Development of immersion gratings and grisms at LLNL

Dispersing elements for astronomy:
New trends and possibilities
Milan, Italy

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October 10, 2017

LLNL-PRES-740702
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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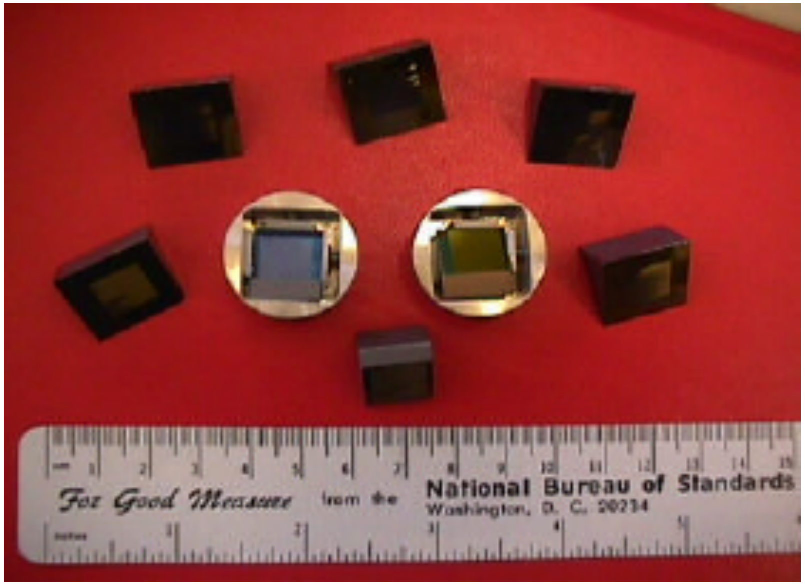
How we got started

- Benefits of immersion derive from the grating equation
  - Dispersion and spectral resolution increase by factor of N, the refractive index of the immersing material.
  - Or else, one can reduce instrument size and maintain resolution.
  - This was known for a long time. Hulthen (1954) Sica (1981 US patent).
- Applied Optics paper (Wiedemann 1993) was first realization of an immersion grating in silicon
  - LLNL got started. So did groups at the University of Texas and ESO.
  - Based on anisotropic etching of silicon, leverages semiconductor R&D.
  - In principle allows very coarse grooves (echelle gratings)
- Etching a groove is easy. Etching a high quality grating is hard.
  - Grating is only as good as lithography mask (periodic error from stitching)
  - Pattern transfer errors (lithography mask-> photoresist-> etch mask-> silicon)
  - Semiconductor tools are designed for wafers not thick silicon.
  - Nanometer errors in groove position have observable effects.

Etched silicon gratings at LLNL (1990's)

- First LLNL grating had predicted dispersion but surface error of 1-2λ @633 nm limited resolution. Work continued to reduce surface error.
- We made some 10 x 10 mm grisms in 1999. R~5000 @ 2.1µm
  - Demonstrated LPCVD Si_xN_y as conformal AR coating on grooves. R < 2%.
  - Tested grisms in IRCAL instrument at Lick Observatory.
  - Surface error 0.035λ @633 nm
- And then…
  - The microfabrication engineer retired.
  - Interests shifted to longer λ, where Si has very poor transmission.
- Time for a new direction
  - Alternative fabrication techniques?



Can immersion gratings be diamond machined?

