Update on the state of technology for a critical-angle x-ray transmission grating spectrometer on the X-ray Surveyor

X-ray Surveyor technology teleconference

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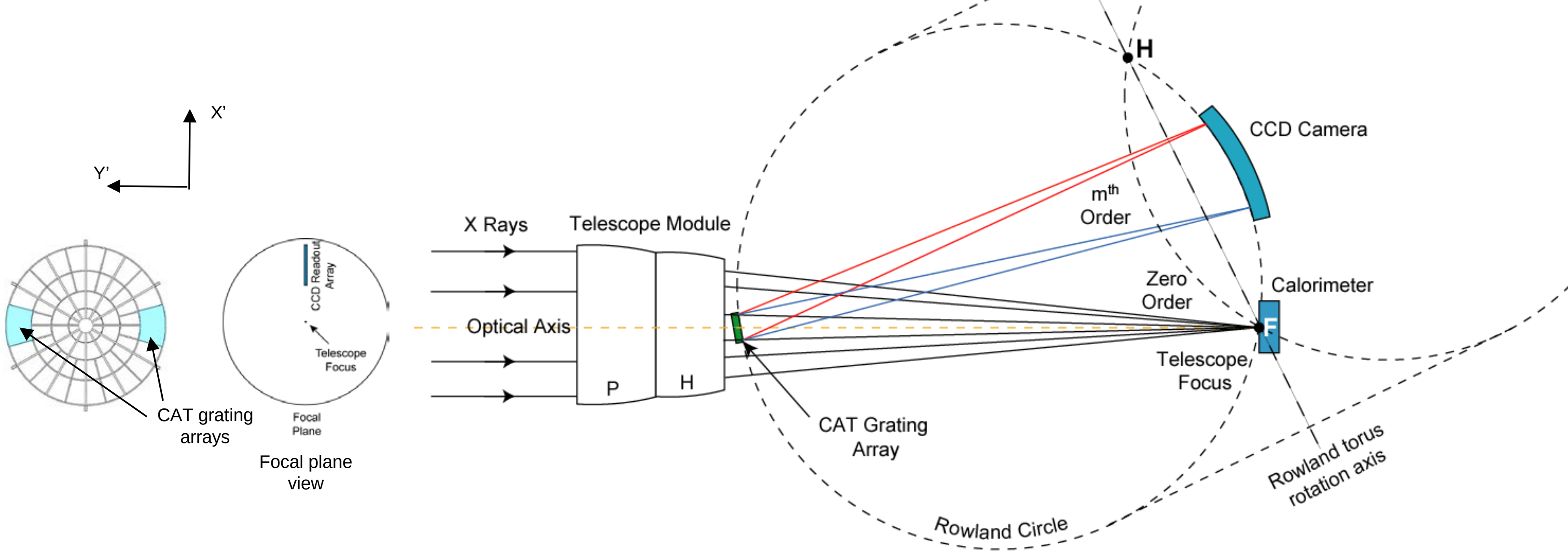
Why CAT Gratings?

- **Combine advantages of transmission and blazed reflection gratings:**
  - Very relaxed alignment and flatness tolerances
  - Low mass
  - Low temperature sensitivity
  - Highly transparent to high-energy x rays
  - High diffraction efficiency
  - Blazing into high orders/to large angles → high resolving power
  - Allows simple design of XGS with minimal resource requirements and orders of magnitude improved performance over existing instruments (HETGS, RGS).

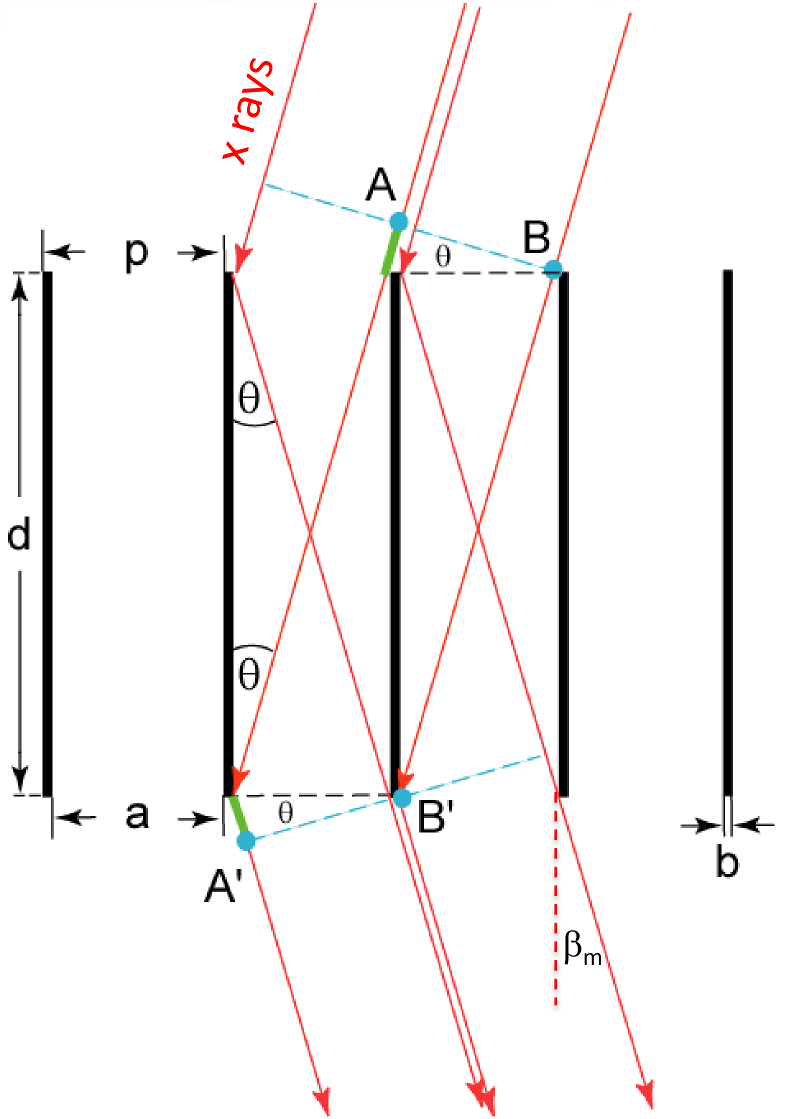
Technical Background: CATXGS Design

Optical Design:

- Wolter I (or similar) telescope mirrors.
- Diffraction gratings in converging beam just aft of mirrors.
- Gratings, camera, and focus share same Rowland torus.
- Blazed gratings; only orders on one side are utilized.
- Only fraction of mirrors is covered: “sub-aperturing”.



CAT Grating Principle



Grating equation:

$m\,\lambda = p\,(\sin(\theta) + \sin(\beta_m))$,
m = diffraction order

Blazing: $\beta_m \sim \theta$

High reflectivity:
$\theta < \theta_c$ = critical angle of total external reflection

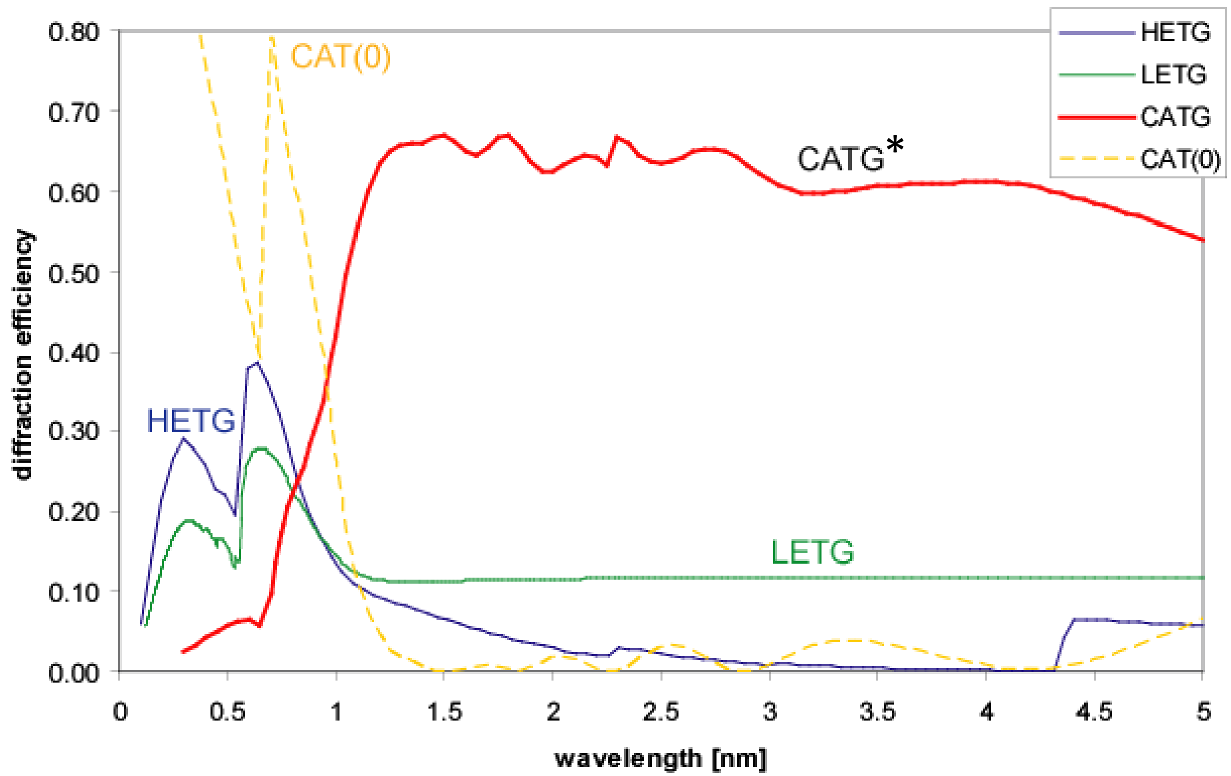
Strawman:

Silicon grating, $\theta = 1.75^o$
p = 200 nm
b = 40 nm
d = 5.2 μm
Aspect ratio d/b = 125

Model Diffraction Efficiencies

Theoretical model: Rigorous Coupled-Wave Analysis (RCWA)
Parameters:
wavelength λ, index of refraction n, period p, depth d, duty cycle b, angle of incidence θ

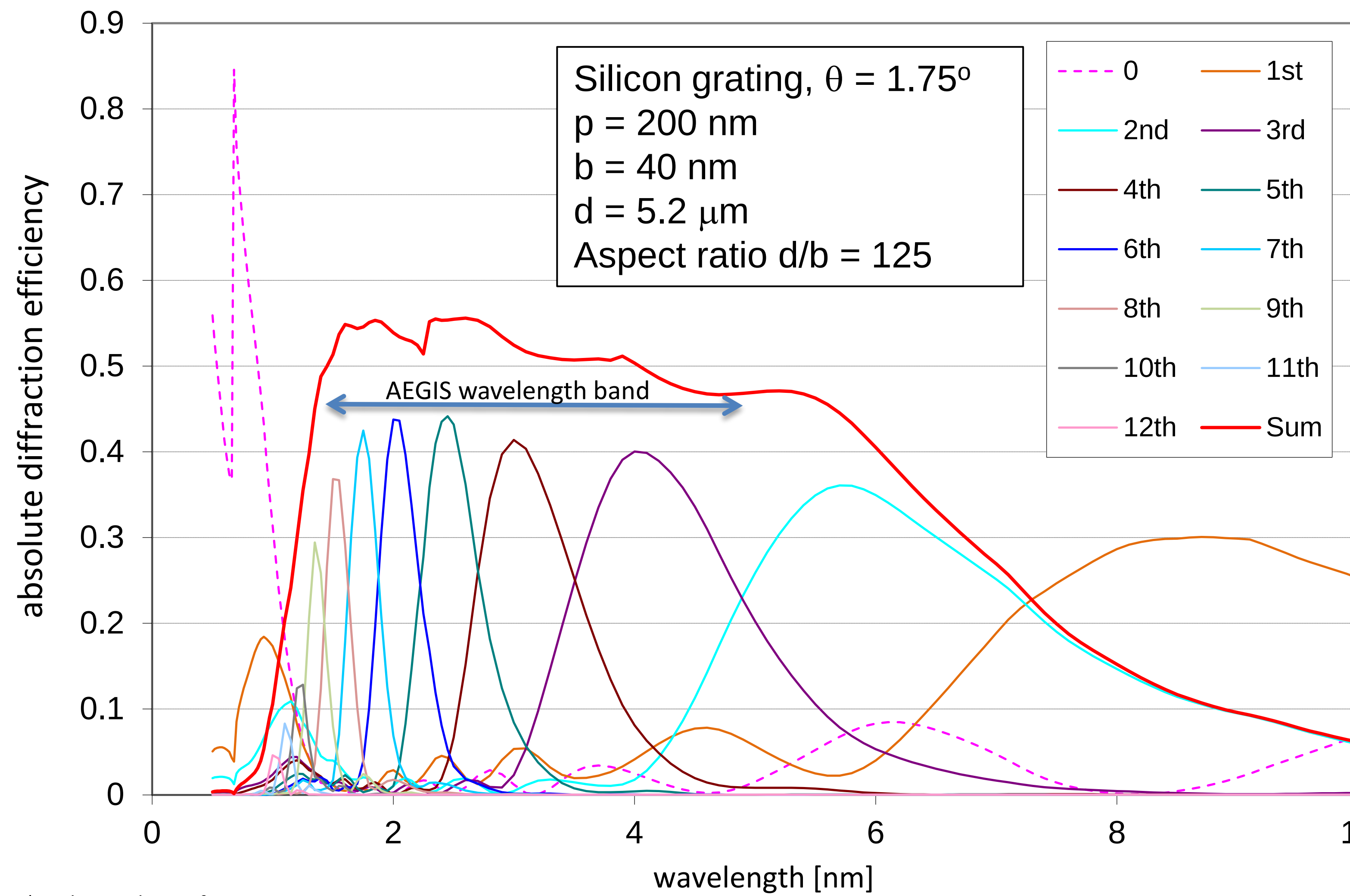
Absorption due to CAT grating bars already included in model, but not losses from additional structural supports (L1, L2, etc.)



