Large-area silicon immersion echelle gratings and grisms for IR spectroscopy

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ABSTRACT

We present design examples for instruments making use of micromachined silicon grisms and immersion gratings. The capabilities of high index grisms, transmission grating-prism hybrids, open up new possibilities in compact IR spectrograph designs with spectral resolving power, R$\sim$500–5000. Coarsely grooved immersion gratings will provide for unique high resolution spectrograph designs in the near and mid-infrared (resolving power, R$\sim 10^4$–10^5). The high refractive index of silicon shortens the required grating depth, to produce a given resolving power, by up to a factor of 3.4. Alternatively, at a given resolving power, an immersion grating can allow a spectrograph slit to be widened by this factor relative to an instrument using a grating illuminated in air or vacuum; this increases the instrument sensitivity without degrading the spectral resolution. Our analysis here illustrates the potential of these devices to improve spectrograph throughput, spectral resolution, and wavelength coverage while reducing the required instrument volume relative to similar instruments using non-immersed diffraction gratings and low index prisms and grisms.

Keywords: diffraction grating:echelle, immersion grating, grism, infrared spectroscopy

1. INTRODUCTION: SILICON DISPERSIVE OPTICS FOR LARGE INFRARED TELESCOPES

Grisms and immersion echelles are grating groove patterns fabricated on wedged substrates (Figure 1).[1] An immersion grating of a given length is equivalent to a vacuum grating that is longer by a factor of the refractive index of the immersion material since the wavelength of incident light shortens upon entering the immersion grating. The result is a grating that, in the case of a silicon substrate (n=3.4 at 2.2 μm), the grating produces $R_{Immersion}=3.4R_{Vacuum/Reflection}$ for equivalent grating lengths. This is equivalent to widening the slit by the same factor at a given R and wavelength. Silicon grisms and immersion gratings allow for IR spectrograph designs that combine high resolution and large spectral range without giving up sensitivity to slit losses.[2–7] Moreover, silicon grisms can turn an existing IR camera into a low to medium resolution spectrograph with out alteration to the instrument optics.

As a general rule, the collimated beam diameter, and therefore the physical volume, of spectrograph optical systems increases with telescope aperture. In fact, though, the information capacity of a telescope-spectrograph system has no direct dependence on the telescope aperture, D, or spectrograph pupil diameter, d. The product, $\epsilon A\Omega RN$, describes the information capacity,[8] where ϵ is the total transmission of the system, A is the system light collecting area, Ω is the solid angle admitted into the system, R=$\lambda/\Delta\lambda$ is the spectral resolving power, and N is the number of resolution elements (spatial times spectral in the case of spectroscopic data) used to sample the data in a given measurement. However, R for a given dispersing element depends on the length of the grating and therefore on the minimum pupil diameter needed to fully illuminate the grating. R also depends on D, since larger telescopes have larger plate scales and the spectrograph slit width, W, must grow with platescale. So, in fact, the information capacity *does* depend, if indirectly, on D and d. Larger instruments are particularly difficult in infrared applications where background radiation levels require cryogenic optical systems. We can get relief from spectrograph inflation by using high index immersed gratings and grisms.

Fabrication of high quality diffraction gratings and grisms in silicon using photolithographic micromachining techniques is now common on substrates with areas 4-75 cm^2.[9–12,3,9,13,2,4,6] We have fabricated high efficiency

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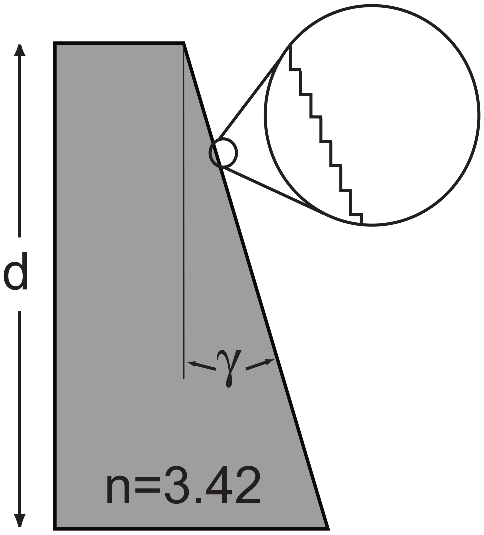

