THE IMPACT OF ARRAY DETECTORS ON HIGH RESOLUTION INFRARED SPECTROSCOPY

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ABSTRACT. Infrared detector arrays implemented for astronomical use during the past few years achieve performance gains which have profound implications for infrared spectroscopy. Arrays are now available with $\sim few \times 10^3$ pixels, each of which is $\sim 10^2$ times more sensitive than previous single element detectors. Depending on the spectral regime, it is now possible to construct infrared spectrometers with limiting sensitivities $10 - 500$ times fainter than in current use.

1. INFRARED DETECTOR ARRAYS, LARGE TELESCOPES AND ADAPTIVE OPTICS

The short history of infrared detector arrays, like the longer history of visible detector arrays, is filled with dead ends, false hopes, and unmarketed one-of-a-kinds. Therefore, this projection of the impact of infrared arrays on spectroscopy will be based on an array which has been manufactured commercially for astronomy and is now available at several observatories. This detector is a 58×62 element MOS Direct Readout InSb array from Santa Barbara Research Center. It is a detector of the hybrid type, with photovoltaic InSb detector material and a bonded silicon readout layer (Orias et al. 1986). Laboratory and telescope tests have been reported by Fowler et al. (1987a,b).

The detector characteristics appearing in Table 1 have been taken from these sources and are based on detectors actually delivered and tested. In addition to the characteristics reported in Table 1, the SBRC InSb array detectors exhibit some nonlinearity. Very preliminary tests show that linearity can be recovered to 5% in a flux ratio of 1700:1, with further improvement expected. Approximately one cosmic ray event is observed per frame and per 500 seconds of integration.

The InSb detector arrays may be compared with single element InSb detectors which are the most sensitive near-IR detectors in general use. These have quantum efficiency similar to the array elements. Normally employed in an analog mode, the performance of these detectors is usually characterized by the Noise Equivalent Power. Except for special and limited situations, the best performance obtained is $\simeq 2 \times 10^{-16}$ W Hz$^{-\frac{1}{2}}$. As an analog detector, the S/N of a measurement improves

[1] National Optical Astronomy Observatories, operated by the Association of Universities for Research in Astronomy, Inc., under contract to the National Science Foundation

G. Cayrel de Strobel and M. Spite (eds.), The Impact of Very High S/N Spectroscopy on Stellar Physics, 61–70.

Table 1: SBRC 58×62 InSb Detector Characteristics

Format	62×58 (3596 pixels)
Pixel Spacing	76×76 μm
Active Area	$\simeq$100%
Readout Noise	400 e^-
Quantum Efficiency	>60%
Well Capacity	>1 × 10^6 e^-
Dark Current	100 e^-/pixel-sec
Good Pixels	>97%
Response uniformity	±25%
Dynamic Range	$\simeq 10^3$

$\propto \sqrt{t}$, where t is the integration time. This differs from the array detector, an integrating device, for which, as long as the measurement is detector noise limited, the S/N improves $\propto t$. Thus a comparison of performance between discrete and array detectors requires an assumed integration time. A single pixel of the array described above has an equivalent NEP of $\simeq 2 \times 10^{-16}$ W Hz$^{-\frac{1}{2}}$ for an integration time of 0.1 seconds. For longer integration times, the array pixel outperforms the discrete detector $\propto \sqrt{t}$. With an integration time of 1000 seconds, the improvement in limiting sensitivity is $\simeq 100$.

The development of large telescope technology offers much to infrared astronomy. In the near infrared, 1–2.5 μm, where the faint limit for high resolution spectroscopy will be set by detector noise for some years to come, the limiting flux improves $\propto (\mathrm{Dd})^{-1}$, where D is the aperture diameter. Several groups (e.g. Beckers et al. 1986; Merkle 1987) are developing adaptive optical systems for large telescopes. The visible light from a point source will be used to measure the wavefront errors, and with this information an active optical element will be adjusted to correct the errors in real time. The correction should suffice to render the telescope diffraction limited at infrared wavelengths $\simeq$ 3–5 μm. Then a smaller acceptance aperture will be selected appropriate to the smaller, diffraction limited images produced by larger telescopes. In this case, the limiting flux also improves $\propto 1/D^2$.

