

# Optical design of a reflectance/Raman confocal microspectrometer

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## ABSTRACT

A miniaturized instrument for systematic planetary mineralogy is presented, and the optical design of the component parts is discussed. The instrument combines the following capabilities: wide field color imaging, confocal imaging at two different resolution/range levels, reflectance spectroscopy in the 400-2500 nm region with a resolution of 10 nm, and Raman spectroscopy over 4000  $\text{cm}^{-1}$  with an average resolution of 3.3  $\text{cm}^{-1}$ . The instrument can also serve as an expandable platform for adding fluorescence spectroscopy, or for examining samples from a distance of several meters while using the same spectrometer.

**Keywords:** optical design, confocal microscopy, planetary mineralogy, reflectance spectroscopy, Raman spectroscopy

## 1. INTRODUCTION

In-situ investigations of planetary materials suffer from a severe handicap: the lack of a human observer to interpret the observations and direct further action. An experimenter typically integrates and considers simultaneously far more data than can be transmitted from another planet to Earth-bound scientists; and of course, s/he does not have to deal with the time delay involved in such transmissions. For this reason, it is important for in-situ planetary instrumentation to provide unambiguous data and operate in an automated fashion as much as possible.

Various types of optical spectroscopy are used to characterize planetary materials, from minerals to organic molecules, but no particular spectroscopic method can claim absolute superiority in unambiguously identifying the broadest possible spectrum of materials. Rather, unambiguous data are more likely to come from correlative spectroscopy, where more than one spectroscopic modality is used to analyze the same sample.

Microscopic examination of rocks and soils yields clues to the geological history of a planet. Such examination needs to be carried out at a relatively fine spatial resolution of less than  $\sim 15 \mu\text{m}$  if it is to include single mineral grains or small deposits. The challenge then is to design an instrument with multiple imaging and spectroscopic capabilities that would be sufficiently compact for integration on a Mars-bound or similar rover. The present instrument combines a color microscopic imager with a 6x6 mm field, a confocal microscope with extended range/resolution, a reflectance spectrometer in the 400-2500 nm range, and a near IR Raman spectrometer, with the optional addition of a UV fluorescence spectrometer. All these instruments are tightly integrated in a compact package. Some optical design aspects of the instrument are presented here.

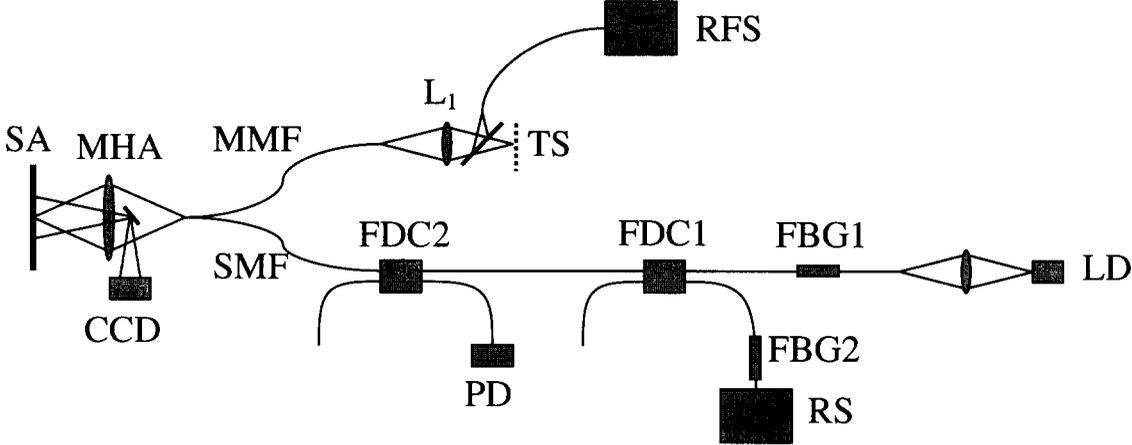
## 2. INSTRUMENT DESCRIPTION

The optical system schematic is shown in Fig. 1. The bottom portion is the Raman spectrometer system. This part has been described elsewhere,<sup>1</sup> with the exception of the Raman spectrometer module itself which is described below. The top part is the reflectance spectrometer portion, which is also described in further detail here, together with the microscope head assembly (MHA). Light is carried from the MHA to the spectrometers through optical fibers, as shown in Fig. 1. The system utilizes the same fiber for illuminating the sample and for collecting light from it. This allows us to position more than one fiber in the optical head without having to align separate illuminating and receiving fibers. It is also more robust against vibrations, thermal excursions, and other similar causes of post-launch misalignment. Not

