Spectroscopy and Spectrophotometry

Why Spectroscopy?

We need to resolve the spectral lines in objects In order to determine radial velocities, composition, stellar atmospheric parameters for a single star or a stellar population in a galaxy, velocity dispersion in a galaxy, see flows or winds, etc, etc. Imaging cannot do ANY of this for us with any accuracy.

Cannot do with narrow filters. Recall that the time it takes to measure in N filters which span some wavelength range to a fixed signal-to-noise goes like N^2. If we could do it all at once, it would only go like N (rhe flux in each filter goes like 1/N, so this is the best we can do.) Doing the measurements simultaneously is said to gain the MULTIPLEX ADVANTAGE.

Note that there is no free lunch. Detectors are 2-dimensional, so gaining resolution in wavelength generally means giving up at least one spatial dimension, though there are partial solutions.

Spectroscopy

Spectroscopy is normally done at wavelngths shorter than a few hundred microns with dispersive techniques—ie techniques which spread the different wavelengths of light out spacially.

The first spectrographs were done with prisms, and one used the decrease of refractive index with wavelength to spread the light out into a spectrum. Will discuss a little a little later.

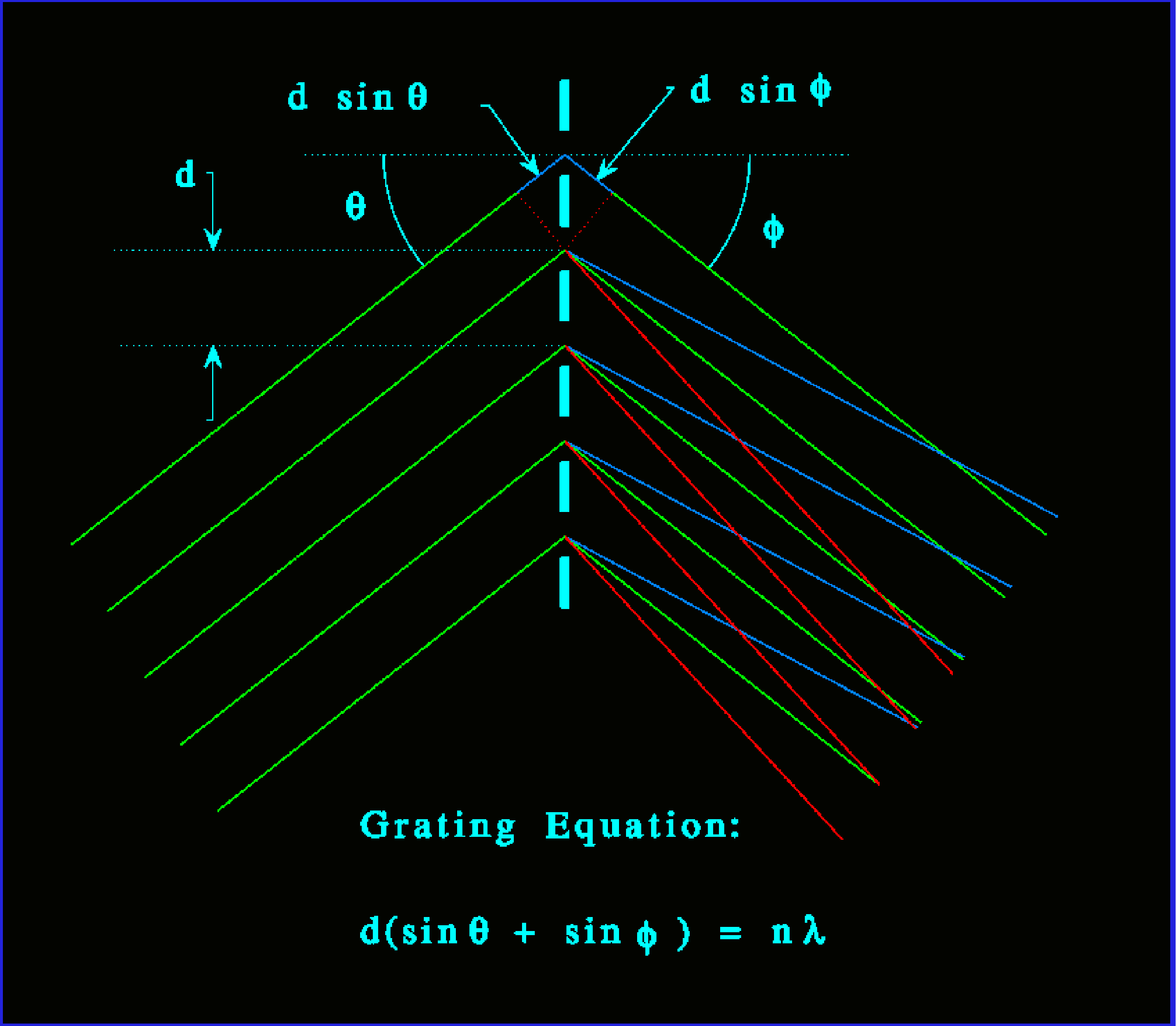
Prisms are still used in special circumstances today, but most work is done with grating spectrographs and spectrometers (used to be different, now the same, and interchangeable words).

Will not discuss history, but be aware that spectroscopy made possible the birth of astroPHYSICS. It offered the first clues into the composition and physical conditions in astronomical objects.

Diffraction Gratings

Gratings are physical optics devices, making direct use of the wave nature of light.

The standard toy model of a grating is a series of slits. The wavelets from all the slits interfere constructively when the path difference from one slit to the next is an integral number of wavelengths, so light of longer wavelengh is DIFFRACTED at larger angles. n is the diffraction ORDER. If the incident angle θ is the same as the diffraction angle ϕ, the grating is said to be in Littrow mode. This is generally advantageous. If the angles are small, gratings have very LINEAR dispersion, $\phi \sim \lambda$



Grating Equation:

$$d(\sin\theta + \sin\phi) = n\lambda$$

Diffraction Gratings—Some Typical Numbers

If $\theta \sim \phi \sim 15$ degrees, then in the visible at 5500A, $2d \sin \phi \sim 0.55$m if the grating is used in 1st order. Then $d \sim 1.1$m, so the grating has ~900 lines per millimeter. A 150mm sq grating then has ~135,000 lines, a total groove length if ruled of 18 km.