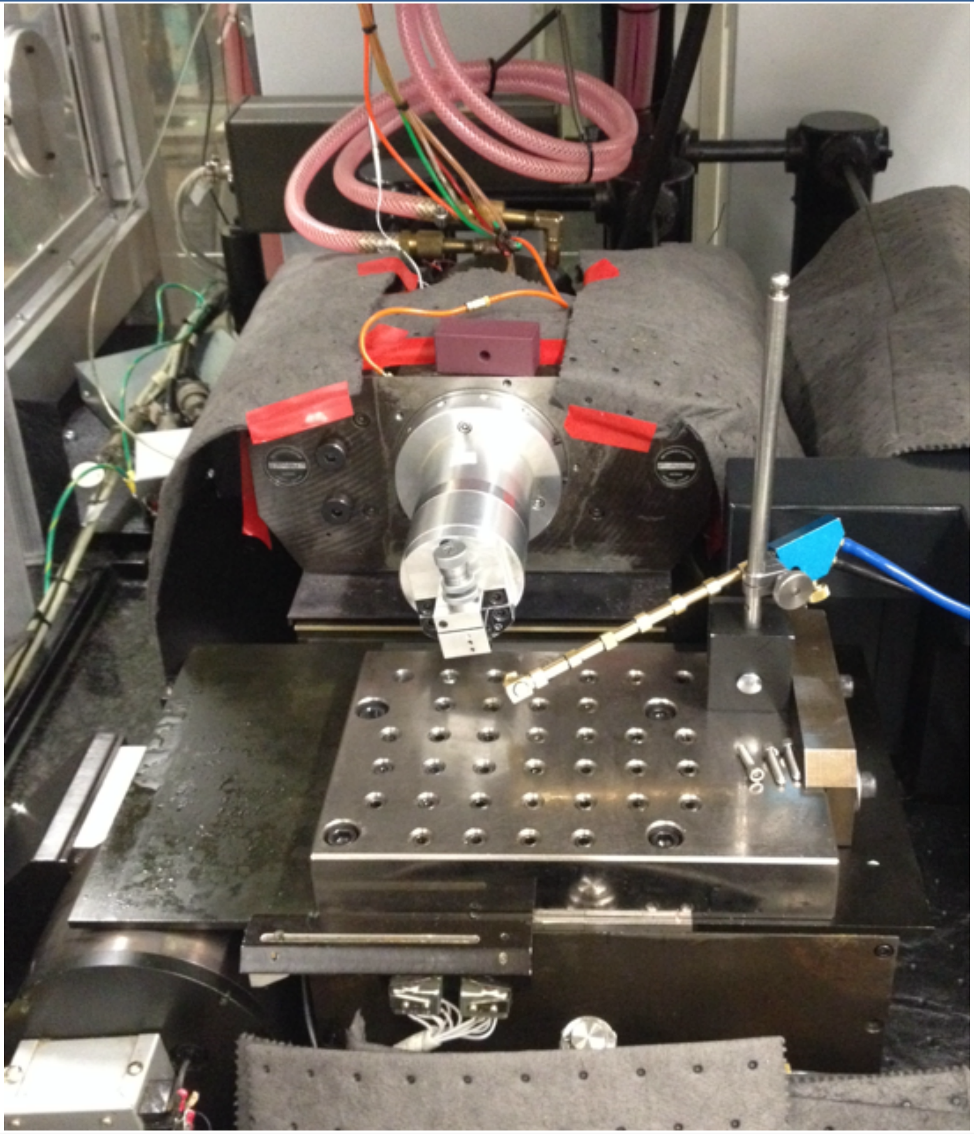
- Fortuitous encounter at SPIE Astronomical Instrumentation 1998
  - Cornell group had test gratings cut in ZnS and ZnSe blanks.
  - LLNL measured < 1λ surface error @633nm, < 10 nm rms roughness.
- Tried to work with commercial vendors on germanium gratings
  - Grooves badly chipped unless feed rates slowed to ~1cm/minute
  - Several waves of surface error due to inadequate temperature control
- Extensive R&D on diamond machining took place at LLNL in 1970’s and 1980’s. Several custom machines were constructed to advance the state of the art of precision machining. One of the smaller machines, PERL II, was available and had several features that made it suitable to attempt to machine a grating.

Diamond machining is versatile

- Groove shape matches tool shape. Allows control of blaze angle and groove apex angle.
- Grating period programmed into machine. Easy to change.
- Works with a variety of materials. Not all optical materials can be diamond machined, but most IR materials work.
- Brittle materials cut as if ductile for very small chip thicknesses.
  - Semiconductors undergo phase transition to ductile state at sufficiently high pressures (several GPa).
  - Requires very stiff mechanical structure, very hard tool, very small area of contact, material in compression.

