GMTNIRS and the Promise of High Resolution Spectroscopy in the Infrared: Part 1

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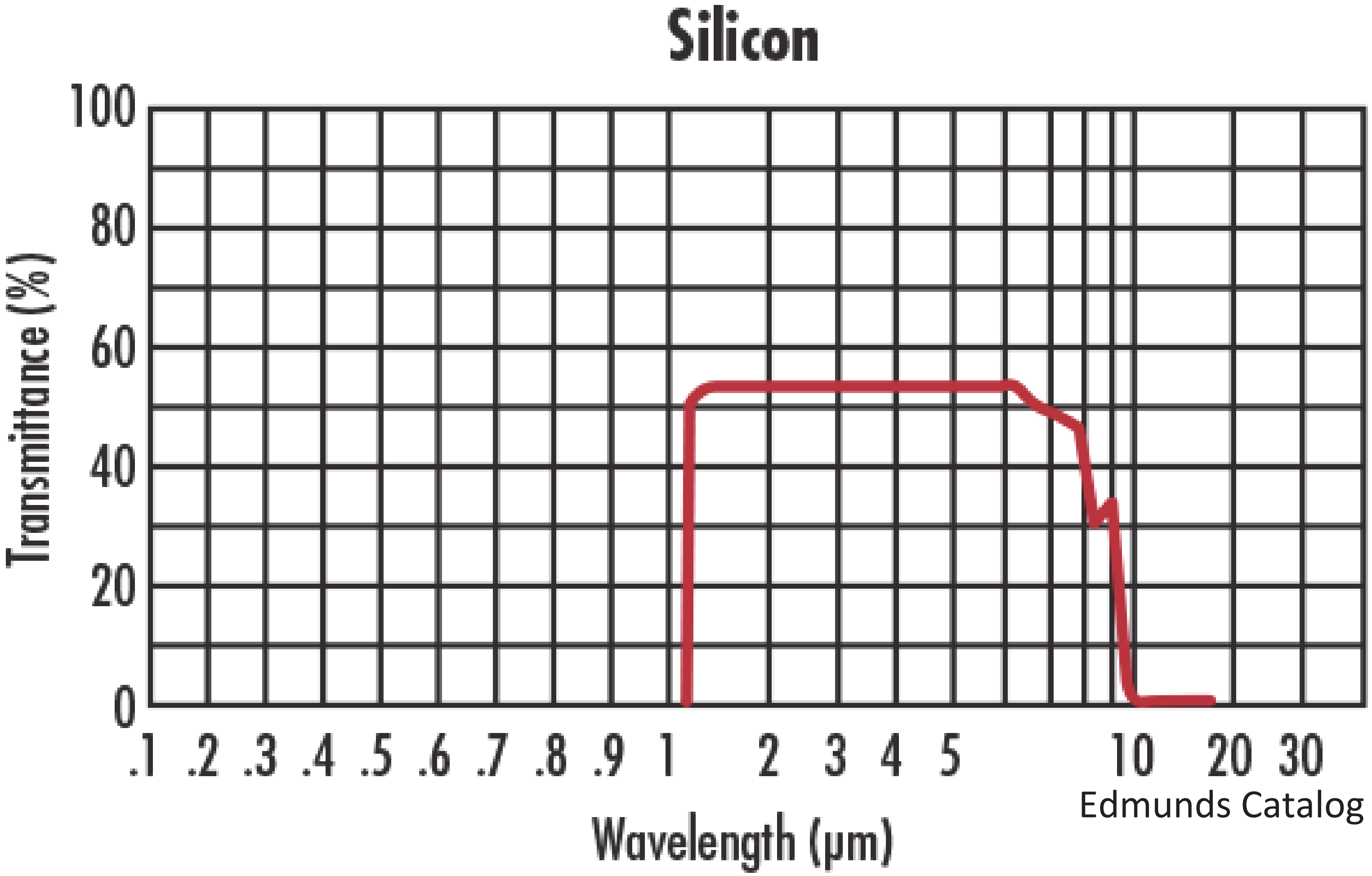
Today:

What is the “infrared”?
State of the art instruments today
Requirements and where they come from
GMTNIRS
Spectrograph basics
Immersion gratings- the “secret sauce”

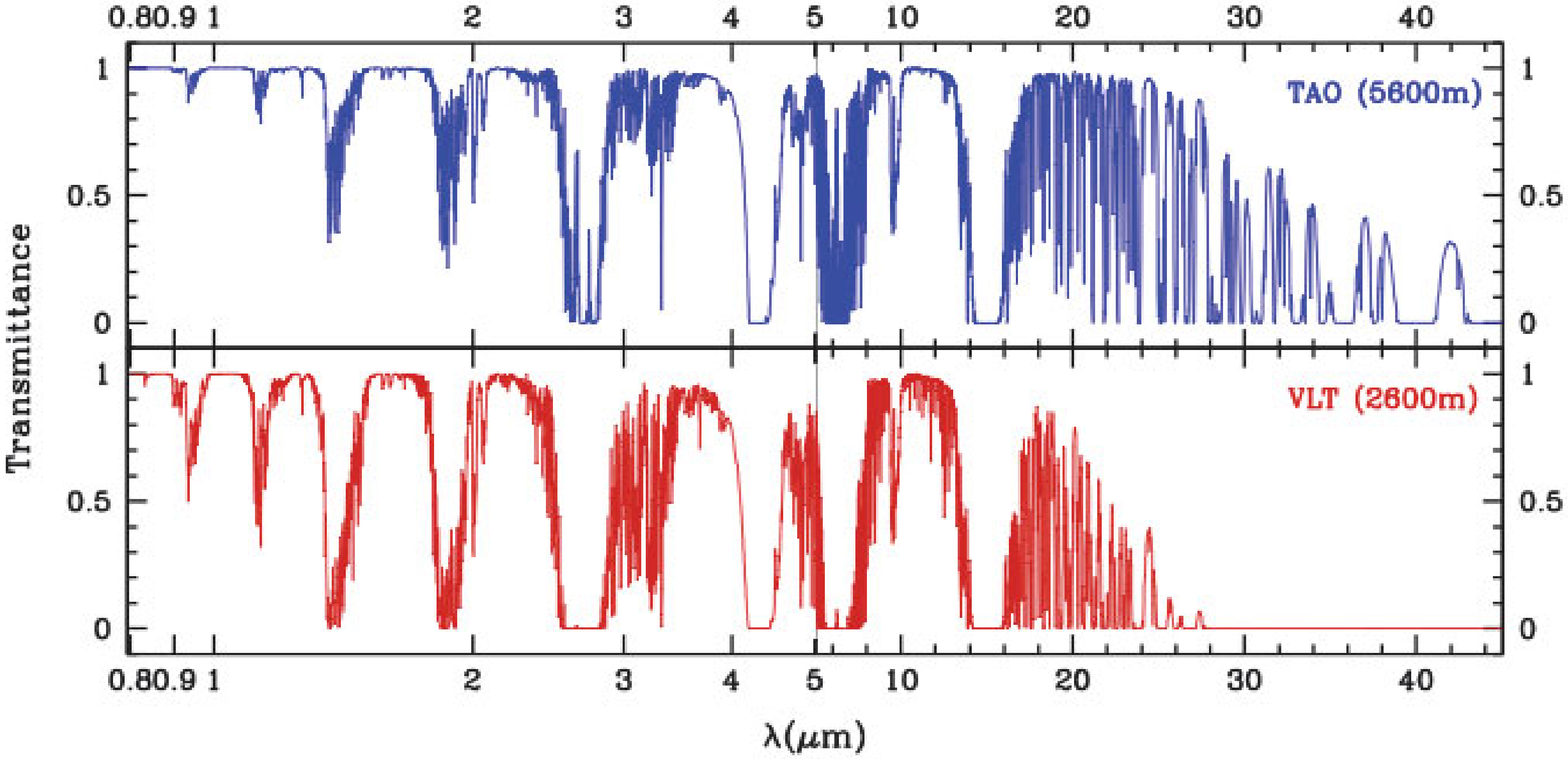
Why are silicon detectors so dominant?



Edmunds Catalog

Dominant IR options are HgCdTe or InSb, both with Si multiplexers.

The infrared divides into windows



University of Tokyo Observatory

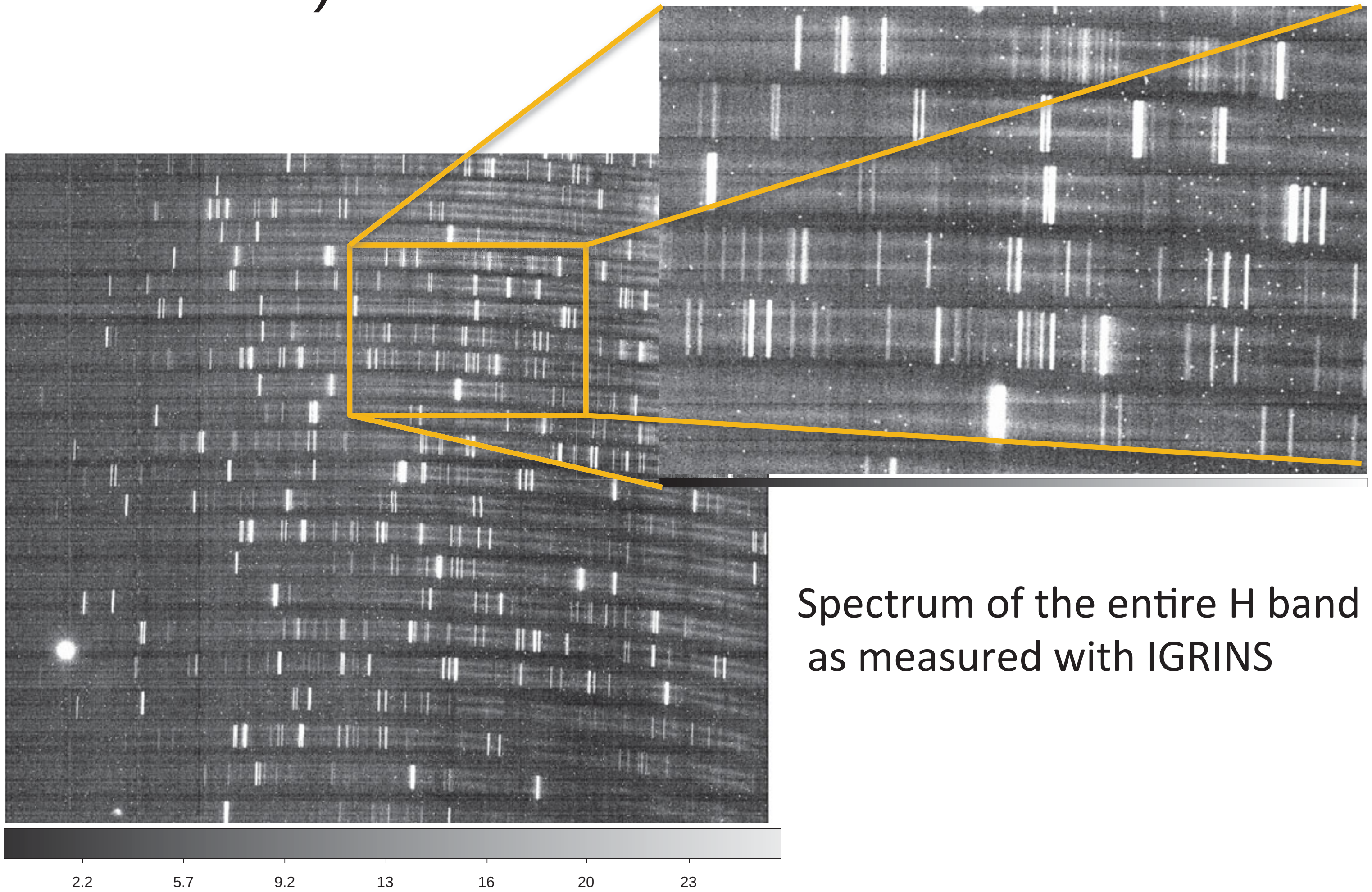
Background from Sky

$$N = B_\nu \, \Delta\nu \, A \, \Omega_{pix} \, \varepsilon/(h\nu)$$

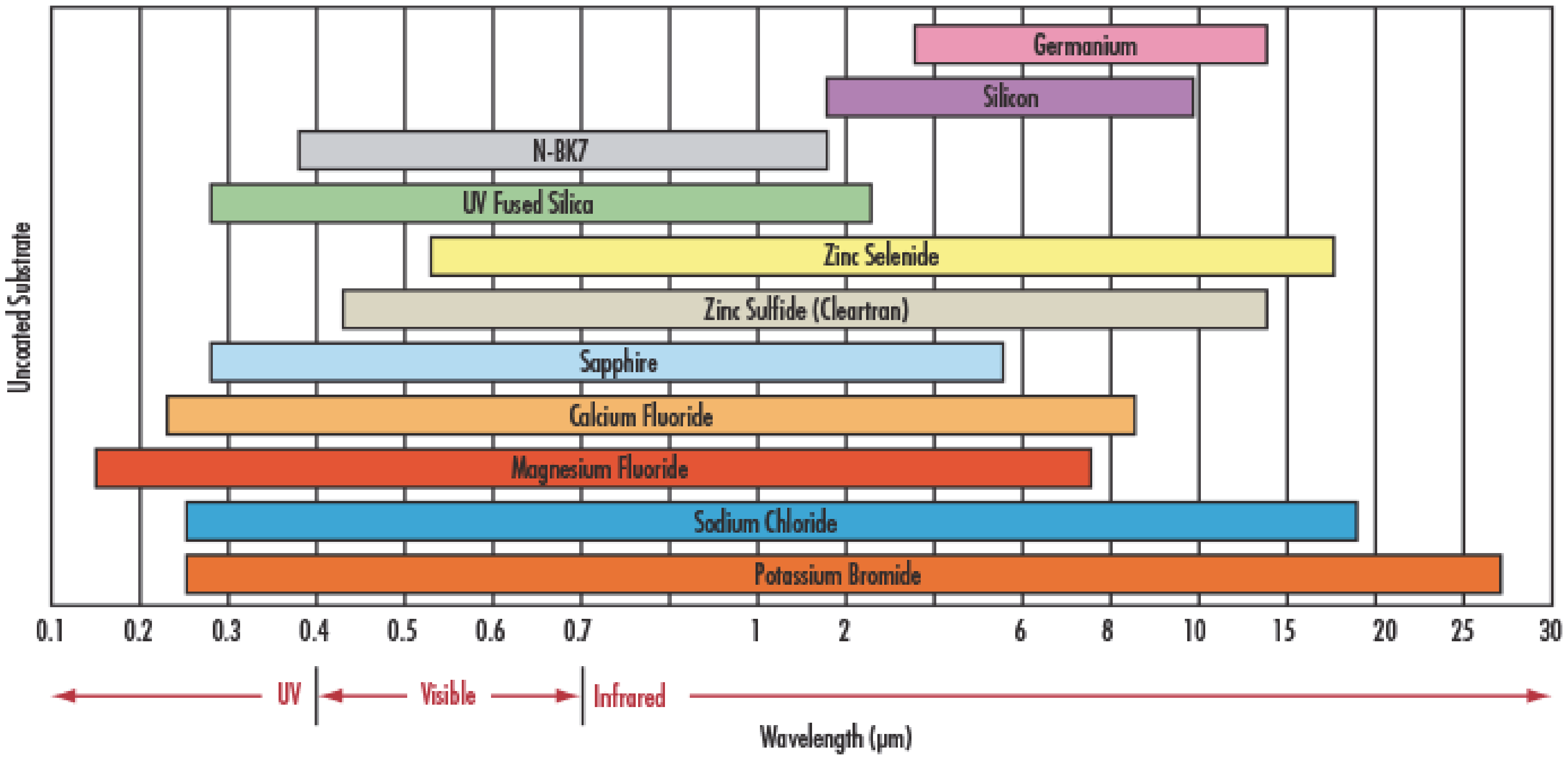
GMTNIRS Background Counts
e/s/pixel

J	H	K	L	M
5e-10	6e-6	1e-2	8	342

OH Night sky in the H band (Chan Park et al.)