Diffraction Gratings

Starting early in the last century, gratings were ruled in aluminum or silver films with a diamond, controlled by very precise machines called ruling engines. They were REFLECTION gratings. All astronomical gratings were made this way until early THIS century, but the old technology has been largely displaced by a new one, called volume phase holography.

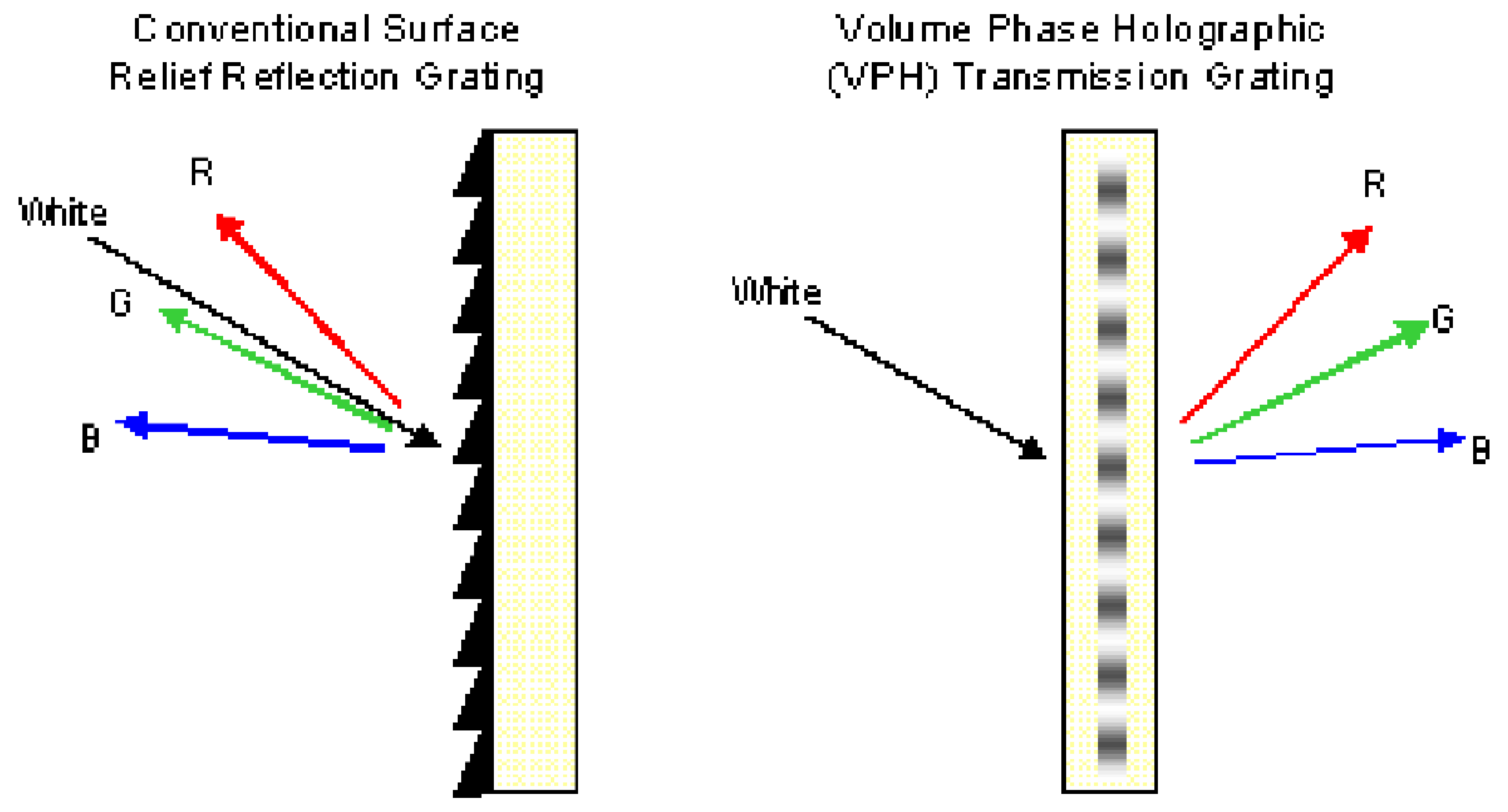


Figure 1. Conventional reflection gratings vs. VPH gratings.

VPH Gratings

VPH gratings are made photographically in a material called dichromated gelatine by a holographic process using interference between two parallel beams generated by a single laser, incident on the gelatine film at a very well-controlled angle under very stable conditions. The gelatine `develops' to have refractive index variations which are functions of the incident intensity. There is no obstruction, simply index and hence phase variations. The gratings work with a combination of the grating equation and the Bragg condition to increase their efficiency. Hence *volume* *phase*. Ruled gratings could be `blazed' for particular wavelengths by controlling the groove angle. VPHs can be `blazed' (tuned) by controlling the depth of the index modulation.

