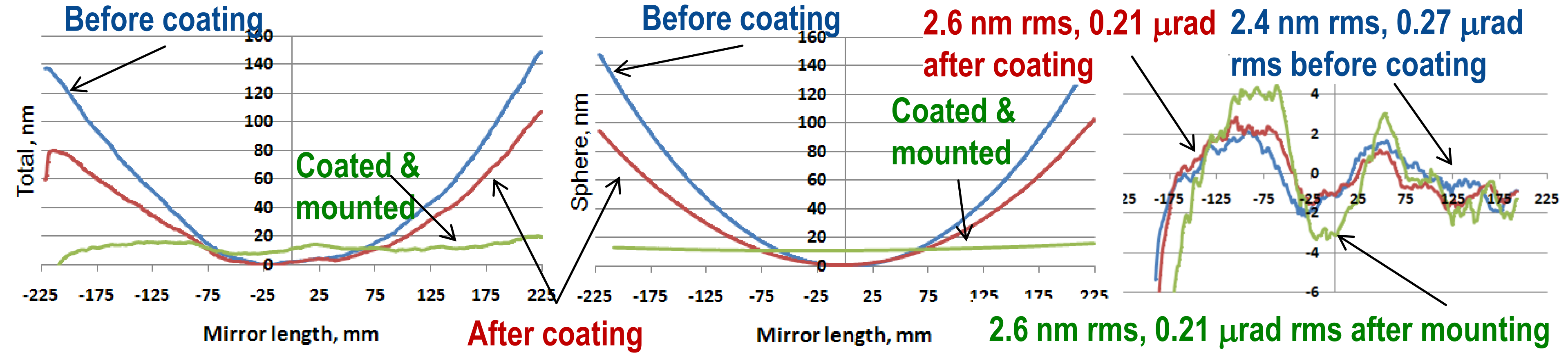


Figure corrections have been made to HOMS mounted mirrors without significantly contributing to aspheric curvature