Therefore, for high resolution infrared spectroscopy (and many other types of infrared observations) the gains in limiting flux for a 10 m (TMT) or 22 m (NNTT) aperture relative to a 4 m aperture will be $\simeq 6$ and $\simeq 22$, respectively (the NNTT is an unfilled aperture, hence the gain is $\propto 1/Dd$, where d is the equivalent filled aperture diameter, and D is the unfilled aperture diameter).

2. PROJECTED SENSITIVITY GAINS FOR INFRARED SPECTROSCOPY

Figure 1 presents the expected gains in limiting magnitude associated with available detectors, expected telescope and optics developments, and possible future detector improvements. Some simplifying assumptions have been made, but the implication of major improvements in limiting magnitude is very accurate.

A gain of more than 2 magnitudes is expected at all wavelengths from the number of pixels across the width of the array (assuming that at least 62 pixels

https://doi.org/10.1017/S0074180900034781 Published online by Cambridge University Press

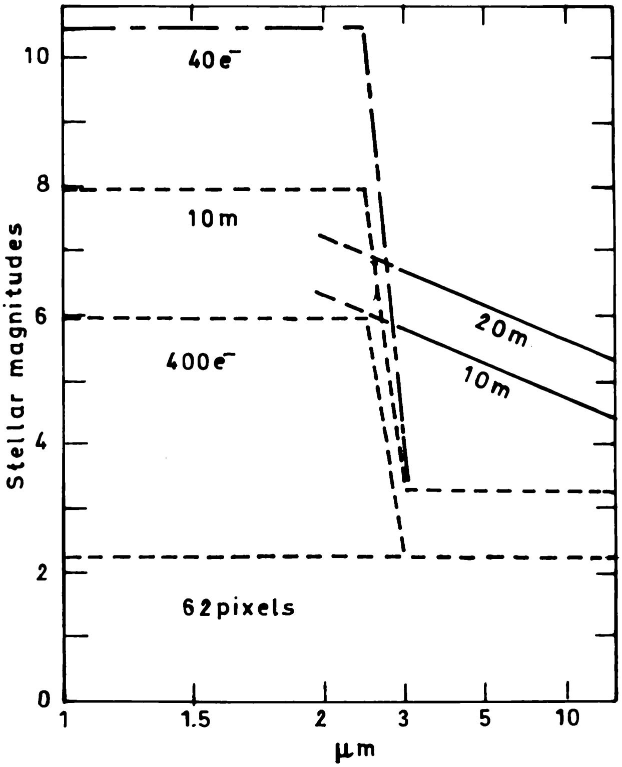

Figure 1. The relative sensitivity gain in magnitudes vs wavelength in μm, arising from use of an integrating InSb array 62 pixels wide instead of a single discrete detector, with integration time 100 seconds, and readout noise of 400 and 40 e^-, and the gains associated with a 10 m effective aperture for flux collection, and a 10 or 20 m effective aperture for diffraction limited imaging.

of spectrum are needed). The available readout noise of 400 e^- provides a gain of more than 3 magnitudes in the near-IR. A 10 m telescope aperture, relative to a 4 m aperture, provides 2 magnitudes gain in the near-IR. It provides less in the longer wavelengths, unless adaptive optics are available, in which case a substantial additional gain is achieved. Reduction of detector read noise to levels associated with CCD's (possible in the not too distant future) would provide another 2.5 magnitude gain in the near-IR.

3. EXPLOITATION OF THE IMPROVED INFRARED DETECTORS

High resolution infrared spectroscopy has brought abundant and detailed astrophysical results during the last decade (e.g. reviews by Ridgway and Brault 1984; Ridgway 1987). Areas of particularly impressive achievements from high resolution infrared spectroscopy have been non-equilibrium chemistry in outer planet atmospheres, atomic and isotopic abundances in cool stars, dynamical structure of pulsating stellar atmospheres, kinematics of mass loss, chemistry in stellar envelopes, mass-motions in molecular clouds, and young stars and star formation.