Spectrum of the entire H band as measured with IGRINS


Germanium
Silicon
N-BK7
UV Fused Silica
Zinc Selenide
Zinc Sulfide (Cleartran)
Sapphire
Calcium Fluoride
Magnesium Fluoride
Sodium Chloride
Potassium Bromide
Uncoated Substrate
0.1
0.2
0.3
0.4
0.5
0.6
0.7
1
2
6
8
10
15
20
25
30
UV
Visible
Infrared
Wavelength (μm)

Edmunds.com

State of the art instruments today

Resolving power and resolution

$R=\lambda/\Delta\lambda$ Resolution = $\Delta\lambda$ or in some cases ΔV

Coverage angstroms, nm, μm –take your pick.

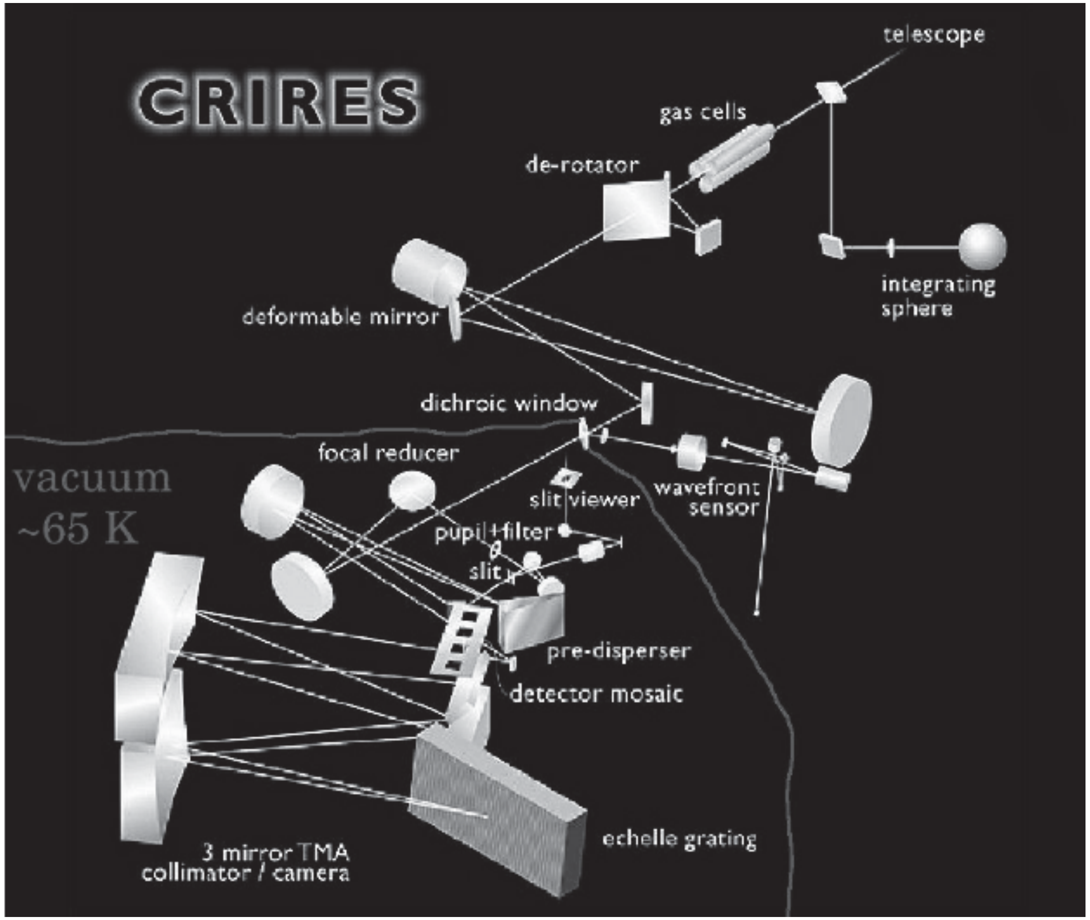
Note Window widths: H and K are each ~400 nm or about $\lambda/5$

First-generation high resolution spectrographs for the IR

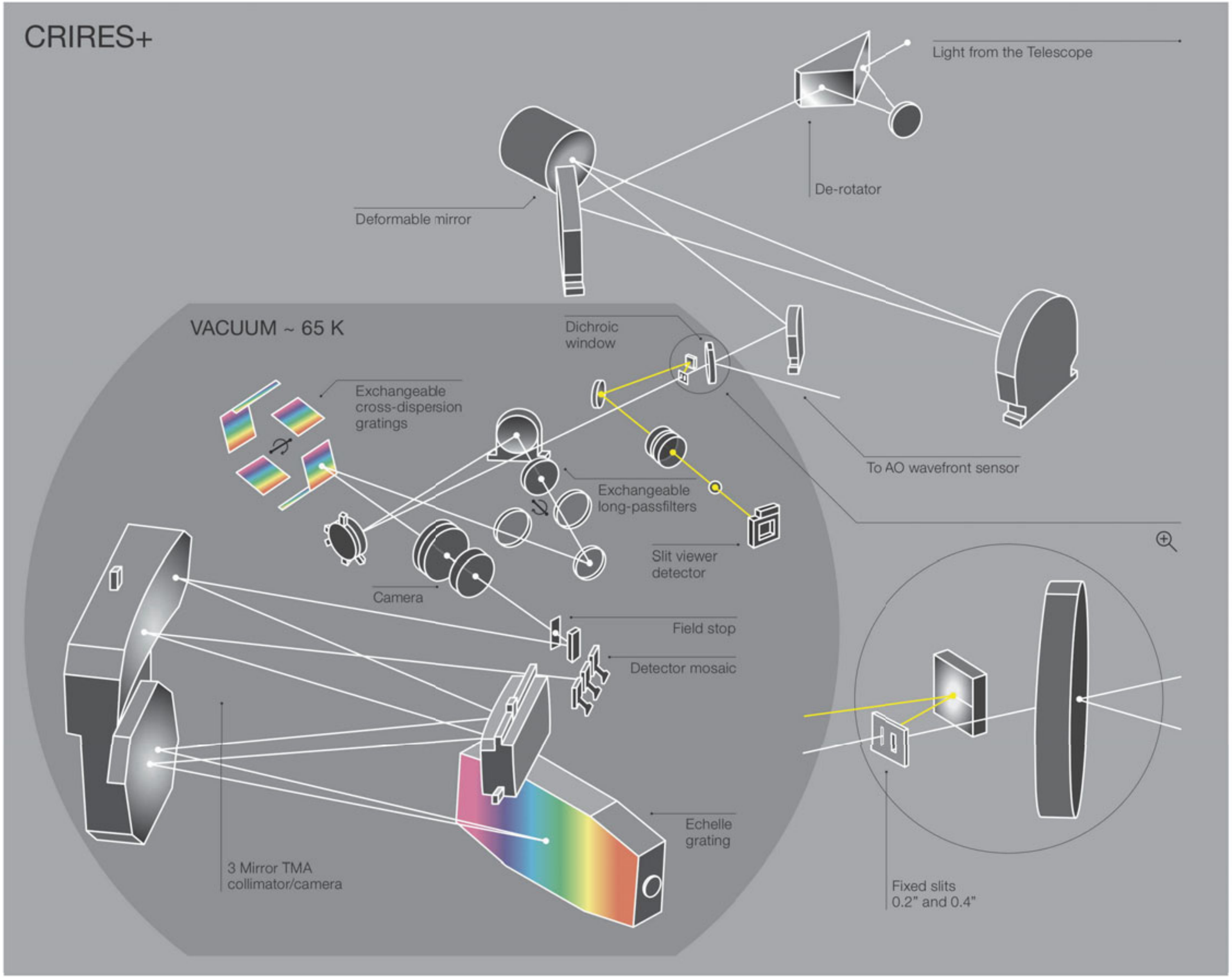
Small wavelength coverage:
CSHELL: $\lambda/200$
Phoenix: $\lambda/100$
CRIRES: $\lambda/70$

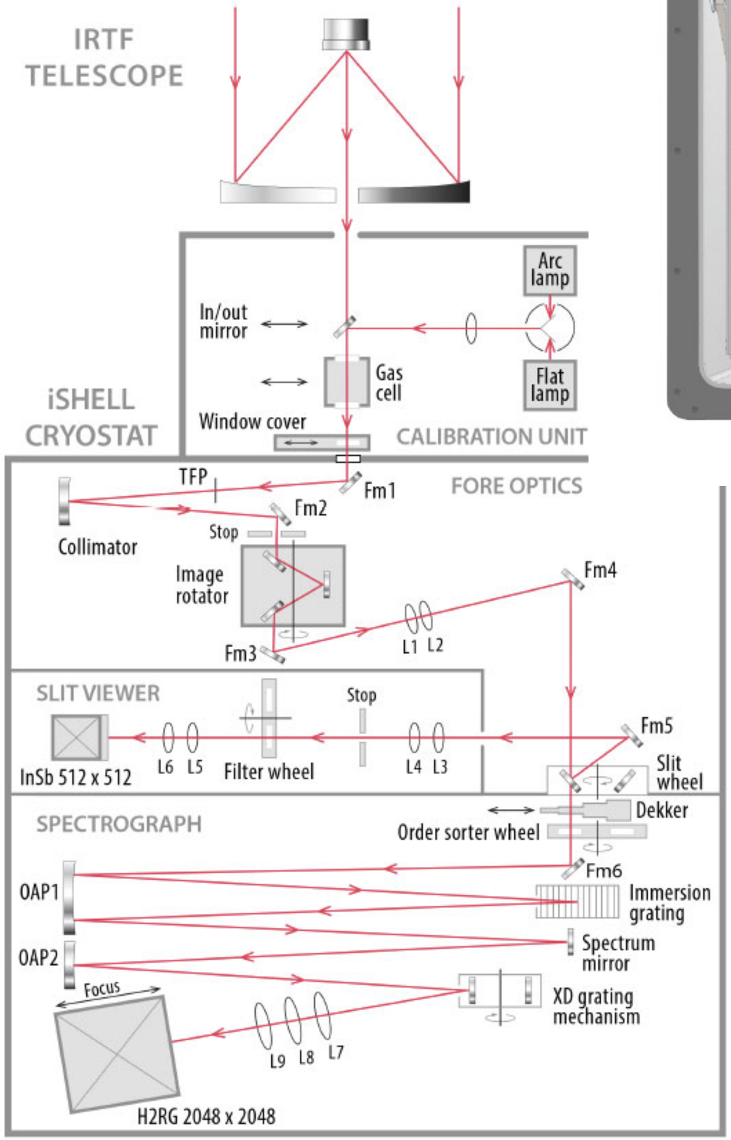
Small coverage means lots of moving parts.

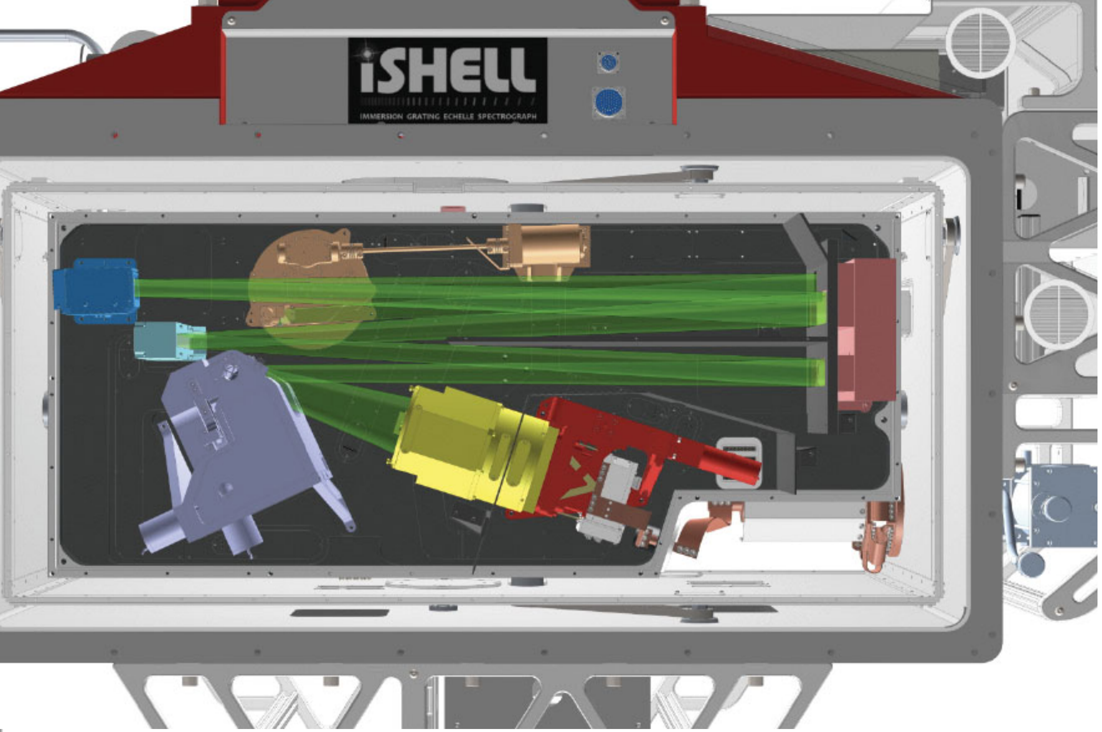
Many surfaces.
Hard to get decent slit sizes at high resolution.
Instruments already quite large and so not too stiff.



VLT CRIRES+ - Full coverage of K







iSHELL on the NASA IRTF

R=70,000 1-5 μm in snippets

Requirements and where they come from

Resolving power
Spectral coverage
Detector,
Background
Throughput
Sampling
Slit length
Spatial resolution,
Spectral stability
Stability overall

Requirements and where they come from

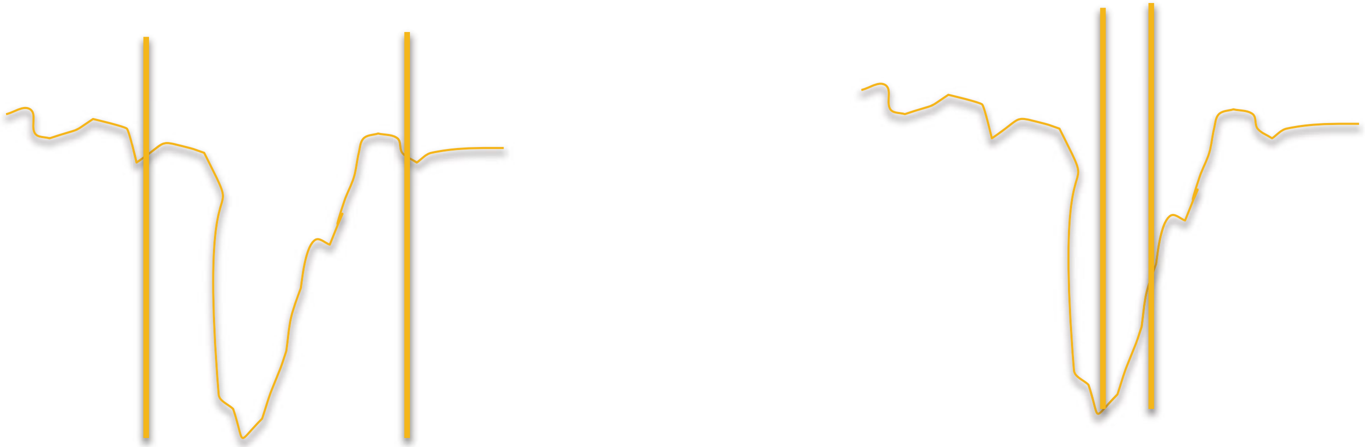
Resolving power

Science driven and technology limited.

$R_{Diff}= 2W\tan\beta/\lambda$

You are limited by the size of the grating and the need to let light into your system. Let’s look at the S/N aspects.

Let’s fix the number of pixels per resolution element:



How does S/N scale with R?

		Short l (low bknd)	**Long l (high bknd)**
Low S/N (=>detector noise limit when background is low)	Continuum	1/R	1/SQRT(R)
	Unresolved	Independent of R	SQRT(R)
	Resolved	1/R	1/SQRT(R)
	Emission unresolved	Independent of R	SQRT(R)
High S/N	Continuum	1/SQRT(R)	1/SQRT(R)
	Unresolved	SQRT(R)	SQRT(R)
	Resolved	1/SQRT(R)	1/SQRT(R)
	Emission unresolved	Independent of R	SQRT(R)

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Which regimes matter?