Figure 1. Grism geometry. The groove pattern is on the exit facet (right hand side in the Figure), γ is the grism apex angle, d is the instrument exit pupil diameter. For a silicon grism substrate, the refractive index at λ=2.2 μm is n=3.4.

diffraction gratings on large mono-crystalline silicon substrates using photolithographic and chemical etching techniques.[9,3,10] Our gratings have excellent optical quality and diffraction efficiency; wavefront error of ∼30 nm rms with 80% diffraction efficiency and <3 percent scattered light at λ=0.632 μm are routine in our tests using them as reflection gratings in a Lithrow configuration. For silicon transmission gratings and grisms having our current optical quality, the efficiency will be >80% down to the transmission cutoff of silicon at λ=1.2 μm. We can produce grisms in silicon with various apex angles, groove spacing, and blaze angles. We have designed round grism substrates to host grating patterns at least 25 mm in diameter to be compatible with a mid-IR camera currently under construction for the Stratospheric Observatory For Infrared Astronomy (SOFIA).

We have also developed further capabilities to extend the silicon grating fabrication process to much larger substrates with the goal of producing large area (200 cm^2) immersion echelles for use in very high dispersion near infrared spectrographs. Why so large if the point is to reduce spectrometer size!? We are interested in designing and building instruments that will take advantage of the new and proposed 8-15 meter telescopes, but that will deliver excellent performance in the seeing limit as well as (but not dependent upon) the diffraction limit of the telescope. Astrophysical kinematic and chemical measurements require high sensitivity to faint light sources in addition to high spectral resolution large spectral range simultaneously. These research goals translate into expensive instrumentation requirements and to engineering trade-offs that directly affect the efficacy of possible observations. We propose to take advantage of silicon immersion echelles to allow spectrographs with seeing disk sized slits. In the end, we will trade instrument compactness for high transmission efficiency without giving up spectral resolving power. When AO is turned on, we'll install the appropriate narrow slits and enjoy even higher spectral resolution.

2. LARGE AREA INFRARED GRISMS

Grisms are diffraction grating-prism hybrids used in transmission as dispersive elements.[1] Using a grism, rather than using a transmission grating or prism alone, allows a direct transmissive system with high dispersion, especially when the grism is fabricated in a high refractive index material. This means that existing cameras can use grisms and filters interchangeably without alteration of the optical systems, producing a spectrograph with relatively little modification of the instrument. In spectrograph designs incorporating grisms from the onset, the devices allow very compact diffraction limited optical systems.[11,12]

The grating equation, for a grism with the geometry illustrated in Figure 1, reduces to:

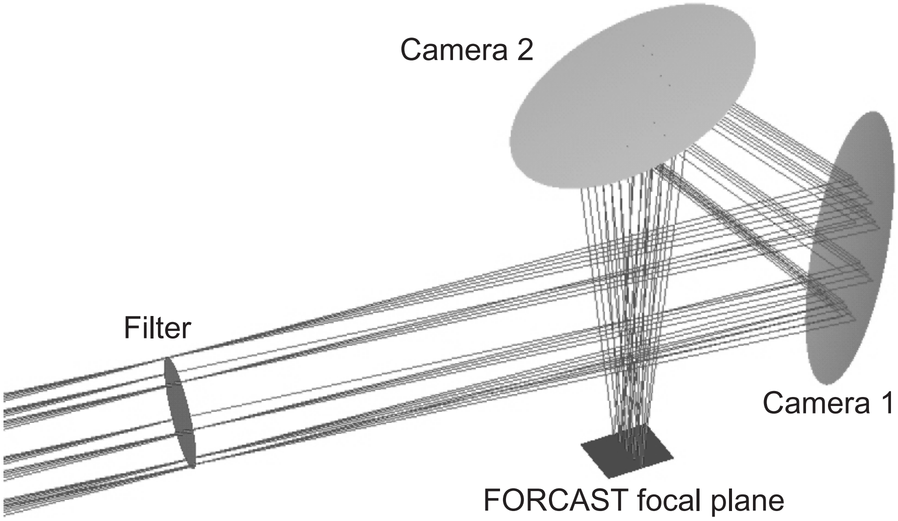

Figure 2. A raytrace of the FORCAST pupil and 2-mirror camera optics layout *without* grisms installed. Interference filters will go just fore and aft of the pupil position. The trace is of a long slit (3.2 arcmin long x 1.9 arcsec wide) located at the SOFIA telescope focal plane and reimaged on the FORCAST focal plane.