The most spectacular improvements projected in Figure 1 are for detector noise limited measurements. As it is in high resolution spectroscopy that this condition is most commonly achieved, implementation of array detectors in a high resolution spectrograph is a natural application of the new technology. The required resolution is determined from the astrophysical objectives. For a high resolution spectrograph the scientific goals normally require that the lines be resolved. The lines in interstellar or circumstellar clouds have intrinsic widths of < 2 km s^{-1} and in addition commonly have multiple components with spacings of a few km s^{-1} (Bernat 1981; Black and Willner 1984). For the photospheres of late-type stars line widths are typically 5 km s^{-1} (Hinkle 1978). High resolution (10 km s^{-1}), long slit spectra of optical emission in the nuclei of a variety of nearby spiral and active galaxies reveal complex line profiles of total widths $\simeq 200$ km s^{-1} but with considerable finer structure (Goad and Gallagher 1985).

Additional insight into selecting resolution can be obtained from experience with the FTS at the KPNO 4 m telescope. The FTS is an excellent learning device for this purpose since the resolution is readily adjusted at the telescope. A majority of observations with the 4 meter FTS are of the photospheres of stellar objects. Here experience with the FTS indicates that resolutions between 40000 and 80000 are requested. Most stellar observations are in the 2.0 to 4.0 μm region, although the oxygen isotopes are best measured using the 4.6 μm CO fundamental. Perhaps 20% of FTS observations are of interstellar or circumstellar clouds. Requested resolutions have been as high as 150000, where for best results in detecting weak lines the resolution should be an approximate match to or exceed the intrinsic width of the line.

In circumstellar or interstellar clouds, not only does the ability to detect weak features depend on high resolution, but important information on the source is gained by resolving the line profiles. For instance, in IRC+10216 CO first overtone lines are obviously present at a resolution of 40000 but at a resolution of 100000 the line profiles reveal that several outflow regions at different temperatures and velocities exist along the line of sight. FTS observations of the BN object in Orion provide a limit on how low the resolution can be for a narrow lined source and still provide useful results. Scoville et al. (1983) were able to use observations at resolution 54000 at 4.6 μm.

Of course, a caveat is that cryogenic echelle projects certainly will be different from those done on the FTS due to the factor of 100 difference in sensitivity between these instruments. While virtually all infrared spectroscopy will enjoy the benefits of the 3–10 magnitude gain in sensitivity, the following areas seem to us particularly promising for rapid progress with improved sensitivity. (Typical spectral resolution in km s^{-1} required by previous similar observations is given in parentheses): molecular clouds (1-2 km s^{-1}), young stellar objects (2-5 km s^{-1}), galactic nuclei (20-50 km s^{-1}), abundances of stars in clusters (2-5 km s^{-1}), and nebulae and novae (5-10 km s^{-1}). We note that all of these areas profit from a long-slit spectroscopic capability, either because the sources are extended, or because several stars may be placed on the slit simultaneously (possibly with fibers, rapidly becoming available in the IR).

We conclude that the scientific goals require that at the longest end of the wavelength range (4.6 μm) the grating size provide a resolution of at least 50000. At resolution 50000 the 2.1 m with cryogenic echelle will reach $\simeq 8$ magnitudes fainter than the 4 m with FTS. (At resolution 50000 the FTS is imited by source or background photon noise at all wavelengths, hence the dispersed spectrometer has as additional advantage of $\sqrt{N_{sp}}$ in addition to the gains in Figure 1, where N_{sp} is the number of spectral elements in the FTS bandpass.) Recognizing the great gains to be achieved, a number of observatories are considering the design of a new generation of infrared spectrographs. At NOAO, design studies have been carried out for the 2.1 m telescope (results described below) and are in progress for the NNTT.