*neglecting losses from supports

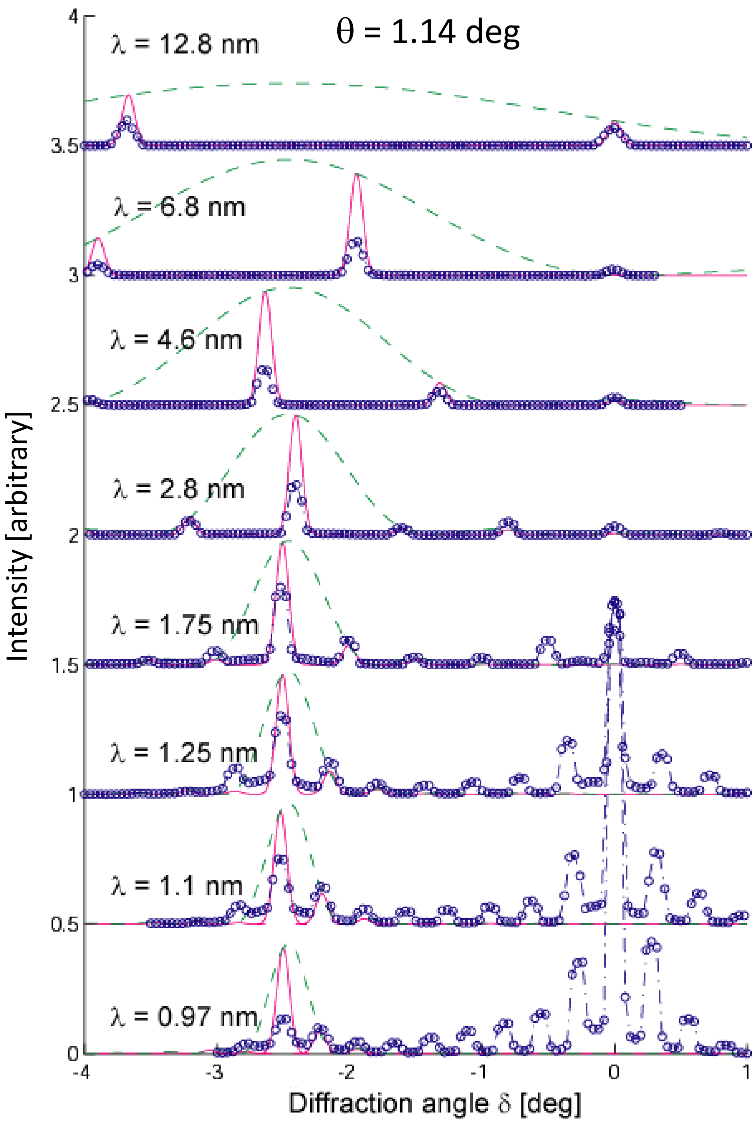
Model Diffraction Efficiencies

for AEGIS design parameters



*neglecting losses from supports

Blazing at Different Wavelengths



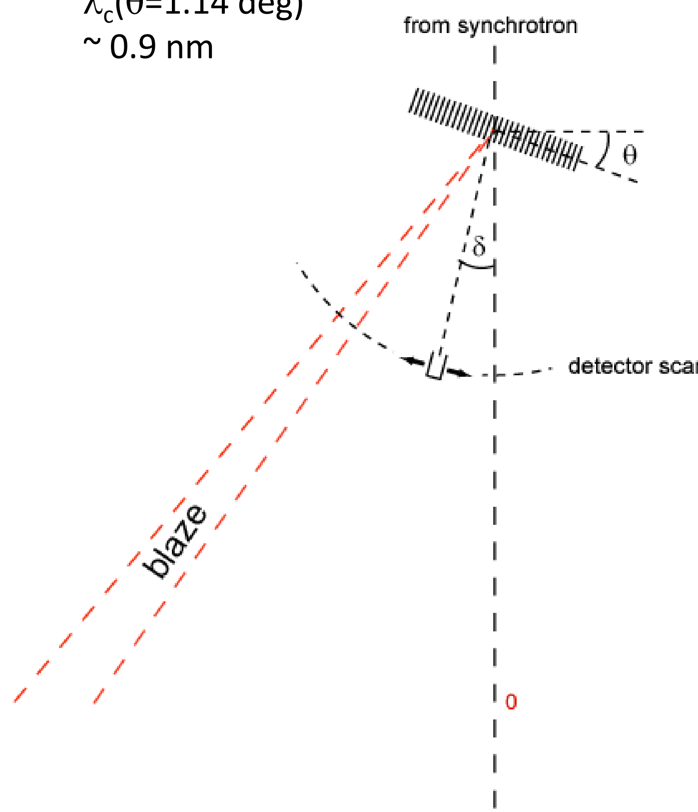
X-ray data

Scanning wavelength:

Blaze peak width ~ λ

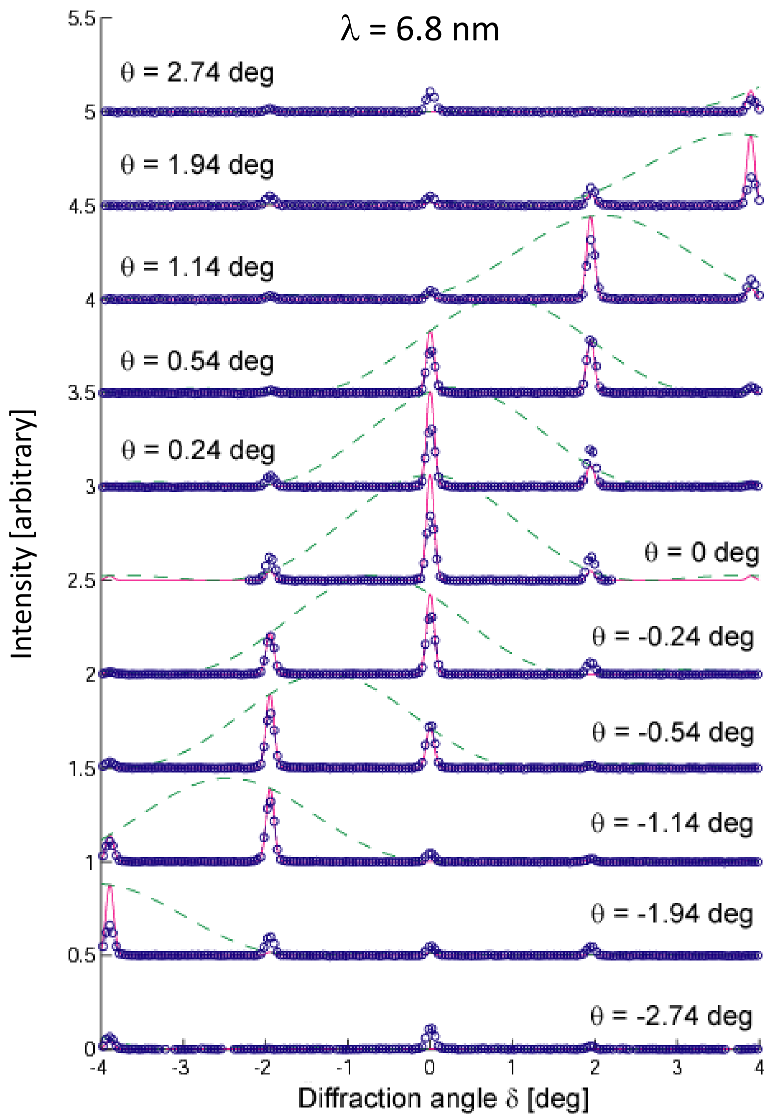
Small λ blaze in higher order *m*

$\lambda_c(\theta=1.14\ \text{deg})$
~ 0.9 nm

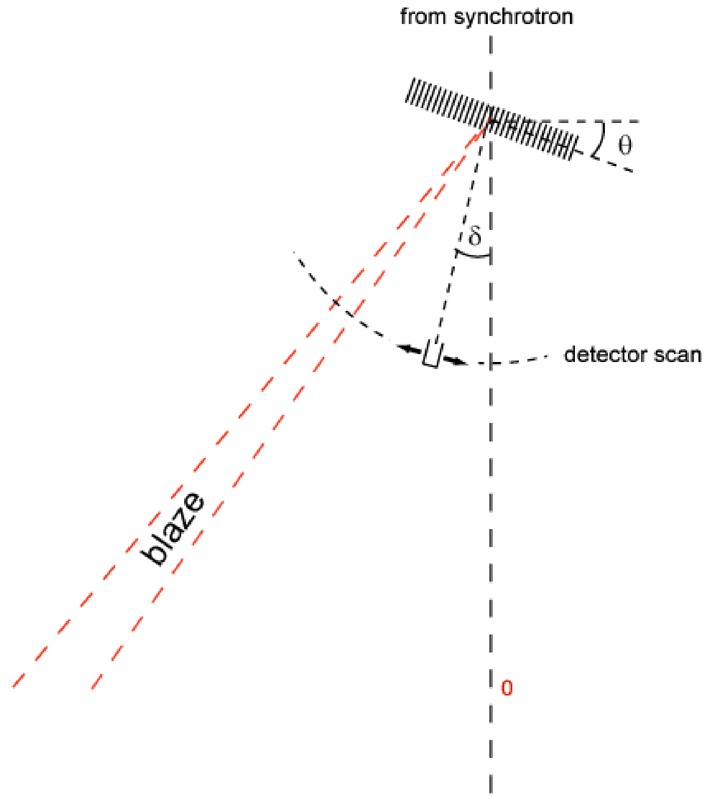


Heilmann *et al.*, Proc. SPIE 74370G (2009)

Blazing and Alignment Insensitivity



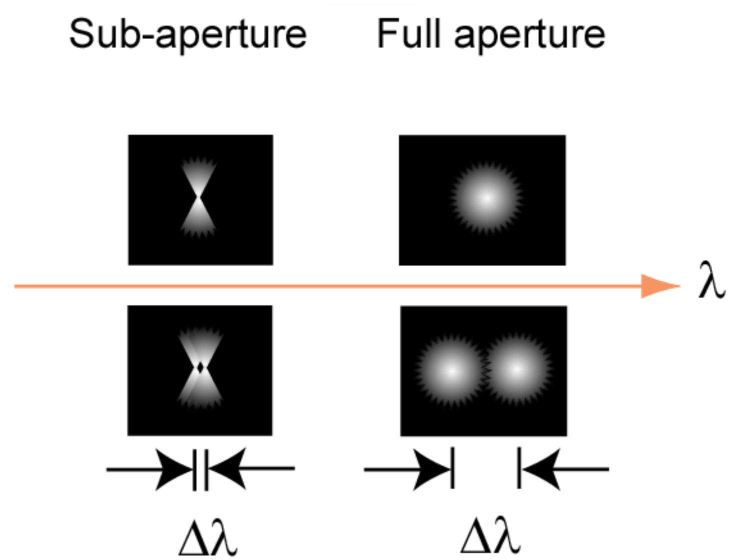
X-ray data
"rocking" the grating:
Blaze angle ~ 2θ
Diffraction angle ~ const.



Heilmann *et al.*, Proc. SPIE 74370G (2009)

Raytracing and Resolving Power

- **Boosting resolving power through sub-aperturing:**
  - Sub-aperturing takes advantage of anisotropic scattering in grazing-incidence reflective optics.
  - Align dispersion direction with narrow dimension of anisotropic PSF → increase spectral resolution by factor 3-5.