		Short l (low bknd)	Long l (high bknd)
Low S/N (=>detector noise limit when background is low)	Continuum	1/R	1/SQRT(R)
	Unresolved	Independent of R	SQRT(R)
	Resolved	1/R	1/SQRT(R)
	Emission unresolved	Independent of R	SQRT(R)
High S/N	Continuum	1/SQRT(R)	1/SQRT(R)
	Unresolved	SQRT(R)	SQRT(R)
	Resolved	1/SQRT(R)	1/SQRT(R)
	Emission unresolved	Independent of R	SQRT(R)

What if you bin?

Requirements and where they come from

Spectral coverage: Which wavelengths?

Short IR
Thermal IR
Mid-IR

Spectral coverage: Grasp
Enough to cover line of interest
Enough to cover group of lines of interest
Enough to cover band or bands

Pan-spectral coverage enables a new mode of science for the infrared

Requirements and where they come from

Detector

Quantum efficiency: As high as possible
Read noise: Below reasonable backgrounds or as low as possible
Dark current: Below reasonable backgrounds or less than read noise in reasonable exposure times.
Wavelength coverage: to as long as necessary but not longer
Readout speed: Not too slow (Fowler sampling)
Size: Big
Pixel Pitch: People may disagree but not small at long λ
Memory and cross-talk: As little as possible
Well depth: Big enough to allow high S/N per exposure
Linearity: Good over full range or calibratable

Requirements and where they come from

Internal background: Basically a requirement on how cold your internal optics need to be.
Has to be less than dark current plus external background at the shortest wavelength you observe with a given channel.

Why do I phrase it that way?

External Background
Good site
As few external surfaces as possible
Cut off where atmosphere or detector does
Cold stop- Must rotate
The trade for AO- more surfaces vs. smaller AΩ
Slit losses vs. Strehl

Requirements and where they come from

Throughput: Obviously more is better. This is particularly true at short wavelengths where you will be source noise or detector noise limited. It matters somewhat less at longer wavelengths where cold throughput affects signal and background both- This tells you which channels to concentrate on.

Requirements and where they come from

Sampling: A combined real estate and noise question.
You want to sample enough that your slit or diffraction are limiting R but oversampling takes up pixels you could use for slit length or spectral coverage and more pixels/resel means higher read noise to overcome.

For high resolution IR spectroscopy, the sweet spot lies between 2.5 and 4 pixels per resolution element.

Requirements and where they come from

Slit length: Needs to be long enough to allow sky subtraction by switching along the slit while always having the object in it.
=>Depends on seeing or AO.

Planetary astronomy and ISM work want to drive you to longer slits.

Requirements and where they come from

Spatial resolution: Why?

ISM, Planets, disks, binaries, confused regions, exoplanets

Limiting Factors:
Seeing- go to AO
Diffraction
Pixel size
Image wander

Requirements and where they come from

Spectral stability: Depends on application. Achievable by mechanics, calibration, or both.

Stability overall: Helps data reduction, calibration. Allows for higher limiting S/N

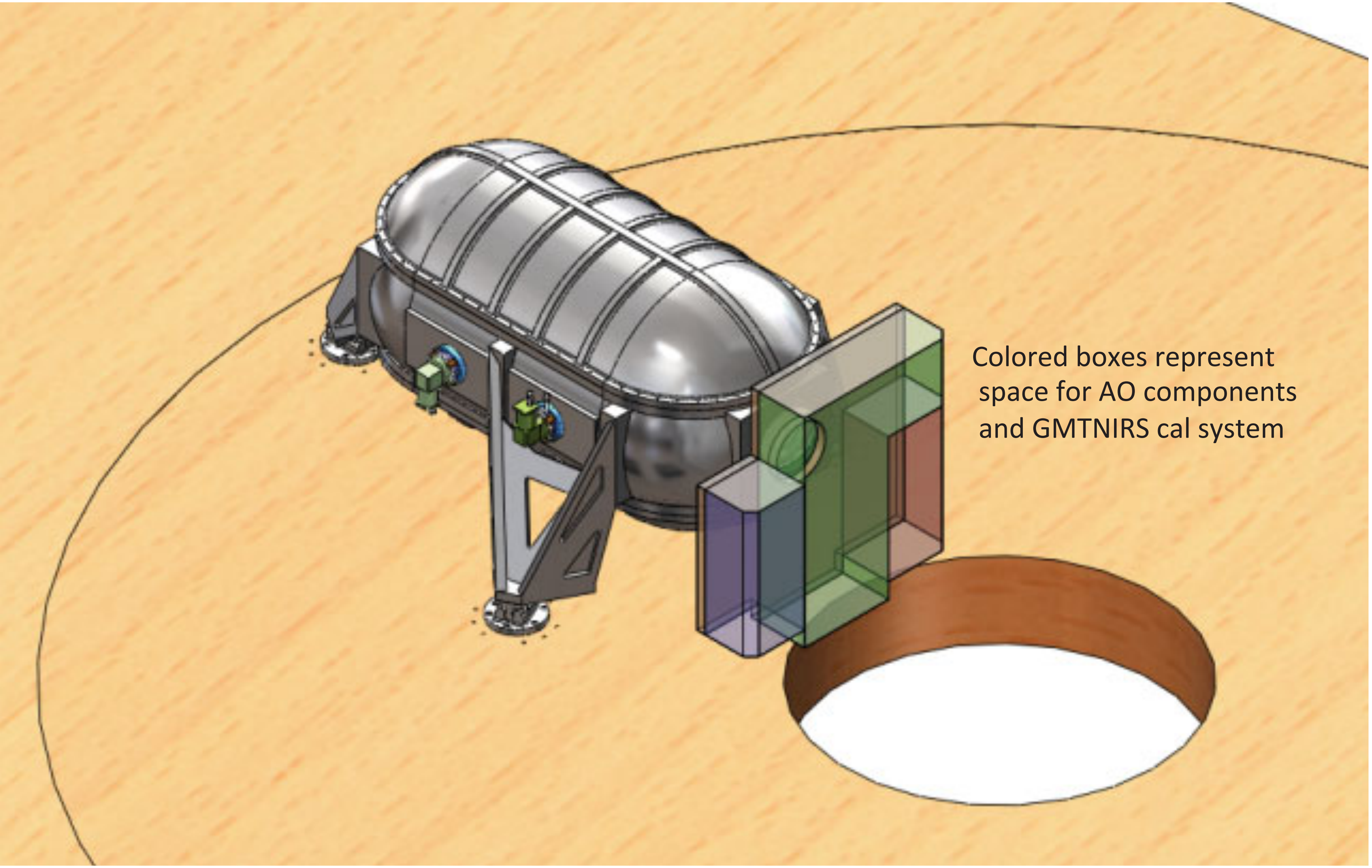
GMTNIRS: GMT's High-Resolution Infrared Spectrograph

-Covers all spectrum transmitted by the atmosphere from 1.07 μm to 5.3 μm in a single exposure.

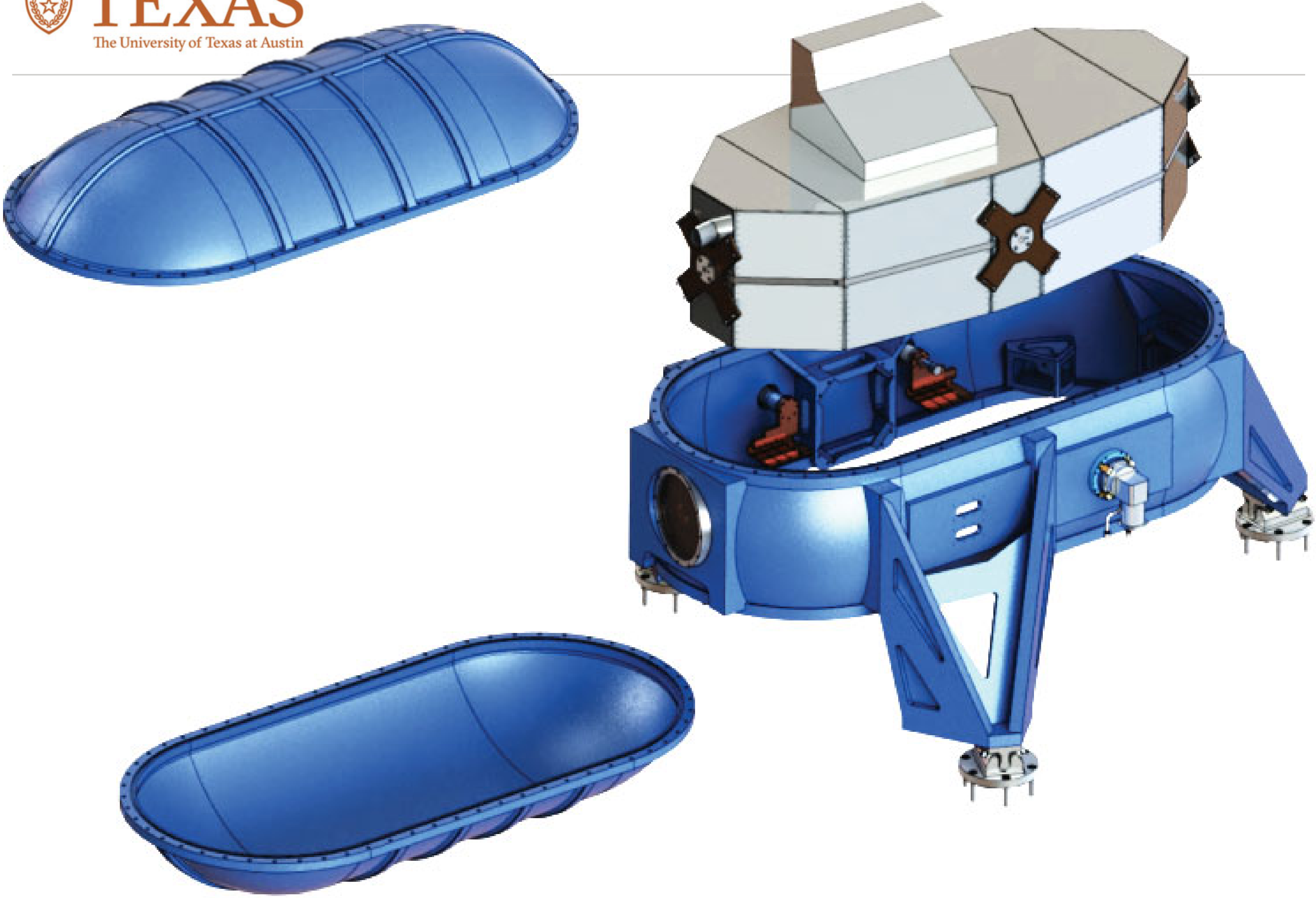
-Resolving power 65,000 at λ< 2.5 μm, 85,000 at λ>2.9 μm.

- 65 mas slit, 1.3" long
- No moving parts after slit
- High throughput leads to high sensitivity
- K-band slit viewing camera
- Automated, near publication quality data pipeline

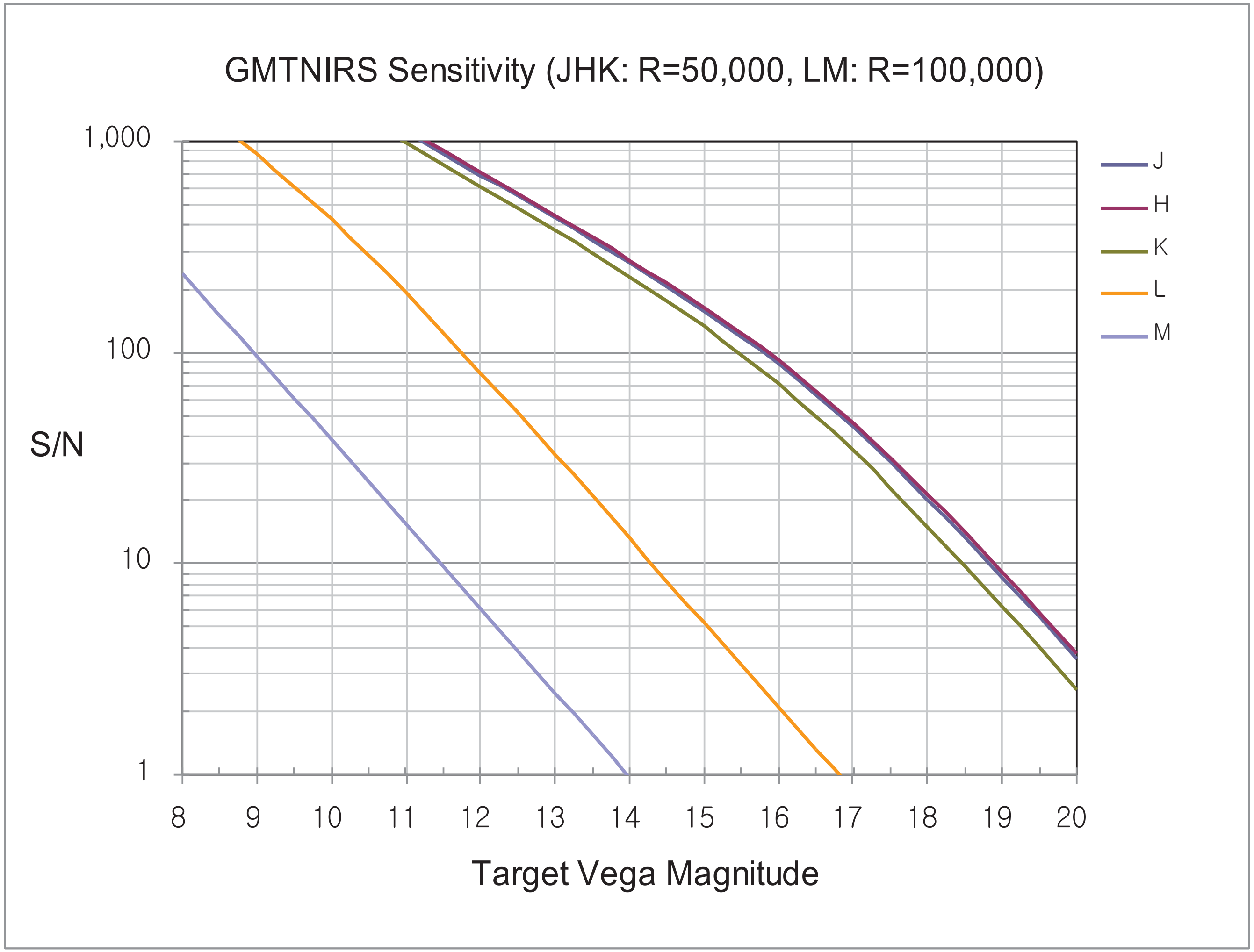
GMTNIRS on rotating instrument platform



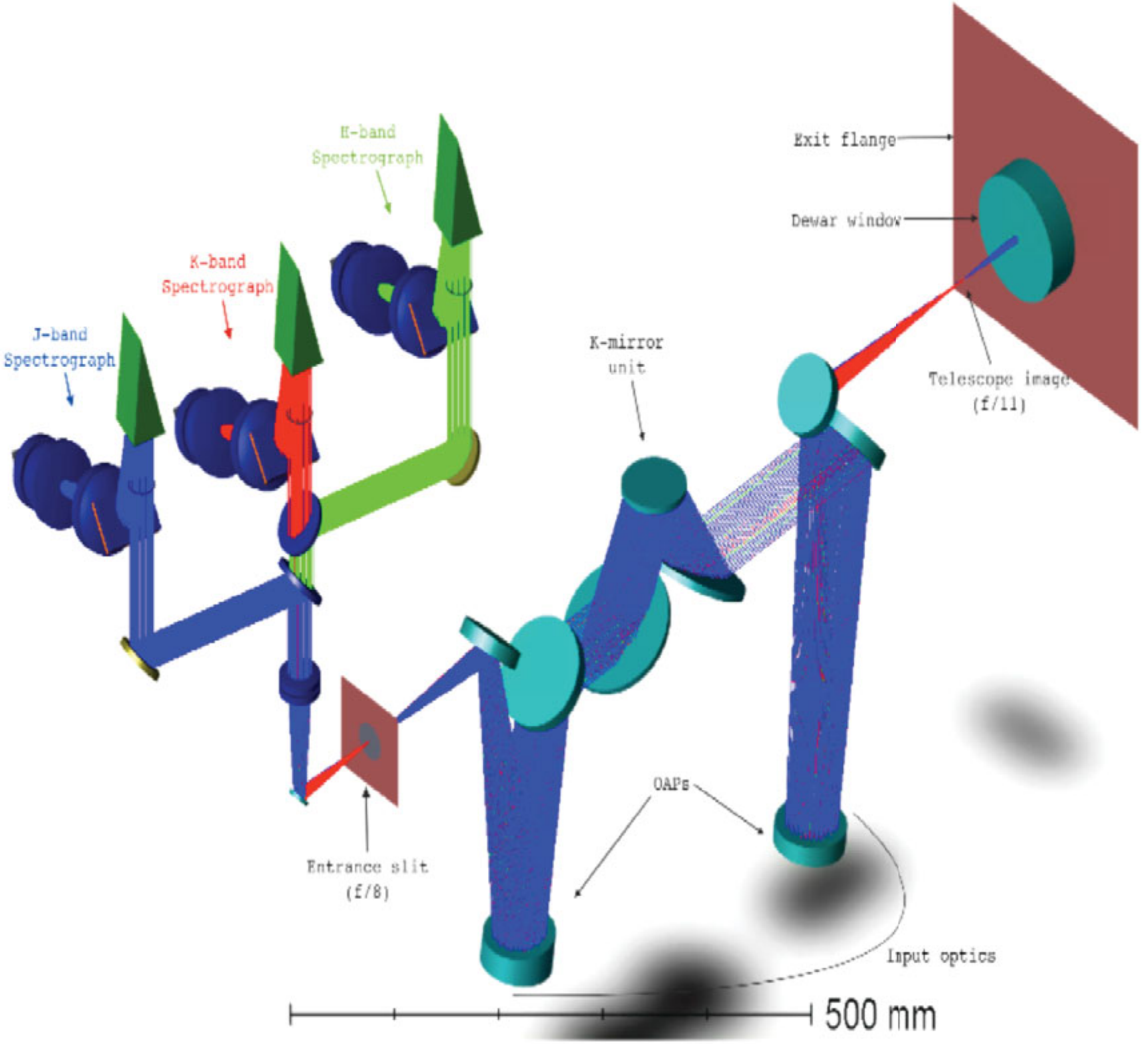
Colored boxes represent
space for AO components
and GMTNIRS cal system