4. THE NOAO INFRARED CRYOGENIC ECHELLE DESIGN

What follows is a discussion of the parameters for an echelle spectrograph matched to a two-dimensional infrared array. We first discuss detector considerations, the wavelength coverage, and the size telescope best suited to the scientific applications. We then outline the arguments specifying the size of the envisaged instrument. Grating size, slit size, and resolution will be reviewed. The size of the optics package is critical because the entire optics assembly must be placed in a dewar and chilled to LN_2 temperature. Finally, we review the various order separation schemes.

4.1. Telescope, Wavelength Coverage and Detector

For the detector we adopt the confirmed performance of the SBRC array described above. The SBRC arrays are relatively small arrays, having only a few thousand elements. We propose designing the spectrograph for a 64 x 256 element array. Owing to thermal stress in detector material, it is unlikely that similar arrays will be much larger than 256 pixels wide for some time. Foreseeable detector improvements should result in pixels no smaller than 50 μm in the lifetime of the cryogenic echelle. Two of the currently available SBRC arrays would take a similar amount of space in the focal plane as a 64 x 256 array and would provide acceptable spectral coverage.

The two dimensional nature of the detector is an important aspect of the operation of the instrument. We propose a slit length of 0.5 to 1 arc-minute which is roughly matched to the height of the current array at 1 arc-second per pixel at the 2.1 meter telescope. This will allow long slit operation on extended sources. On point sources the sky background will be determined by observing the source at various positions along the slit, saving a factor of two in observing time compared with conventional beam-switching. Arguments presented below will demonstrate why we do not favor a cross dispersed output format.

Several considerations dictate the wavelength range of the instrument. At NOAO there is considerable experience with detector arrays for the 1-5 μm region. The 1-5 μm infrared is a natural extension of the visual and near-infrared capability provided by CCD's. Intense usage of the KPNO FTS (Hall et al. 1979) over the last decade has generated considerable interest in and experience with 1-5μm spectra among the NOAO user community. The 2-5 μm infrared contains transitions of light molecules, especially CO and H_2, that are of great astrophysical importance. The CO fundamental and first overtone bands are unique probes of cool regions. The 2-4 μm region also contains bands from essentially all the light diatomic molecules of astrophysical interest (CN, CH, OH, SiO, HCl, HF, NH, C_2), and contains bands from several polyatomic molecules (most notably HCN, C_2H_2, and CH_4. The broad region of telluric absorption between 5 and 8 μm naturally limits the 1-5 μm region. The last factor is that in the 2.3-5 μm region the instrument need only be cooled to LN_2 temperature. At longer wavelengths cooling to LHe temperature becomes necessary and the dewar technology is much more complex.

The NOAO cryogenic echelle is intended for the f/8 Ritchey-Chrétien focus of both the KPNO 2.1 m and 4 m telescopes. A prime focus instrument was removed from consideration because of space limitations and cryogen handling problems in the prime focus cage. A prime focus instrument also would be restricted to the 4 meter and S/N calculations indicated that many projects could best be done at the 2.1 meter. Prime focus does have the unique advantage of only one warm reflection. Placing the instrument at f ratio foci larger than f/8 was removed from consideration because of the resulting increase in the instrument's size. One arc second at f/8 on the 2.1 m is 78 μm, easily matched to the detector pixel size. Background subtraction will be done by moving the telescope to alternately place the star at different positions along the slit.

The FWHM seeing disk on Kitt Peak typically is about 1 arc second. The corresponding (predicted) values at 2.2 and 5 μm are 0.89 and 0.76 arcsec. For a Gaussian image profile, a slit width equal to the FWHM will accept 77% of the source flux. Clearly slit widths of 0.5 arcsec or less are highly inefficient.