Total figure = Spherical curvature + Aspheric residual



Before coating

Coated & mounted

After coating

Before coating

Coated & mounted

2.6 nm rms, 0.21 μrad after coating

2.4 nm rms, 0.27 μrad rms before coating

2.6 nm rms, 0.21 μrad rms after mounting

# HOMS #2 figure coated and installed on mount

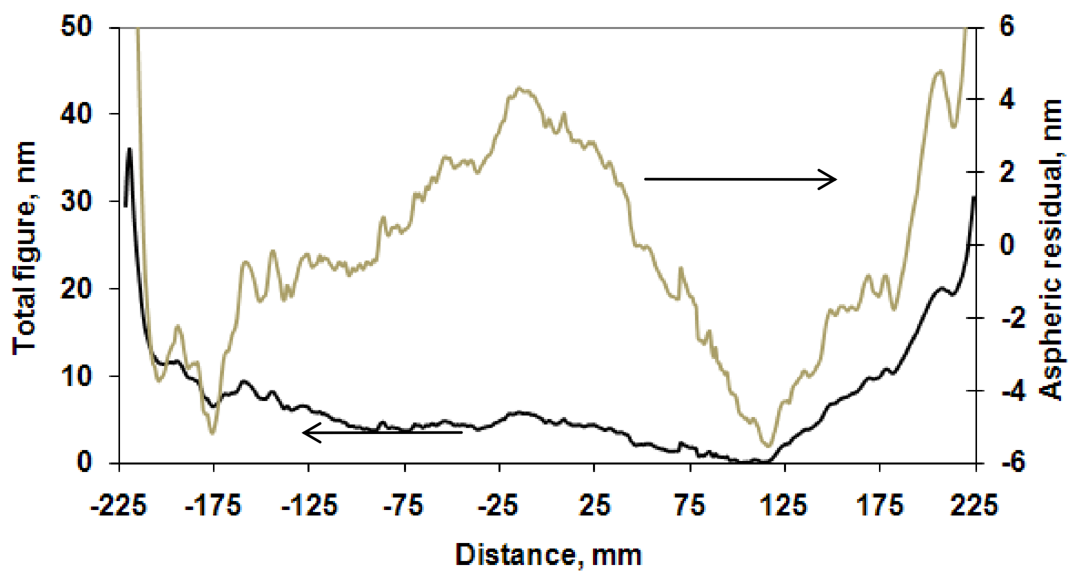
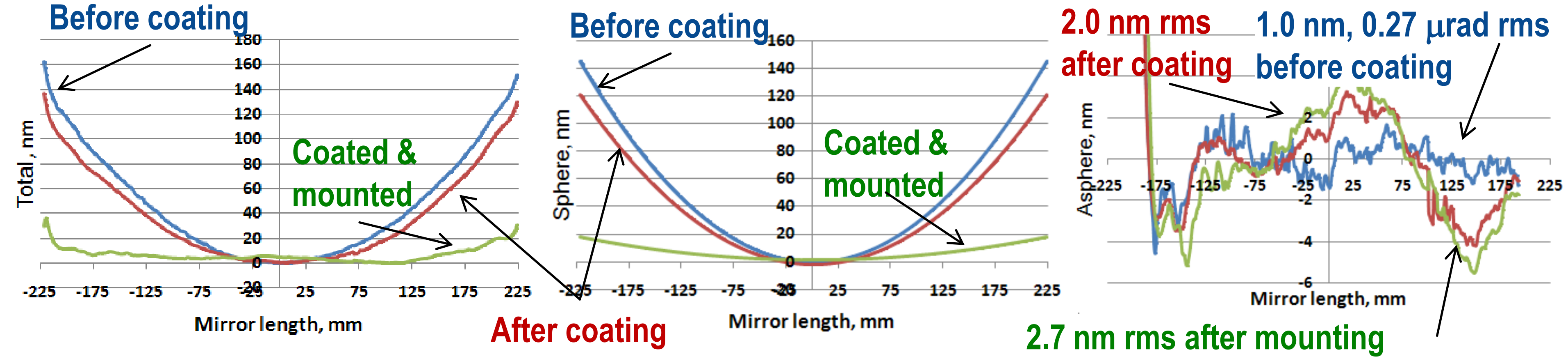


Figure corrections have been made to HOMS mounted mirrors without significantly contributing to aspheric curvature