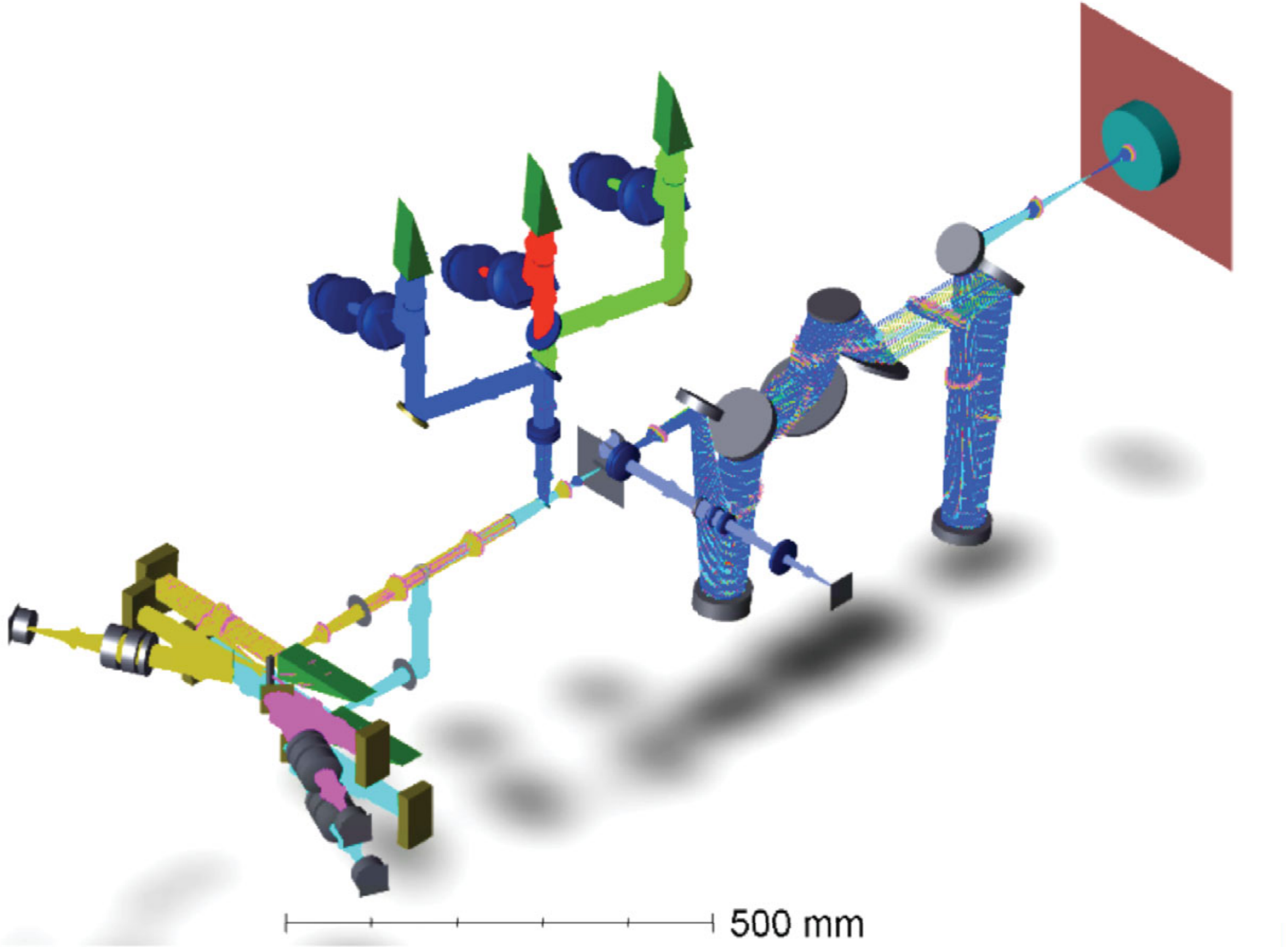


GMTNIRS sensitivity calculated conservatively: Average position along the blaze of both the echelle and the cross-disperser, 6x600 second exposures, image size = slit size.



In J,H,K, GMTNIRS can take a S/N> 100, R=50,000 spectrum of basically anything in the 2MASS catalog in under an hour


H-band
Spectrograph
K-band
Spectrograph
J-band
Spectrograph
Exit flange
Dewar window
K-mirror
unit
Telescope image
(f/11)
OAPs
Entrance slit
(f/8)
Input optics
500 mm


500 mm

Spectrograph basics: Spectrograph design without the grating equation:

$R_{diff} = Nm$

#of diffraction limited resels/order = # of grooves

Diffraction limited spot size at focal plane = f/ • λ

Diffraction limited spatial and spectral spot sizes the same.

Real resolving power:

$$R = R_{diff} \bullet (\theta_{diff}/\theta_{slit}) = Nm\,(\lambda/D)\,(\theta_{slit})^{-1}$$

(where in the right-hand version θ_{slit} is in radians)

Trial Spectrograph Design (use these rules)

Let's design a spectrograph that can cover the entire K band (2.0-2.5μm) in a single exposure at R=50,000 for use on GMT.

Givens:
Detector is 2048x2048 with 18 μm pixels (standard Teledyne product)
Diffraction limit of telescope = 0.08*2.2 = 18 mas.

We need a slit of 70 mas (this is about 4λ/D)
This protects against phase errors and image wander, allows long wavelength use of same slit.

Let's also decide that we want to sample with 4 pixels per slit width.

Trial Spectrograph Design (use these rules)

The $4\lambda/D$ slit implies that R_{diff}=200,000 to get R=50,000

With 4 pixel sampling R_{perpix} = 4x50,000 = 200,000

The two together mean that $R_{perpixel}$= 200,000 or λ/D
i.e. one R_{diff} for each pixel.

This also means that each pixel is one diffraction limited spatial element, or 18 mas.

Trial Spectrograph Design (use these rules)

Because of the length of a free spectral range varies across the band, we cannot use the full detector width at 2.2 microns. Better to use about 80% or 1600 pixels.

So, **N=1600 grooves** which will make the 2.2μm order free spectral range cover 1600 pixels.

How long does the grating have to be?

R_{diff}= 200,000. $L=\lambda R_{diff}/(2\sin\delta)$

For reasonable values:

$L = 2.2x10^{-4} \bullet 2x10^{5}/(1.8) = 24$ cm

Trial Spectrograph Design (use these rules)

What is the groove pitch we need?

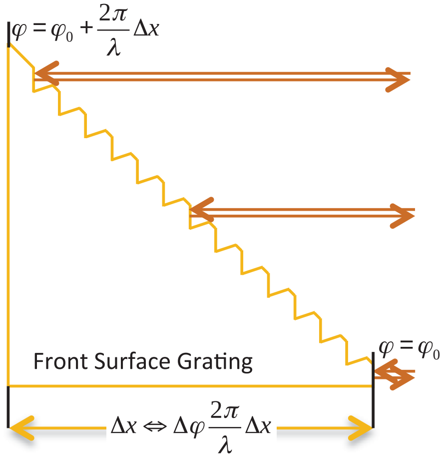
$2.4\times10^{-1}/1600 = 1.6\times10^{-4}$m= 160 μm => 6 grooves/mm
THIS IS IMPOSSIBLY COARSE

What camera f/ number do we need?
f/ • λ needs to equal the pixel size of 18 μm,
so we need f/8. THIS IS PRETTY EASY.

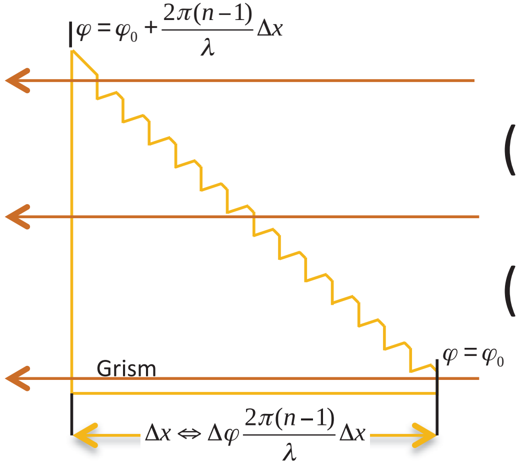
Now, the only question is the cross-dispersion.

The window is about $\Delta\lambda/\lambda = 0.22$, so we need 0.22*50,000= 11,000 individual resolution elements. Our central order has 400 elements, so we need 28 orders. If we spread these across 2000 pixels, we have 71 pixels per order for a mean separation of 0.018*71= 1.3”.

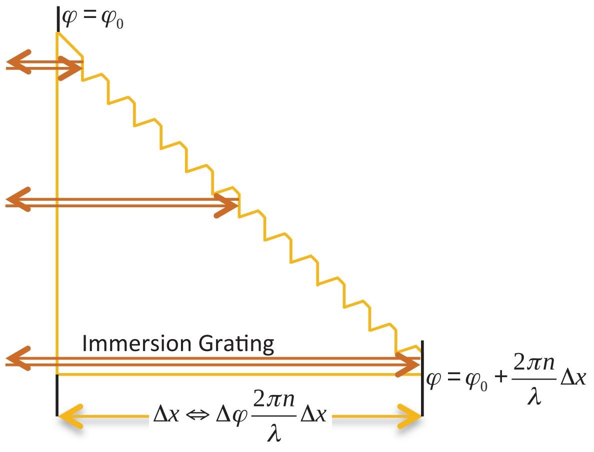
In practice, we will need to leave some space between orders so the slit length will be closer to 1”. Good thing this is an AO instrument.



n_{Si} ~ 3.4



(see our grism instrument design paper: Deen et al. (2017), PASP)



Resolving power is equal to phase delay across the beam measured in wavelengths divided by the ratio of the angular size of the slit to the diffraction limited angular scale.

$R = \lambda/\Delta\lambda = (2L\sin\delta)/\lambda \bullet \theta_{diff}/\theta_{slit}$

Where L is the grating length and δ is the grating angle.

$$m\lambda = n_G \sigma(\sin\alpha + \sin\beta)$$

In immersion, the internal wavelength shrinks by a factor of n, the refractive index

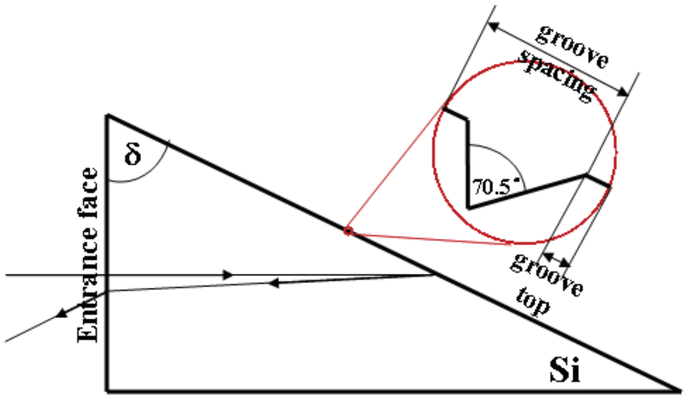
$$R_{\max} = \frac{2n_G L \sin\delta}{\lambda}$$

$$\frac{d\beta}{d\lambda} = \frac{2n_G \tan\beta}{\lambda}$$

The invention of the immersion grating by Dan Jaffe

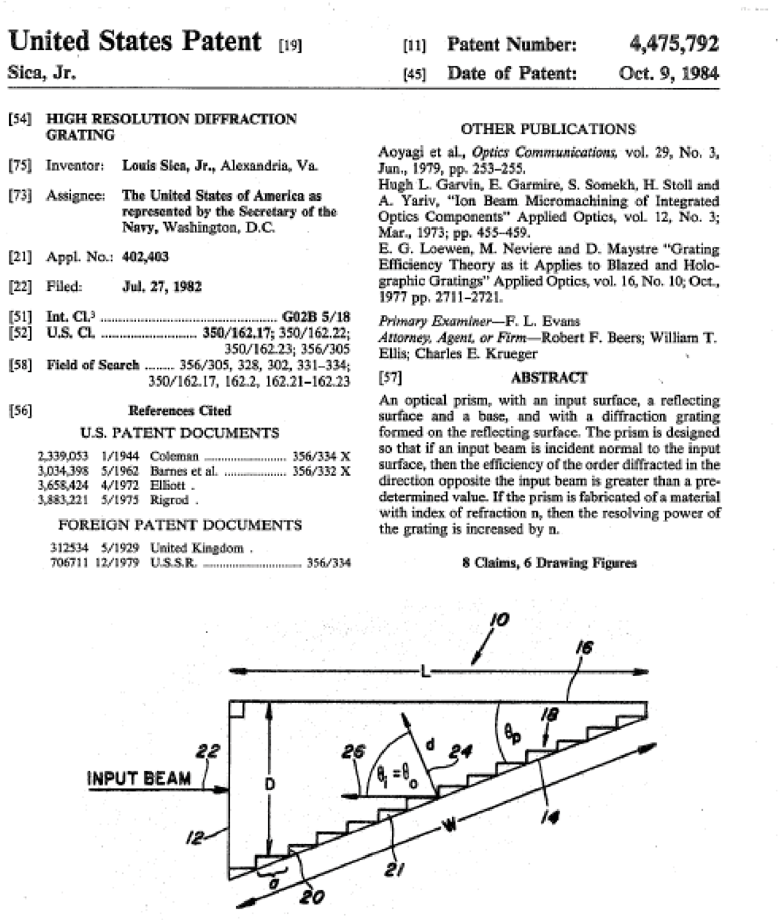
1. The “eureka moment”- Spring 1992

If you illuminate a grating from inside a transparent medium, the density of the medium leads the light to see the grating as “longer”, that is, bigger by a factor of the refractive index, n, which is 3.4 for silicon



The invention of the immersion grating by Dan Jaffe

2.The “oh” moment – discovering a US patent from 1984



United States Patent [19]
Sica, Jr.

[11] **Patent Number: 4,475,792**
[45] **Date of Patent: Oct. 9, 1984**

[54] **HIGH RESOLUTION DIFFRACTION GRATING**

[75] Inventor: Louis Sica, Jr., Alexandria, Va.