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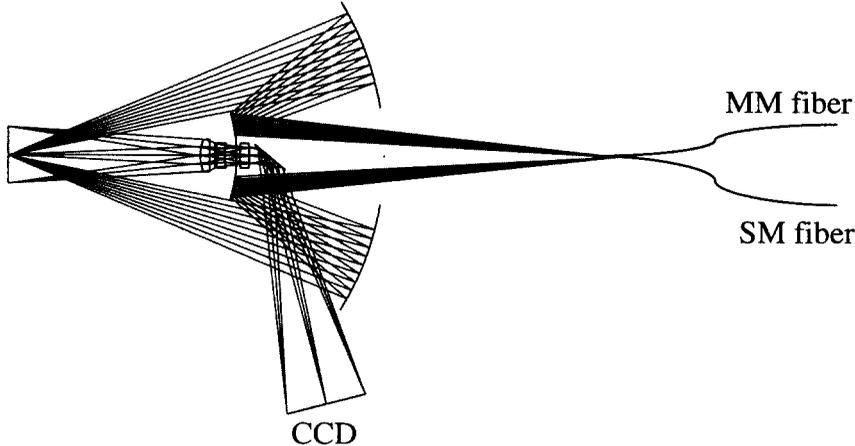
shown in the figure is a fiber switch, which chooses the fiber input to the reflectance spectrometer (RFS). Depending on requirements, two or three different fibers can be selected. For example, one more fiber can carry light from a remote optical head that scans the surrounding area searching for interesting targets. Or, if a UV-laser is added to excite the sample, a corresponding fiber could collect the fluorescence signal.



**Figure 1:** System schematic. SA: sample, MHA: microscope head assembly, MMF, SMF: multi/single mode fiber, TS: tungsten source, RFS: reflectance spectrometer, FDC1: fiber coupler 50-50%, FDC2 fiber coupler, 10-90%, FBG1, 2: fiber Bragg gratings, RS: Raman spectrometer, LD: laser diode, PD: photodiode.

**2.1 Microscope head assembly**

The microscope head combines a confocal part and a wide field lens, as shown in Fig. 2. Light is carried onto the sample by the illumination fiber and focused through the reflecting (Schwarzschild) objective. Light reflected/scattered from the objective is collected by the objective and is focused onto the same fiber from which it emerged. This return light is carried to the spectrometer for analysis. In order to provide context information and to be able to identify quickly sites of interest on the sample, a color CCD camera is integrated into the same head, by taking advantage of the obscuration of the reflecting objective. Illumination for the CCD camera is either ambient at daytime or through a ring of white LEDs during the night.



**Figure 2:** Optics of the microscope head assembly, scale 1.

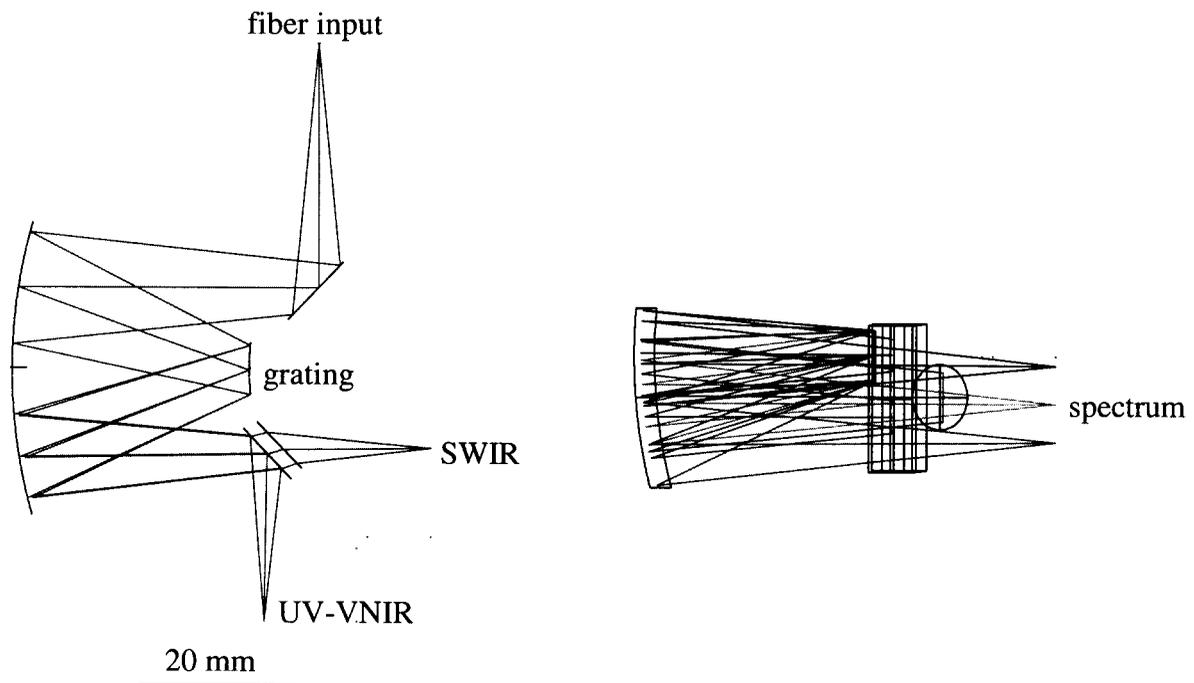
The Schwarzschild objective is a fairly standard design with two spherical surfaces and ~27% area obscuration. It demagnifies the fiber face onto the sample by a factor of 3.5, so it has NA = 0.35 on the sample side. It is fully diffraction-limited (Strehl ratio of 0.99 at 450 nm).

