WaFIRS, a Waveguide Far-IR Spectrometer:

Enabling Space-Borne Spectroscopy of High-z Galaxies in the Far-IR and Submm.

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ABSTRACT

The discovery of galaxies beyond z~1 which emit the bulk of their luminosity at long wavelengths has demonstrated the need for high-sensitivity, broadband spectroscopy in the far-IR/submm/mm bands. Because many of these sources are not detectable in the optical, long-wavelength spectroscopy is key to measuring their redshifts and ISM conditions. The continuum source list will increase in the next decade with new ground-based instruments (SCUBA2, Bolocam, MAMBO) and the surveys of HSO and SIRTF. Yet the planned spectroscopic capabilities lag behind, primarily due to the difficulty in scaling existing IR spectrograph designs to longer wavelengths.

To overcome these limitations, we are developing WaFIRS, a novel concept for long-wavelength spectroscopy which utilizes a parallel-plate waveguide and a curved diffraction grating. WaFIRS provides the large (~60%) instantaneous bandwidth and high throughput of a conventional grating system, but offers a dramatic reduction in volume and mass. WaFIRS requires no space overheads for extra optical elements beyond the diffraction grating itself, and is two-dimensional because the propagation is confined between two parallel plates. Thus several modules could be stacked to multiplex either spatially or in different frequency bands. The size and mass savings provide opportunities for spectroscopy from space-borne observatories which would be impractical with conventional spectrographs. With background-limited detectors and a cooled 3.5 telescope, the line sensitivity would be better than that of ALMA, with instantaneous broad-band coverage. We have built and tested a WaFIRS prototype for 1-1.6 mm, and are currently constructing Z-Spec, a 100 mK model to be used as a ground-based $\lambda/\Delta\lambda \sim 350$ submillimeter galaxy redshift machine.

1. Scientific Motivation

The advent of large-format bolometer arrays for wavelengths around 1 mm (SCUBA, MAMBO) had revealed a new class of galaxies which are likely at medium to high redshift. These sources are cosmologically significant – their counts reproduce much of the diffuse far-IR / submillimeter background radiation, representing the energy generated by all galaxies over the history of the universe (Blain et al.1999, Barger et al, 1999). These submillimeter galaxies are luminous systems similar to the nearby IR galaxies discovered with IRAS. Of the nearly 200 submillimeter galaxies discovered thus far, only a small fraction have confirmed spectroscopic redshifts and well-determined properties at other wavelengths. This is because the sources are very dusty with high extinction at short wavelengths, the optical and UV energy is almost entirely reprocessed and reradiated between $\lambda = 50$ μm and 1 mm, making the optical counterparts too faint to be detectable. While there are spectral features that could be used in the millimeter / submillimeter, the instantaneous bandwidth of heterodyne millimeter-wave receivers is currently a small fraction of unity, so searching for lines in sources with unknown redshifts is impractical.

The long-wavelength continuum source list will only increase in the next decade with new ground-based instruments (SCUBA2, Bolocam) and the confusion-limited surveys of HSO and SIRTF. The recently discovered submillimeter galaxies, and their soon-to-be-discovered far-IR cousins demonstrate the need for broad-band spectroscopy in the far-IR / submillimeter / millimeter bands. Long wavelength spectroscopy with large instantaneous bandwidth is the key to measuring these sources' redshifts, which constrain their luminosities, sizes, and masses. Moreover, the wide variety of spectral features in the mid- and far-IR provide information on the conditions in the interstellar medium and contrain the luminosity source(s). The types of spectral features include:

Fine Structure Lines. Species include Ne^{+}, S^{++}, Si^{+}, C^{+}, C^{0}, O^{0}, O^{++}, with luminosities from 10^{-4} to 3×10^{-3} of the total bolometric luminosity. These lines also measure the gas conditions and UV field properties in regions where stellar or AGN luminosity is input into the ISM. Mid- and far-IR fine structure lines have been used to study the starburst conditions in nearby galaxies (Stacey et al., 1991, Lord et al, 1994, Colbert et al. 1999, Carral et al. 1994, Malhotra et al, 2001) and recently, in as an AGN / starburst discriminator in ULIGs (Genzel et al, 1998).