[73] Assignee: The United States of America as represented by the Secretary of the Navy, Washington, D.C.

[21] Appl. No.: **402,403**

[22] Filed: **Jul. 27, 1982**

[51] **Int. Cl.**³ **G02B 5/18**
[52] **U.S. Cl.** **350/162.17**; 350/162.22; 350/162.23; 356/305
[58] **Field of Search** 356/305, 328, 302, 331–334; 350/162.17, 162.2, 162.21–162.23

[56] **References Cited**

U.S. PATENT DOCUMENTS

2,339,053 1/1944 Coleman .... 356/334 X
3,034,398 5/1962 Barnes et al. .... 356/332 X
3,658,424 4/1972 Elliott .
3,883,221 5/1975 Rigrod .

FOREIGN PATENT DOCUMENTS

312534 5/1929 United Kingdom .
706711 12/1979 U.S.S.R. 356/334

OTHER PUBLICATIONS

Aoyagi et al., *Optics Communications*, vol. 29, No. 3, Jun., 1979, pp. 253–255.
Hugh L. Garvin, E. Garmire, S. Somekh, H. Stoll and A. Yariv, “Ion Beam Micromachining of Integrated Optics Components” Applied Optics, vol. 12, No. 3; Mar., 1973; pp. 455–459.
E. G. Loewen, M. Neviere and D. Maystre “Grating Efficiency Theory as it Applies to Blazed and Holographic Gratings” Applied Optics, vol. 16, No. 10; Oct., 1977 pp. 2711–2721.

Primary Examiner—F. L. Evans
Attorney, Agent, or Firm—Robert F. Beers; William T. Ellis; Charles E. Krueger

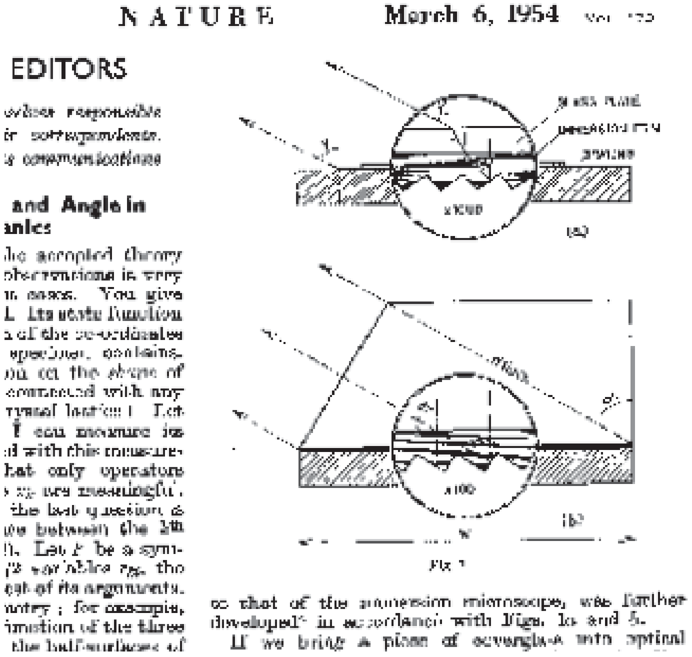
[57] **ABSTRACT**

An optical prism, with an input surface, a reflecting surface and a base, and with a diffraction grating formed on the reflecting surface. The prism is designed so that if an input beam is incident normal to the input surface, then the efficiency of the order diffracted in the direction opposite the input beam is greater than a predetermined value. If the prism is fabricated of a material with index of refraction n, then the resolving power of the grating is increased by n.

8 Claims, 6 Drawing Figures

The invention of the immersion grating by Dan Jaffe

3.The “hah” moment- finding an article from Nature, 1954



NATURE March 6, 1954

EDITORS

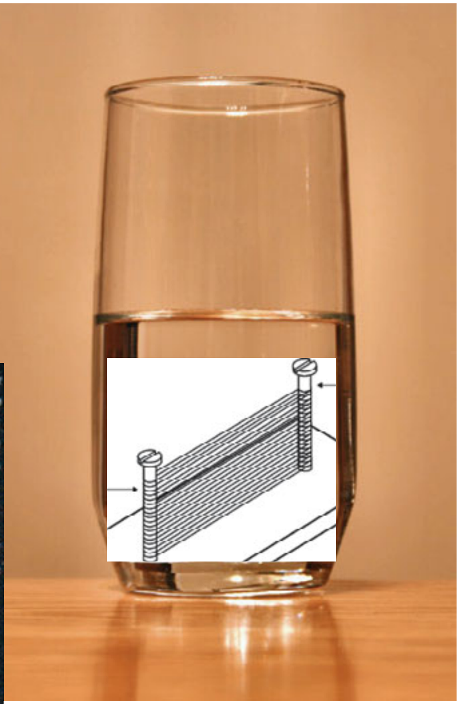
and Angle in

The invention of the immersion grating by Dan Jaffe

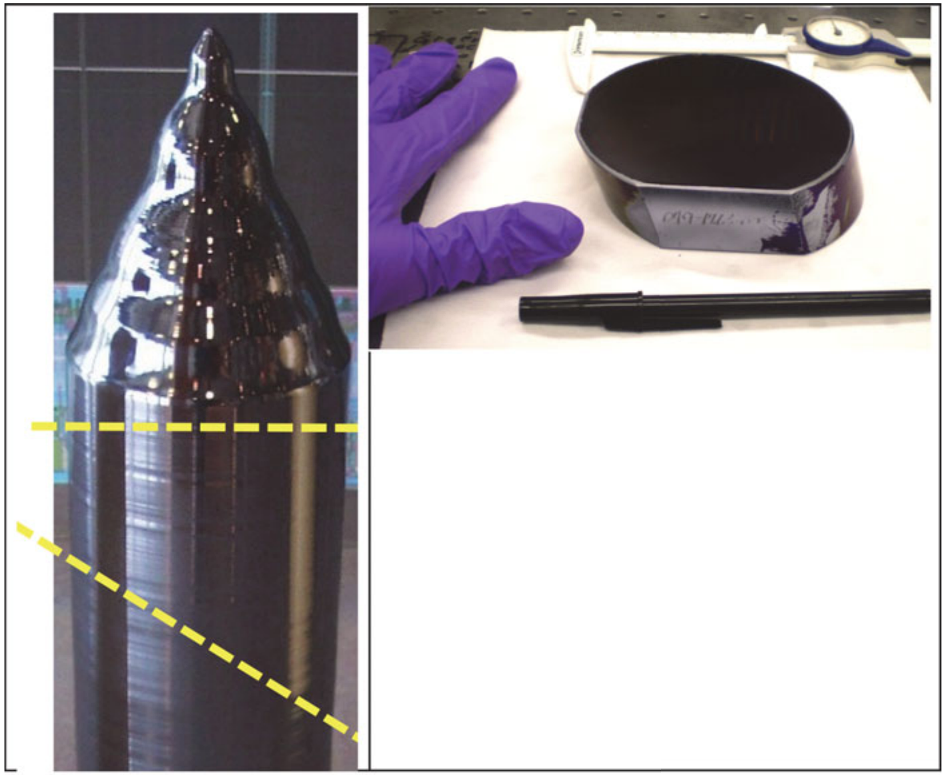
4. The "duh" moment: *Gegenseitige Einwirkung der im Wasser und anderen brechenden Mitteln gebeugten Strahlen* Joseph Fraunhofer 1823

The interaction of diffracted radiation in water and other refractive media.

Fraunhofer immersed his gratings in water, linseed oil, and turpentine. We immerse ours in solid silicon but the physics is the same.

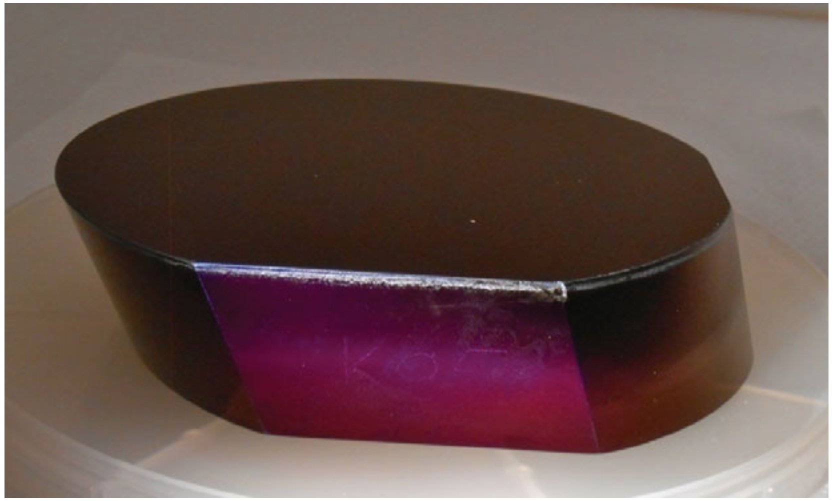


The thick substrates require a completely independent process chain from what wafers require.

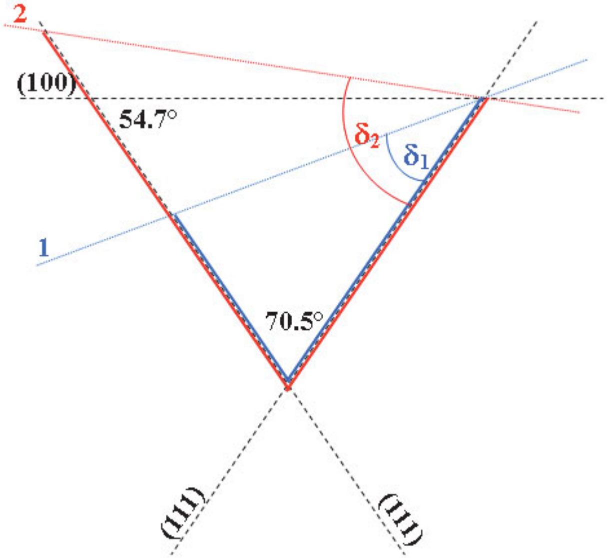


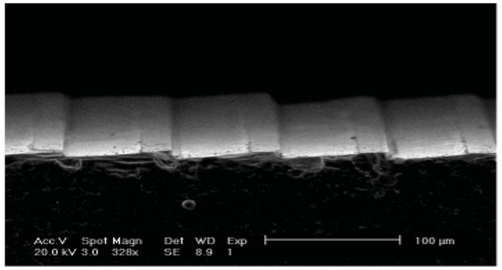
Material preparation requires coordination of:

1. Float-zone silicon boule, resistivity of >10,000 ohm-cm.
2. X-ray crystallography to orient to 0.04°. Tilt and slice boule.
3. Chemically mechanically polished to λ/10
4. LP-CVD silicon nitride 600 Å ± 5%

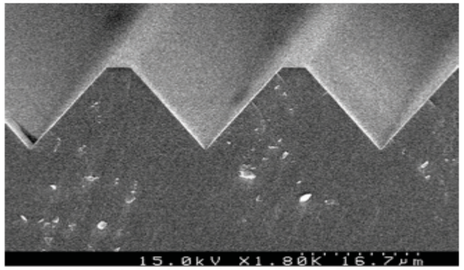


By correctly orienting the disk surface with respect to the silicon crystal planes, we can produce a grating with any blaze angle.

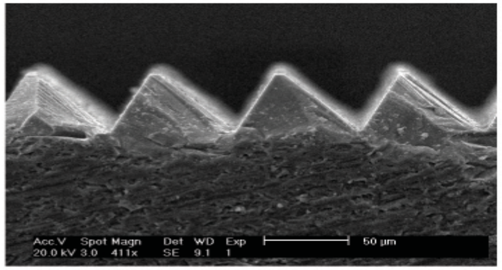




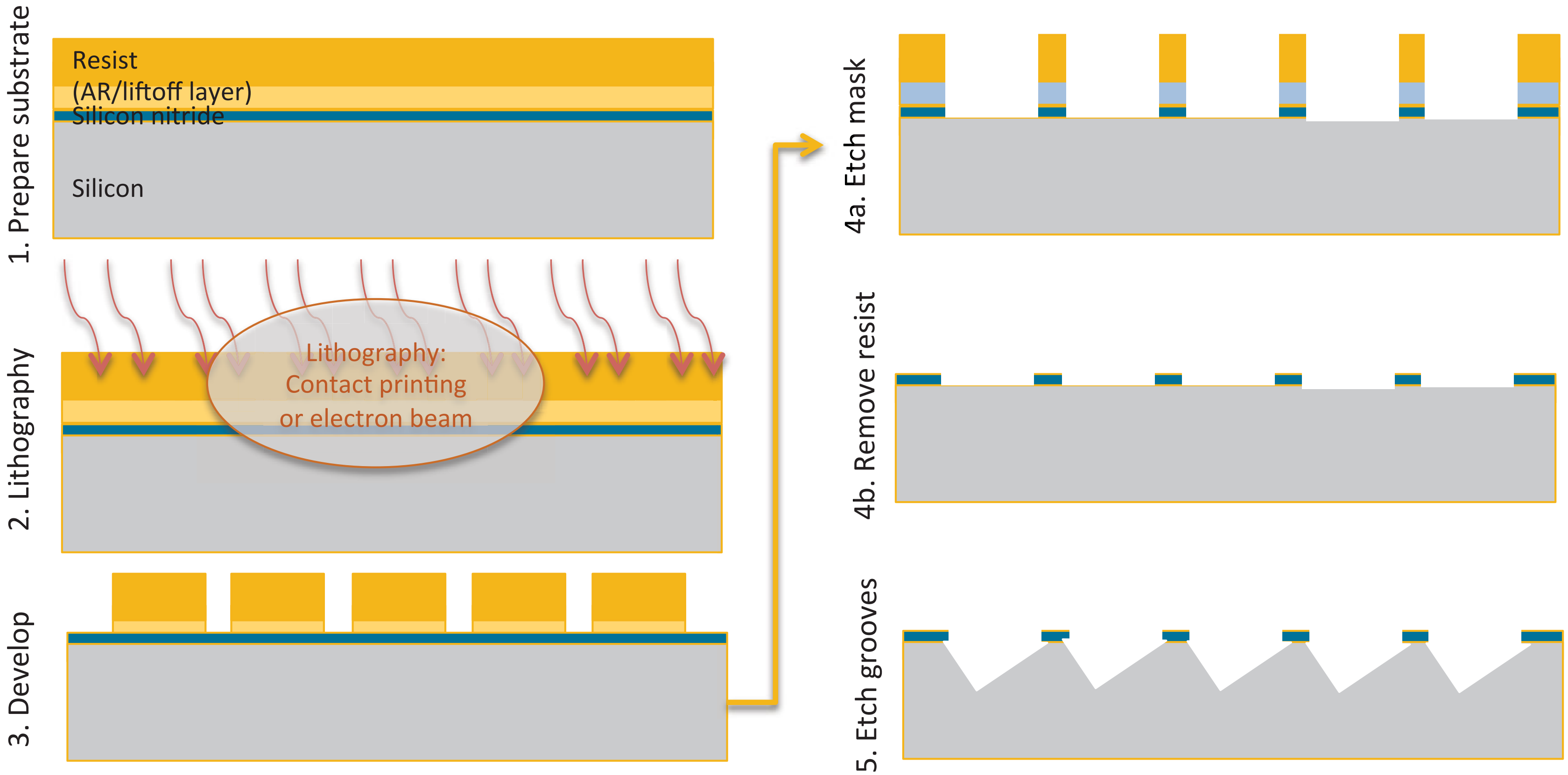
6.16°



54.7°



63.4°



1. Prepare substrate

Resist
(AR/liftoff layer)
Silicon nitride
Silicon

2. Lithography

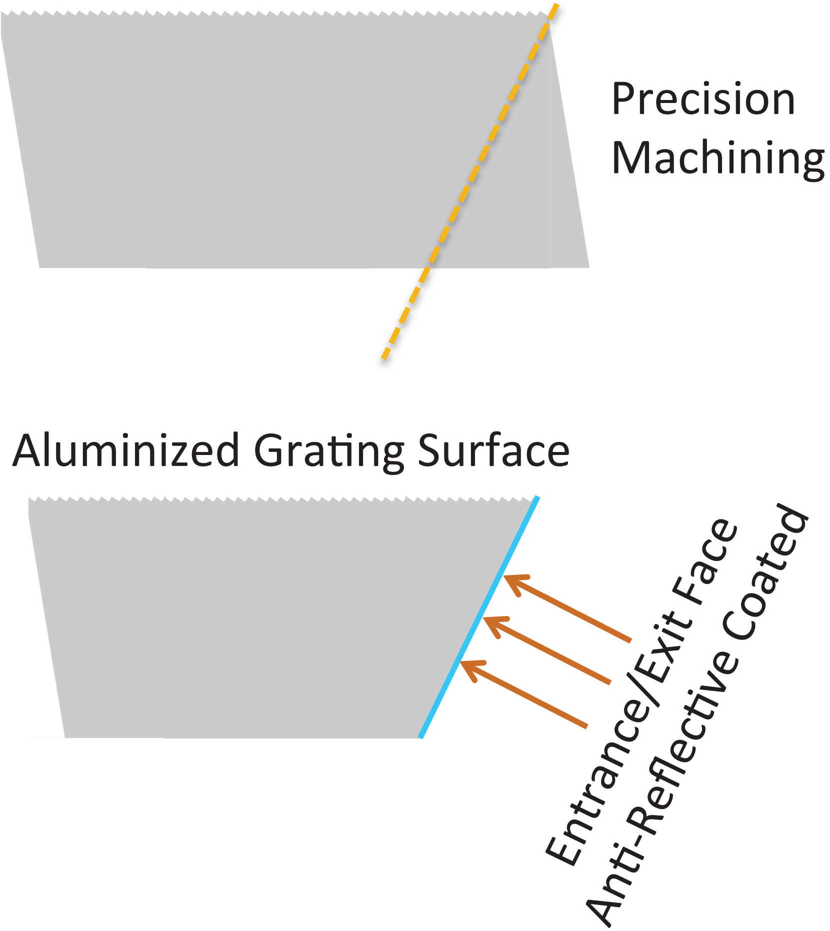
Lithography:
Contact printing
or electron beam