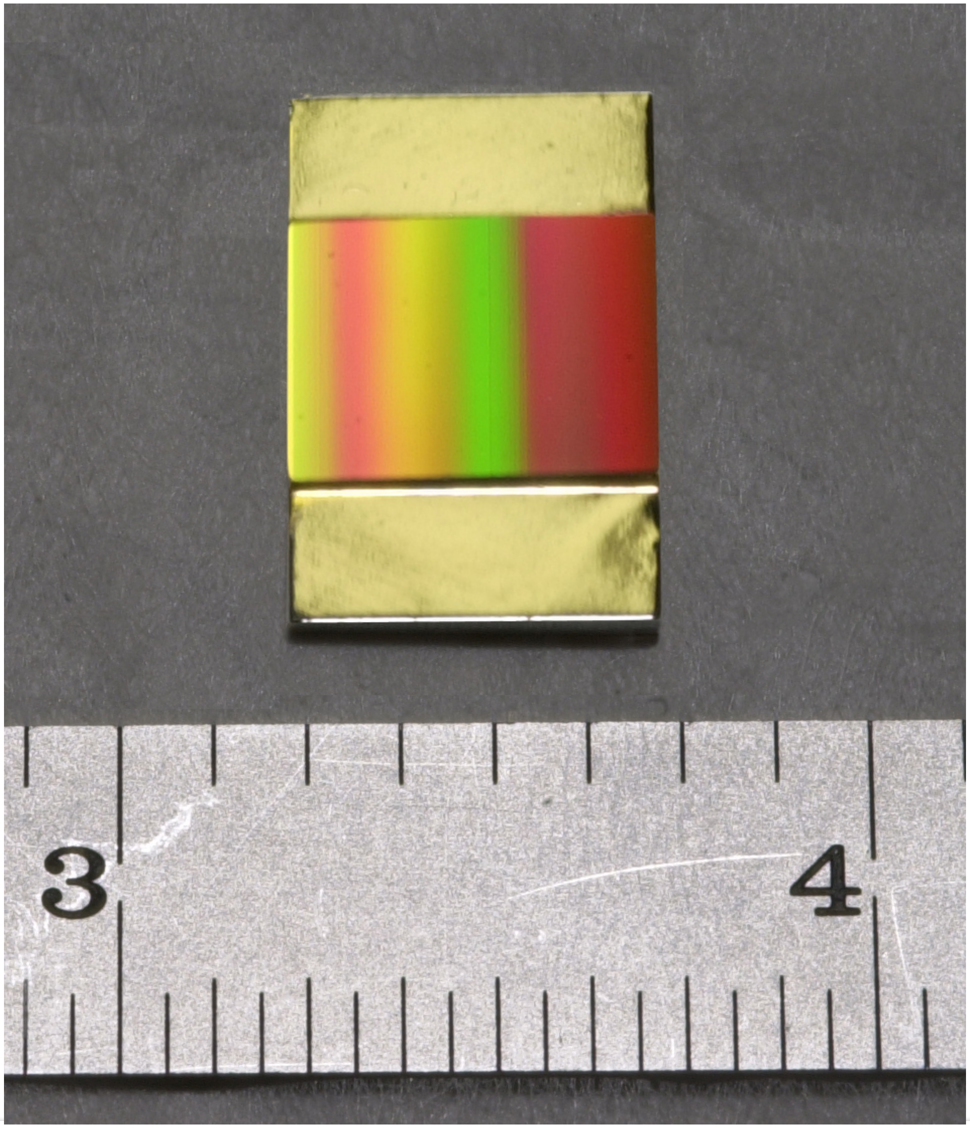
Precision Engineering Research Lathe (PERL II) at LLNL machines immersion gratings and grisms

- Numerically controlled precision lathe. 100 mm travel in radial and axial directions. Air bearing spindle.
- Laser interferometers control position with 2.54 nm resolution.
- Ultra-stiff linear hydrostatic slide ways with capstan drive.
- Temperature controlled (±0.01ºF) spindle and machine enclosure.
- Machine components rest on pneumatically isolated granite slab (122 x 122 x 46 cm).