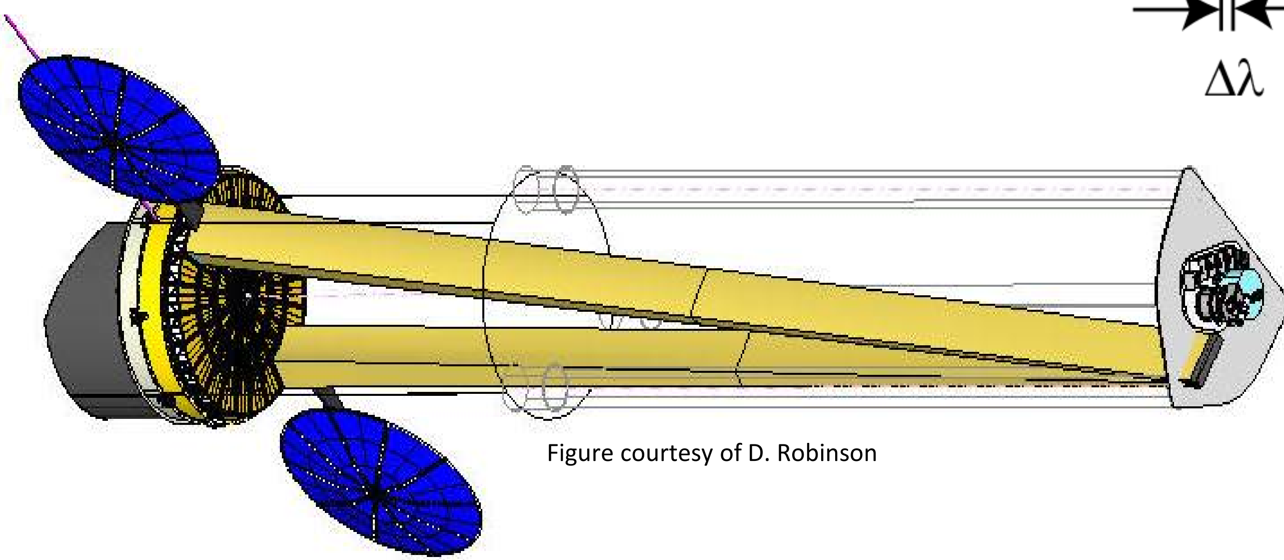
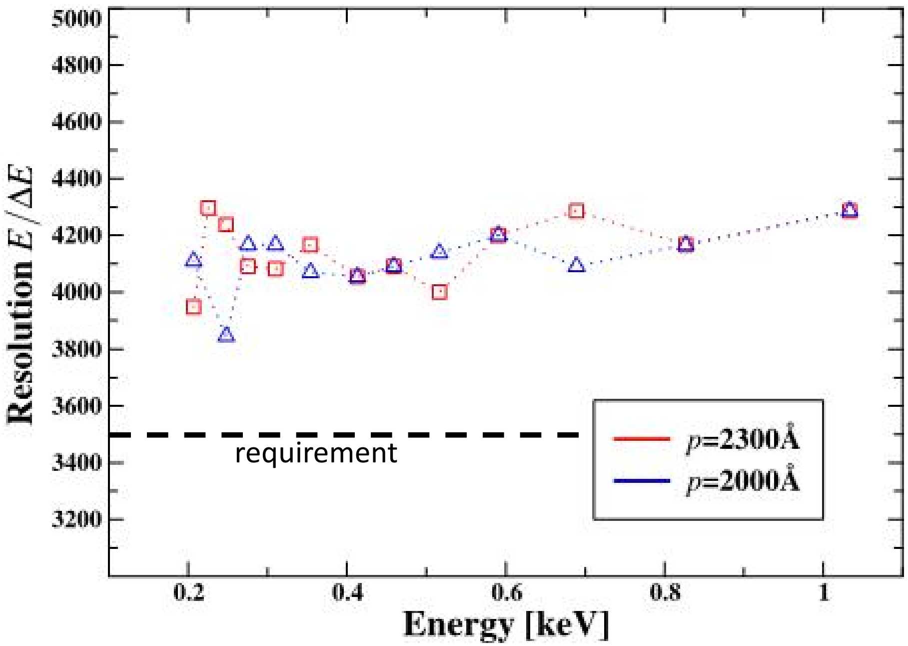
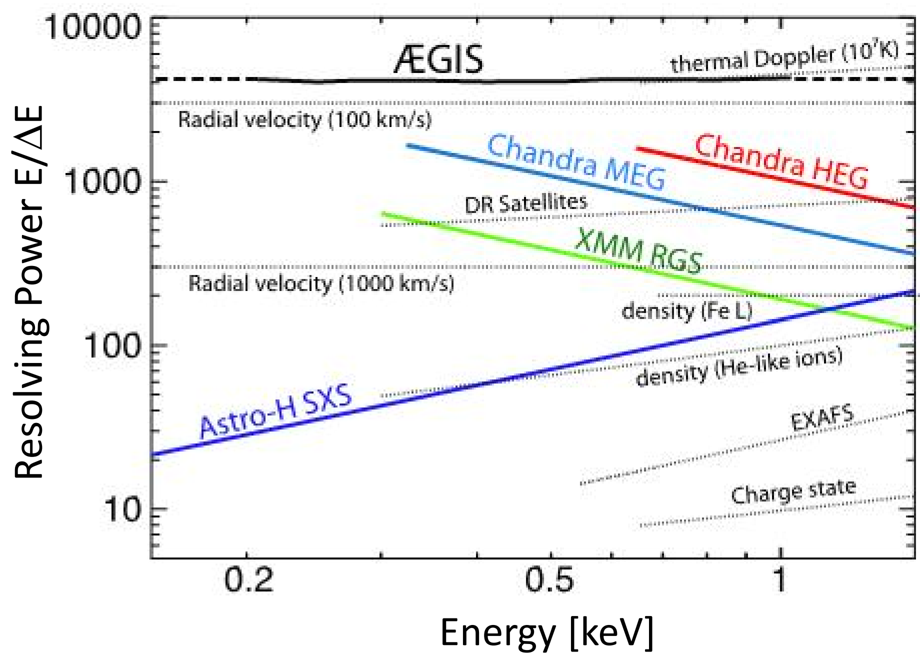


Figure courtesy of D. Robinson

Raytracing and Resolving Power

AEGIS as a probe-size reference mission (10” mirror PSF)

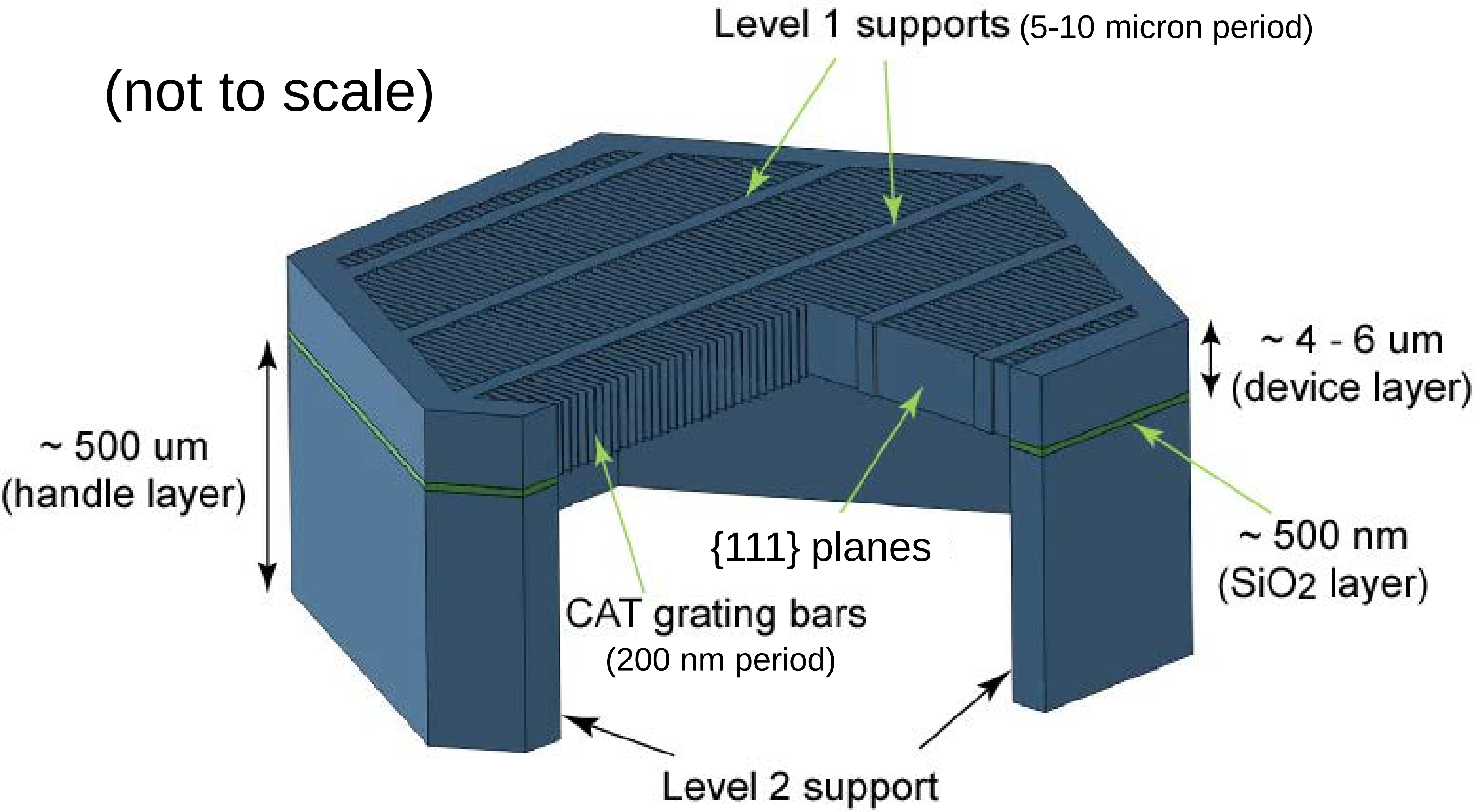




http://pcos.gsfc.nasa.gov/studies/rfi/Bautz-Marshall-RFINNH11ZDA018L.pdf

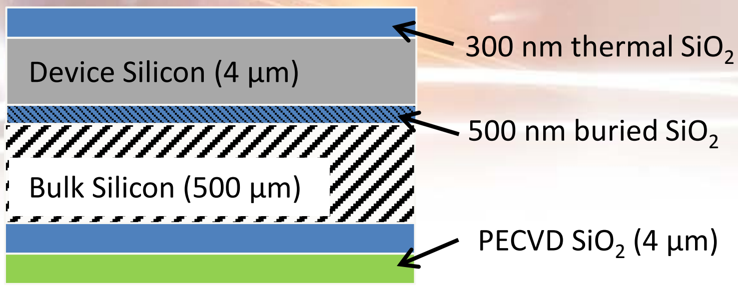
CAT Grating Structure: "Unit Cell"

(not to scale)