3. Develop

4a. Etch mask

4b. Remove resist

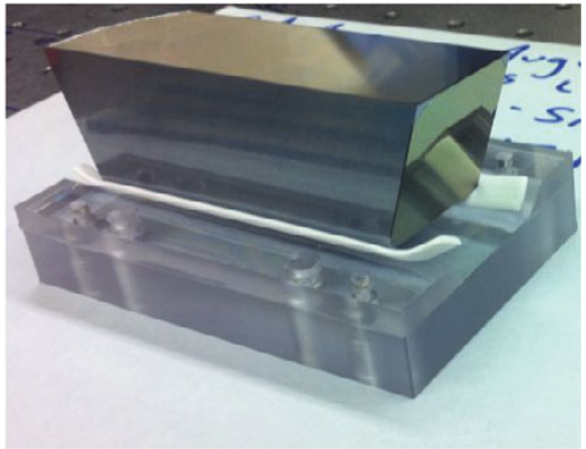
5. Etch grooves



Precision
Machining

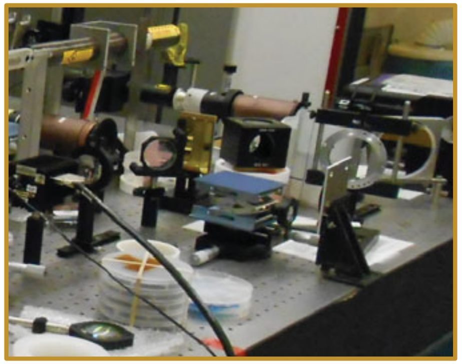
Aluminized Grating Surface

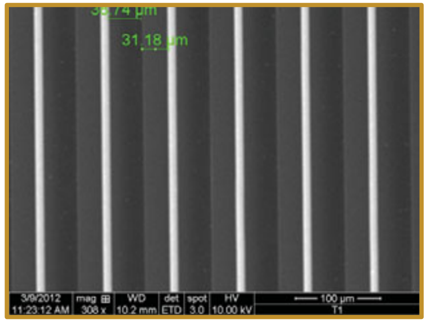
Entrance/Exit Face
Anti-Reflective Coated

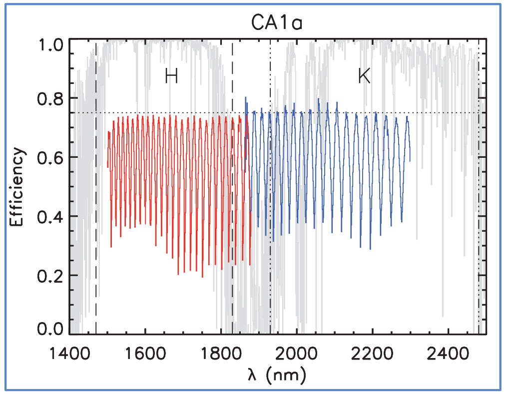


IGRINS immersion grating

Test	Specification
Front surface interferogram in Littrow at 633 nm (Equivalent to~2.15 µm in immersion)	λ/4 in immersion at operating wavelength
Laser spectrum	Ghosts < 2 x 10^{-3}
Imaging with scanning electron microscope (SEM)	Smooth surface, <<1% defect area
Efficiency in immersion over wavelength range	>= 75%

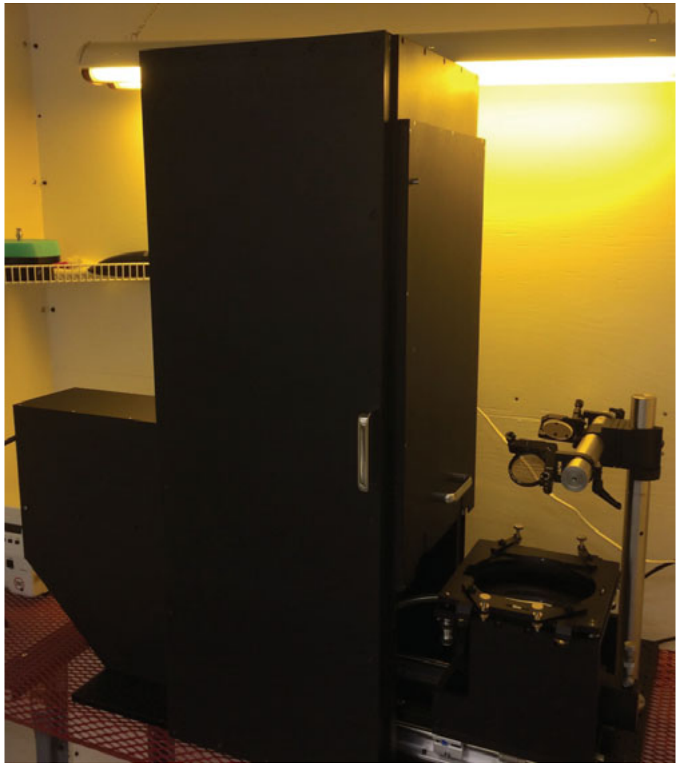


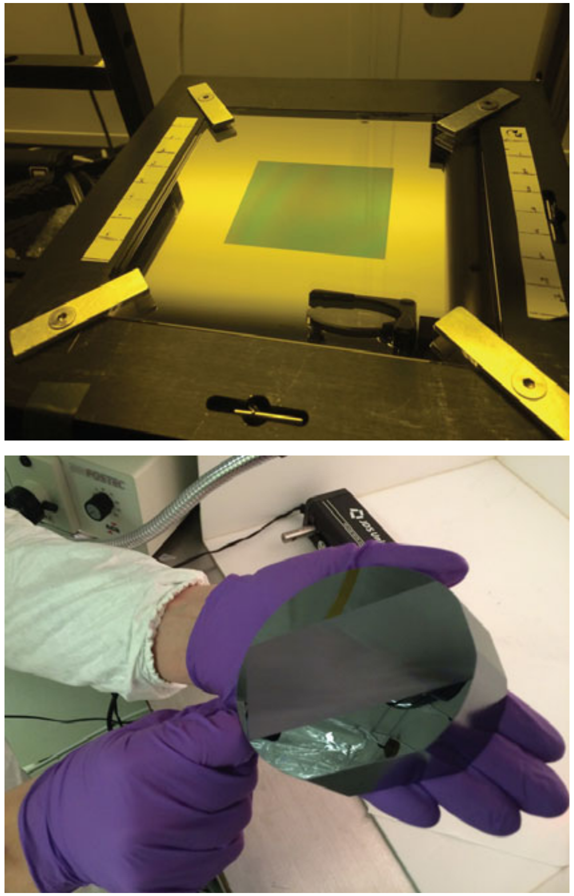




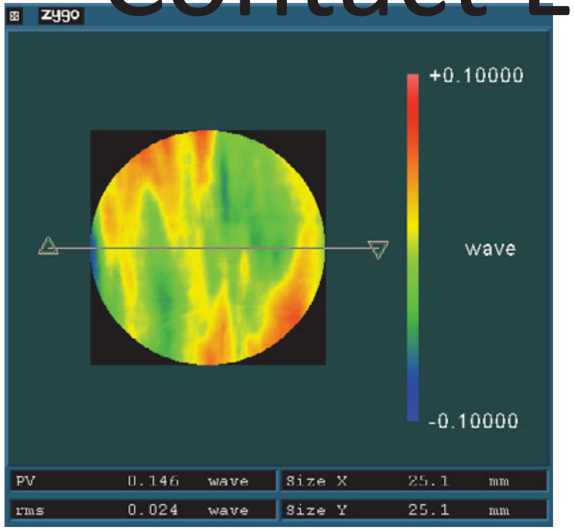
Contact Lithography

UTexas Grating Contact Aligner



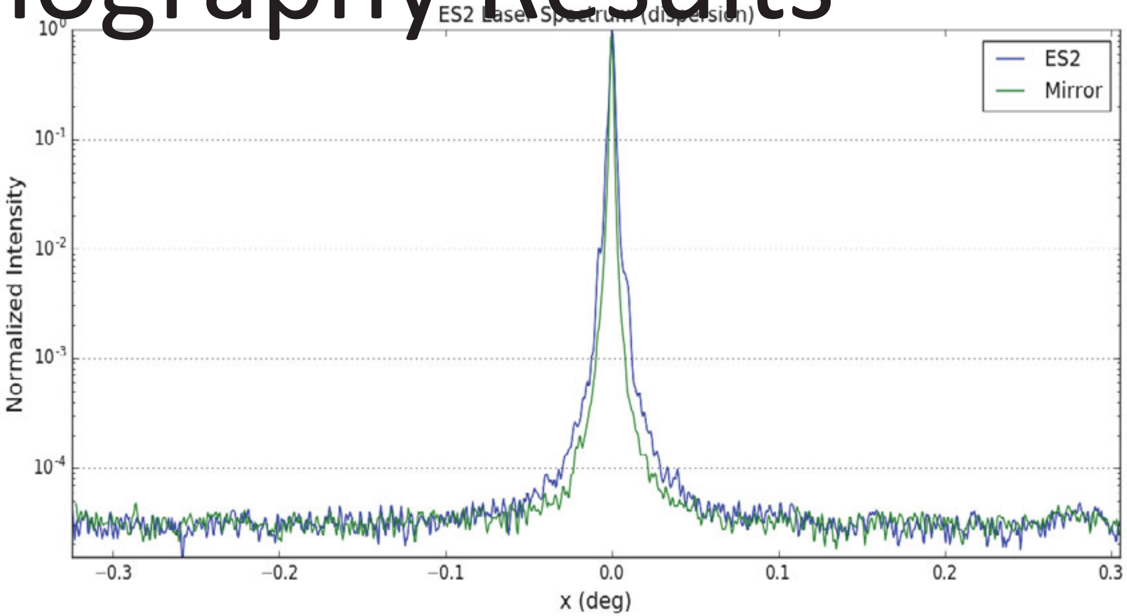


Contact Lithography Results



PV 0.146 wave
Size X 25.1 mm
rms 0.024 wave
Size Y 25.1 mm

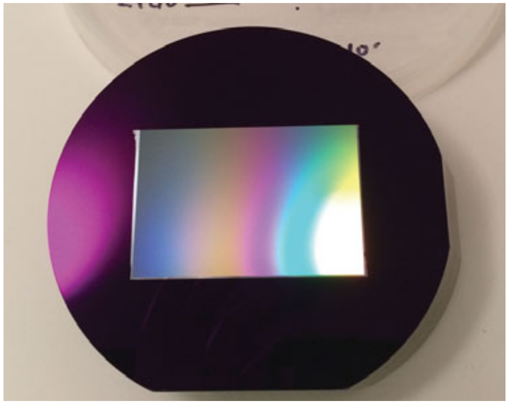
- Front surface interferogram in Littrow at 71.6° for a 25 mm beam.
- Phase PV is 0.146 waves at 633 nm, corresponding to ~2.0 µm in immersion.

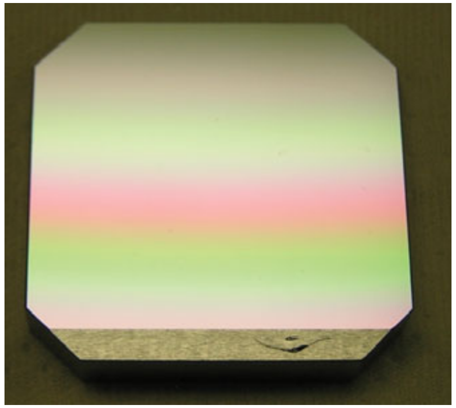


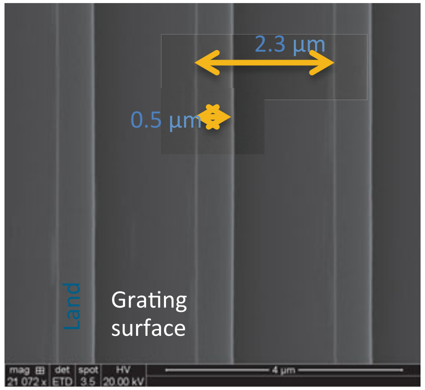
- High dynamic range, front surface monochromatic spectrum of same grating.
- Contact gratings can be as coarse as 5 l/mm

JPL electron beam lithography tool

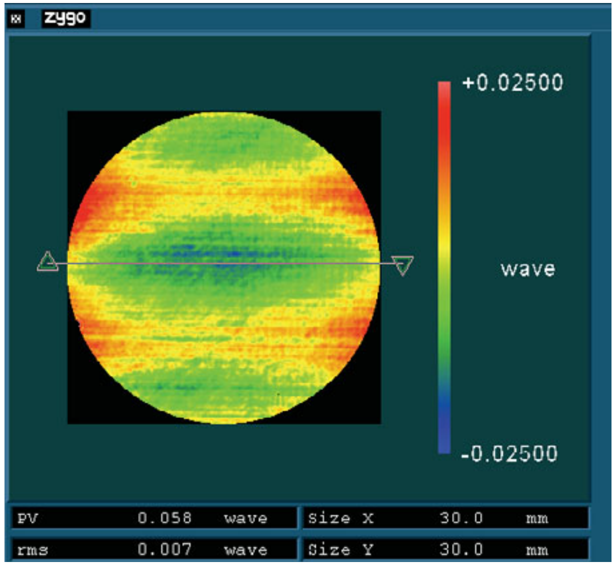
MDL's World-Class JEOL JBX-9300FS Electron-Beam Lithography System uses a focused beam of electrons to write patterns directly on wafers. This powerful capability allows MDL technologists to create atom-sized features as small as 4 nanometers.