PAH Bands. These features are very prominent in starburst systems, a well-studied redshift template with luminosities typically 1-4 % of L_{bol}. (see Helou et al., 2001, Tran et al., 2001.)

Molecular Rotational Transitions. Millimeter and submillimeter CO rotation is the dominant coolant of molecular gas and a probe of its temperature and density. Mid- and high-J lines trace warm gas associated with UV or shock heating of dense molecular gas (Jaffe et al, 1985, Harris et al, 1993 Ward et al., 2002, Bradford et al., 2001). Though not energetically important, other abundant species such as OH and

CH, constrain molecular gas column densities and abundances through absorption transitions (Bradford et al, 1999, Smith et al, 2001, Fischer et al 2001). These lines also have potential as a redshift probe for extremely obscured sources (those weak in fine structure lines) like Arp 220.

Table 1 (below) examines the various ISM probes available in the far-IR and submillimeter. The redshift range is that which would be observable with a spectrometer operating from λ = 20 μm to 1 mm.

TABLE 1. Far-IR SPECTROSCOPIC PROBES

SPECIES	WAVELENGTH	DIAGNOSTIC UTILITY	REDSHIFTS
		IONIZED GAS	
O IV	54.9	Primarily AGN.	0 - 17
S IV	10.5	Probes of the gas density and	0.9 - 100
O III	51.2, 88.4	UV field hardness in star-	0 - 18
S III	18.7, 34.8	formation H II regions.	0 - 50
N III	57.3	Provides effective temperature	0 - 16
Ne II	12.8	of hottest stars.	0 - 75
N II	122, 205	Diffuse interstellar H II regions.	0 - 7
		NEUTRAL ATOMIC GAS	
C II	158	Density and temperature probes	0 - 5
Si II	34.81	of photodissociated neutral-gas	0 - 30
O I	63, 145	interface between H II regions	0 - 15
C I	370, 610	and molecular clouds.	0 - 1.7
		MOLECULAR GAS	
H2 rotation	28.1 and shortward	Arises in dense, 100 - 1000 K molecular gas - often shock heated. Coolant of first gravitational collapse.	0 - 100
CO rotation	2600 and shortward	Primary coolant of molecular gas - probes pressure and temperature. Isotopes provide column densities, total gas mass	0 - 3
		DUST	
PAH	7.7, 11.3	Indicates star formation	0.8 - 100

2. Sensitivity from Space

Unfortunately, though there are a wealth of diagnostics for dusty galaxies in the far-IR and submillimeter, the wavelength range is not generally accessible from the ground. The atmospheric windows shortward of λ~700 μm are accessible only occasionally from mountaintop sites. Between 30 and 200 μm, the atmosphere is completely opaque from all terrestrial sites. While there are space missions planned to observe these wavelengths in the continuum (SIRTF, HSO), there is very limited spectroscopic capability planned for these wavelengths from space. The sensitivity attainable from a modest (diameter ~ 3.5 m) cool (T < 15 K) space telescope is dramatically better than what is currently planned between SIRTF and ALMA (see Figure 1). The effective line survey speed, proportional to the inverse of the sensitivity squared divided by the instantaneous bandwidth shows a more