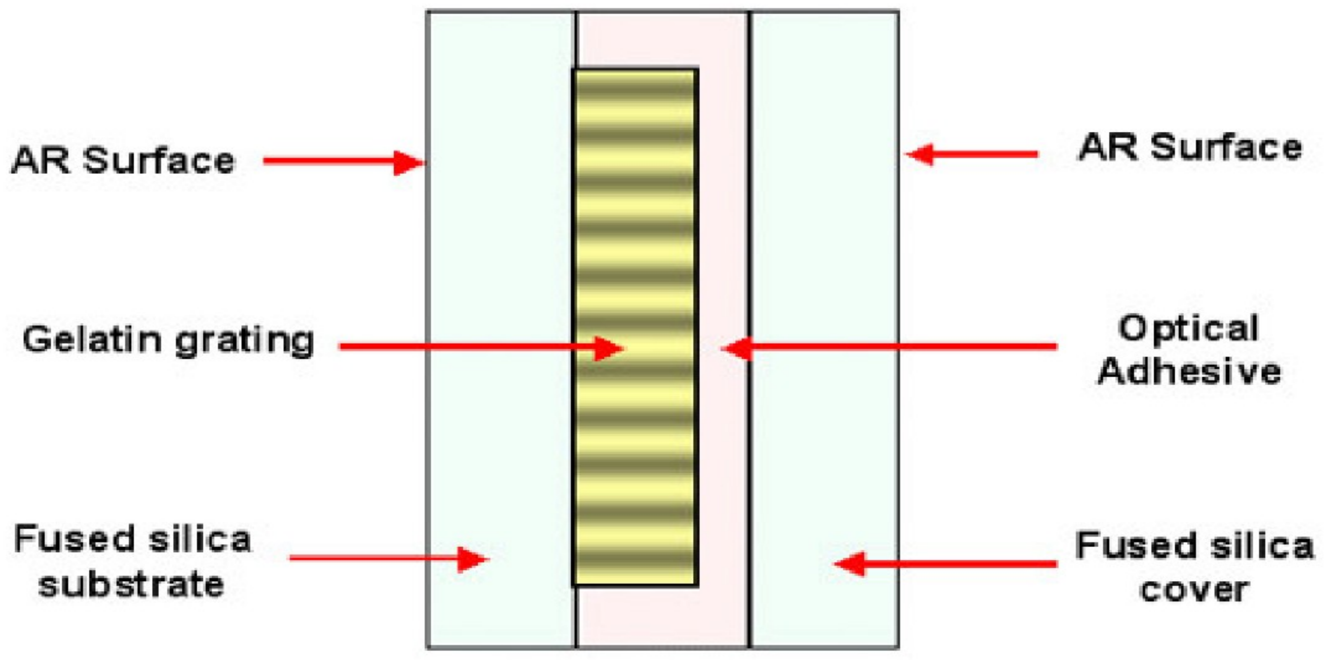
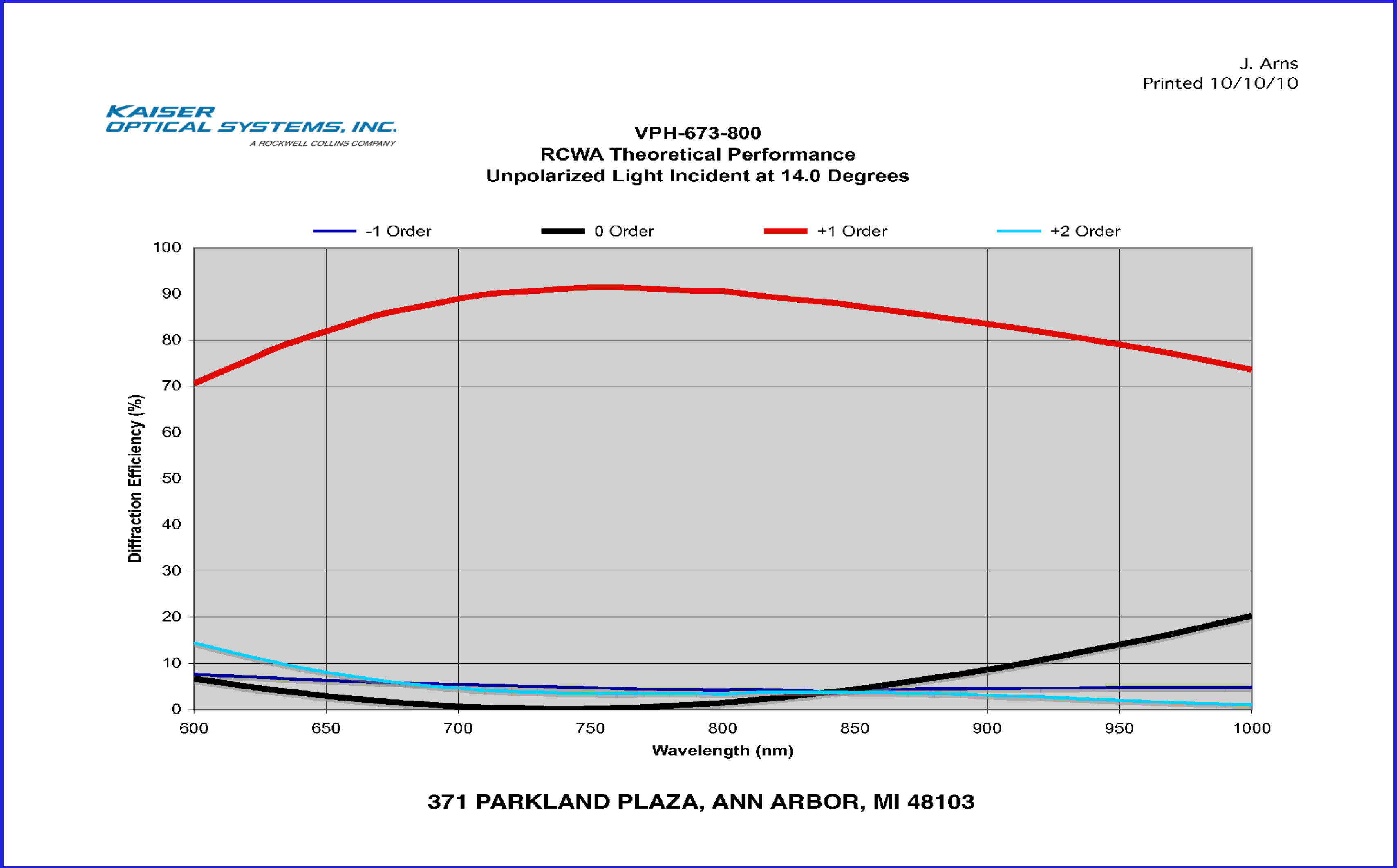


Figure 3. Structure of a VPH Grating.