$$\frac{m\lambda}{\sigma} = nsin(\gamma) - sin(\beta) \tag{1}$$

where m is the spectral order, λ is the wavelength of light, σ is the grating pattern groove spacing, n is the refractive index of the prism, γ is the apex angle of the prism, and β is the angle of the dispersed beam relative to a beam entering the grism normal to the entrance facet. If the grooves are blazed, the blaze wavelength λ_{blaze} occurs where $\gamma = \beta$:

$$\lambda_{blaze} = \frac{\sigma(n-1)sin(\gamma)}{m}. \tag{2}$$

Alternatively, the expression can yield the required opening angle, γ, given a desired λ_{blaze} and groove spacing:

$$\gamma = sin^{-1}[\frac{m\lambda_{blaze}}{\sigma(n-1)}]. \tag{3}$$

For a pupil diameter d, the resulting diffraction limited resolving power of such a grism is:

$$R_{diff} = \frac{dtan(\gamma)(n-1)}{1.22\lambda}. \tag{4}$$

For a given desired diffraction limited resolving power, the pupil diameter will be:

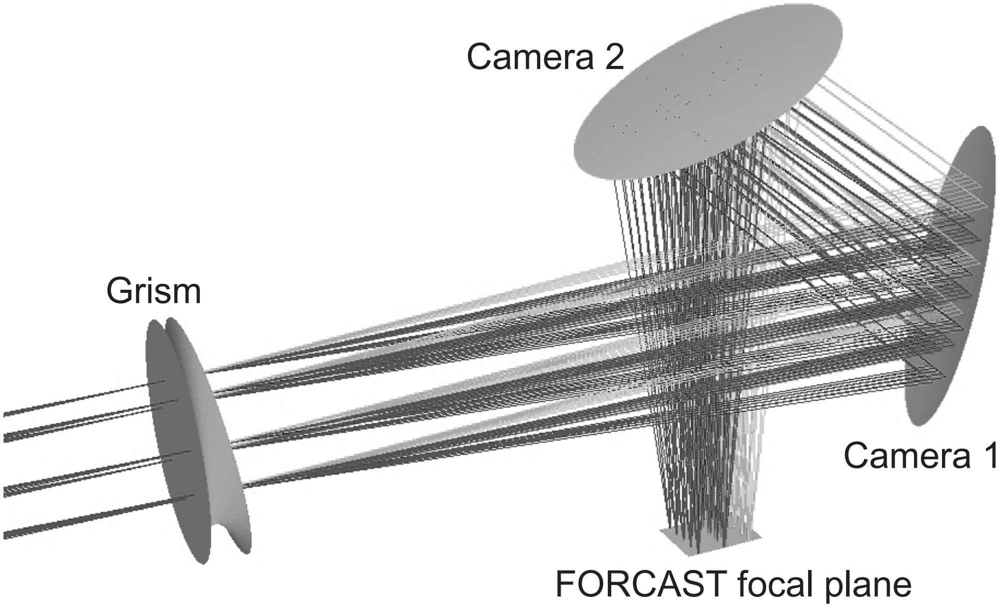

Figure 3. A raytrace of the FORCAST camera optics with a grism installed in place of a filter. The camera optical configuration is identical to that shown in Figure 1. The grism has γ=6.73^o, groove spacing σ=25 μm, and is 25 mm in diameter. The dispersed spectrum is of 4 lines at 6.000, 7.000, 7.035, and 8.000 μm (see raytrace detail in Figure 3 and simulated spectrum in Figure 4.

$$d = \frac{1.22 R_{diff} \lambda}{tan(\gamma)(n-1)}. \tag{5}$$

Note that R is directly proportional to (n-1) and that d decreases with increasing n. Thus, by using a grism substrate with a very high refractive index, we can increase the spectral resolving power of an instrument without increasing the pupil diameter.