Small germanium immersion gratings

- 10 x 9 mm clear aperture, 2.5 mm thick, 5.5º blaze.
- Typical surface error 0.020λ rms at 633 nm. (0.010λ best)
- Minimal ghost intensity.
- Very low scatter.
  - rms roughness ~3 nm



ZnSe gratings for WINERED, near IR (λ= 0.9-1.35 µm), high resolution ($R\sim10^5$) spectrometer

- Very ambitious goals
  - Much larger grating (90 x 90 mm entrance aperture, 70º blaze) than anything previously attempted.

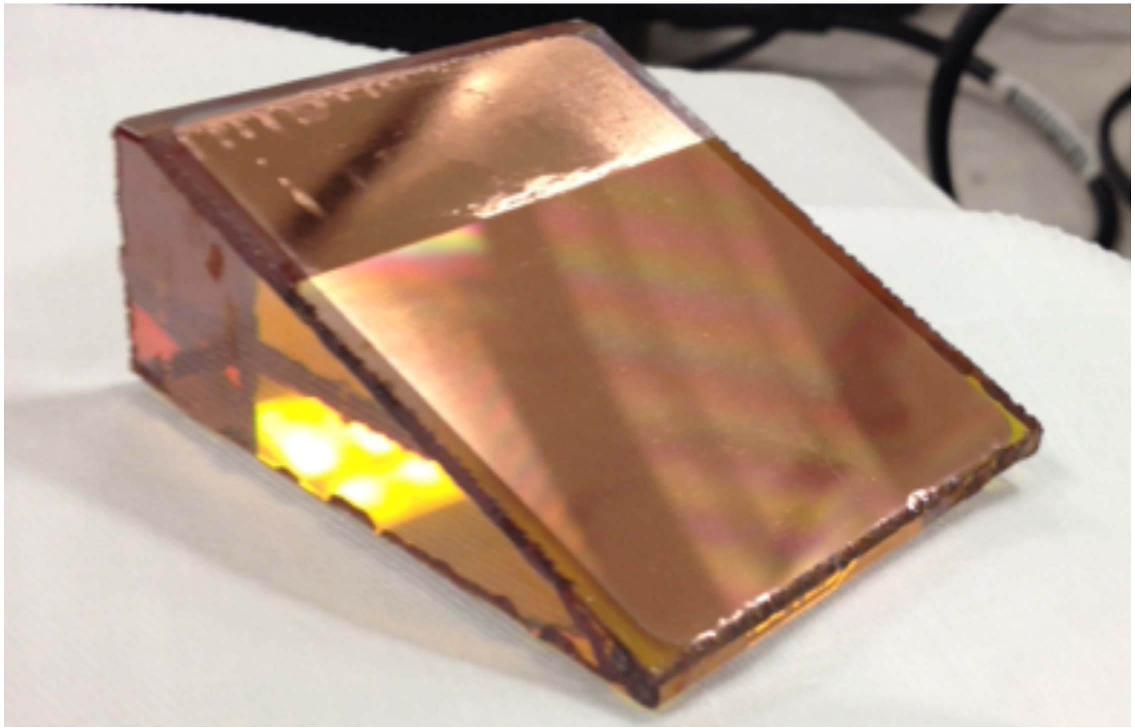
- Subscale prototype 23 x 50 mm aperture, 31.8 µm pitch
  - Estimate 9 days machining time, using a unidirectional cut.

- Many problems to overcome
  - Infrastructure: electrical brownout cut short machining; inadequate building temperature control produced large surface error.
  - Bad groove chipping due to subsurface damage, need better surface prep
  - Interorder ghosts remedied by unidirectional cutting.