The camera objective is a Cooke triplet derivative, but the stop is placed on the last surface. This minimizes the diameter of the last lens as well as the size of the fold mirror and prevents vignetting of the rays within the reflective objective. All curvatures are fit to existing testplates from a single supplier and the front element is plano. This objective has a focal length of 15.8 mm, imaging a 6x6 mm area onto the Kodak CAI-1010 CCD array, which is approximately 9x9 mm, 1024x1024 pixels of 9 μm size. It is achromatized over the visible range and is fully diffraction-limited, although at ~f/15 the diffraction spread means that the resolution is effectively halved, to 512x512. This is not detrimental since the resulting sample resolution is perfectly adequate, and the increased depth of field allows tolerance in positioning and thermal drifts between the two lenses. The camera lens is focused using the confocal property of the fiber confocal portion. This is important for remote operation when one cannot rely on a human observer.

The use of both a single mode and a multimode fiber is advantageous, especially when rough, unprepared samples are to be examined. For this reason, the coarse resolution provided by the multimode fiber is just as useful as the finer one provided by the single mode fiber. Through the use of both fibers, the system provides the ability to scan larger volumes fast, as well as smaller volumes in high-resolution mode.

## 2.2 Spectrometers

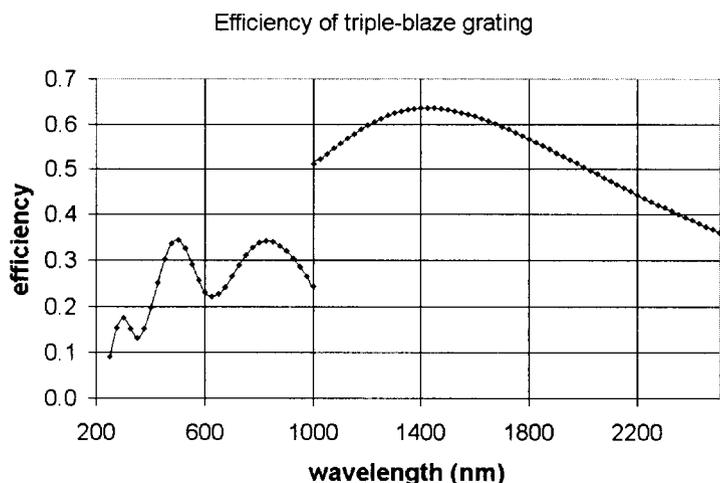
Since the requirements for reflectance spectroscopy are very different from those of Raman spectroscopy, it is necessary to use two different spectrometers. Both are convex grating designs.<sup>2,3</sup> The reflectance spectrometer is shown in Fig. 4. Its response can be extended to the UV as shown later. Otherwise, it operates over the 400-1000 (VNIR) and 1000-2500 nm (SWIR) range simultaneously, by utilizing both the first and second order of diffraction.



**Figure 4:** Miniature UV-VNIR-SWIR spectrometer, shown in actual size. A dichroic beamsplitter reflects wavelengths below 1000 nm and transmits those above. Left: y-z section, shows more clearly the size (spectrum into the page). Right: x-z section, shows the extent of the SWIR spectrum.

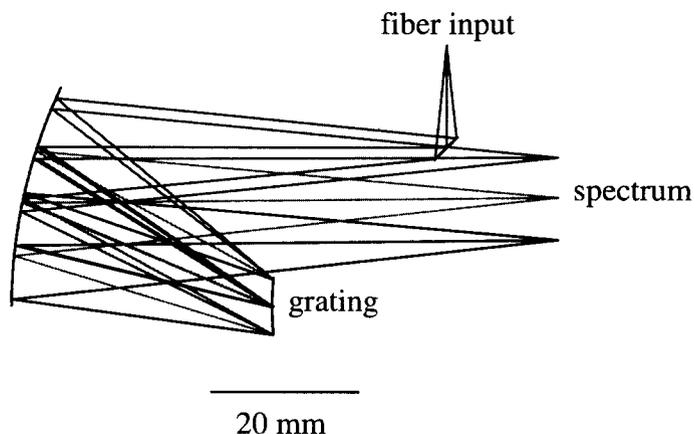
The fiber core diameter is 50  $\mu\text{m}$ , matched to the pixel size of the arrays. There is a trade between f-number and size, with the present design having been settled on after preliminary experiments indicating sufficient signal to noise performance even with an f-number of 5. The design can be operated at  $f/4$  without any changes, if the element apertures are appropriately sized. However, any change in the fiber NA must also be reflected in the design of the microscope head assembly.