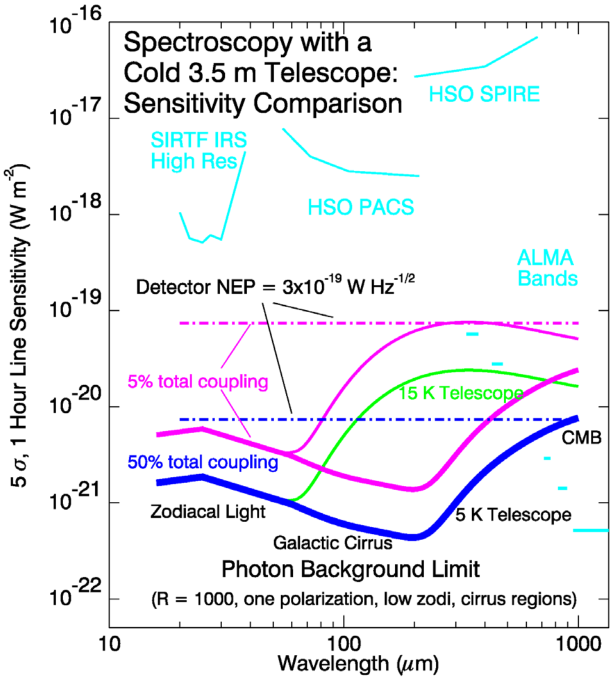


Figure 1. Spectral sensitivity on a cold 3.5 m space telescope. The 50% and 5% total couplings are conservative bounds to what might be achieved with a real spectrometer. Background noise is calculated from the fluctuation in the Zodical and cirrus backgrounds, toward patches of low intensity. If historical trends continue, background-limited performance at these frequencies will be possible, and gains of 2-4 orders of magnitude in sensitivity could be achieved.

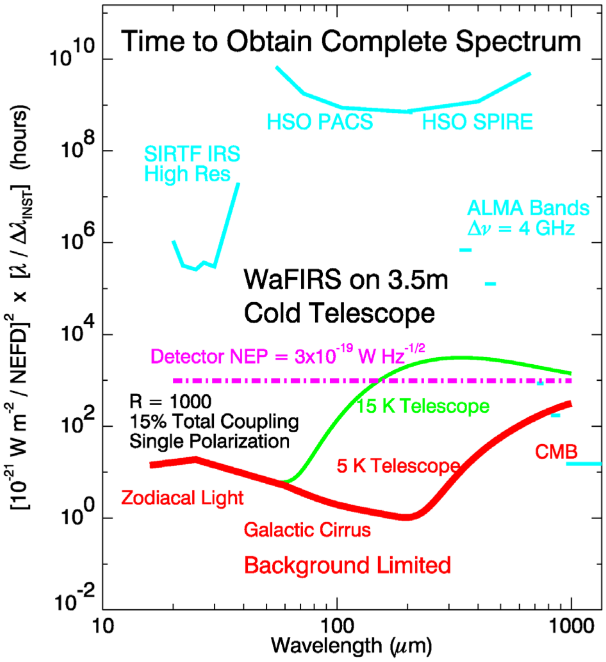


Figure 2. Sensitivity calculations similar to those of Figure 1, but including the effect of instrumental bandwidth. Under reasonable assumptions (15% efficiency, one polarization only), a broad-band spectrometer on a cold 3.5 meter telescope will have line survey speeds 6 or more orders of magnitude faster than the spectrometers of HSO, making far-IR line surveys practical. Such an instrument would be faster than ALMA for λ<600 μm.

dramatic gain of several orders of magnitude (see Figure 2). These large potential gains are possible in part because the raw sensitivity improves substantially by cooling the telescope to 15 K or lower (HSO is expected to operate at about 60 K). Another key aspect for observing sources with unknown redshifts is that the spectrometers on HSO are not optimized for line surveys. PACS is an imaging spectrometer with only a 1% instantaneous bandwidth, and SPIRE is a Fourier transform instrument with noise from the full band on the detectors at once. For an 8 meter class cold telescope such as SAFaIR, the sensitivity advantages are improved an additional factor of more than 5 beyond what is plotted in Figures 1 & 2.