Figure 1 also illustrates the Littrow grism configuration that we have chosen. We locate the grism at the exit pupil of the optical system. The beam enters the grism normal to the entrance facet. The grooves are blazed so that the groove facets are plane–parallel to the entrance facet in the dispersion direction, but slightly tilted perpendicular to the dispersion to attenuate internal reflections and ghosts. The zeroth Littrow order (corresponding to the blaze wavelength) for a given grism set up this way exits the grism undeviated along the optical axis of the system. This configuration is perfect for retrofitting an existing imaging camera with spectroscopic capability.

2.1. Design example: grisms for the SOFIA mid-infrared camera

The Faint Object infraRed CAmera for the Sofia Telescope (FORCAST[14]) is the facility mid IR camera for the airborne observatory. FORCAST, sensitive in the wavelength range λ=5–40 μm, will provide for diffraction limited imaging longward of λ=15 μm. Currently the SOFIA first light instrument compliment does not cover the FORCAST wavelength range with spectral resolving power in the range, R=500–2000.[14] An obvious solution to this hole in observational phase space is to provide an instrument with low and medium resolution spectroscopic capability in the FORCAST wavelength range. A much less expensive solution is to provide dispersive capability to FORCAST as long as it does not require significant (read expensive) alterations to the camera. We have designed and are in

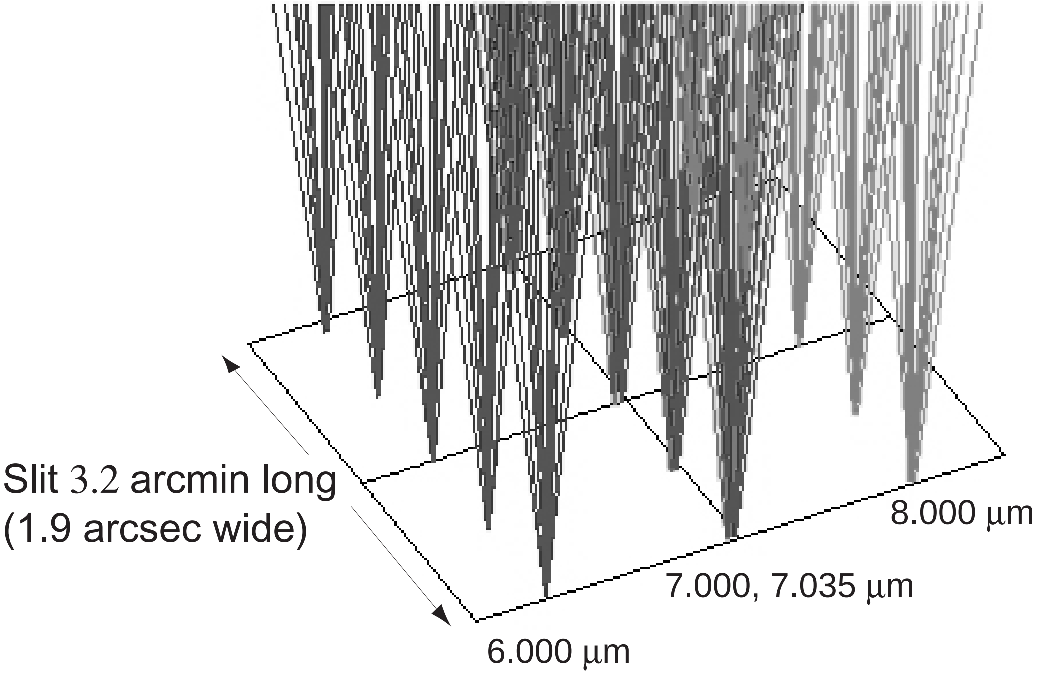

Figure 4. A detail view of the FORCAST focal plane illustrated in Figure 2. Four slit images form the grism spectrum. The tipped square represents the FORCAST 256 x 256 pixel focal plane array, which measures 3.2 arcmin (12.8 mm) on a side.

the process of producing grisms that can provide FORCAST several low and medium resolving power spectroscopic modes throughout its wavelength coverage.