- Developed a copper-based coating with immersed R>90%
  - Aluminum reflectivity dips near 900 nm

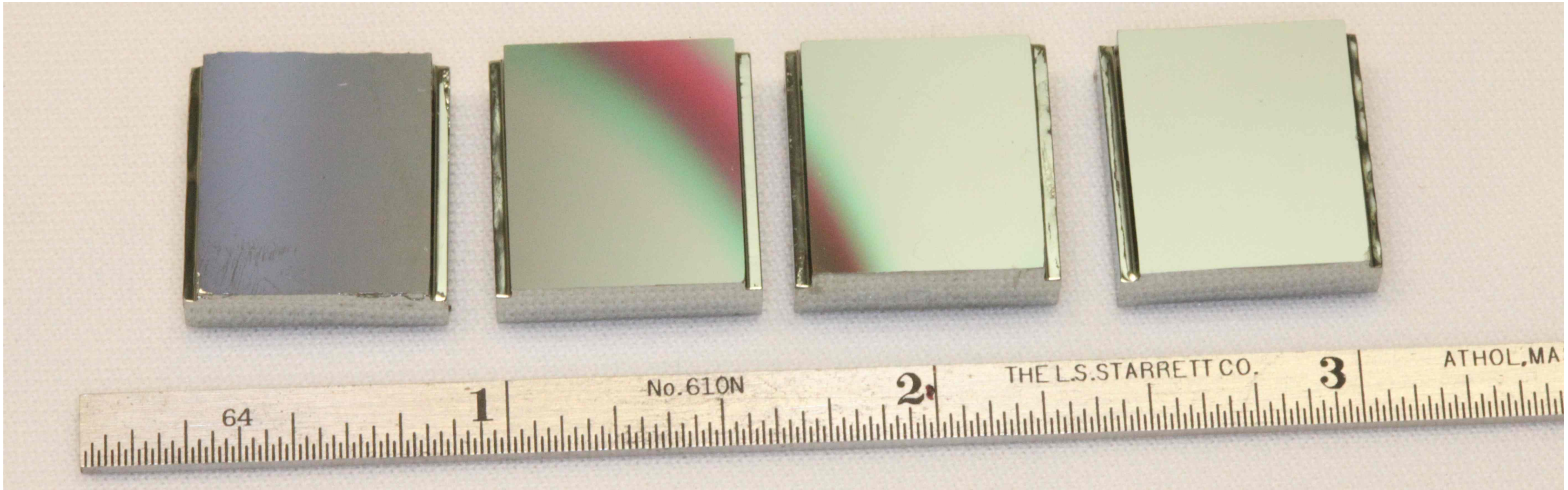
WINERED grating did not work out as expected

- Final attempt achieved R=91,200@1 µm, 0.086λ rms surface error @ 633 nm immersed, but poor diffraction efficiency ~27% on 70º facets. Much better on 20º facets. Machining issues?