3. Technical Background: Why a Waveguide Spectrometer

While there are a variety of options for a far-IR and submillimeter spectrometer, some are better suited to the science goals outlined above – observing high-redshift dusty galaxies with high sensitivity. Sources will be taken from preceeding continuum surveys, and will be spatially unresolved, so that imaging is not particularly important. In most cases, the redshifts will not be known in advance and the diagnostic lines are distributed over a broad spectral range, so a large instantaneous spectral bandwidth is critical. Given that in the far-

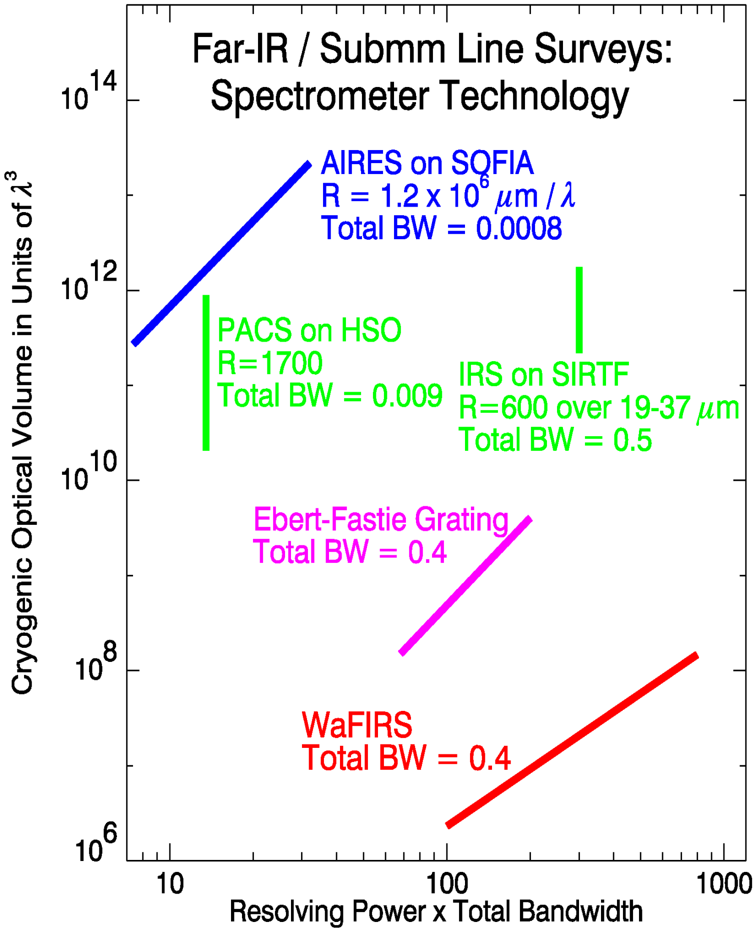


Figure 3. Sizes of existing spectrometer modules compared with their survey capability. The spectral survey capability of an instrument is given by its resolving power X total bandwidth. Modest resolution, broad-bandwidth systems exist (eg the SIRTF IRS modules) but are prohibitively large when scaled to far-IR and submillimeter wavelengths. WaFIRS offer a compact broadband system for longer

IR and submillimeter, the total number of detectors is typically a constraint, it therefore desirable to have the detectors arrayed spectrally rather than spatially, and an imaging monochromator such as a Fabry-Perot is not the instrument of choice. For ultimate sensitivity, a Fourier transform spectrometer (FTS) is not ideal because it places the entire spectral bandwidth and its associated photon noise onto a single detector. An FTS is appropriate only when using a detector which is not background-limited at the spectrometer resolution.