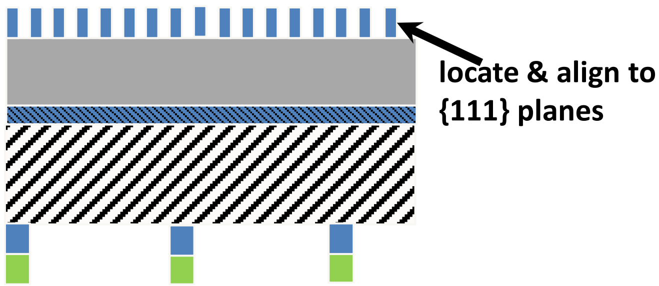


Fabrication Process

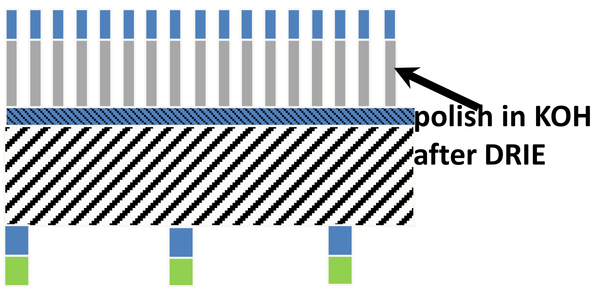
Combining DRIE with KOH Polishing



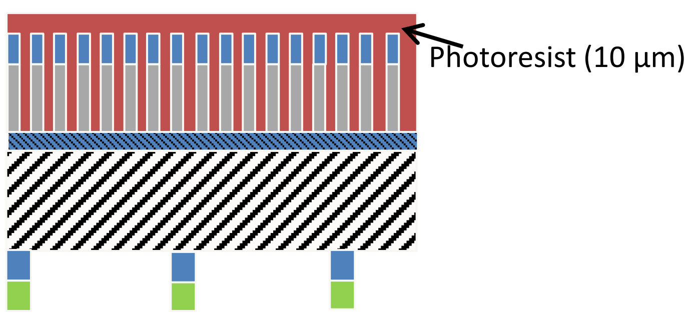
1. Start with SOI wafer



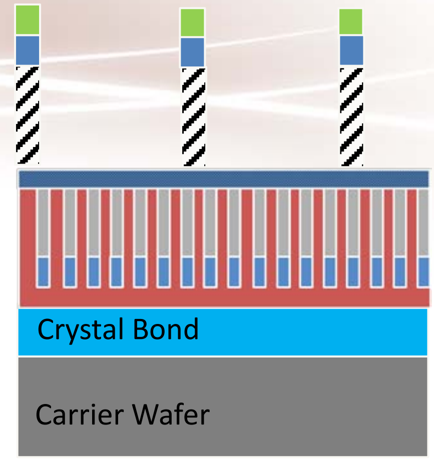
2. Pattern front and back side SiO_2



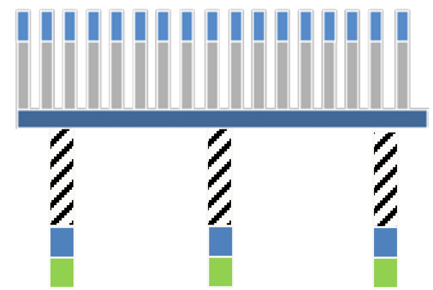
3. DRIE front side and stop on SiO_2



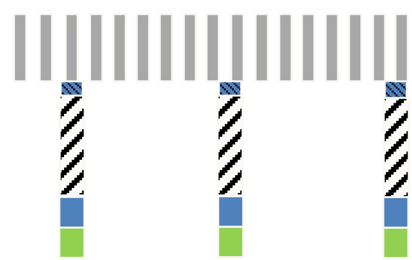
4. Fill front side gratings with photoresist



5. Flip over, bond to carrier wafer with crystalbond under vacuum, DRIE handle layer



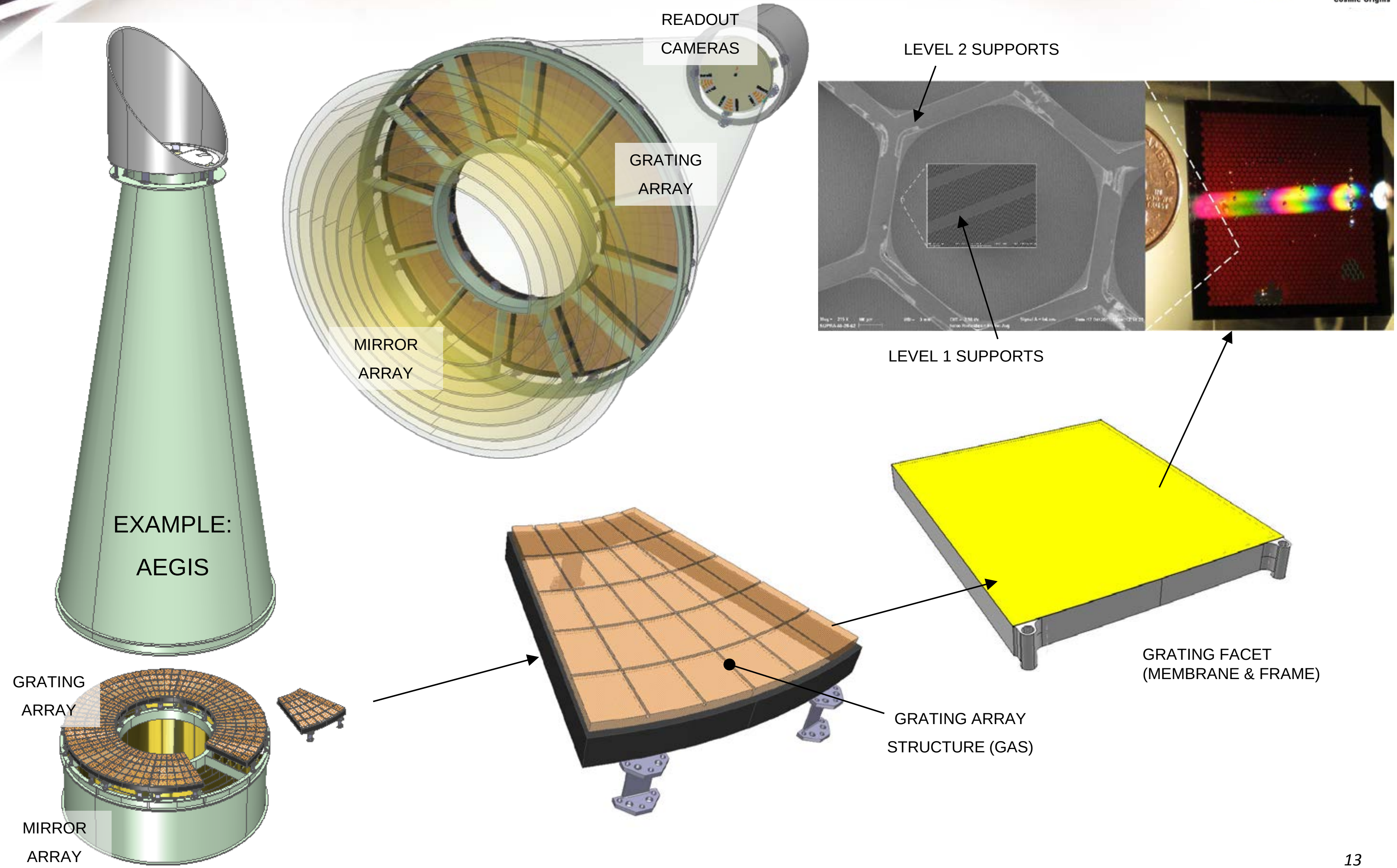
6. Separate from carrier in hot water, piranha clean twice and critical-point dry



7. Remove buried SiO_2 and SiO_2 front side mask via vapor HF

Heilmann *et al.*, Proc. SPIE 960314 (2015)

CATXGS Structural Hierarchy



Key Performance Parameters/Technical Targets

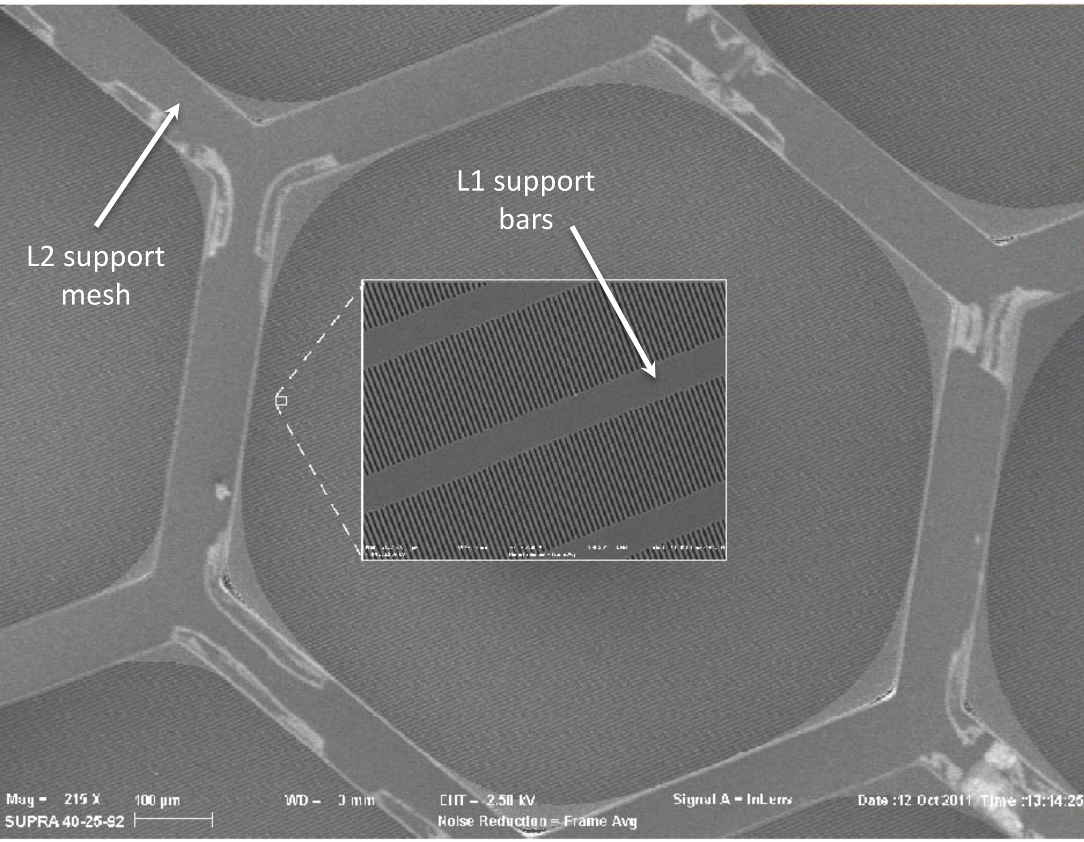
- Grating "throughput" (effective area)
  - Flow down from science requirement for effective area.
  - Mirror design gives mirror effective area and aperture to be covered by gratings.
  - Losses reduce mirror effective area:
    - Blockage from grating support structures (GAS, facet frames (L3), L2, L1)
    - Gaps between grating facets
    - Diffraction efficiency < 100%
    - Detector size and readout/quantum efficiency
  - Realistic grating throughput goal: > 0.3
- Resolving Power
  - Flow down from science requirements
  - Requirement: $R = \lambda/\Delta\lambda = 3500$
  - Determined by
    - Mirror design, mirror PSF, error distribution within mirror PSF
    - Assembly and alignment errors
    - Optical design (focal length, Rowland torus parameters, sub-aperture azimuth, grating size, blaze angle)
    - Grating period variation $\Delta p/p$
    - Detector pixel size
    - Thermal expansion
    - Spacecraft pointing

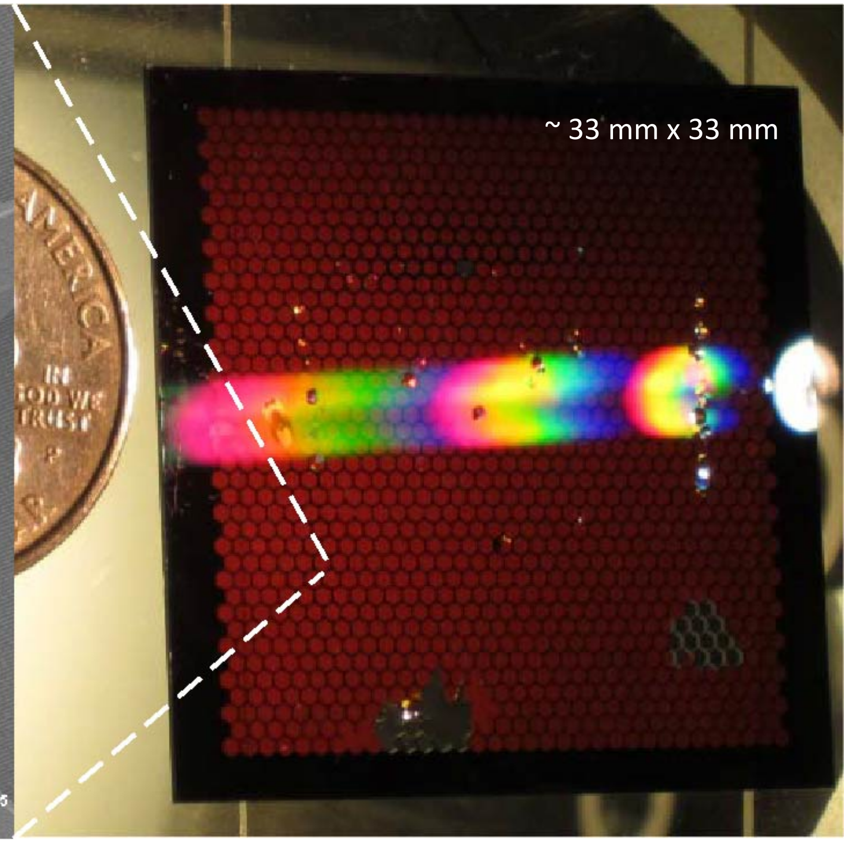
Technical Status

- Major milestones
  - Developed front and backside DRIE process -> freestanding gratings with narrow L1 supports
  - Integrated KOH polishing into process for smoother sidewalls
  - Confirmed theoretical diffraction efficiency predictions with synchrotron measurements over wide band of wavelengths, angles, and grating parameters (several publications in peer reviewed literature; see http://snl.mit.edu)
  - Fabricated and x-ray tested metal-coated extended-bandpass CAT gratings for resolving power measurements at MSFC Stray Light Facility (SLF)
  - Performed resolving power measurements: demonstrated R > 10,000
- Technology Readiness Level 4 (vetted by PCOS Technology Board)