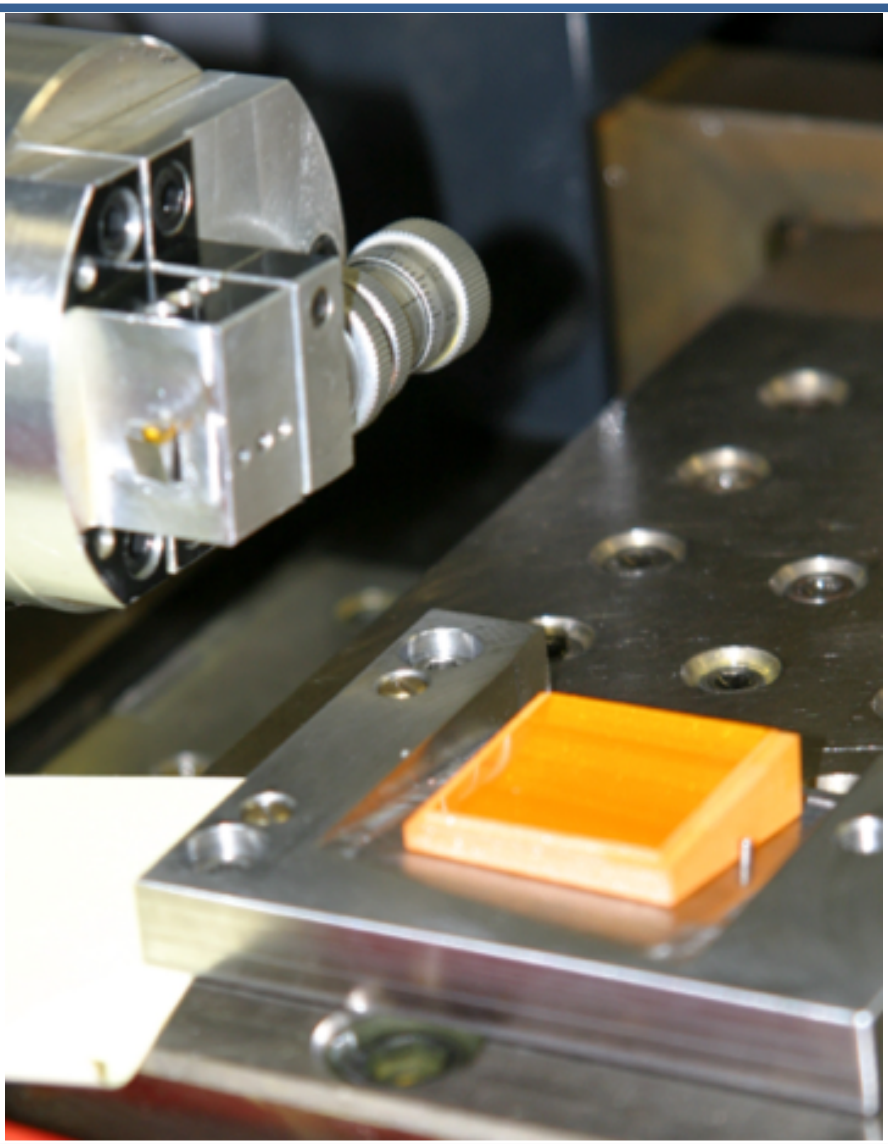
2 Sets of 3 germanium grisms for LMIRCam on the Large Binocular Telescope. In use since 2012.

- 2.89º blaze, 14 x 16 mm grating area
- 40 grooves/mm (L-band); 32 groove/mm (K and M bands)
- Surface error 0.10 to 0.14 λ PV (0.012 λ rms best one) @633 nm
- Grating surface successfully AR coated.



We made the GR700 ZnSe grism for NIRISS (JWST) Launch date spring 2019.

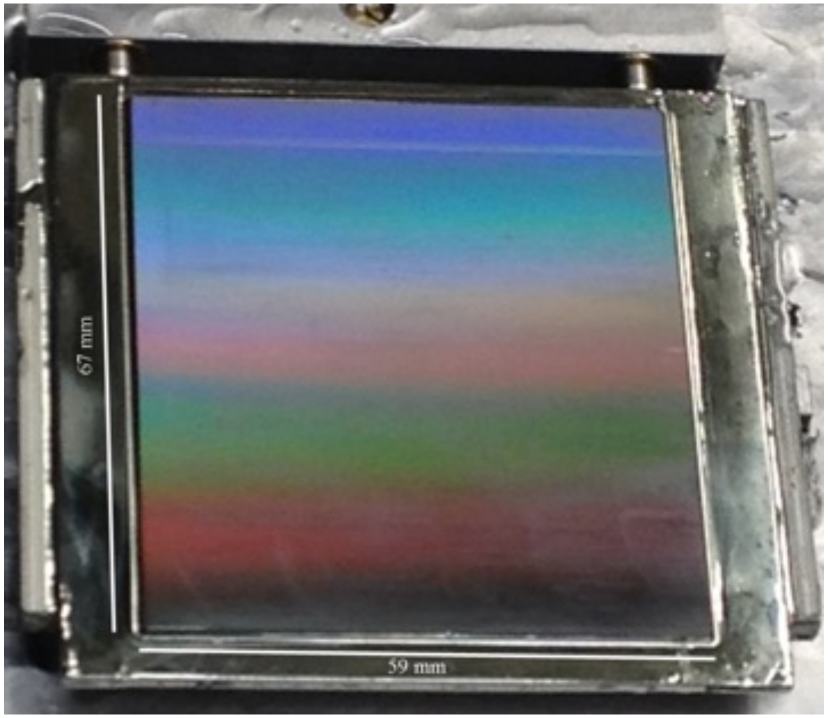
- 30 x 29 mm clear aperture, 11 mm thick, 2.6º blaze.
- 56% diffraction efficiency @633 nm, uncoated.
- Surface error 0.21λ P-V and 0.030λ rms @633 nm.
- No visible ghosts in transmitted beam.
- Very low scatter.
  - rms roughness ~3 nm