2.2. Incorporating dispersion into the camera design

We present a list of possible FORCAST grisms in Table 1. Although we had the grism upgrade in mind as we finalized the FORCAST optical design, the upgrade will involve two minor alterations to the instrument system: we must add slits to the existing aperture stop collection at the telescope focal plane in the FORCAST cryostat, and we must remove bandpass filters to make room for grisms. The major effort in this upgrade, other than producing the grisms, will be in developing additions to the existing data acquisition and data analysis pipeline software for FORCAST. We note that grism spectroscopy is *not* currently part of the FORCAST baseline design and is not funded. However, the FORCAST design leaves room for slits and grisms in the aperture and filter wheels, respectively, and our grism fabrication efforts (funded independently of SOFIA) will benefit from tests in actual instruments. We will provide test grisms to the FORCAST team as part of our silicon dispersive optics research program.

Figures 2 and 3 illustrate the FORCAST pupil and camera optics without and with a grism installed. Because the FORCAST filter set in each channel is divided between two parallel filter wheels, we can install grisms in pairs to allow for low and medium spectral resolving power long slit spectra, using one or the other of two grisms, and for cross dispersed spectra, using both grisms in series with their dispersion planes rotated 90^o with respect to one-another. Figure 4 shows a detailed view of the FORCAST focal plane in Figure 3 and illustrates the use of the unaltered FORCAST optical system to image the grism spectrum. We have used these raytrace data to simulate a FORCAST mid-IR long-slit spectrum (6-8 μm in this example, see Figure 5). The spectrum is the raytrace data of light through a 1.9 arc-second wide slit dispersed with a single silicon grism (σ=25 μm, γ=6.73 ^{o}) and sampled with a 256 x 256 pixel array. The two lines in the center of the spectrum are separated in wavelength by 0.035 μm and are easily resolved (R=200).

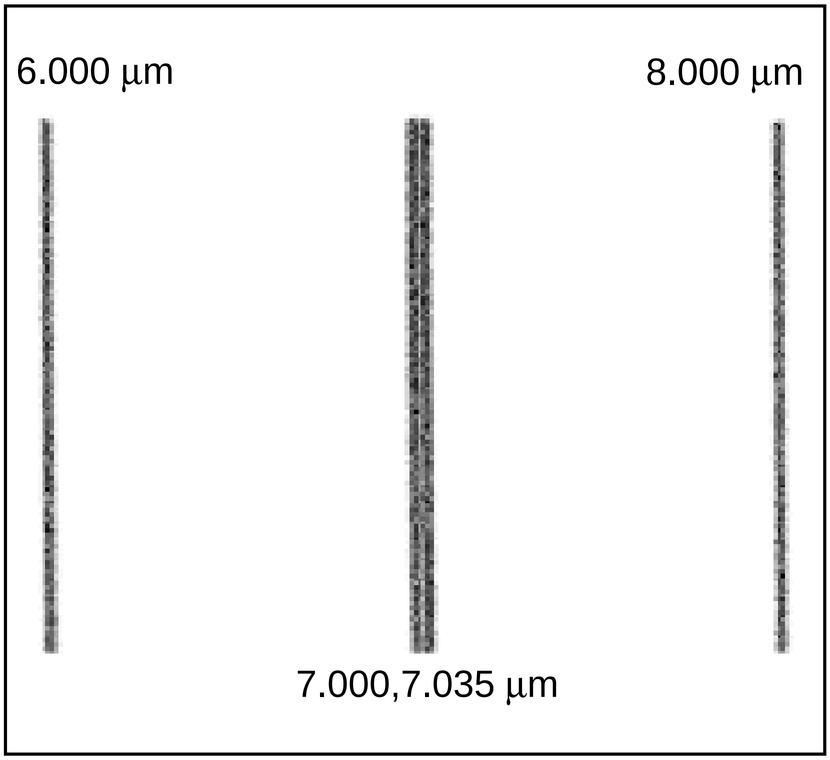

Figure 5. A simulated grism spectrum derived from the raytrace data shown in Figures 2 & 3. Wavelengths of the individual lines are labeled; the barely resolved pair in the center are separated by 0.035 μm (R=200).