Results

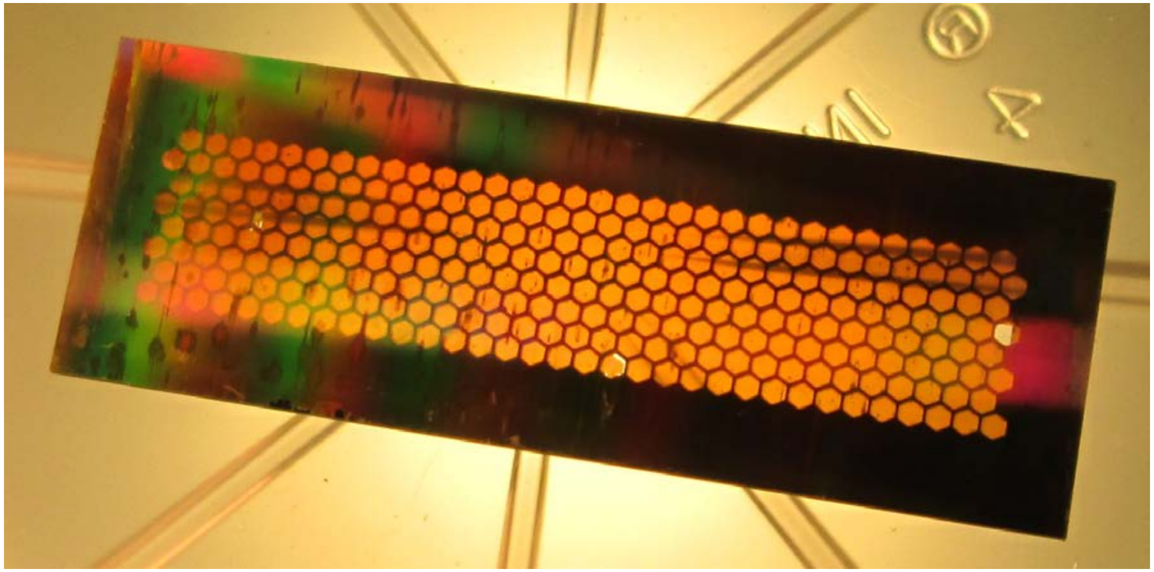
- Product: 200 nm-period silicon CAT grating membrane with integrated L1 and L2 supports, > 30x8 mm^2.

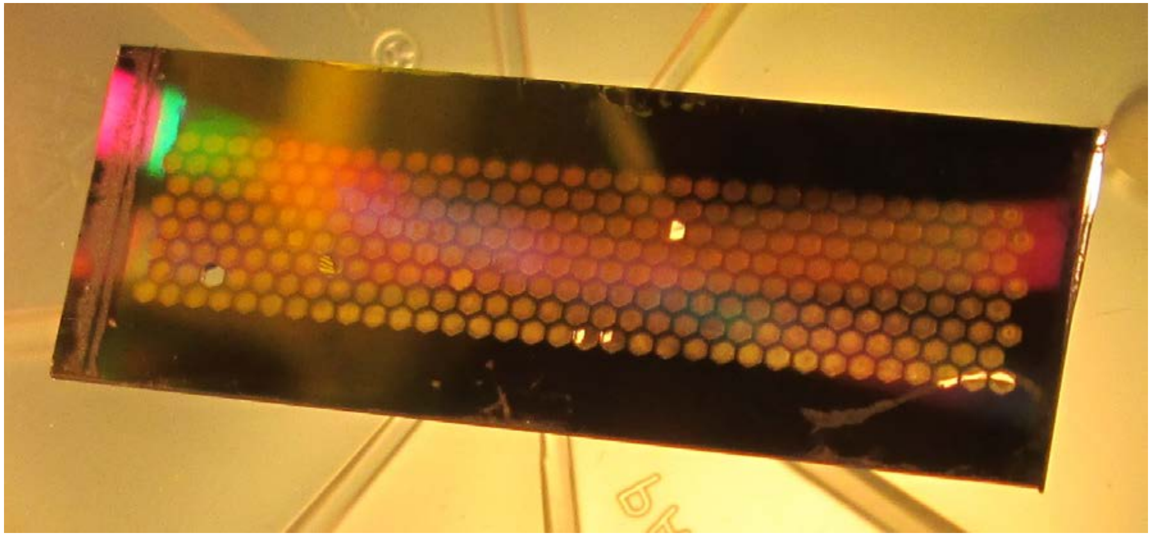


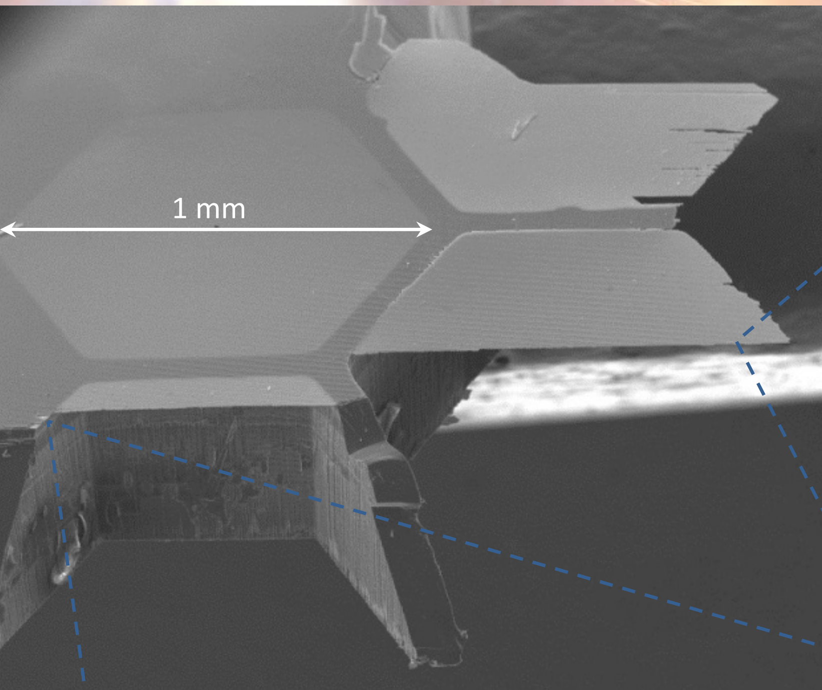


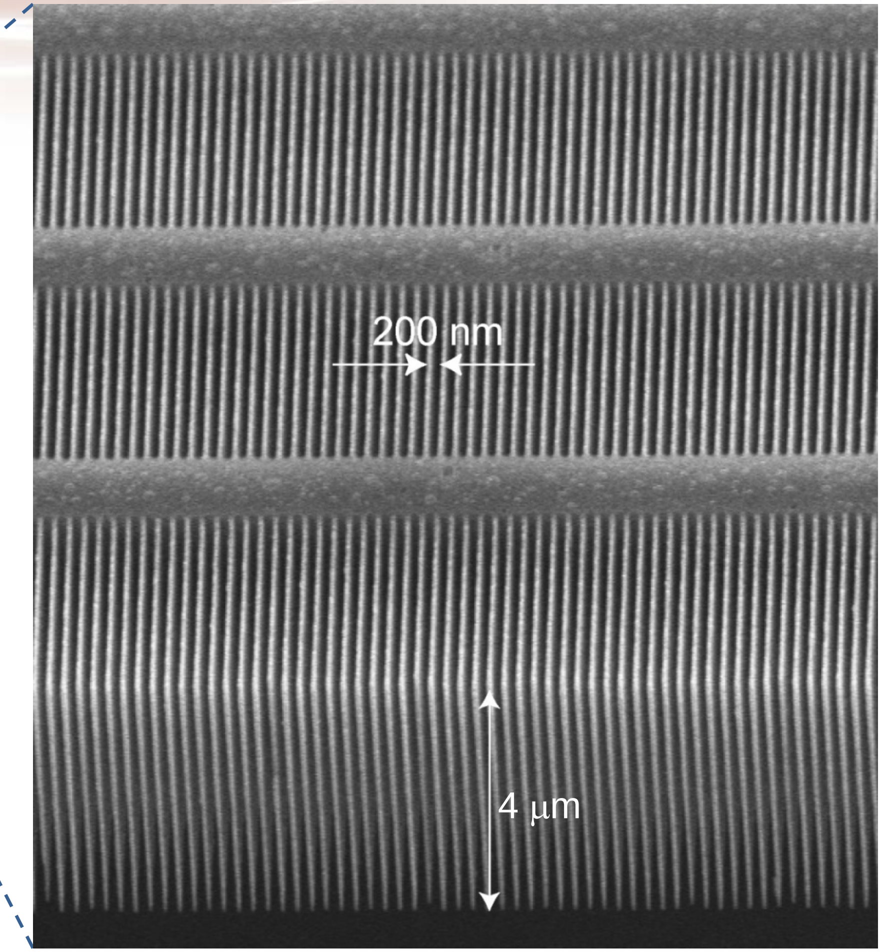
(DRIE only)