Large germanium immersion grating

- 59 x 67 mm area, 11.36 µm pitch, 32º blaze required 28 days of machining. Negligible tool wear observed.
- Building chiller unit failed 24 days into cut. Caused loss of PERL temperature control.
- Increased surface error
  - 1.2 λ PV, 0.33 λ rms @633 nm
  - Met requirements

Ref. Montesanti (2016)



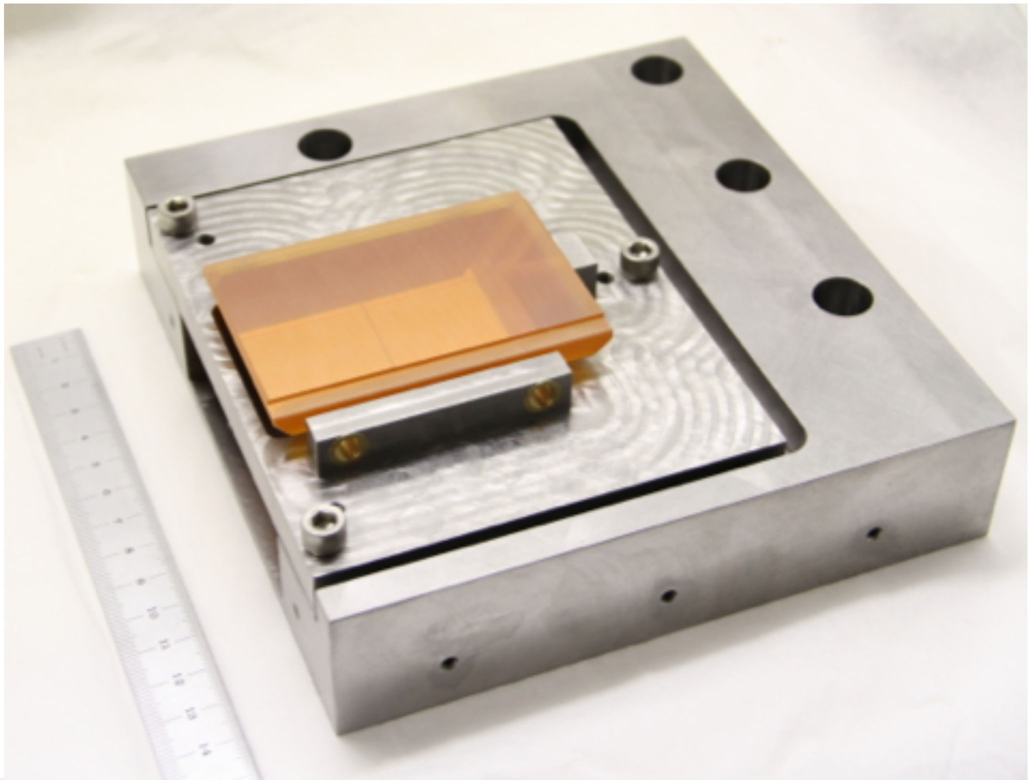
Fine pitch germanium immersion grating

- 30 x 30 mm area, 3.13 µm pitch, 15º blaze required 24 days of machining. Minor chipping started halfway through cut and increased until end of cut. But still met requirements.
- Spindle air compressor failed after 20 days. Machine halted then restarted with loss of position.
- Acceptable surface error
  - 0.55 λ PV, 0.081 λ rms @633 nm