Table 1. Possible grism configurations for FORCAST.

Wavelength Band (μm)	Resolving Power (2" slit width)	Grism Properties
6.0–9.0	250–600 (long slit)	σ=33 μm, γ=10.0, m=2
6.0–9.0	1500–2000 (X-dispersed)	σ=100 μm, γ=44.35, m=19–32
18–25	250–600 (long slit)	σ=142 μm, γ=11.07, m=3
18–25	R>1000 (X-dispersed)	σ=330 μm, γ=54.7, m=26–34
25–33	250–600 (long slit)	σ=142 μm, γ=11.07, m=2
25–35	1775 (X-dispersed)	σ=550 μm, γ=54.7, m=28–39

3. IMMERSION ECHELLES: SOME ISSUES TO CONSIDER FOR LARGE GROUND BASED TELESCOPES

As we have illustrated in our grism designs for FORCAST and SOFIA, silicon immersed dispersion devices are useful not only in the diffraction limit, but in the seeing limit as well if the gratings are made large enough. We have shown that such large area grisms and immersion gratings are possible. This makes the retrofit FORCAST grisms possible, but is even more profoundly useful in contemplating spectrograph designs for very large ground based telescopes.

Large telescopes designed to have wide fields of view for direct imaging necessarily have larger plate scales (arc seconds on the sky per millimeter on the telescope focal plane). Larger plate scale produces a seeing disk that, imaged on the telescope focal plane at a given observatory site, covers a larger area. For slits narrower than the seeing disk, the spectrograph sensitivity only increases linearly with telescope aperture, rather than as the collecting area, since light is transmitted along the slit but lost to vignetting in the dispersion direction. Narrow slits require adaptive optics (AO) or image slicers to avoid introducing these transmission losses. To maintain high spectral resolving power with a widened slit, we'll need to lengthen the grating since resolving power is directly proportional to the number of grooves of a given width that are illuminated. A longer grating requires a larger collimated beam diameter. To produce a larger diameter pupil, the spectrograph optics must grow.

An additional trade-off arises when the diligent optical designer wishes to optimize the use of a two dimensional detector focal plane array to image a cross-dispersed spectrum. The larger telescope plate scale must be reduced in the spectrograph to avoid over-sampling the slit image at the spectrograph focal plane and losing spectral range. To minimize the number of optical components in the system–especially important for thermal infrared applications–the most direct focal reduction is with a faster spectrograph camera.

We now have a big, expensive instrument *and* we require AO to get the required spatial resolution to avoid substantial slit losses. An alternative is to immerse the diffraction grating surface in a high index material.

Providing near and mid-IR instruments for large ground based telescopes is a contortionist balancing act. On one hand the telescope plate scale is necessarily quite large. For example, for a 15 meter, f/15 telescope (f/1.4 primary mirror) the plate scale will be 0.85 arc-seconds mm^{-1}. To sample a 1 arc-second slit (nearly 1 mm wide at the telescope focal plane) will require focal reduction at magnification 18 to Nyquist sample with 27 μm wide pixels. On the other hand we must minimize instrument weight and cost since observatory budgets and instrument platforms are finite. The advent of large area silicon immersion gratings provides an alternative to the large, multi-purpose and therefore extremely complex and expensive spectrographs currently designed for and in use at existing large telescope facilities.

Immersion echelles allow for a new approach to fitting telescopes with high dispersion IR spectrographs. We have described such a spectrograph design in detail elsewhere.[2] This design can produce resolving power up to R=70,000 with a 1 arc sec wide slit and cover an entire near infrared atmospheric window in a single cross dispersed spectrum (e.g K or M band). We have adapted this design for as a first light instrument for the Large Atacama, Telescope[15,16] which is expected to be a 15 m, f/15 IR optimized telescope. A very important point that we illustrate with this design is that we have *not* assumed a diffraction limited PSF. Using the median seeing limit for the LAT site (0.7 arc sec FWHM) rather than the diffraction limit (0.016 arc sec) degrades the resolving power, but vastly improves the overall efficiency of the instrument. We do not rely upon AO to to science with this instrument.