The obvious choice for background-limited point-source spectroscopy is a diffraction grating. Gratings have been used in astronomy for decades, and recently in the Infrared Space Observatory (ISO) as cryogenic, space-borne infrared spectrometers. When operated in first order, a grating naturally provides an octave of instantaneous bandwidth, and the resolution can be increased by increasing the grating size, roughly $d \sim \lambda \times R/2$. At far-IR and submillimeter wavelengths, this size quickly becomes prohibitively large, especially since real instruments are typically larger than the fundamental limit because they include collimating and imaging mirrors as well as order-sorting elements. For example, each of the spectrometer modules on SIRTF, measures about 40 x 15 x 20 cm, with a maximum $\lambda \times R$ product of 2 cm (R = 600 at 37 μm). To scale such an instrument up for a wavelength of 200 μm would result in a long dimension of over 2 meters, prohibitive for a space mission. Another example is the PACs spectrometer for HSO, an image slicing spectrometer which provides R=1500 out to 200 μm. The size of the cryogenic enclosure is quite large, roughly 80 cm x 80 cm x 30 cm, and because the instrument is designed for imaging spectroscopy; it only provides 16 spectral resolution elements, or 1% instantaneous bandwidth. The sizes of existing spectrometers are shown in Figure 3 in units of λ^3, plotted against the total number of spectral resolution elements.

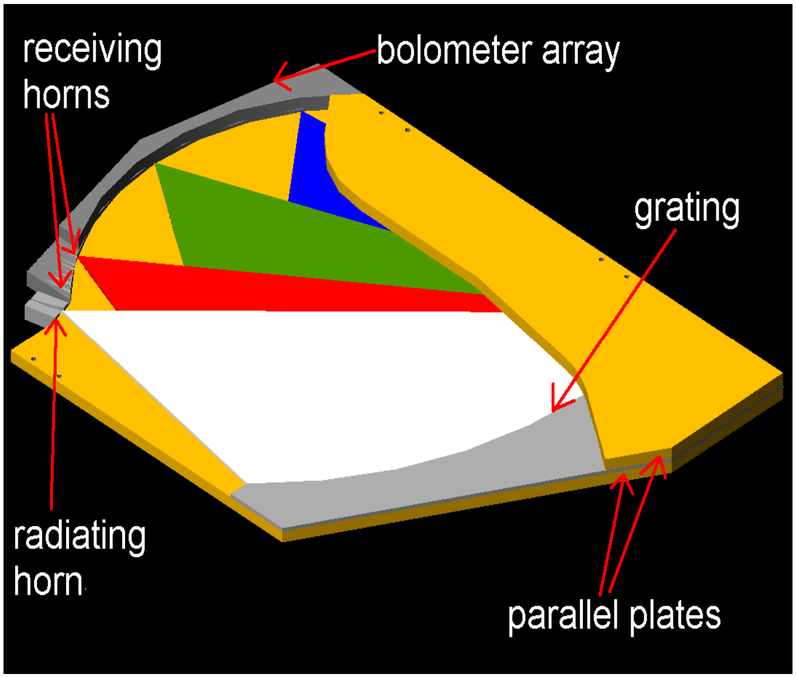


Figure 4. WaFIRS Concept: Rowland grating in parallel plate waveguide.
The light enters the parallel plate medium from the radiating horn and illuminates the curved diffraction grating. Each facet of the grating is individually positioned. Bolometers are positioned behind receiving horns on the focal curve.

To provide spectroscopic follow-up capability for the continuum surveys and to provide the foundation for further spectroscopic study, we are developing a new technology for a compact, broad-band spectrometer for the far-IR and submillimeter. WaFIRS, the Waveguide Far-IR Spectrometer, consists of a curved diffraction grating, entrance feed horn and detector feed horns all inside a parallel-plate propagation medium (see Figure 4). The spectrometer need be only a few wavelengths thick due to the two-dimensional geometry. Several spectrometers could easily be stacked to provide multiple wavelength bands, multiple spatial pixels, or both. The curved diffraction grating is the most space-efficient grating configuration possible because it both disperses and focuses the light. The grating can be nearly as large as the largest spectrometer dimension, with very little overhead, thus providing the maximum resolving power for a given cryogenic volume. Furthermore, the grating is used in first order which provides up to an octave of instantaneous bandwidth for any given module. The dramatic reduction in volume relative to conventional spectrometers is illustrated in Figure 3. The design has no moving parts and, once assembled, is completely light tight. While the concept has not been applied in the far-IR or submillimeter before, similar systems have been produced for near-IR and optical applications. The compact, lightweight geometry and robust construction make WaFIRS extremely well-suited for airborne, ballon and space-based spectroscopy.