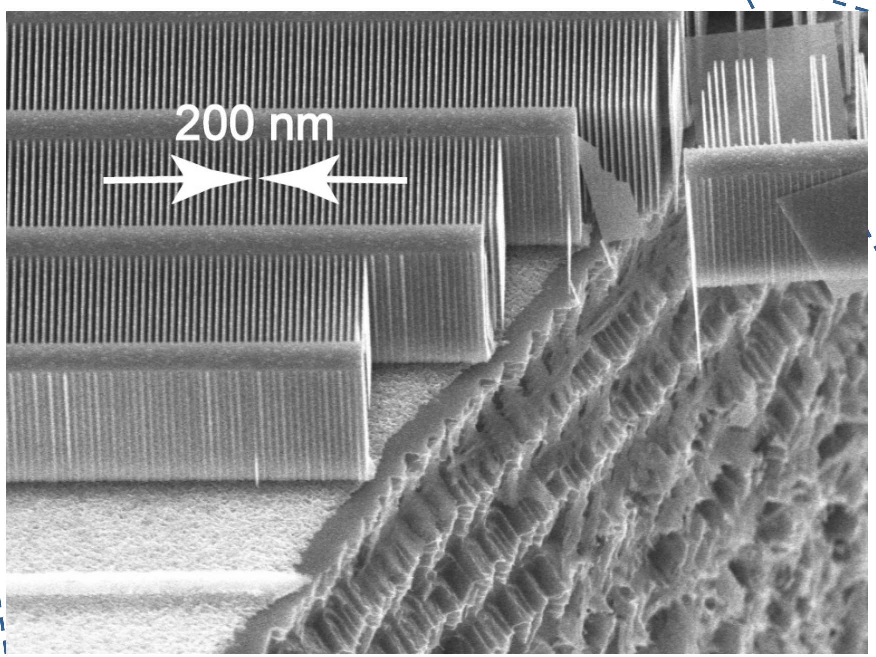
Recent Samples







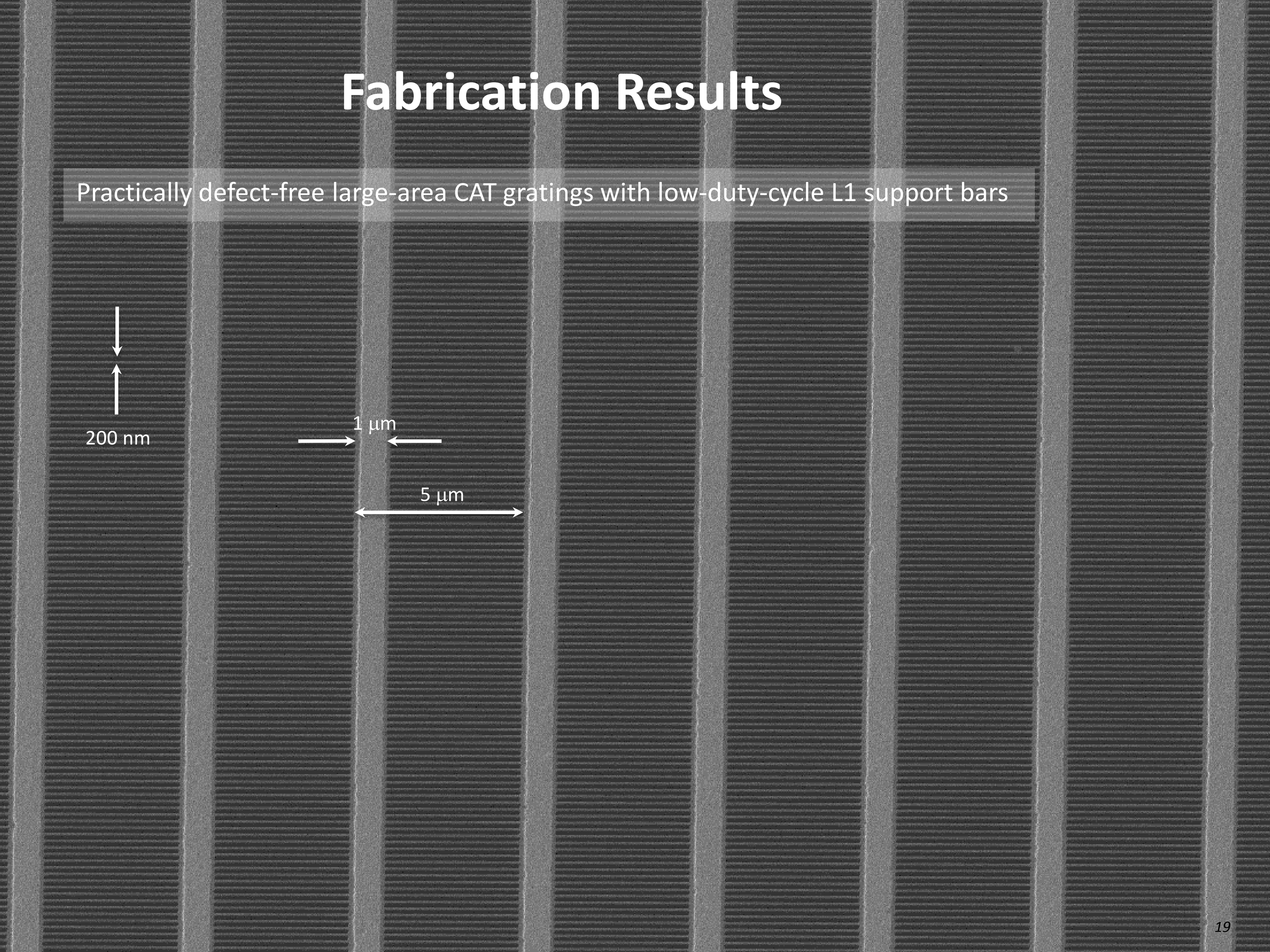




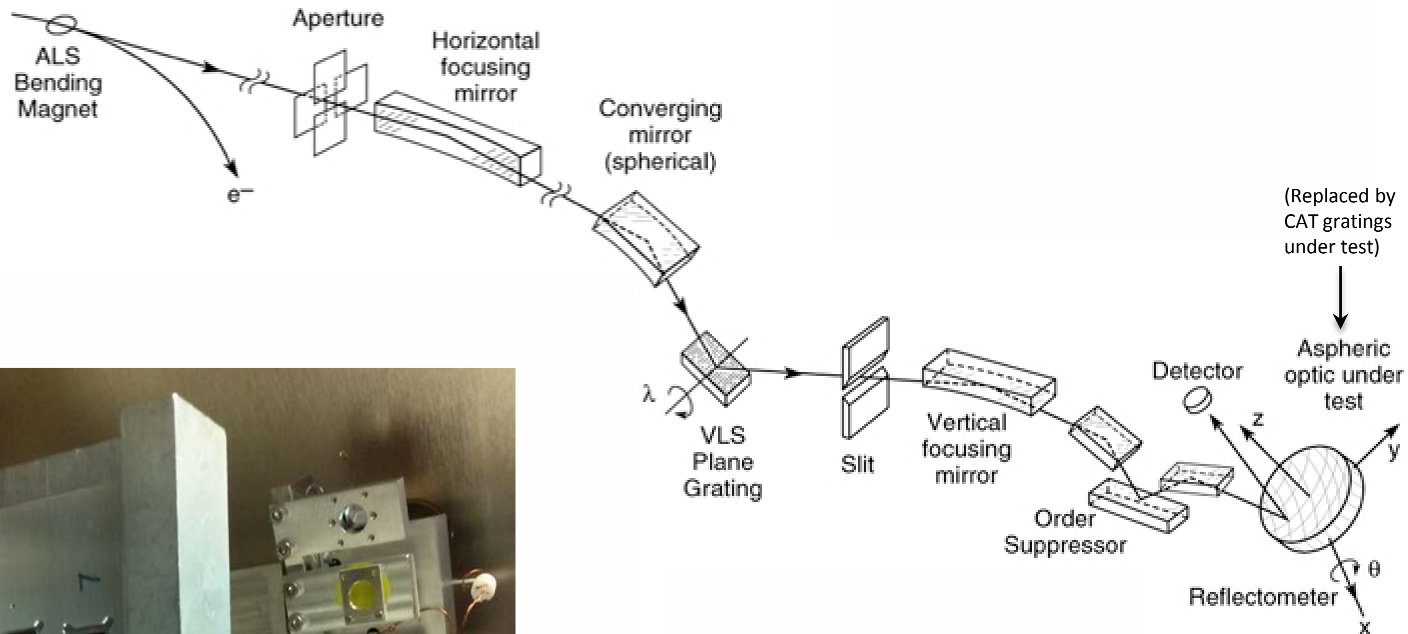
Scanning electron micrographs of cleaved freestanding CAT grating samples

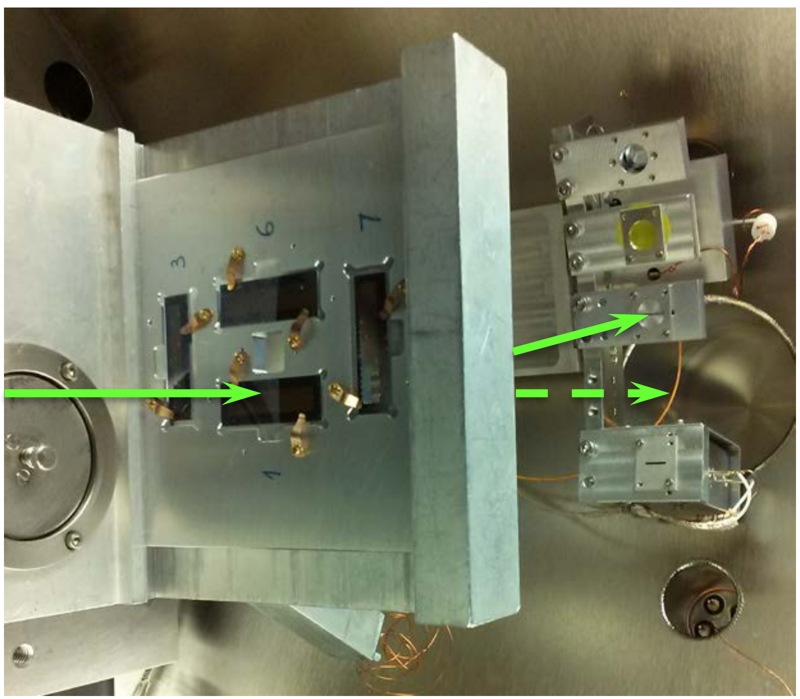
Fabrication Results

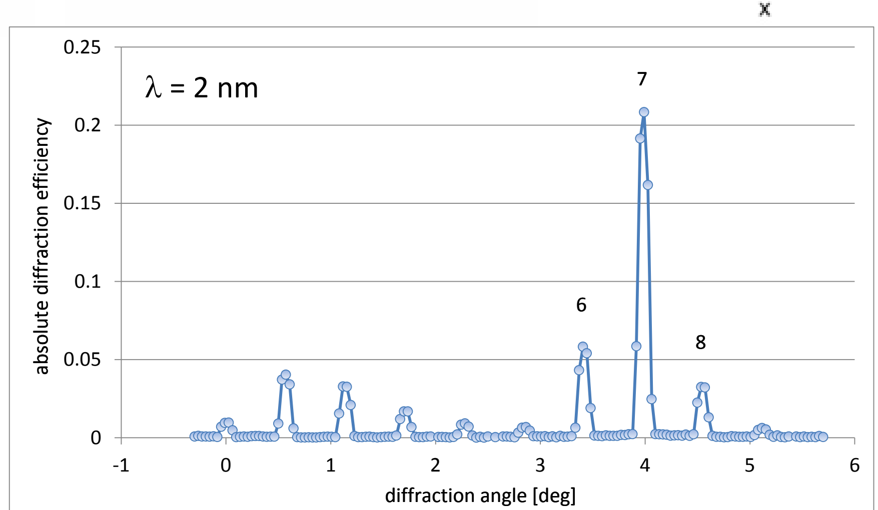
Practically defect-free large-area CAT gratings with low-duty-cycle L1 support bars



Diffraction Efficiency: ALS Beamline 6.3.2

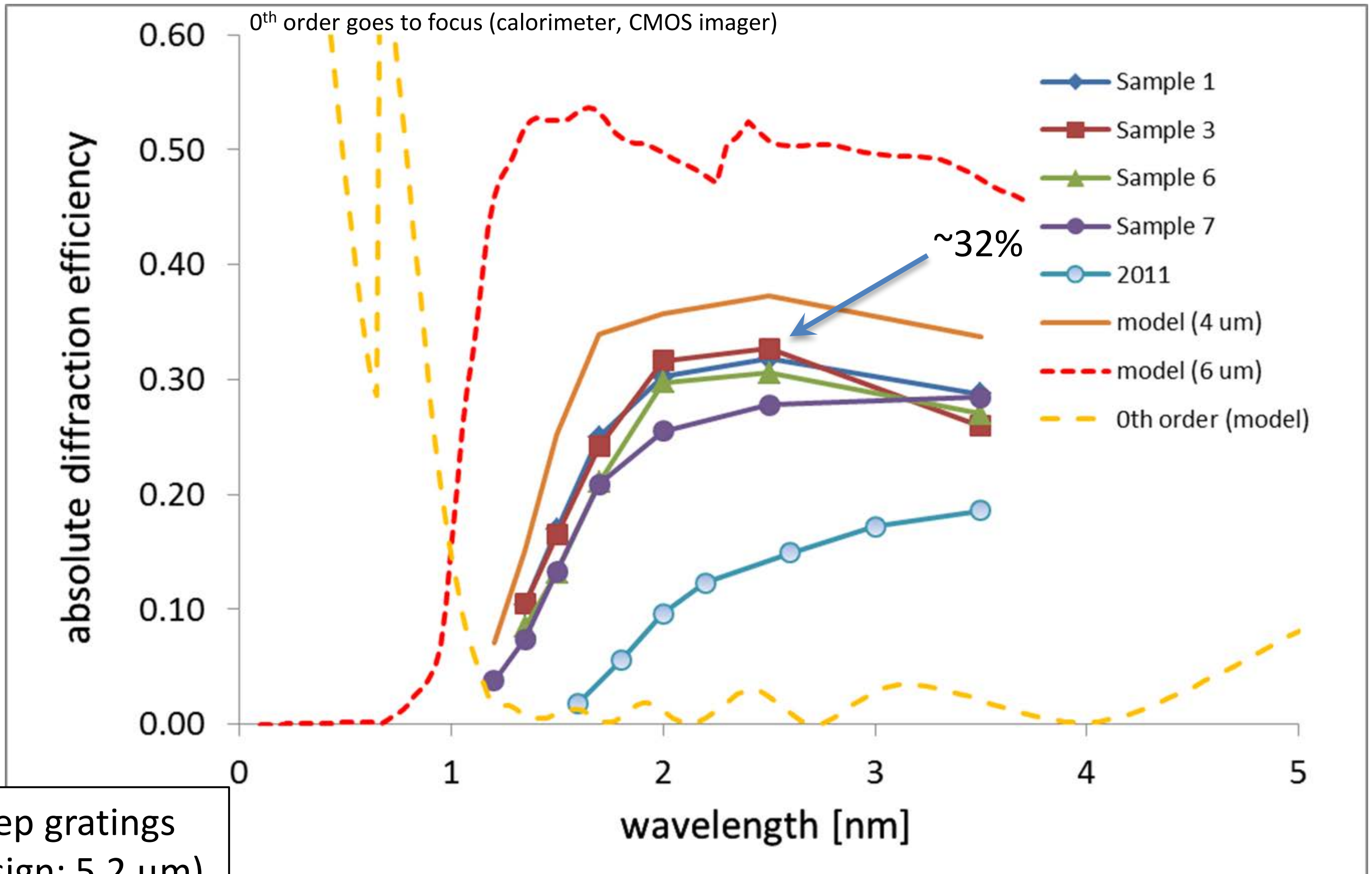






Diffraction Efficiency

- Synchrotron data: Sum of efficiencies in blazed orders, reduced by L1 absorption.
- Achieved 88% of model prediction at λ = 2.5 nm.
- Repeatable fabrication process leads to repeatable performance.