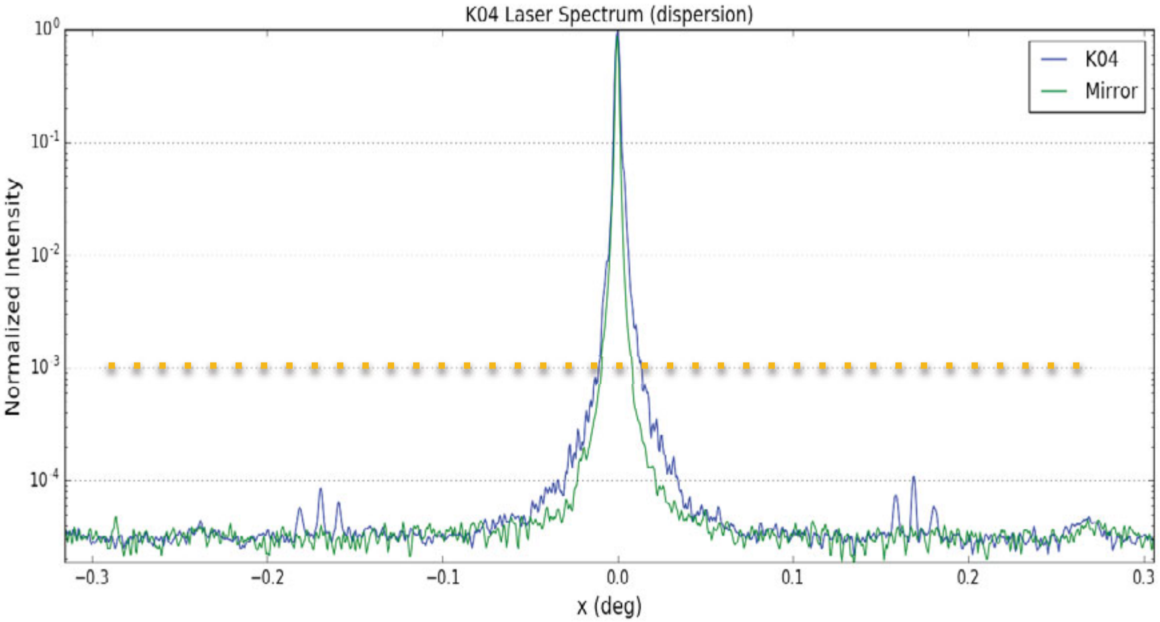




Electron beam lithography allows us to make very fine-pitch gratings of 1 µm or below.



PV	0.058	wave	Size X	30.0	mm
rms	0.007	wave	Size Y	30.0	mm



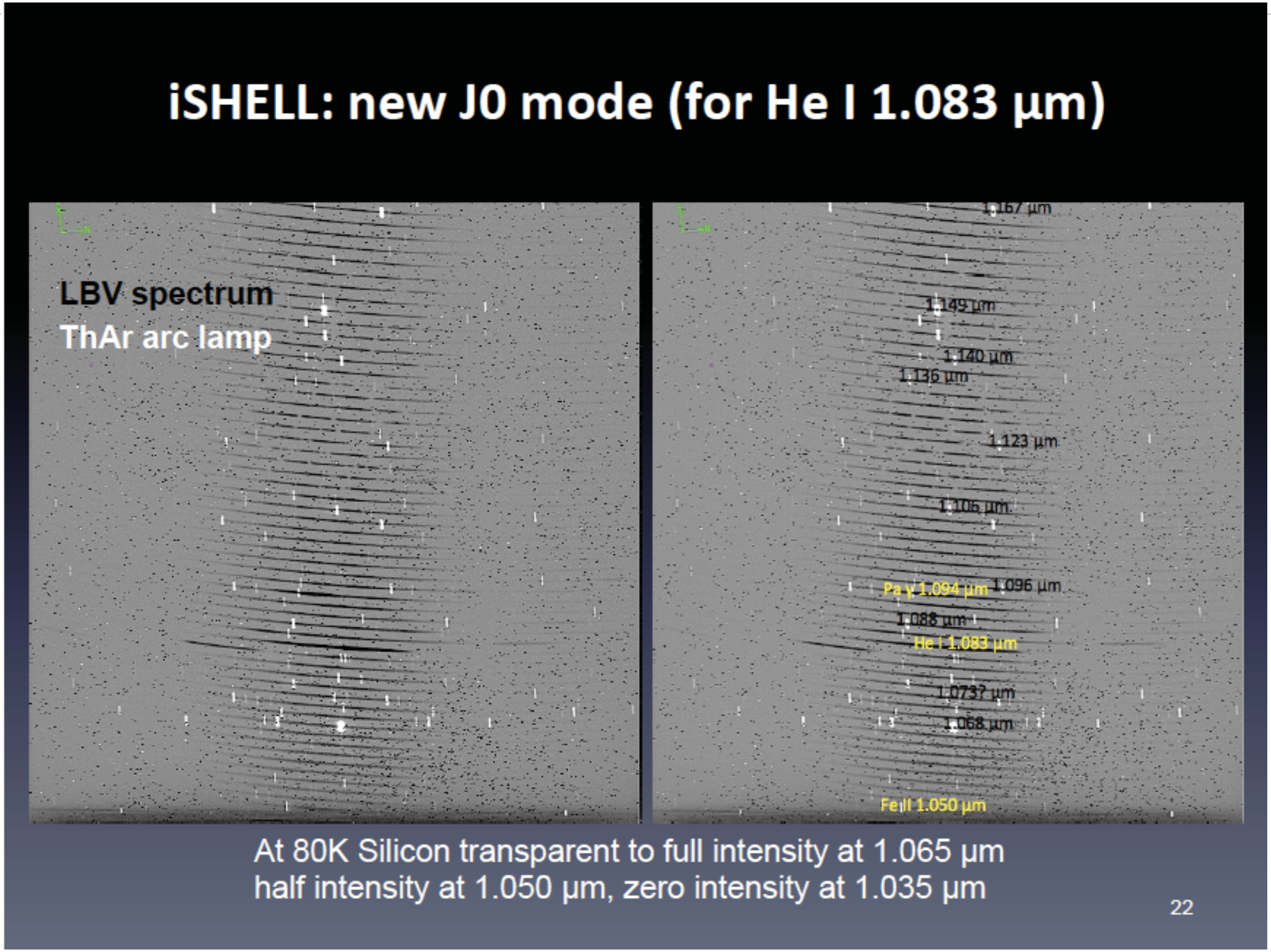
- Front surface interferogram in Littrow at 18° for a 30 mm beam.
- Phase PV is 0.06 waves at 633 nm, corresponding to ~2.0 μm in immersion.

- High dynamic range, front surface monochromatic spectrum of same grating.
- Ghost specification is $<10^{-3}$ of the central peak; these are $<10^{-4}$.

Degree of Difficulty

Degree of difficulty: scales with $[(n-1)\sin\delta]/\lambda$ for grisms and with $[2n\sin\delta]/\lambda$ for immersion gratings. Scales with length of grating divided by width of slit in units of diffraction limited width.

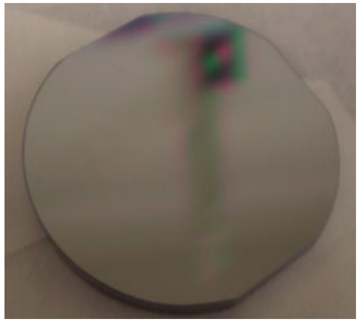
Forcast grism 1: $\delta=11^o$ $\lambda= 30$ μm, DD=1
Other Forcast grisms: DD=1-10
JWST grisms: DD= 9
IG for IGRINS: DD=120
IG for GMTNIRS: DD= 250



iSHELL: new J0 mode (for He I 1.083 µm)

At 80K Silicon transparent to full intensity at 1.065 µm
half intensity at 1.050 µm, zero intensity at 1.035 µm

Deployed Technology

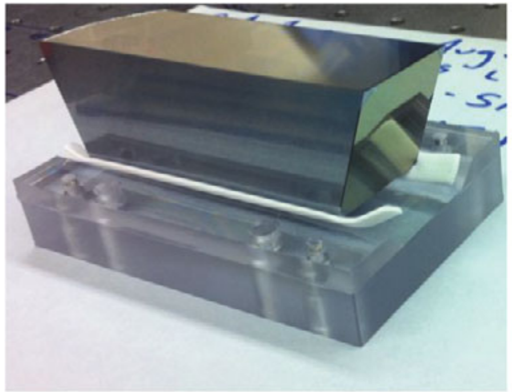


Silicon grism flight parts:

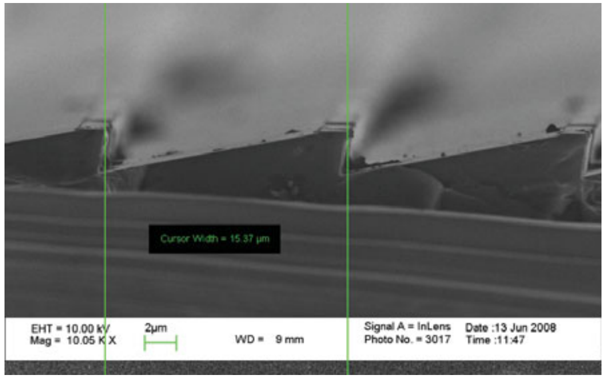
- James Webb Space Telescope NIRCam
- FORCAST on SOFIA Telescope

Echelle immersion gratings:

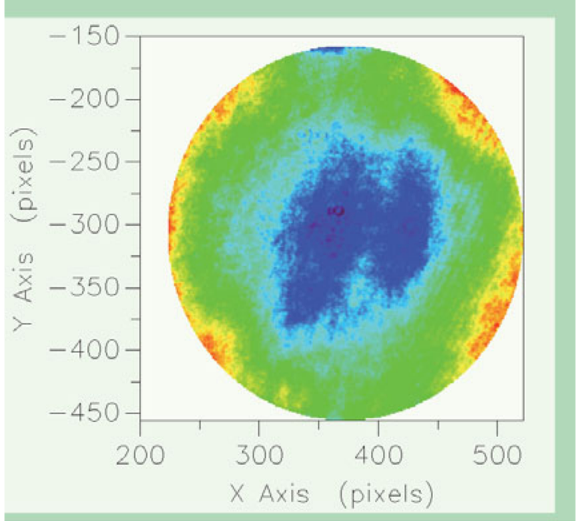
- Immersion GRating Infrared Spectrograph (IGRINS) installed at McDonald Observatory
- iShell for the NASA InfraRed Telescope Facility
- Planned GMT Near InfraRed Spectrograph (GMTNIRS) for the Giant Magellan Telescope.



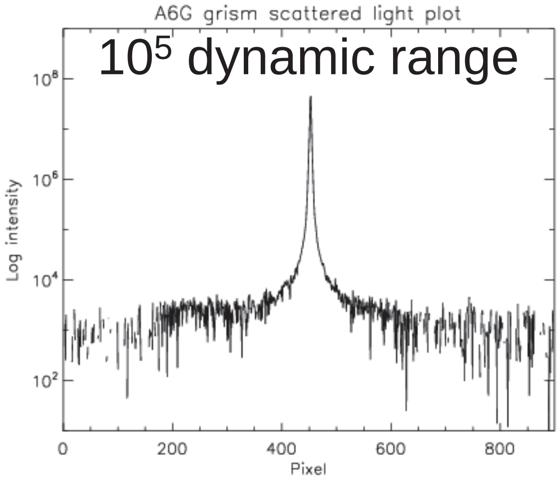
JWST NIRCam Grisms



λ/100 rms grating surface

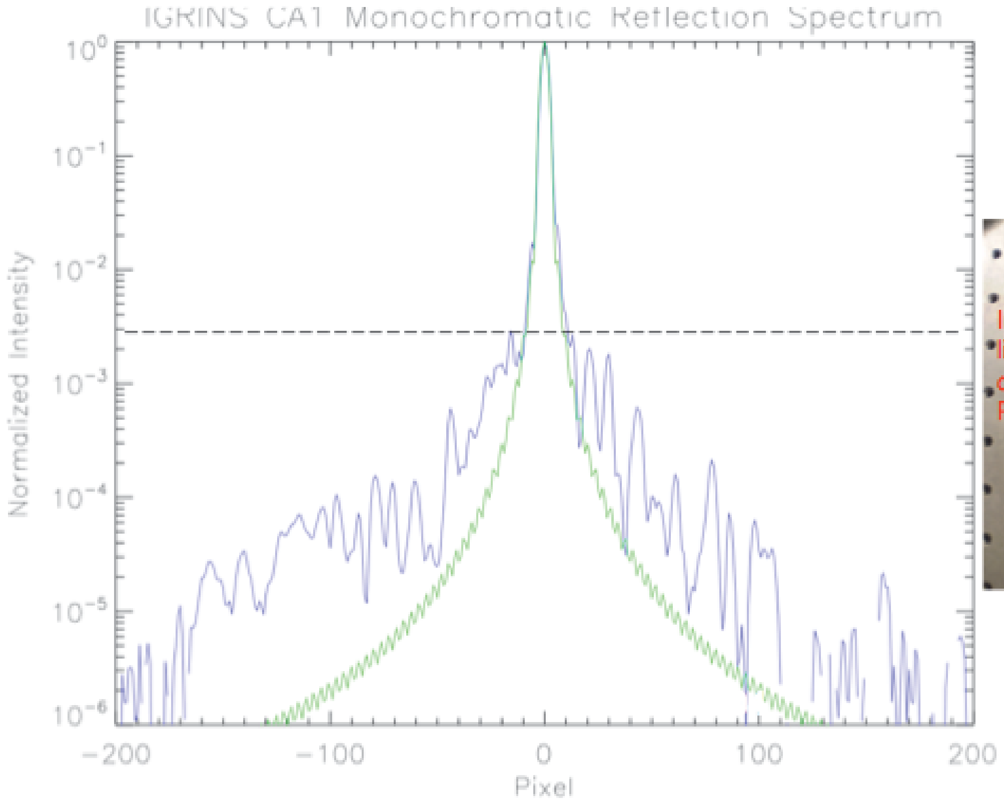


10^5 dynamic range

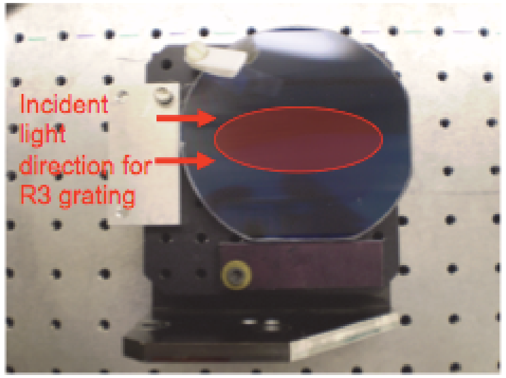


Flight Part

IGRINS Immersion Grating- Complete 2011



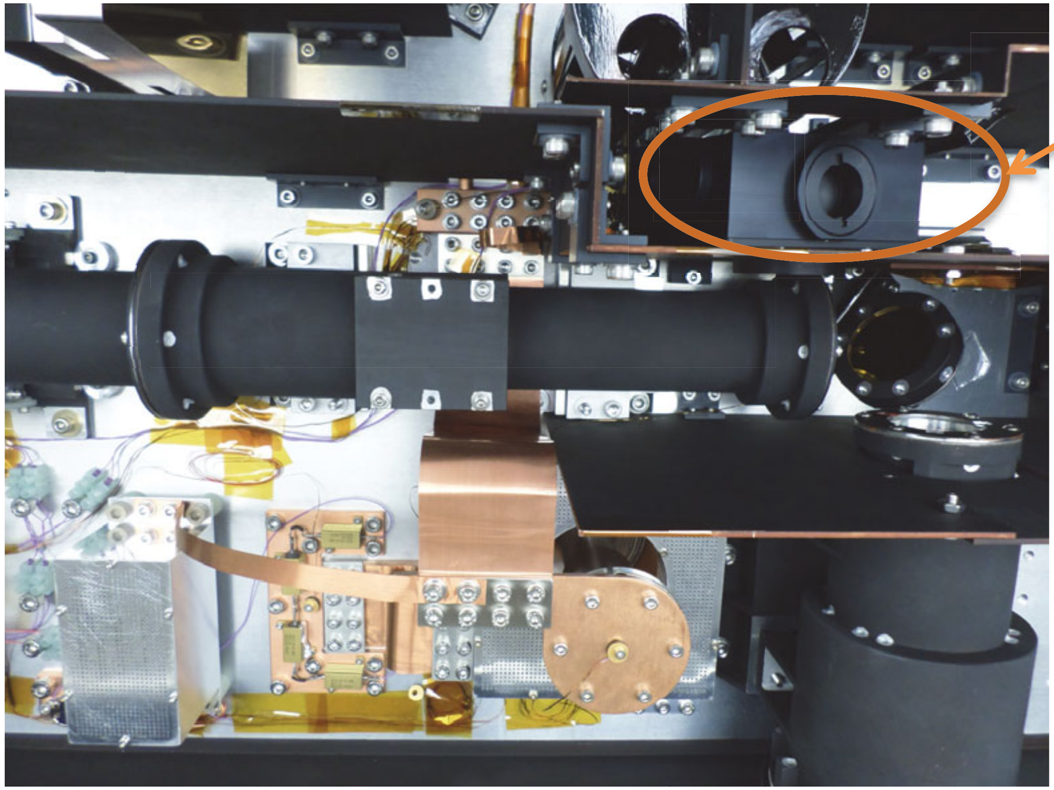
- wavelength - 543 nm
- beam size – 20 mm
- logarithm scale