**Total figure = Spherical curvature + Aspheric residual**



Before coating

Coated & mounted

After coating

Before coating

Coated & mounted

2.0 nm rms after coating

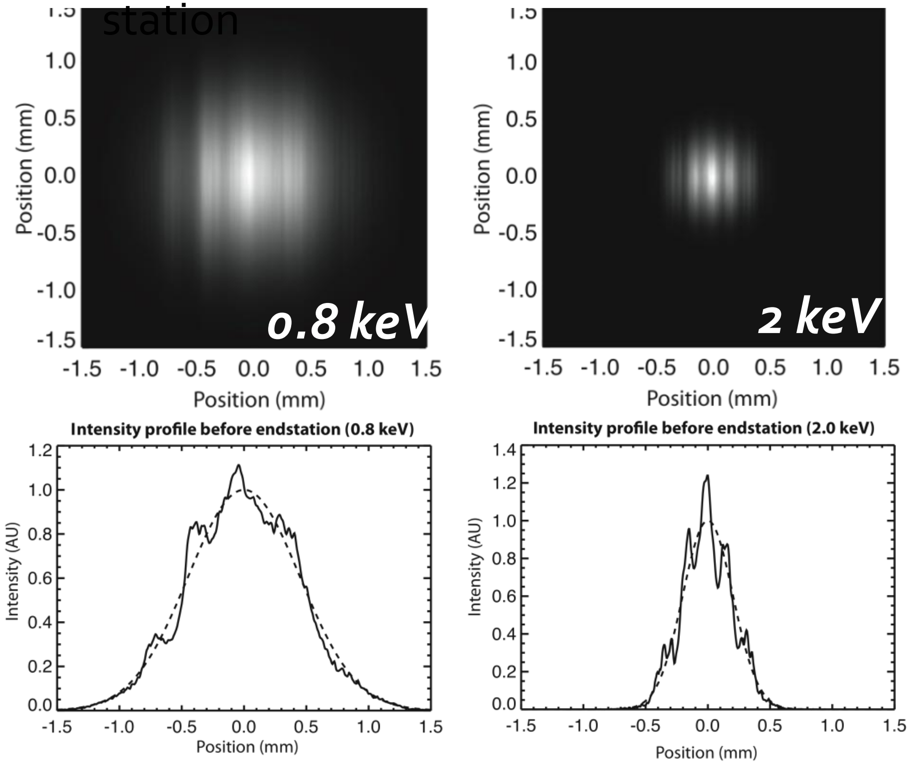
1.0 nm, 0.27 µrad rms before coating

2.7 nm rms after mounting

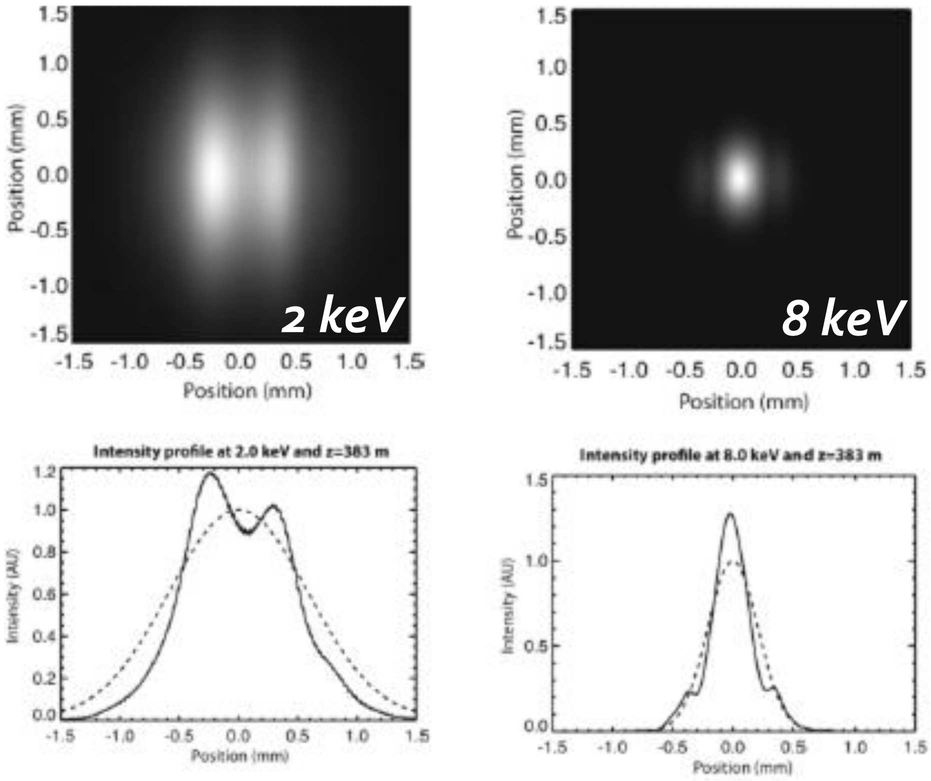
# SOMS & HOMS performance predictions

- LLNL metrology data, coupled into coherent wavefront propagation code, used to predict HOMS & SOMS focal spot structure
  - Scalar diffraction model was employed
  - Same methodology to select order of SOMS and HOMS elements for optimum performance

**SOMS branch line before AMO end station**



**HOMS branch line before CXI end**



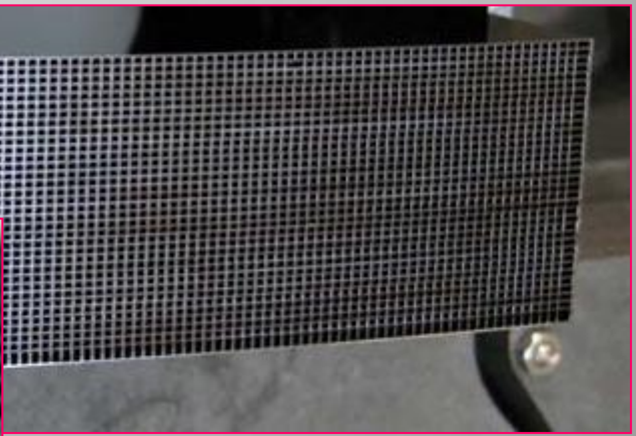
A. Barty *et al*. *Optics Express*, **17**, (2009)

# FUTURE TRENDS

# X-ray astronomy

- ESA (and NASA?) pursuing large missions

- ESA now pursuing L-class mission ATHENA (**A**dvanced **T**elescope for **H**igh **EN**ergy **A**strophysics)
- Technologies
  - Silicon pore optics
  - Slumped glass
  - Replication ?