4. WaFIRS Technical Discussion:

WaFIRS is conceptually similar to the slit spectrometers with curved gratings used by Rowland, Wadsworth, Eagle and other shortly after Rowland made the first curved grating around the beginning of the 20th century (see Born & Wolf, 1999). Though WaFIRS uses the same basic layout, it is based on propagation of a single electromagnetic mode in a two-dimensional medium bounded by parallel, conducting plates. The propagation mode is analagous to the TE_10 mode in rectangular waveguide -- the electric field is normal to the direction of propagation, with a half-wave vertical profile which vanishes at the top and bottom. [The dispersion relation is that of waveguide, namely as the frequency decreases toward cutoff, the wavelength increases infinitely.] Light is injected into a WaFIRS module with a horn which provides a suitable illumination pattern on the grating. The grating is in first order, and diffracts the light to a circular focal curve which extends over nearly 90 degrees of arc, on which the feed-horn coupled bolometers are arrayed. Figure 4 shows a sketch of the WaFIRS concept.

We have designed and built a prototype for wavelengths of 1-1.6 mm. The spectral resolving power is between 180-250 and the overall size only 56 cm x 42 cm x 2.5 cm. The key to the design is the placement of each facet individually such that for two frequencies, the change in propagation phase from the input to the output is exactly 2π between two adjacent facets, providing perfect (stigmatic) performance at these two frequencies. In our λ=1-1.6 mm prototype, there are 400 facets, and the resulting grating curve has a length of 51 cm. To evaluate the spectrometer designs, we perform diffraction calculations which account for the amplitude and phase produced by the input horn at each facet, then sum the contributions from all the facets at each output location. The model therefore includes diffraction and geometric optics, at a scalar approximation. The illumination of the grating is important -- a larger pattern from a smaller input horn produces higher spectral resolution, but lower efficiency, due to power which is lost beyond the edges of the grating. For the first prototype, we have chosen a 3.5 mm input horn which illuminates the grating with a power pattern of FWHM = 110 (180) facets at 1.0 mm (1.6 mm). The spectral resolution ($\nu / \Delta\nu_{FWHM}$) that results is 180 (250) at 1.0 (1.6 mm). Because the facet positions are individually calculated, the geometric aberrations are completely negligible, and the system is strongly diffraction limited.

4.1 Spectrometer Efficiency

Estimates of the spectrometer efficiency must include losses from: 1) Waveguide propagation with finite-conductivity plates, 2) diffraction efficiency into the proper order (i.e. blaze efficiency), and 3) illumination losses. Figure 5 plots our calculations of these contributions, and their product. The waveguide propagation loss is given by standard expressions (see Pozar, 1998), the 3 % loss for total propagation from input to detector can be achieved by polishing and gold-plating the parallel plates. In our prototype operated