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REFERENCES

1. D. J. Schroeder, *Astronomical Optics.* Academic, San Diego, Calif., 1987.
2. L. D. Keller, D. T. Jaffe, and G. Doppmann, "Design for a near-infrared immersion echelle spectrograph: breaking the r=100,000 barrier from 1.5 to 5 μm," in *Astronomical Telescopes and Instrumentation*, *Proc. SPIE* **3354**, 1998.
3. L. D. Keller, D. T. Jaffe, O. A. Ershov, T. Benedict, and U. U. Graf, "Fabrication and testing of chemically micromachined silicon echelle gratings," *Applied Optics* **39**(7), 2000.
4. U. U. Graf, D. T. Jaffe, E. Kim, J. H. Lacy, H. Ling, J. T. Moore, and G. Rebeiz, "Fabrication and evaluation of an etched infrared diffraction grating," *Applied Optics* **33**, 1994.
5. G. Wiedemann and D. E. Jennings, "Immersion grating for infrared astronomy," *Applied Optics* **32**, 1993.
6. P. J. Kuzmenko, D. R. Ciarlo, and C. D. Stevens, "Fabrication and testing of a silicon immersion grating for infrared astronomy," in *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research*, *Proc. SPIE* **2266**, 1994.
7. H. U. Kaufl, K. Kuhl, and S. Vogel, "Grisms from germanium/silicon for astronomical instruments," *Proc. SPIE* **3354**, 1998.
8. K. Taylor, "Spectroscopic techniques for large optical/ir telescopes," in *Instrumentation for large telescopes*, Cambridge, 1995.

9. D. T. Jaffe, L. D. Keller, and O. A. Ershov, “Micromachined silicon diffraction gratings for infrared spectroscopy,” in *Astronomical Telescopes and Instrumentation*, *Proc. SPIE* **3354**, 1998.
10. O. A. Ershov, D. T. Jaffe, J. Marsh, and L. D. Keller, “Production of high-order micromachined silicon echelles on optically flat substrates,” *Proc. SPIE* **4440**, 2001.
11. J. Ge, D. Ciarlo, P. Kuzmenko, B. Macintosh, C. Alcock, and K. Cook, “Etched silicon gratings for ngst,” *Proc. NGST Science & Technology, ASP Conf.* **207**, 2000.
12. J. Ge, D. Ciarlo, P. Kuzmenko, C. Alcock, B. Macintosh, R. Angel, N. Woolf, M. Lloyd-Hart, R. Q. Fugate, and J. Najita, “Adaptive optics high resolution spectroscopy: present and future direction,” *Proc. SPIE* **3762**, 1999.
13. P. J. Kuzmenko and D. R. Ciarlo, “Improving the optical performance of etched silicon gratings,” in *Astronomical Telescopes and Instrumentation*, *Proc. SPIE* **3354**, 1998.
14. L. D. Keller, T. L. Herter, G. J. Stacey, G. E. Gull, B. Pirger, J. Schoenwald, H. Bowmann, and T. Nikola, “Forcast: a facility 5–40 micron camera for sofia,” *Proc. SPIE* **4014**, 2000.
15. R. Giovanelli, J. Darling, M. Sarazin, J. Yu, P. Harvey, C. Henderson, W. Hoffman, L. D. Keller, D. Barry, J. Cordes, S. Eikenberry, G. Gull, J. Harrington, J. D. Smith, G. Stacy, and M. Swain, “The optical/infrared astronomical quality of high atacama site. i. optical seeing,” *PASP* **submitted**, 2001.
16. R. Giovanelli, J. Darling, M. Sarazin, J. Yu, P. Harvey, C. Henderson, W. Hoffman, L. D. Keller, D. Barry, J. Cordes, S. Eikenberry, G. Gull, J. Harrington, J. D. Smith, G. Stacy, and M. Swain, “The optical/infrared astronomical quality of high atacama site. ii. infrared transmission,” *PASP* **submitted**, 2001.