VPH Efficiency

VPH gratings can have very high efficiencies compared to ruled gratings. In first order, their efficiency can be greater than 90 percent; ruled gratings seldom exceed 60 percent. Shown is the design for the PFS red grating; the finished products generally are at most two or three percent worse than the design.



J. Arns
Printed 10/10/10

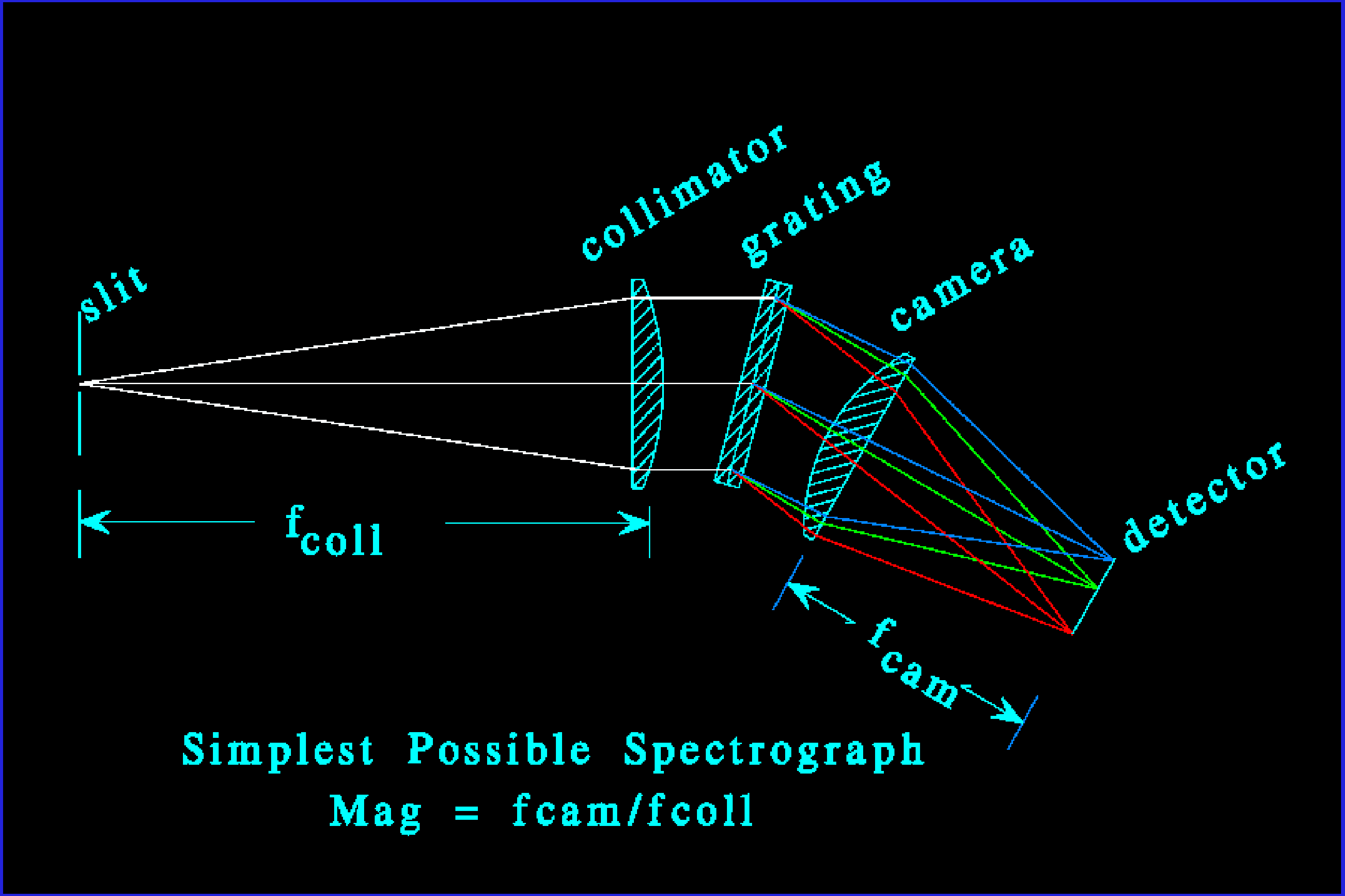
KAISER OPTICAL SYSTEMS, INC.
A ROCKWELL COLLINS COMPANY

VPH-673-800
RCWA Theoretical Performance
Unpolarized Light Incident at 14.0 Degrees

371 PARKLAND PLAZA, ANN ARBOR, MI 48103

Spectrographs

The diagram shows a very simple spectrograph layout. The light enters the instrument through a slit of fixed or variable size, is made parallel by a collimator lens, goes through a dispersing element (grating or prism), and is focussed onto a detector with a camera lens. The slit is imaged onto the detector at each wavelength, demagnfied by the ratio of camera to collimator focal lengths.



Simplest Possible Spectrograph

Mag = fcam/fcoll

Spectrograph Design: Resolving Power

There are many design criteria for spectrographs, including efficiency, detector real estate, admissible slit size, and resolving power—that is, how detailed the resulting spectrum is.

If the minimum resolved wavelength interval is $\delta\lambda$ (set by the slit width, or, heaven forbid, the pixel size) the RESOLVING POWER, R, is

$R = \lambda/\delta\lambda$.

for PFS, for example, in the red at 7500A, the resolution is about 2.5A (FWHM) so the resolving power is ~3000.