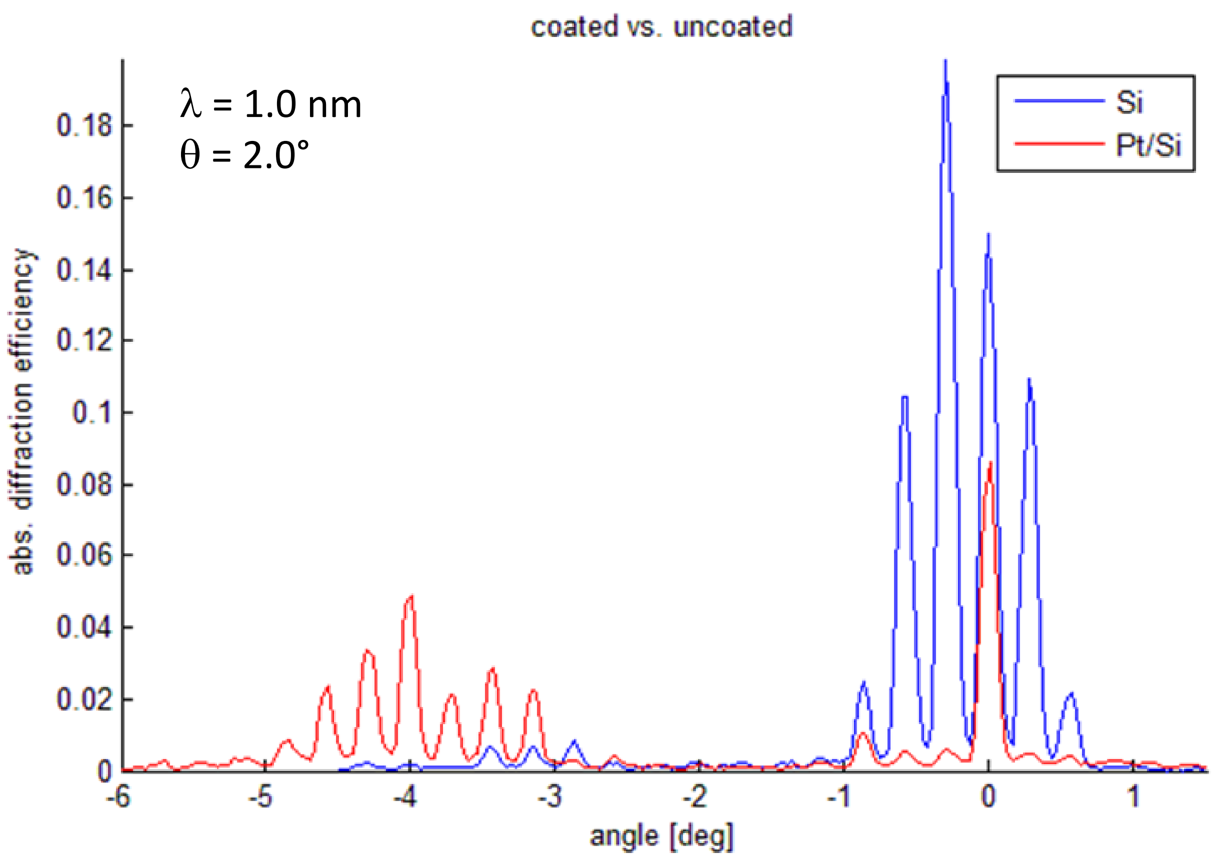


4 μm deep gratings
(AEGIS design: 5.2 μm)

Heilmann *et al.*, Proc. SPIE 960314 (2015)

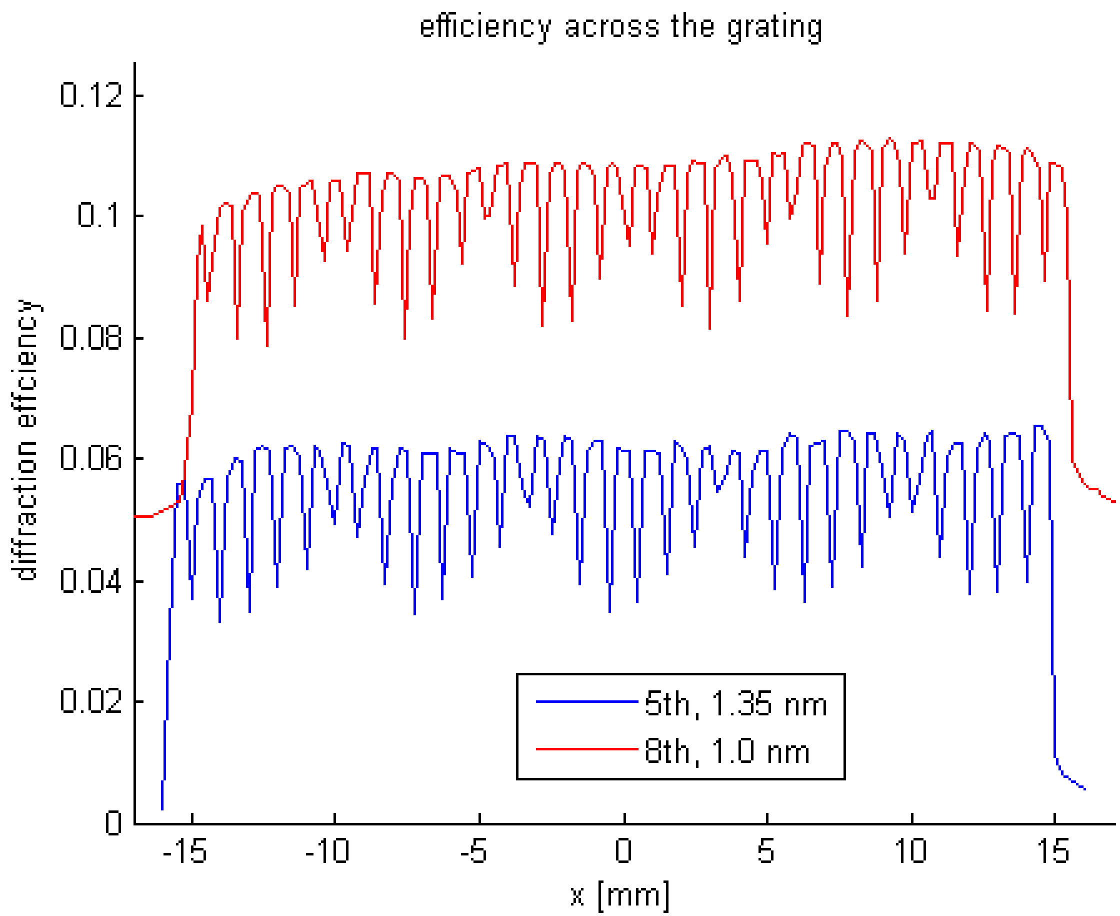
Extended Bandpass CAT Gratings

- Blaze angle limited by critical angle for silicon.
- Conformally coat CAT gratings with nm-thin layers of materials with higher electron density/critical angle → extended bandpass CAT gratings



Grating Uniformity

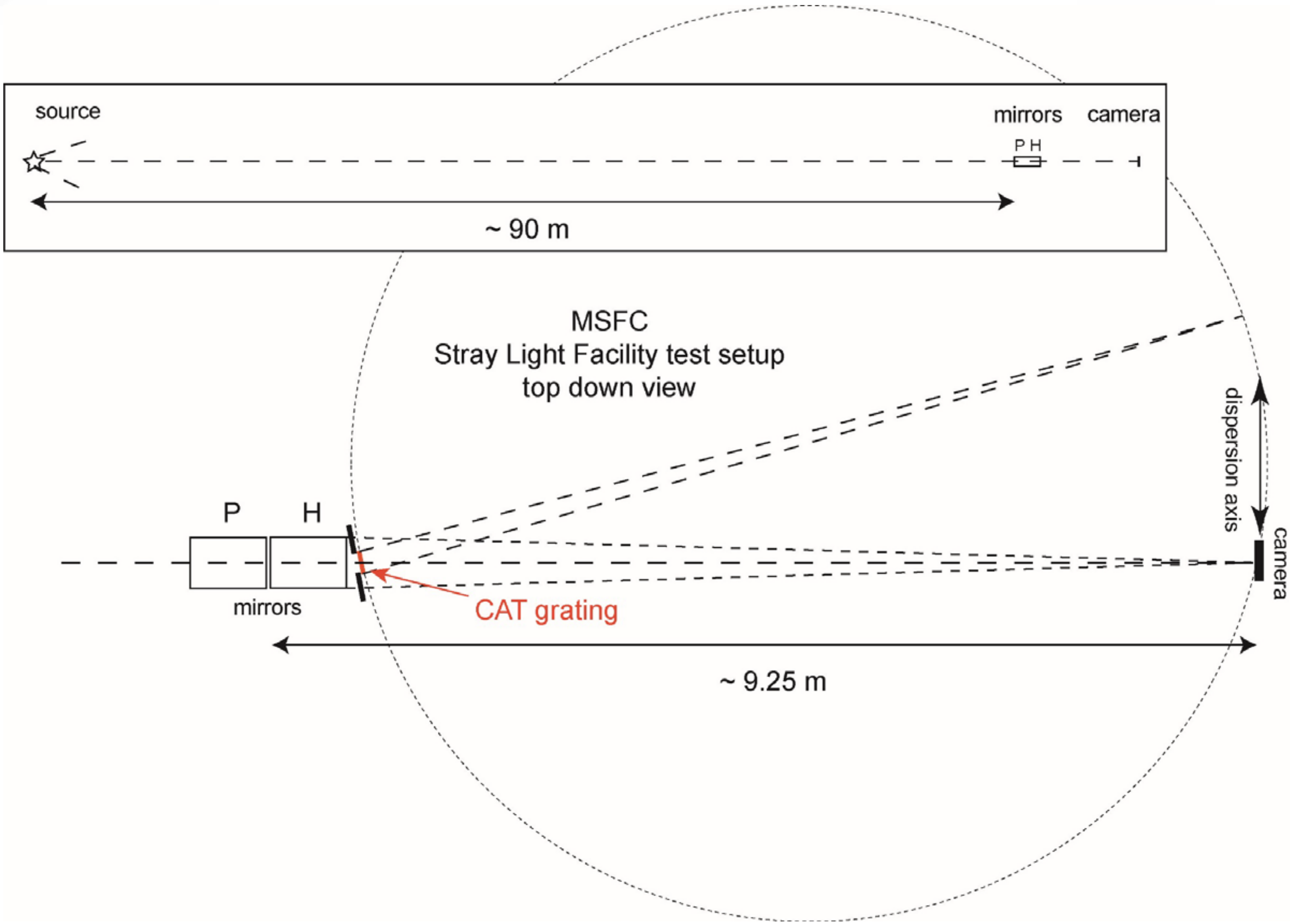
- Measure diffraction efficiency of blazed order while scanning grating through the x-ray beam (red curve shifted for clarity, dips due to L2 mesh blockage)



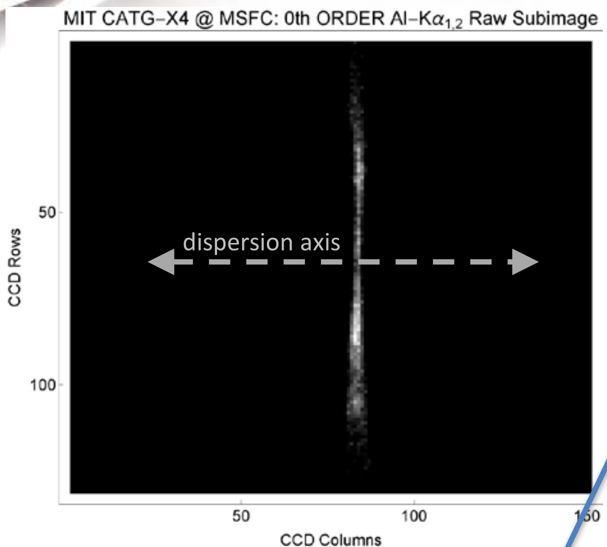
Resolving Power

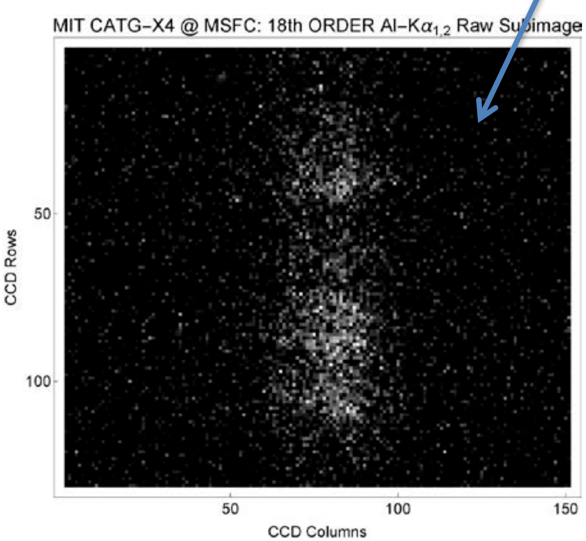
MSFC Stray Light Test facility: Al K_α source (λ ~ 0.83 nm, $\lambda/\Delta\lambda$ ~ 3400), ~ 90 m beam line
Focusing Optic: GSFC Technology Development Module (~ 8.5 m focal length)
Sub-apertured LSF: ~ 1.5" FWHM in dispersion direction
AEGIS requirement: R > 3500.
Dispersion angle 1^o : R = $\lambda/\Delta\lambda$ ~ 2400
Dispersion angle 3.5^o (AEGIS): R = $\lambda/\Delta\lambda$ ~ 8400!
<u>Problem</u>: Θ_c ~ 1.1^o for Si CAT gratings at λ = 0.83 nm;
current 4 μm deep gratings optimized for ~ 2.0^o
<u>Solution</u>: Coat Si gratings with PT using ALD -> extended band CAT gratings