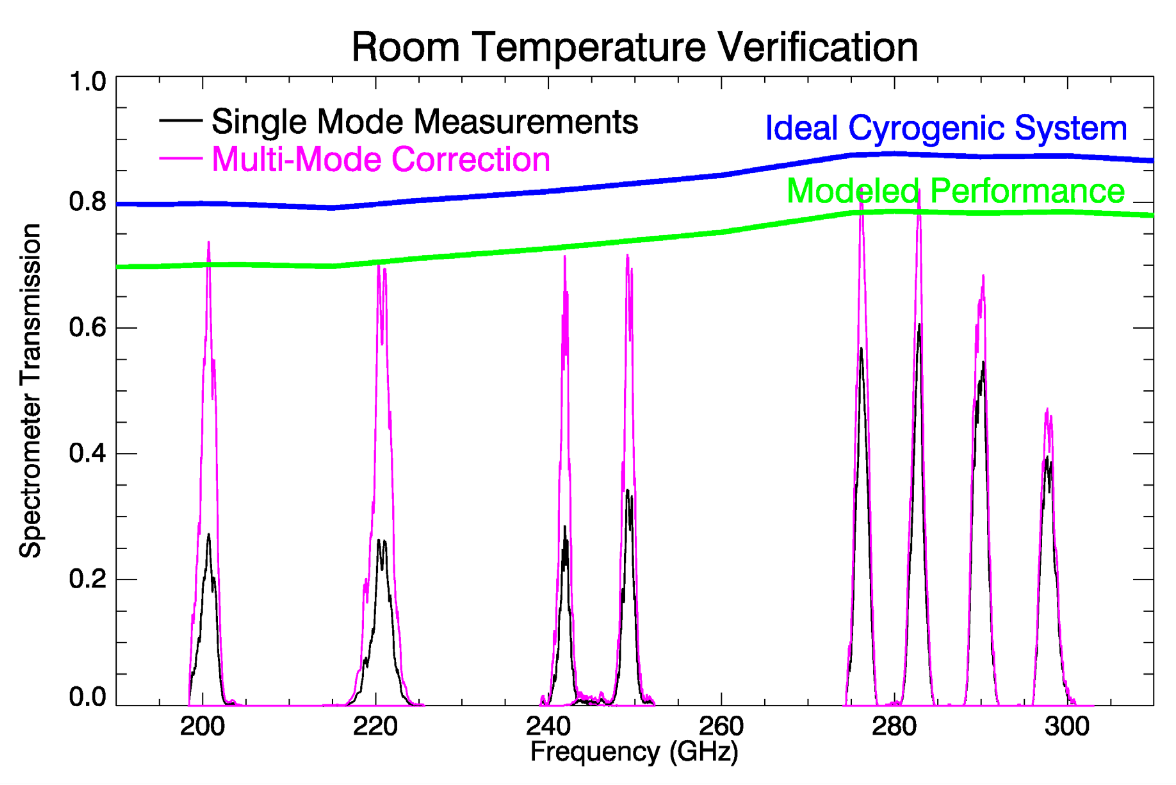
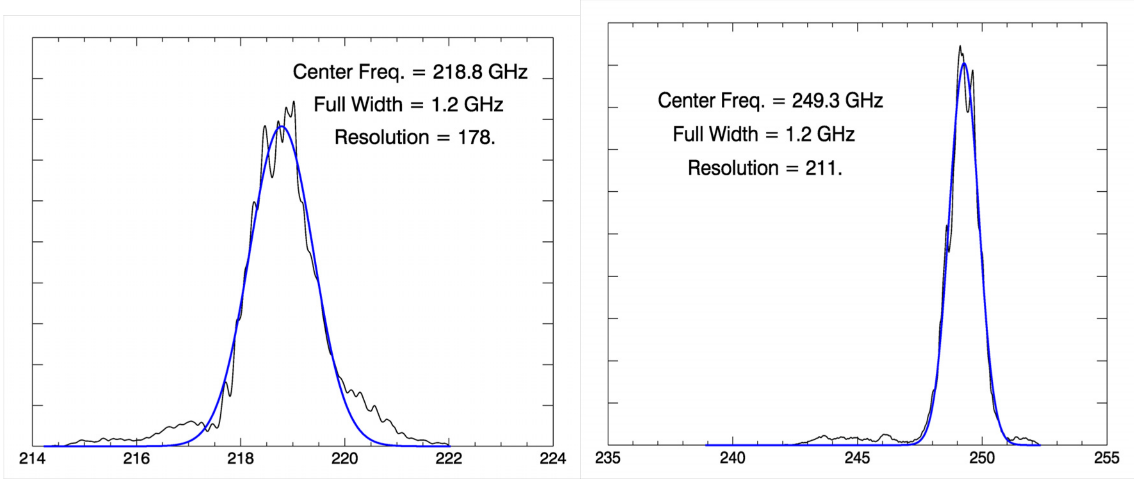