Ref. Montesanti (2017)

Pair of ZnSe grisms for RIMAS

- Just getting started on these.
- 43º blaze, 25 groove/mm (60 x 45 mm grating area) and 50º blaze, 20 groove/mm (75 x 45 mm grating area)



Coatings for immersion gratings and grisms

- As cut grooves have Fresnel reflectivities of 11% for N=2, and 36% for N=4).
  - Want R-> 100% immersion gratings; R-> 0% for grisms.
- Metals are a good choice for broadband HR coating.
  - Immersed reflectivity will be less than reflectivity in air, $[(n_1-n_2)/(n_1+n_2)]^2$
  - Often need an adhesion layer under metals like Au. Absorption in the adhesion layer can be significant at shorter wavelengths.
- Can you AR coat grooves for grism application?
  - Issues of uniformity on inclined surface; effects of shadowing
  - Successfully demonstrated by Jaffe group (2006)
  - They have worked well on LMIRCam grisms (Ge) and NIRISS grism (ZnSe)

Limitations on PERL machined gratings

- Stage travel limits grating area to 90 x 90 mm.
- Cutting unidirectionally eliminates periodic error (ghosts), but increases machine time.
- No barometric compensation of interferometer. This can affect groove spacing and surface error. Mitigated by pausing cut during storms and frontal passage.
- Practical limits to machining time (one month?)

Fundamental size limitations on machined gratings & grisms

- Limits on available size of optical quality blanks
  - Limitations on crystal growth, limits on CVD thickness (ZnS, ZnSe)
- Size also limited by absorption and scatter loss in blanks.
  - Loss reduces transmission and limits spectral resolution
  - Measured by Kuzmenko (2008), Ikeda (2009), Kaji (2014, 2016)
  - Mitigate by mosaic of several gratings?
- Limits set by blank inhomogeneity, stress induced birefringence
  - Thermal gradients present in CZ crystal growth freeze in radial compressive stress and tangential axial stress.
  - Refractive inhomogeneities (Δn) measured in Ge up to few parts in 10^{-4} .
  - Birefringence measured in Ge up to one part in 10^{-4} .
  - Partially mitigated by annealing.
  - CVD material homogeneous to few parts in 10^{-6} .

Fundamental limitations on machined gratings & grisms (cont.)

- Total length of high quality grooves limited by tool wear.
  - Depends on substrate hardness, chemical interaction with diamond.
- Starting material must be free of subsurface damage
  - Prepare surface by chemical etching or damage-free polishing
- For single crystal materials there is an optimal orientation for highest feed rate. Should cut across not along cleavage planes.

Benefits of working with LLNL

- A great deal of expertise in precision engineering and metrology developed over the years can be brought to bear on problems.
- Many facilities in a single location (e.g. optical shop, coating chambers, materials analysis capability, optical testing, etc.)
- Ongoing work to improve/upgrade diamond machining capabilities.

Many people contributed to this work over the years

- Etched silicon gratings and grisms- Dino Ciarlo, Jian Ge, Marcia Kellam
- PERL machinist - Steve Little
- People who built and maintain LLNL's diamond machining capabilities
  - Steve Bond, Steve Bretz, Charlie Cass, Rich Cobiseno, Pete Davis, Dave Hopkins, Travis Martin, Rick Montesanti, Mario Montoya, Jim Morton, Darron Nielsen, Doug Owens, Steve Patterson and Timm Wulff, and Brian Yoxell
- Coating, modeling, polishing and testing
  - Jennifer Alameda, Elaine Behymer, Kerry Bettencourt, Jay Bixler, Jeff Carr, Jackie Crawford, Jim Ferriera, Tim Graff, Marcia Kellam, Liesl Little, Paul Mirkarimi, Rick Montesanti, and Peter Thelin
- Outside collaborators
  - Löic Albert, David Aldridge, Mathilde Beaulieu, René Doyon, Yuji Ikeda, Naoto Kobayashi, Alexander Kutyrev, Matt Richter, Driss Touahri, John Wilson, and Peter Zell