What sets the resolving power? Clearly some combination of the projected slit width w and the angular dispersion $d\phi/d\lambda$. If the grating is used in Littrow mode, so that the central value of ϕ is the same as the incident angle θ, then it is trivial to show from the grating equation that

$d\phi/d\lambda = 2 \tan \theta / \lambda$. But $\delta\phi = w/f_{cam}$, and $\delta\lambda = (d\lambda/d\phi)\delta\phi$, so

$$R = \lambda/\delta\lambda = \lambda/ (w/f_{cam})d\lambda/d\phi = 2f_{cam} \tan \theta/w$$

Spectrograph Design: Resolving Power

$R = \lambda/\delta\lambda = \lambda/\ (w/f_{cam})d\lambda/d\phi = 2f_{cam} \tan\theta/w$

This is a quite remarkable formula. It does not depend directly on the gratring spacing d, nor on the wavelength, ONLY on dimensions in the spectrograph optics and the angle of diffraction.

The projected slit width w and the pixel size clearly should be related. If the projected width is much smaller than a pixel, the slit is too narrow and you are probably not letting in enough light.

More seriously, the spectrum is UNDERSAMPLED. Imagine an infinitely narrow slit. Then the line is somewhere on the pixel, but you do not know where. If the line is two pixels wide, then by the ratios of signal in adjacent pixels, you can figure out where the centroid is to a fraction of a pixel. This is a simple statement of the Nyquist theorem, that one can reasonably reconstruct an input signal if you have at least two samples per FWHM. For a gaussian LSF, (the 1-D PSF in the wavelength direction), you can reconstruct the spectrum to about 1% if you have 2 pixels per FWHM; to about 0.1% if you have 3, and to about 10% if you have 1.7—it is exponentially dependent on the ratio.

Spectrograph Design: Camera f-ratio

*Subaru is a very large telescope. At prime focus, the focal ratio is 2.24 with the HSC corrector, so the focal length is 8200mm * 2.24 = 18400mm, and an arcsecond subtends 18400mm/206265 arcsec/radian = 89μ.*

Miyazaki-san is lucky. Detectors these days all have 15μ pixels, and astronomers do not have enough political/economic power to change this. This pixel size corresponds to 0.17 arcseconds, just about right for good sampling in 0.4 arcsecond seeing, which he would like to take advantage of. (Think about 20 or 30 meter telescopes).

Think about a spectrograph. You have a telescope, a collimator, and a camera. What determines the scale on the final detector?

*Scale at telescope = (diameter * f-ratio)/206265 mm/arcsec.*
The collimator has the same f-ratio as the telescope, or you lose light; if it is faster, you waste glass, because you only GET the f-ratio of the telescope. The scale at the detector is the input scale times the ratio of the camera focal length to that of the collimator, which is the same as the ratio of the f-ratios. so the collimator f-ratio=telescope f-ratio cancels, and

*Scale at spectrograph detector = (diameter * camera f-ratio)/206265 mm/arcsec*

Spectrograph Design: Camera f-ratio, cont.

Scale at spectrograph detector = (diameter * camera f-ratio)/206265 mm/arcsec

and depends only on the camera f-ratio, not at all on where the spectrograph is deployed (prime, cass, nasmyth, etc, all of which have different f-ratios at the input.) This is

scale = 40μ*camera f/ratio/arcsecond

We mentioned last lecture that there is an optimum aperture size which is of order 1.5 times the FWHM at which the sky noise and object flux are such that the S/N is optimal. For a spectrograph, we cannot do matched filter photometry, and must be content with the optimum aperture if we are using fibers (more in a bit) or a slit. The optimum aperture (fiber) size is about 1.1 arcseconds for a barely resolved galaxy in 0.7 arcsecond seeing. This corresponds to 44μ*camera f/ratio on the detector, or ~ 3 pixels * camera f-ratio on a modern 15μ detector.

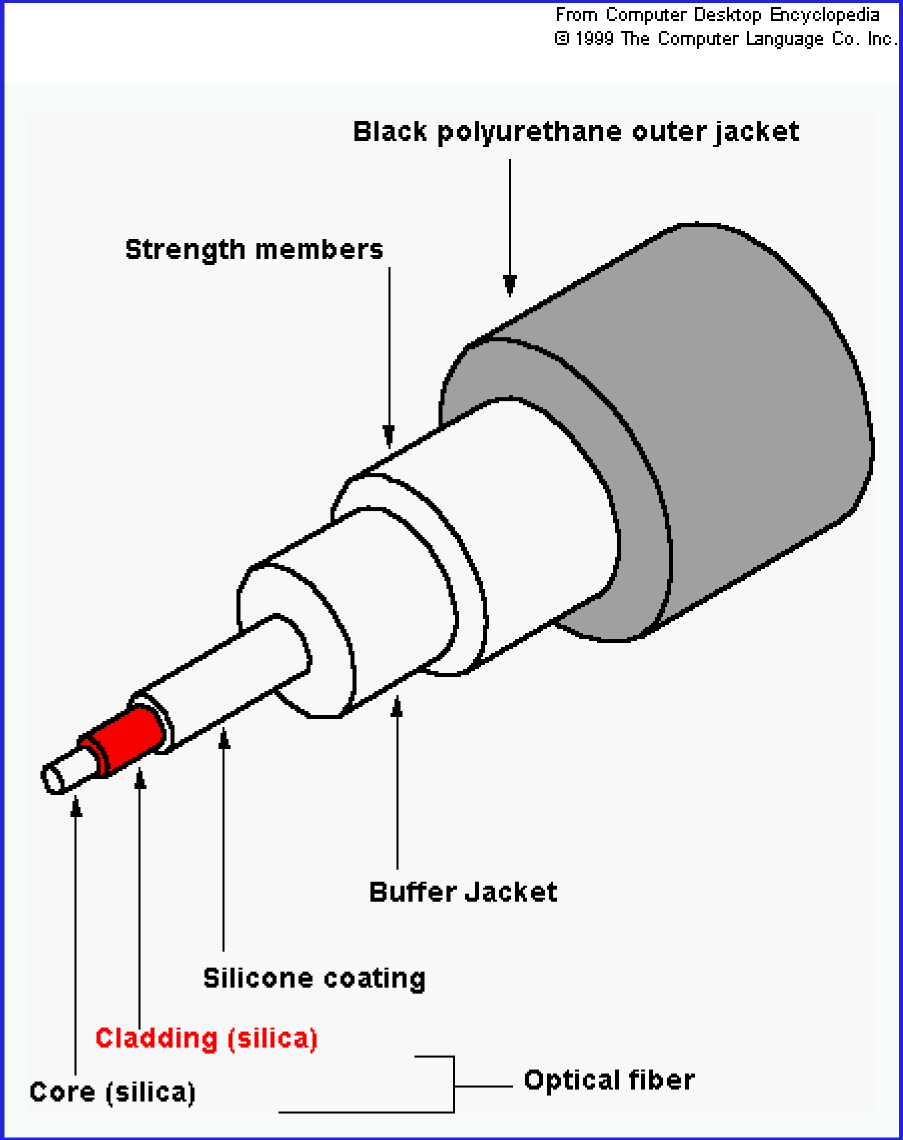
This is fine, you say. IF the camera f-ratio is 1.0. 1.0 is VERY, VERY hard. We will try 1.1 on PFS. (Think about a 20 or 30-m telescope).