4.2. Grating Size, Slit Width, and Resolution

The grating size is set by two constraints, the theoretical resolution R, for an echelle

$$R = \frac{2W}{\lambda} sin\theta_B cos\theta \tag{1}$$

and the slit width S (in seconds of arc)

$$S = 206265 \frac{Wm\lambda}{aDR} \tag{2}$$

(Bingham 1979). The symbols used above have the following meanings: λ is the wavelength, R is the resolving power, $\lambda/\Delta\lambda$, m is the order number, θ_B is the blaze angle, a is the groove spacing, D is the diameter of the telescope primary, and W is the width of the used area of the grating in the plane of the grating. θ is defined so that the angle of incidence $\alpha = \theta_B + \theta$, and at the peak of the blaze the angle of diffraction $\beta = \theta_B - \theta$. Hence the grating equation may be expressed

$$m\lambda = 2a \sin\theta_B \cos\theta \tag{3}$$

Equation (2) is best restated by substituting this form of the grating equation,

$$S = 412530 \frac{W \sin\theta_B \cos\theta}{DR} \tag{4}$$

From equation (1), the grating size required to provide a resolution of at least 50000 at 4.6 μm, assuming standard values of $\theta_B = 63.4^o$ and $\theta = 6^o$ (Schroeder, 1970), has a length of $\simeq$ 12.9 cm. However, the grating size also controls the slit width (equation 4). The following discussion of slit width is for the 2.1 meter telescope. For R=50000, W=12.9 cm , and D=2.1 m the slit width is 0.45 arc second. This is unacceptably small, especially if higher resolutions are to be used at shorter wavelengths. Note that S and W are directly proportional, so 1 arc second corresponds to W=28.7 cm. Echelle gratings are available commercially in sizes up to 8 x 16 inches with 5 x 10 inches being in common use. A 5 x 10 inch grating will give a

0.87 arc second slit for R=50000 and a 0.43 arc second slit for R=100000. A 8 $\times$ 16 inch grating provides a gain of 1.6 in slit width, i.e. 1.4 arc second for R=50000.

A 8 $\times$ 16 inch grating appears to be the optimal choice because of the large slit width that it provides. However, size of the grating also is limited by the need to keep the instrument size and weight under control. Use of a 5 $\times$ 10 inch grating could be a desirable option to limit instrument size and weight if R$\leq$100000 is emphasized. A third alternative is to use a 5 $\times$ 10 inch grating and over fill it, providing a larger slit size (Diego and Walker 1985). This is done on the 4 meter echelle and results in only a small amount of lost light. In the thermal IR it would improve cold baffling as well. With any choice of echelle size the grating can be shaped to match the collimated beam size. This may save space in the dewar depending on the mechanical design.

4.3. Order Separation

In wavenumbers, the length of an order (free spectral range) of an echelle is given by

$$\frac{1}{2a \sin\theta_B \cos\theta} \tag{5}$$

(Loewen 1970). For a 31 line mm^{-1}, 63.4^o echelle, the free spectral range in Littrow is 175 cm^{-1}. In the 1-5 μm infrared using this echelle grating, the order number ranges from 12 to 60. Thus some scheme is needed to separate the order we wish to observe from the other 47$^+$ orders visible to the detector.

The basic order separation device for any spectrograph is a filter. If a narrow filter is selected one order may be observed or if a broader filter is selected several orders may be observed by using a cross dispersing element. Echelles in the visual when used with a two dimensional detector (CCD, photographic plate) often use a cross disperser.

To examine the usefulness of a cross disperser in the infrared we will consider a best case: the lowest resolution at which the cryogenic echelle will be used, $R \simeq 20000$, i.e. 0.2 cm^{-1} at 4300 cm^{-1}, combined with the an array of 256 $\times$ 256 elements, the largest array we foresee. This combination would sample about 25 cm^{-1} (at 2 pixels per resolution element) out of the free spectral range of 175 cm^{-1}. Thus it is possible to detect only about 15% of the spectrum in each order. From the example above, we conclude that: cross dispersion gains little additional information in the infrared because less than 20% of each order may be sampled (array improvements foreseeable in the next 10+ years are covered by this statement!). To make cross dispersion useful the free spectral range needs to be $\simeq$ 50 cm^{-1}. This would be possible if gratings could be made at $\leq$10 lines mm^{-1}. Rulings this coarse are not possible now or in the foreseeable future. (Note that at 5000 Å the 175 cm^{-1} free spectral range of a 31 line mm^{-1} echelle grating corresponds to $\sim$ 40 Å. At 0.1 Å resolution, the entire free spectral range will fit on 800 pixels so cross dispersion is very desirable in the visual.)