Setup example for R3 grating

Green – theoretical line
Blue – measurement

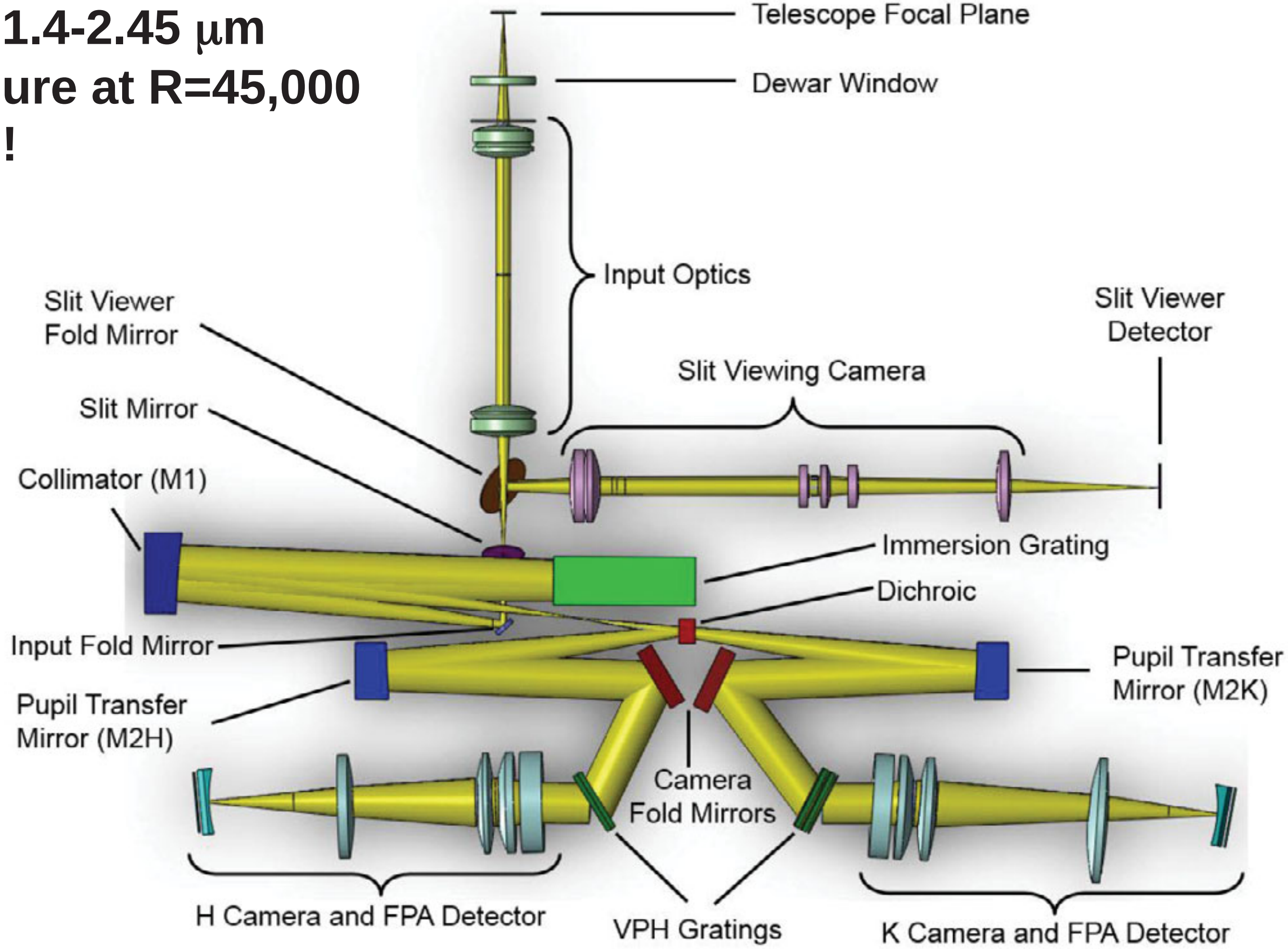
Surface is $\lambda/6$ peak to valley. Efficiency ~80%



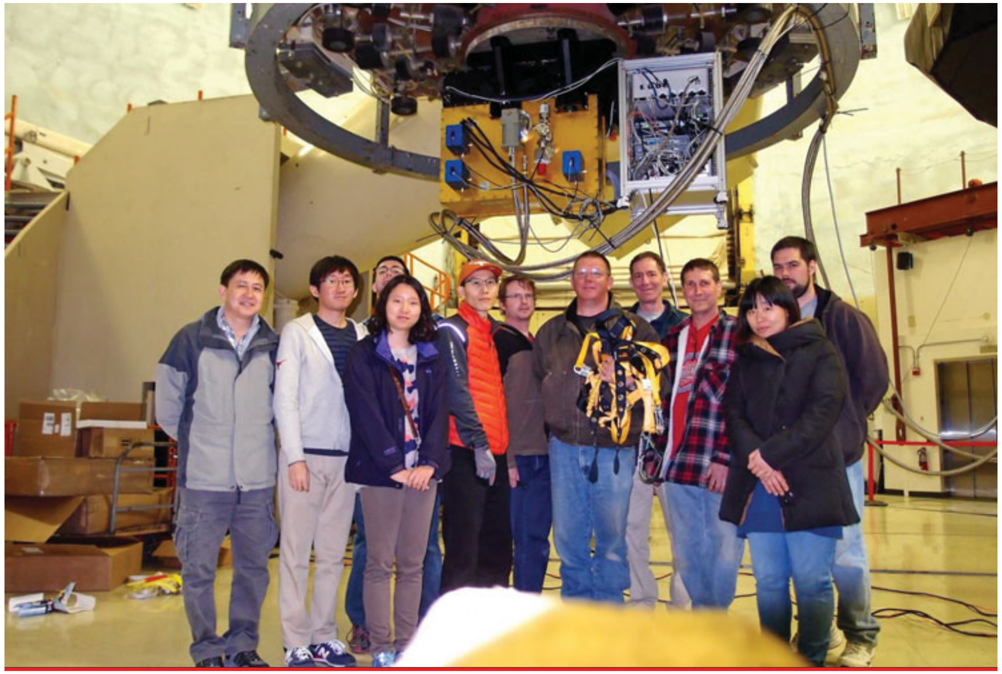
IGRINS
Immersion Grating

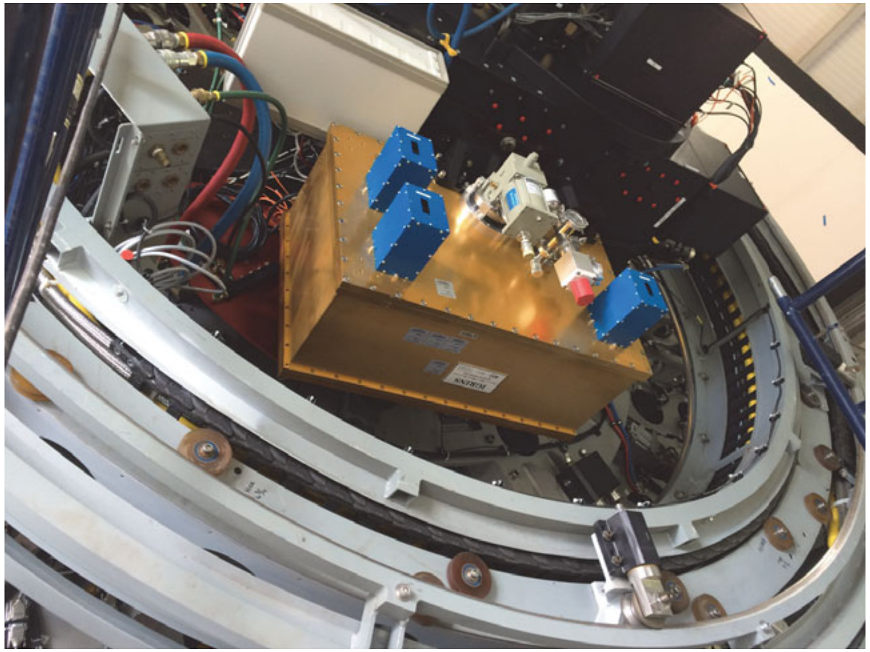
INfrared

IGRINS (UT and KASI) covers all of 1.4-2.45 μm in one exposure at R=45,000 with no gaps!



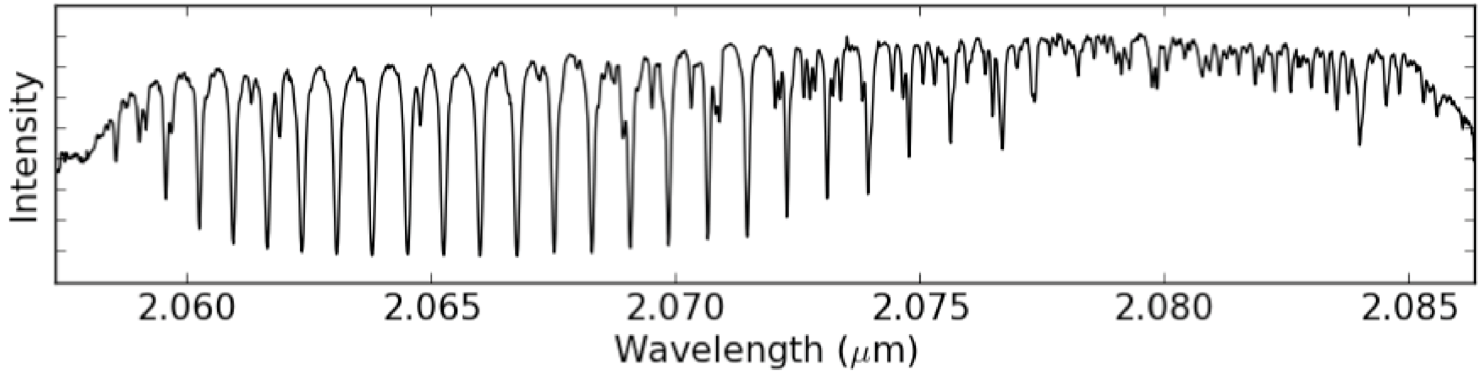
IGRINS on McDonald 2.7m 2014-2016, no cold moving parts, warm calibration system with moving mirrors

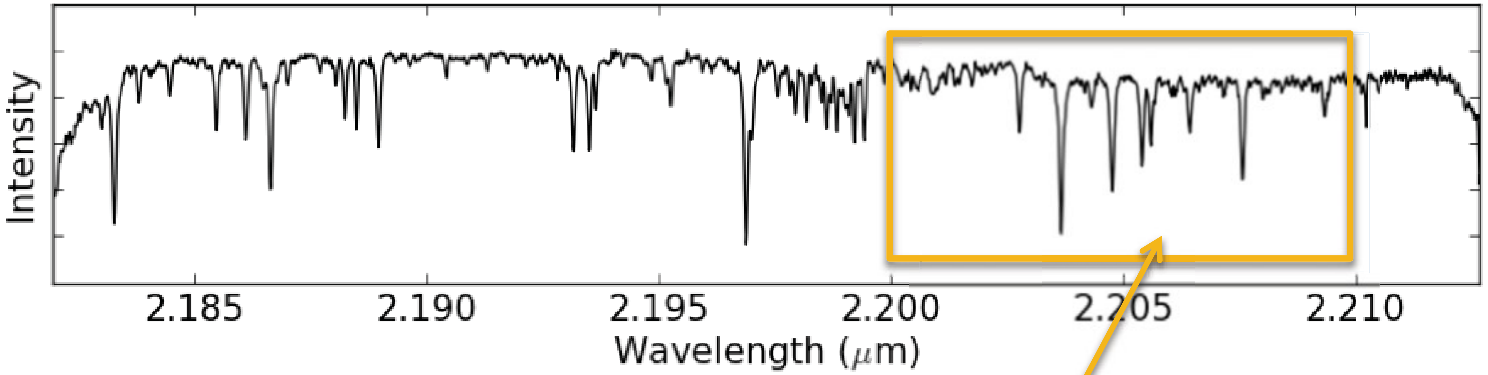




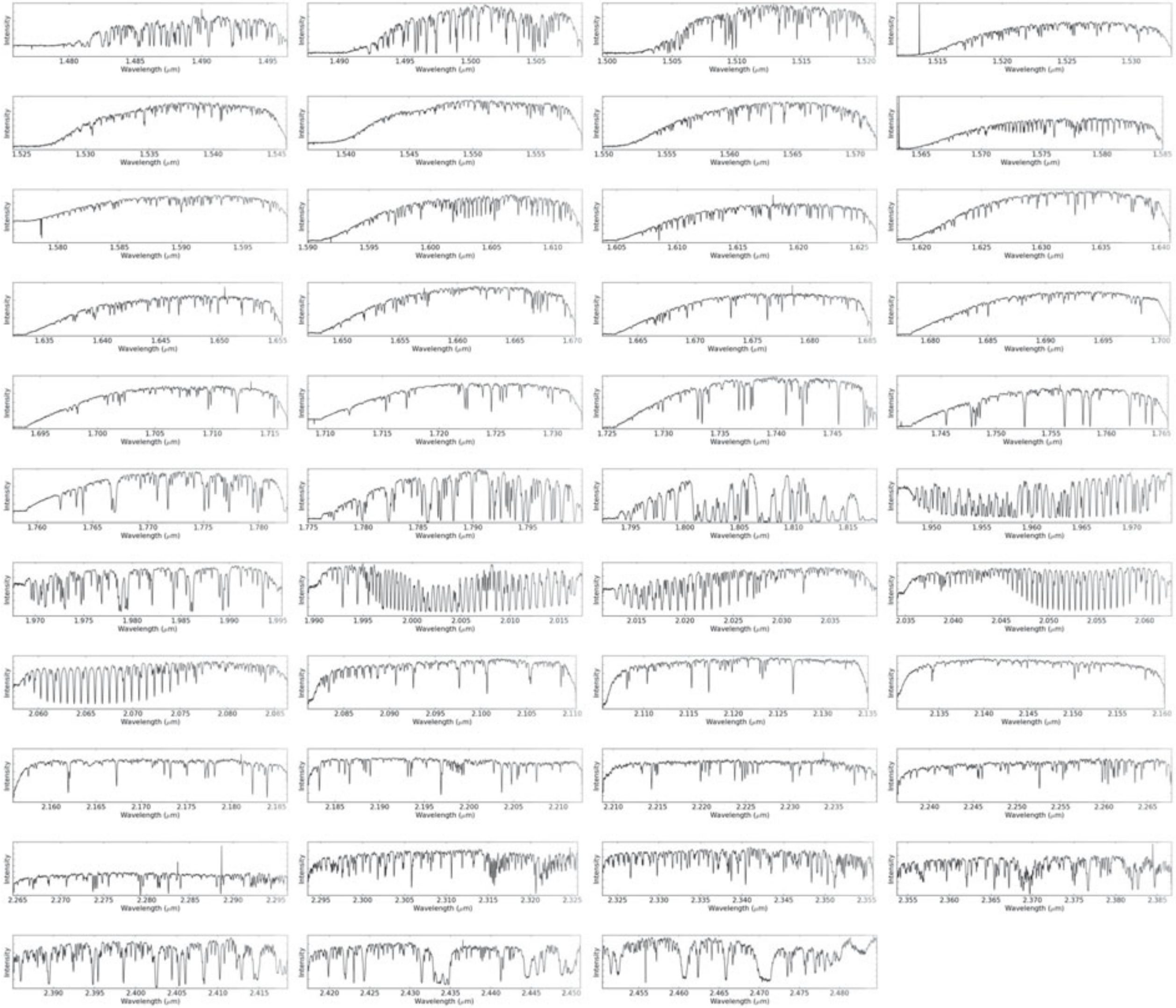
IGRINS on 4.3m DCT 2016- and McDonald 2.7m 2017-
No moving parts, sky emission and absorption lines, white spot

IGRINS Spectrum of a star, not corrected for telluric absorption





Region covered by the Phoenix spectrograph


Intensity
Wavelength (μm)