But even this is not straightforward. We will use FIBERS.

Fiber Spectroscopy

Optical fibers for telecommunications became common in the 1970s, first proposed by Nishizawa (Tohoku) in 1963. Development waited on pure silica glass technology to reduce attenuation to acceptable levels.

First tried in astronomical spectrographs in the 1980s. Here need not only low absorption, but need to preserve focal ratio—ie must have very small angular scattering, so telescope f-ratio is preserved. Otherwise either lose light or must have very fast collimator to collect and an EVEN faster camera, and cannot do this on large telescopes.


From Computer Desktop Encyclopedia
© 1999 The Computer Language Co. Inc.

Fiber Spectroscopy, cont.

How do fibers work? Let ε be the angle between a ray and the fiber axis. The core of the fiber has index n_1, the cladding which surrounds the core index $n_2<n_1$. Let ζ be the angle of the ray in the cladding. Then Snell's law says

$$n_1 \cos \varepsilon = n_2 \cos \zeta$$

Total internal reflection occurs when $\zeta=0$, or

$$\cos \varepsilon = n_2/n_1.$$

remember $\sin \varepsilon = NA$, the numerical aperture.

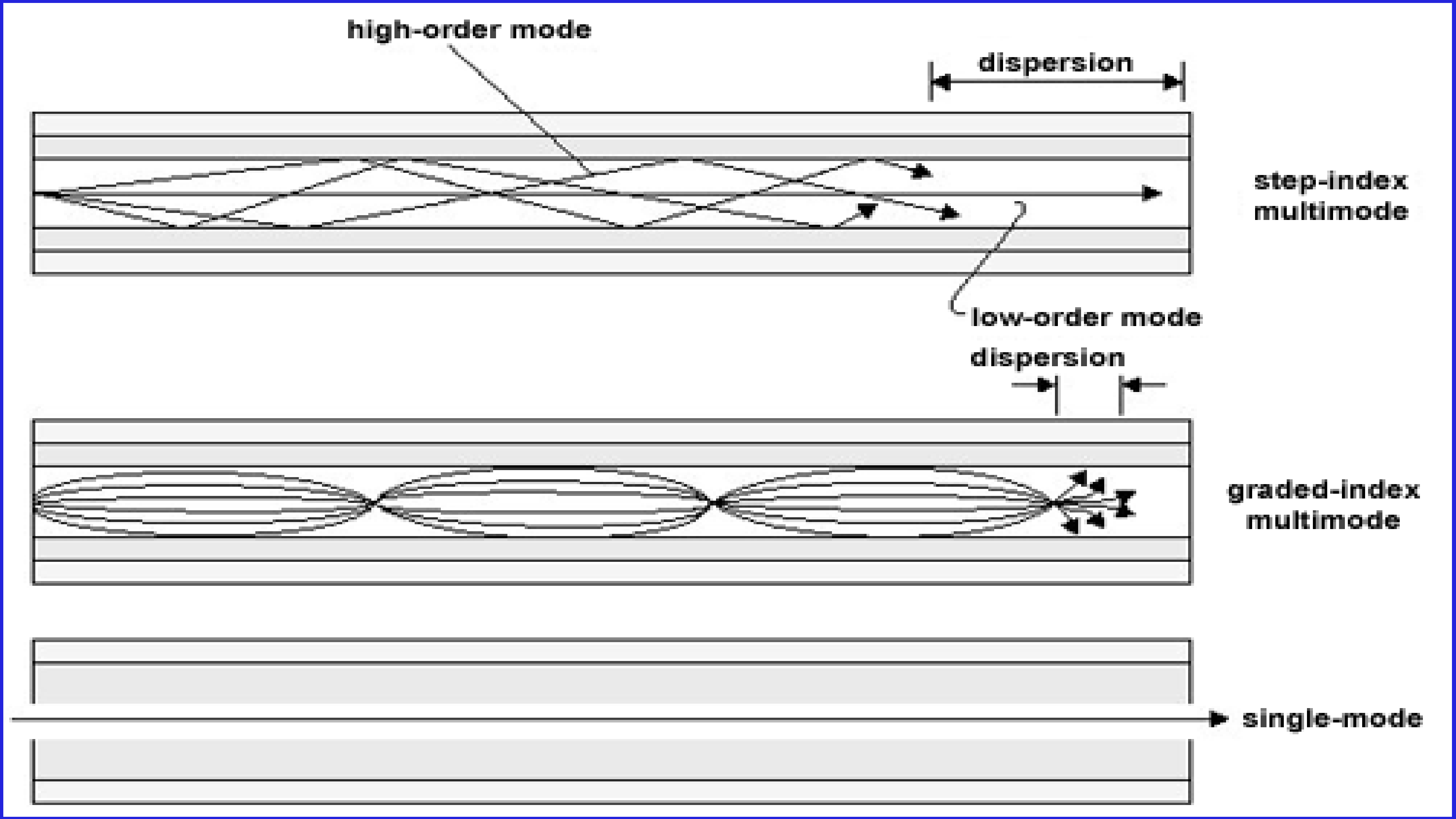
so $\mathrm{sqrt}\,(1 - NA^2) = n_2/n_1$,

and $NA = \mathrm{sqrt}(1 - n_2^2/n_1^2)$

represents the largest angle which can propagate by total internal reflection in the fiber; typically $NA \sim 0.24$, so $n_2/n_1 \sim 0.97$; the index difference is very small.