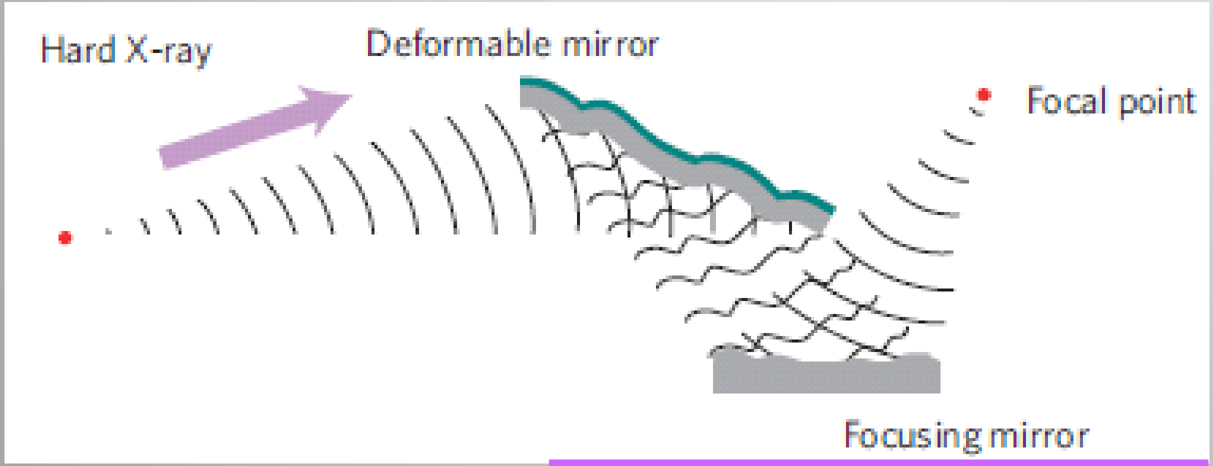


Marcos Bavdaz, “Silicon Pore Optics”, (MPE: 17-19 Sep 2008)

# Adaptive x-ray optics

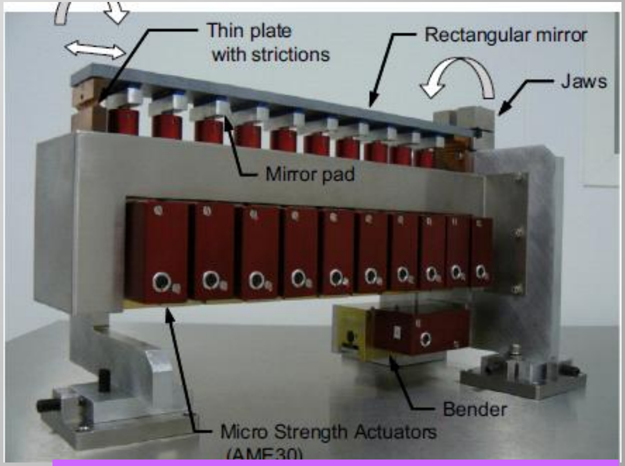
- Light sources will place ever more stringent requirements on optics
- Traditional fabrication and metrology approaches may not work
- One approach: closed-loop, *in situ* monitoring (*e.g.*, using at-wavelength sensing) and correction using actuated mirrors
- Some state-of-the-art efforts:

***Osaka consortium***



H. Mimaru *et al.*, *Nat Phys*, **6**, 123, (2010)

***SOLEIL***



M Idir *et al.*, *NIM A*, **616**, 162, (2010)

- LLNL has a nascent effort underway that leverages strong visible light AO expertise and LCLS x-ray optics development effort