MSFC SLF Optical Layout



Resolving Power



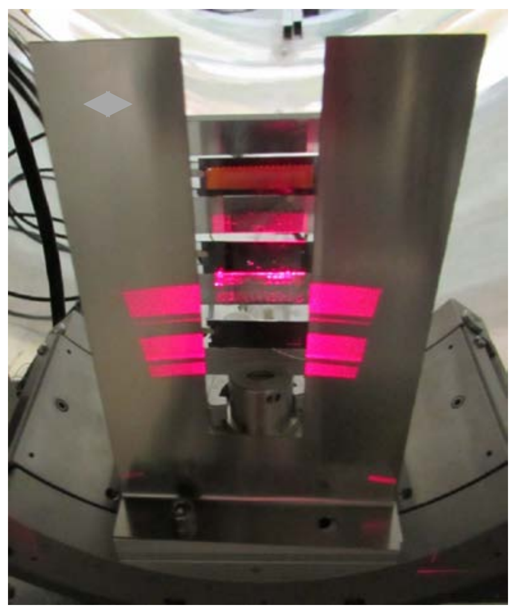


TDM and CAT gratings

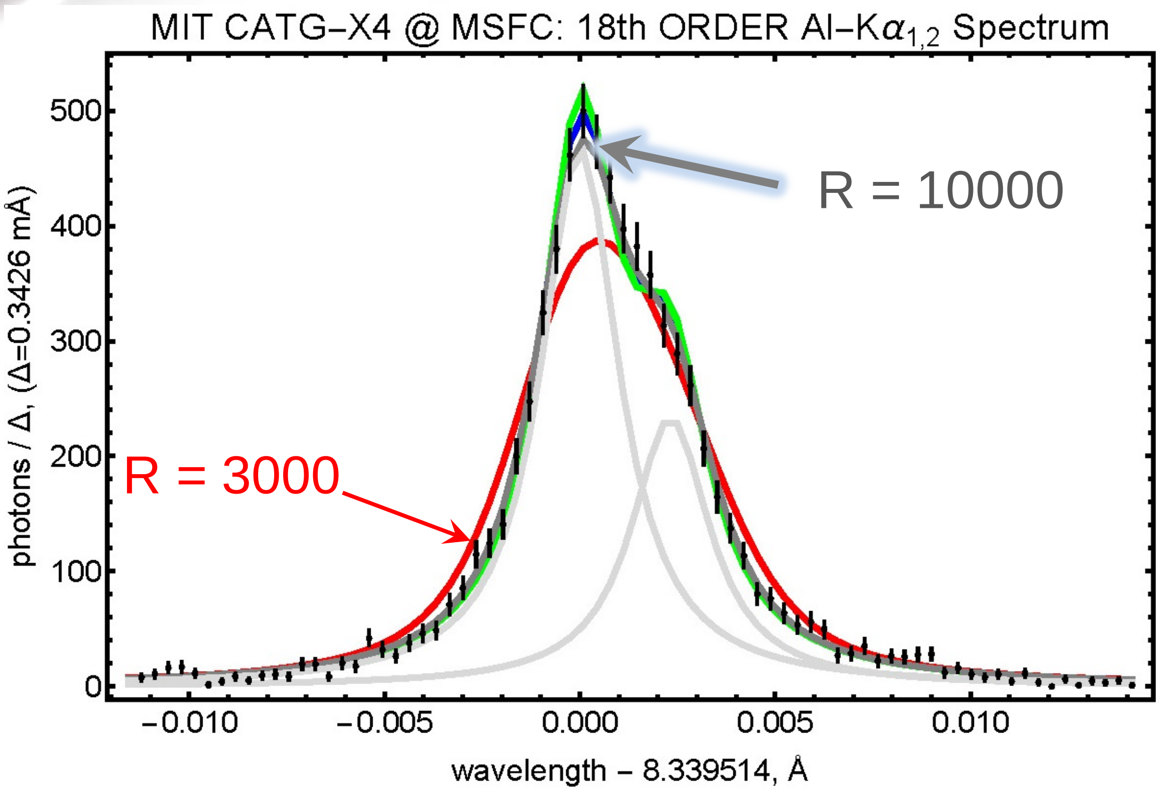
0th order image
(~ 1.2” LSF)

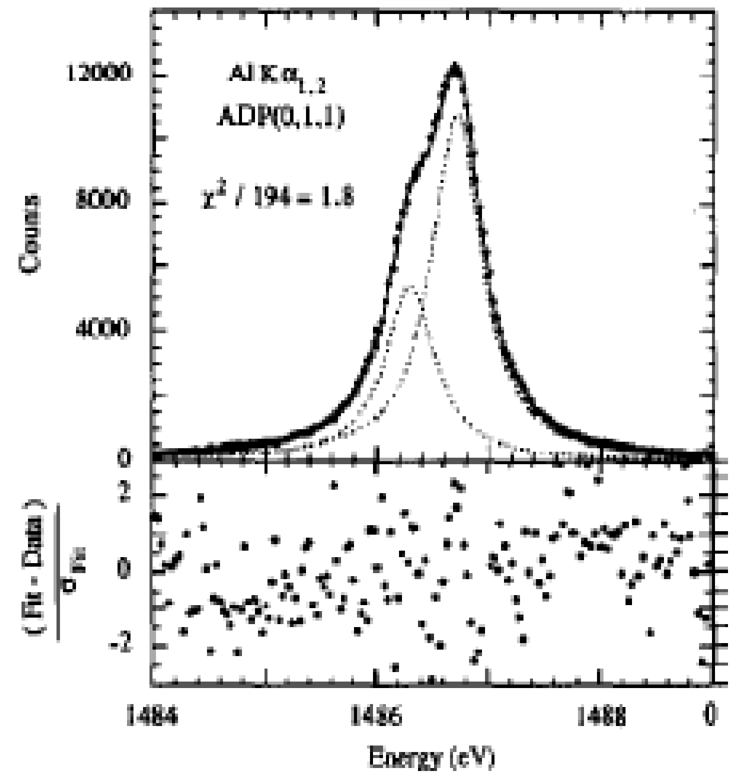
18th order image
(~ 1.2” LSF)

CAT gratings during
optical alignment



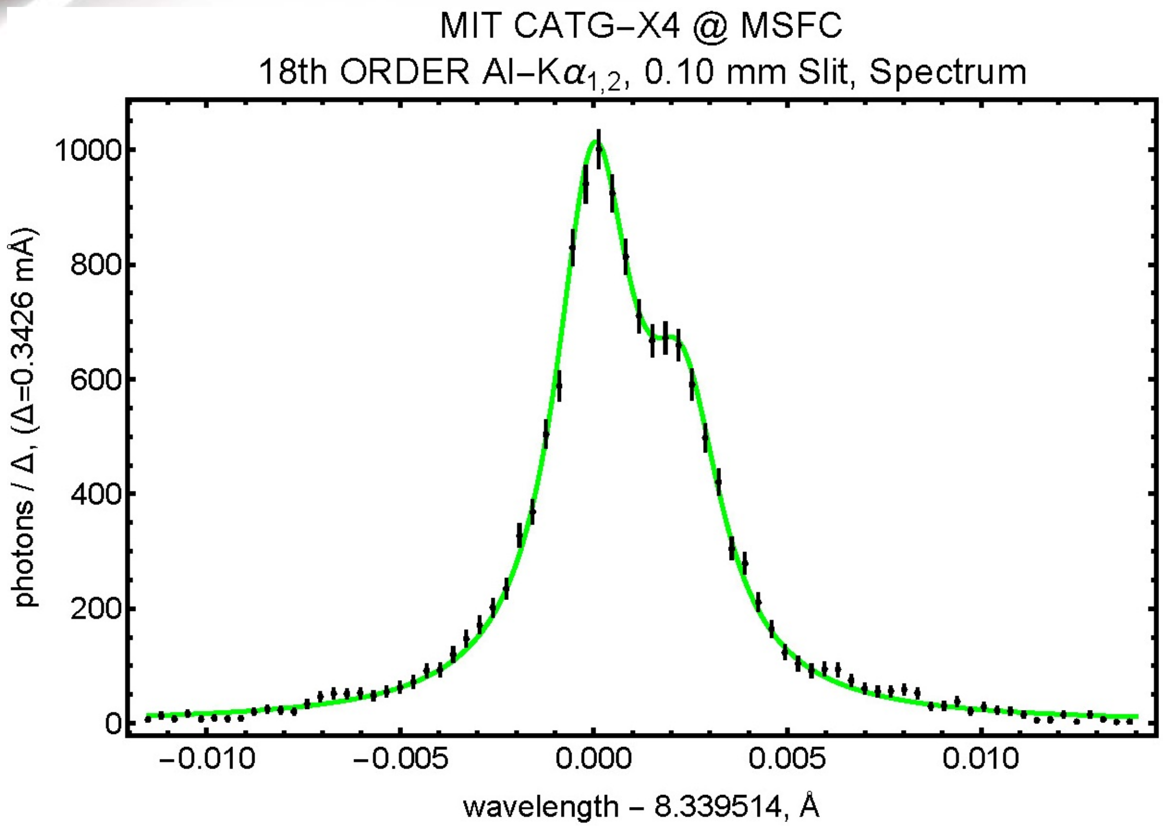
Resolving Power





Measured Al K$\alpha_{1,2}$ spectrum in 18th order with 0.15 mm slit. Vertical lines are the error bars around the number of photons in a given bin. Light gray are the two K_α components with their natural Lorentzian widths, green is their sum. Blue is the convolution with the measured source/mirror 1-D LSF. Dark gray is the blue curve convolved with broadening due to a Gaussian $\Delta p/p$ distribution that would limit R to 10,000. It still falls short at the peak. The red curve also assumes a Gaussian $\Delta p/p$ distribution, but corresponding to R = 3000. Right: Measurements of the Al K$\alpha_{1,2}$ spectrum with a double crystal monochromator by Schweppe *et al*. (J. Schweppe *et al., J. Electron Spectrosc. Relat. Phenom* **67**, 463 (1994)).

Resolving Power



Measured Al $K\alpha_{1,2}$ spectrum with 0.10 mm slit (8 hour exposure). The green curve is a simple one-parameter fit to the sum of two Lorentzians with their quoted natural widths (0.002412 Å), a 2:1 amplitude ratio, and 0.002317 Å spacing. There is very little room for a convolution with the measured LSF (1.0”), and even less room for any broadening due to contributions from the grating.

Preliminary analysis strongly suggests that the tested CAT gratings, illuminated across 30 mm width, are not a limiting factor in the design and construction of blazed transmission grating spectrometers with resolving power on the order of $R = \lambda/\Delta\lambda$ = 10,000.

Future Plans

- Performance demonstration planned
  - Demonstrate resolving power of GAS with three CAT gratings simultaneously illuminated with x rays from focusing. Perform pre and post environmental tests.
  - Demonstrate effective area with pencil-beam synchrotron measurements of individual gratings; extrapolate from diffraction efficiency and designed and measured dimensions of larger structures (L2, L3, gaps, GAS).
    - Maximize throughput for both L3 & GAS, and/or
    - Increase diffraction efficiency by making deeper gratings & narrower bars/L1/L2
- Notional schedule or timeline: TRL5 by end of 2018, based on renewal of SAT funding.

Summary

- Technology for large-area, high-resolution soft x-ray CAT grating spectrometer stands at TRL4. Rapid recent progress and performance improvements.
- Status of technology meets/exceeds TRL4 in many respects.
  - Diffraction efficiency > 85% of maximum at 0.5 keV.
  - Gratings contain full structural complexity of goal design.
  - Uniform over surface, reasonable size.
  - Demonstrated R > 10,000 possible with CAT gratings at 1.48 keV.
- Path forward
  - Clear and feasible path to TRL5.
  - Attach gratings to frames and develop alignment technology for CAT grating array (polarization of visible light, adapted from Chandra HETGS).
  - Want to improve fabrication yield and x-ray "throughput" further.
  - Proposed for SAT funding beyond 2016.