Fiber Spectroscopy, cont.

Types of fibers:



Fibers for astronomical spectroscopy are step-index multimode (single-mode fibers cannot be larger than a few wavelenths in diameter)

Fiber Spectroscopy, cont.

$n_2/n_1 \sim 0.97$; the index difference is very small.

This is a problem. The indices are sensitive to stress in the fiber, so the fiber cannot be bent or stressed very much, or light is lost. Worse, small stresses cause FRD (focal ratio degradation).

FRD is caused by

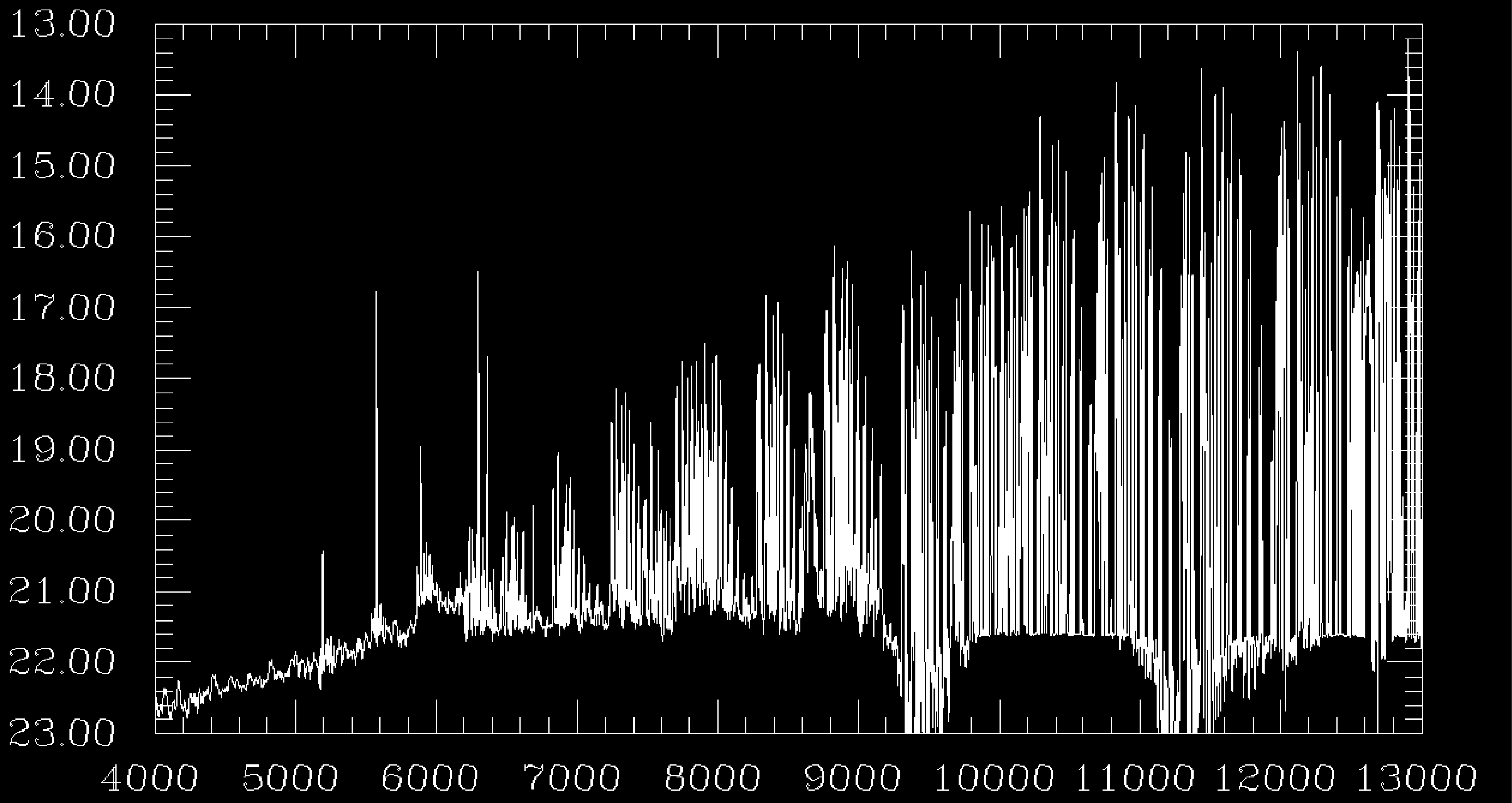
a) small diameter variations in the fiber, corresponding to some structure function in the angle the core-clad interface makes with the axis. The angle scattering should grow like the square root of the fiber length. May or may not be observed.

b) Stresses in the fiber run or in the fiber terminations. This seems to be the largest contributor, and typically the NA is degraded by of order .025, so f/5 in becomes f/4 on the output. For PFS, f/2.8 in becomes f/2.5 out. (lenses on the fiber input transform f/2.2, which is faster than the fiber will accept, to f/2.8)

The fiber run of 50m will transmit 85-90% of the light, and have this FRD. We hope.