Figure 5. Testing of the first WaFIRS prototype. Measurements were made with a detector behind a single-mode feed, which does not couple all the power in the profile. Accounting for this coupling inefficiency produces the corrected curves which are close to performance predicted by the waveguide propagation loss, spillover loss. The high-frequency degradation is due to a blaze inefficiency, which will be corrected in future designs.

with only nickel coated plates and an aluminum grating, the propagation efficiency is somewhat lower. The blaze efficiency is calculated with commercially available software, applicable since with the waveguide propagation mode, the radiation is effectively in TE grating mode. These same calculations are the basis of our choice of a 29° blaze angle. Spillover losses are discussed above, they range from 89% to 94%. The net efficiency of a gold-plated cryogenic system is expected to be higher than 80% across our band.

4.2 Prototype Testing

We have measured the performance of our prototype using a backward wave oscillator (BWO) as a sweeping millimeter wave source (Figure 5,6, below). The power was measured with a diode detector in single-mode waveguide. At each frequency, a very small feed horn was used to measure the size of the intrinsic profile, then the total coupling as measured with a larger (but still single mode) feed is deconvolved using this profile. The results are quite close to our predictions over much of the band. We are investigating the reason for the loss in performance at the highest frequencies, it is likely a blaze efficiency.



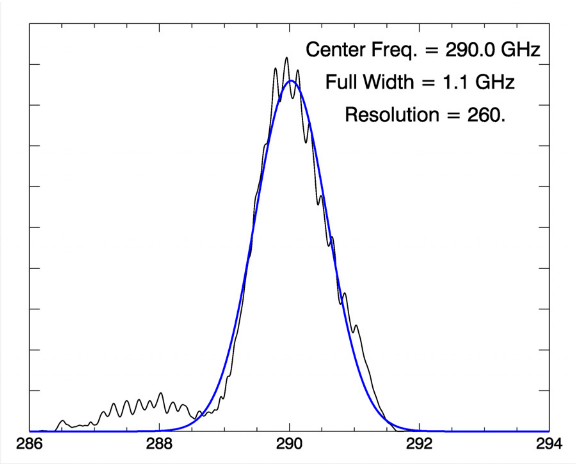


Figure 6 a,b,c .
Measured resolving power of the first WaFIRS prototype. To within the measurement uncertainties, profile widths are equal to those calculated in the design model. The second generation spectrometer will have resolving power between 250 and 400.

5. Scalability: Ground Based Observations and WaFIRS Modules for the Far-IR

In addition to our λ=1 mm prototype, we are constructing a cyrogenic version, Z-Spec for observations from ground-based submillimeter / millimeter observatories. Z-Spec will demonstrate the capability of WaFIRS to provide broadband spectroscopy with background-limited sensitivity. Z-Spec is discussed in more detail by J. Glenn et al in these proceedings (Glenn et al (2001)). We have produced designs with the same size and shape for a variety of shorter wavelengths, including a system which provides R=2000 at λ=100 μm. As wavelength is shortened, the number of facets and spectral resolution elements increases while the facet size and the physical size of a resolution element decrease. The grating remains in first order and the total fractional instantaneous bandwidth is constant. This extension to shorter wavelengths is possible because the design produces a stigmatic geometry for the grating, and geometric aberrations are small. The table below shows three examples of spectrometer designs:

Design Parameter	**1st Prototype**	**Z-Spec Module**	**Far-IR Module**
Frequency Range	195-310 GHz	195-310 GHz	1.9-3.0 THz
Stigmatic Frequencies	273, 204 GHz	296, 199 GHz	2.8, 2.0 THz
Number of Detectors	------------	160	~500
Number of Facets	400	500	4000
Resolving Power	180-250	250-400	1000-2000
Plate Spacing	2.5 mm	2.5 mm	0.6 mm
Spacing Tolerance	0.08 mm	0.04 mm	0.005 mm
Longest Dimension	50 cm	61 cm	55 cm
Illumination Efficiency	.87-.91	.78-.85	.9

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