Several other problems with cross dispersion in the infrared are readily apparent. In the thermal infrared the 175 cm^{-1} free spectral range is large enough that different orders will have large differences in background radiation making optimization of integration time impossible for more than one order at a time. Tokunaga (private communication) has investigated cross dispersion in detail and notes that 3 different cross dispersing gratings would be required to provide optimum performance across the 1-5 μm range. Some of these gratings have unobtainable groove spacings. The possibility of fringing is not removed by using a cross disperser since the cross disperser also obeys the grating equation and must have its other orders blocked.

https://doi.org/10.1017/S0074180900034781 Published online by Cambridge University Press

To summarize, cross dispersion does not seem appropriate in the infrared because it adds little information, greatly increases the complexity and size of the instrument, and does not improve throughput or eliminate the possibility of fringing.

The most obvious choice for a filter to pass the individual orders of an infrared echelle is a circular variable filter (CVF). CVF's are available with bandpasses from 1 to 10%. The 175 cm^{-1} free spectral range provided by a 31 line mm^{-1} echelle is 1.9% at 1.1 μm and 8.5% at 5 μm. A 31 line mm^{-1} echelle appears well matched to the range of bandpasses available with a CVF. A 23 line mm^{-1} echelle has a free spectral range of 1.4% at 1.1 μm and could be blocked with a CVF but pushes harder on the narrow bandpass end of CVF technology.

An alternative to a CVF would be a refractive order separator. This option has the advantages of no possible fringing and potentially high throughput. The disadvantage is that refraction is not linear with wavelength making such an order separator optically and mechanically complex. This is especially true since the cryogenic echelle will operate over a factor of 5 in wavelength.

The following table summarizes the conclusions and recommendations based on this design study.[2]

- Resolutions of 100000, 50000 and 25000.
- 8 $\times$ 16 inch echelle grating (preferred), 5 $\times$ 10 inch (alternate).
- Slit width of 1.4 arc seconds for resolution of 50000 and 0.7 arc seconds for resolution 100000 on the 2.1 meter telescope for 4.6 μm.
- Cross dispersion is not useful at wavelengths much longward of 1 μm with foreseeable echelle grating technology. Improvements in the technology are not expected on a time scale relevant to this project.
- Order separation with CVF's.
- A 31 line mm^{-1} echelle is well matched to a CVF order separator.

We wish to acknowledge very fruitful discussions with Alan Tokunaga and Don Hall on IR echelle spectrometers, and with Richard Joyce on the InSb detector arrays. STR thanks the University of Paris and the Meudon Observatory for their hospitality when this review was under preparation.

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[2]These parameters and other aspects of the cryogenic echelle are under review at NOAO at the time of this writing.

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DISCUSSION

LINSKY Will the proposed NOAO cryogenic échelle spectrometer operate at 10 μm and if so what will be the sensitivity gain over the 4 m FTS spectrometer.

RIDGWAY We plan to restrict the spectral range to $\lambda \leqslant 5$ μm. Operation at 10 μm would require cooling to much lower temperature, and exchangeable detectors and gratings. A 10 μm spectrometer can be simpler if constructed separately from the 1 – 5 μm unit. The gain over an FTS should be considerable, on the order of the square root of the ratio of the FTS bandwidth to the dispersive spectral resolution. Gains of 2 – 3 magnitudes should be easily obtained.

ANDERSEN Did your comparison of performance figures between the spectrograph and the 4m FTS include the wavelength range included in a single observation ?

RIDGWAY No.