Spectroscopy: The Sky Background

You have probably seen this twice before. No matter how much resolving power we might WANT for our astronomical objects, we MUST have enough in the red and near IR to work between the lines in the forest of OH lines. This demands R~4000 in the 1-1.3 micron region and about 3000 in the red (7200A-1 micron)



Spectroscopy: Resolving Power Requirements

What real consequences does a requirement on R have?

You have a finite number of pixels on your detector. You can mosaic detectors, but generally if you use a 4x4 array, say, the camera and collimator and spectrograph become twice as large and eight times as expensive, and fast cameras even more difficult.

So stick with a single large detector, say 4000 15-micron pixels. The fiber footprint is degraded by FRD and is about 54 microns; the FWHM of a round fiber image is sqrt 3/2 = .866 of its diameter, so about 46 microns, 3 pixels. So there are 4000/3 ~ 1330 resolution elements across the detector.

What can R be? 1/R is $\delta \ln \lambda = (1/N) \ln \lambda_2/\lambda_1$, *where* λ_2 *and* λ_1 *are the ends of the FREE SPECTRAL RANGE on the detector. So the maximum R you can have if you demand some FSR is*

$R = N/\ln \lambda_2/\lambda_1 = 1330/\ln \lambda_2/\lambda_1$ *in our case.*

Spectroscopy: Resolving Power Requirements

$R = 1330/\ln \lambda_2/\lambda_1$ for us.

If we need 4000, the log can be 1/3, or $\lambda_2/\lambda \sim 1.4$, and we cannot cover much wavelength. The same computation in the red, R~3000, gives $\lambda_2/\lambda \sim 1.55$. This is where the three channels and the wavelength coverage of PFS comes from:

blue 3800-6500 A (no sky driver)
red 6500-9800 A R=3000
IR 9800-13000 A R=4000

Spectrophotometry: Limitations and SotA

Briefly.

We do not know the SED of any astronomical object to better than ~ 2 percent.

Calibration is very difficult. There are no calibrated sources in orbit; doing the work from the ground (using radiance standards like platinum furnaces) is hard to impossible.

Best prospect is use of astronomical objects for which SEDs can be calculated with the required (sub 1%) accuracy.

Best prospect for THIS is dA white dwarfs. They have
a. No convection
b. High densities, so non-LTE effects are negligibly small.
c. The atmospheres are PURE HYDROGEN. Everything heavier has settled by diffusion.

Only two parameters. T_{eff} *and log g, separable by the spectrum itself.*

But the models are not good enough because we do not understand the HYDROGEN ATOM. This will get better. Soon. Maybe. (Pierre Bergeron)

Stellar Spectral Synthesis

Briefly.

The problem: Given a galaxy spectrum, calculate

1. **The current stellar mass**

2. **The star formation history**

3. **The metallicity distribution**

4. **The dust extinction**

If this sounds impossible, that is because it is.

An entire industry has grown up pretending that it is not, but that does not make it possible. It is not possible to estimate the errors in the current models, or even if they are vaguely applicable. There is some reassurance In that M/L ratios which can be checked with dynamics come out semi-reasonable if one uses current estimates for stellar mass, but that is a very crude check.

Stellar Spectral Synthesis, cont.

The problem sounds difficult; It SHOULD be straightforward if it is, in fact, mathematically well posed, which is not obvious (ie is there a unique solution). One can make SSPs (Simple Stellar populations) of any age and metal abundance, and a galaxy is a linear combination of these, so all one has to do is find the weights of these and evaluate the desired quantities. This is a deconvolution of sorts, and its mathematical nature is not clear. But worse is that the inputs to the problem are, if not garbage, at least seriously flawed, because we do NOT understand stellar evolution very well.

1. *We do not understand convection, semiconvection, convective overshoot, and these are important energy transport/mixing process at most stellar masses, but particularly in high-mass stars which produce most of the heavy elements.*

2. *We cannot make good cool model atmospheres, and much of the light from old populations comes from giants and AGB stars*

Stellar Spectral Synthesis, cont.

3. We do not understant either AGB evolution or the production of dust in AGB atmospheres. Most of the luminous AGB stars in the Galaxy are invisible at optical wavelengths, but this does not happen at lower metallicies. We do not understand why or where. 20% of the energy is produced by AGB stars in populations a few Gyr old.

4. Most stars are binaries, many close enough that they interact profoundly when they enter the giant branch. We understand next to nothing about binary evolution.

5. The most metal-rich cluster in the Galaxy that we know about, NGC6791, has a metallicity of at least twice solar. It has a BLUE horizontal branch, which it is not `supposed' to have. It has an anomalous population of white dwarfs, which seem to be younger than the cluster, but may just be helium white dwarfs instead of carbon, and may have been produced by direct evolution from the giant branch instead of the AGB. These metallicities are common in big ellipticals. We do not have a clue what is going on.

Stellar Spectral Synthesis, cont.

6. We do not understand the IMF in the solar neighborhood very well. There is a very religious view that it (whatever it is) is constant throughout the universe, for which there is not a shred of evidence. Now there is convincing evidence that it is NOT the same in the central parfs of big ellipticals as it is in the solar neighborhood; there are very many more cool M dwarfs than In the solar neighborhood per unit stellar mass.

7. We have no empirical evidence about how either very low-metallicity stars evolve (we see only old, low-mass ones) or how super-solar stars evolve (cf NGC6791), but we happily make models with both... and there is good evidence from 6791 that we do NOT understand.

8. The models currently have a single metallicity, but we know there is a distribution in the Galaxy, and havng a wide spread significantly modifies the spectrum. We cannot calculate what we expect, even if we knew what stars produce, because galaxies blow winds which carry away gas and metals, doubtless have infall of clean gas, and we understand neither.

Stellar Spectral Synthesis, cont.

I do not wish to be discouraging, but this is a field in which tiny changes in the inputs produce very large changes In the outputs, and we do not understand the inputs well enough to produce them accurately. I do not know what is believable in the current models, but it is strictly a garbage-in/garbage out situation with the answer to ANY detailed question. You asked, Masataka.