The spectrometer is fully diffraction-limited throughout the visible and infrared range (minimum Strehl ratio of 0.89 at 400 nm). Both curved surfaces are spherical. The spectral sampling is 8 nm in the SWIR, and 4 nm in the VNIR (2<sup>nd</sup> order). The grating needed to cover the VNIR/SWIR band would be a dual-blaze design, similar to the one that has been demonstrated in ref. 4. A triple blaze would be necessary to cover the UV. The anticipated efficiency from such a grating is shown in Fig. 5.



**Figure 5.** Triple-blaze grating theoretical efficiency in the 2<sup>nd</sup> order (< 1000 nm) and in the first order (>1000 nm).

The Raman spectrometer ray trace is shown in Fig. 6. Both curved surfaces are spherical and nearly concentric. The small fold mirror does not vignette the return beam because it is out of the plane of the paper. As shown, the spectrometer has a total range of 4000  $\text{cm}^{-1}$  and an average resolution of 3.3  $\text{cm}^{-1}$  (realizing that it is linear in wavelength, not wavenumber). The f-number is 5, matched to that of the single mode fiber. The wavelength of operation is the near infrared, such that the excitation laser does not cause fluorescence in the minerals under examination.



**Figure 6.** Raman spectrometer ray trace.

In practice, the spectral range is expected to be limited by the fiber and couplers to more like  $2000 \text{ cm}^{-1}$ . A benchtop prototype spectrometer with this more limited range is under construction at present, utilizing stock lens and mirror substrates, with the limited curvature choices ultimately restricting image quality. With the original (or even testplated) curvatures, the spectrometer is diffraction-limited throughout (Strehl ratio  $>0.94$ ).

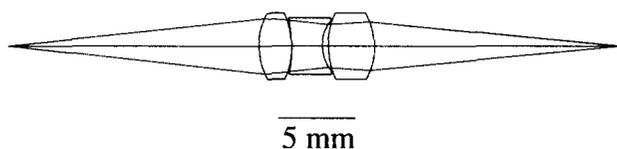
The grating for this spectrometer is fabricated through electron-beam lithography. It was made to operate in the second order, and has a pitch of  $1.7 \text{ }\mu\text{m}$  and a blaze angle of  $27^\circ$ . Preliminary results show very good characteristics, but a full report will await a future publication.

### 2.3 System considerations

When using the same fiber for the illumination as well as the signal path, reflections from the fiber end faces can overwhelm the signal. Thus all fibers must be terminated by polishing at an angle such that the return light is coupled into radiative modes. In this sense, restricting the MM fiber NA to that of the spectrometer helps ensure that small angles are needed. Appropriate fiber holders must be designed to pre-align the fiber axes in such a way that the chief rays from all fibers are aligned with the microscope lens axis.

The focusing lens ( $L_1$  in fig. 1) has an important function and an interesting design. First, it must transmit between 400-2500 nm (and even possibly down to  $\sim 270 \text{ nm}$  if UV-fluorescence is to be included), as well as minimize reflection losses. In the forward direction, image quality is irrelevant, since the tungsten filament is many times larger than the fiber diameter, and all one needs to ensure is that the Lagrange invariant of the fiber is overfilled. Therefore, a tilted plate beamsplitter can be inserted without affecting the light coupling efficiency (apart of course from the beamsplitting function), even though it has a significant detrimental effect on image quality. In the return direction, image quality is important because it might cause light loss upon coupling into the final fiber leading to the spectrometer. However, in this direction the beamsplitter only acts as a front-surface mirror, if the reflective facet is properly oriented. The lens must also be achromatic over the complete 400-2500 nm range.

The design is shown in Fig. 7. The lens operates at unity magnification. The two outer elements are  $\text{MgF}_2$  and the middle one is fused silica. These low index materials minimize reflection loss even without any coating. Additional features intended to facilitate fabrication are identical curvatures on the two convex lenses ( $c_1 = c_6$ ,  $c_2 = c_5$ ), all curves testplated to existing testplates from a single supplier, and center contact between the first and second elements. This facilitates positioning by allowing the distance between first and third element to be set with a spacer that can be easily fabricated.



**Figure 7:** Focusing lens ray trace, shown without beamsplitter.

Three elements are needed for achromatizing and correcting this lens over the wide wavelength range (400-2500 nm) using only low-index materials. The performance of the design is summarized in Table 1 in terms of encircled energy.

**TABLE 1**

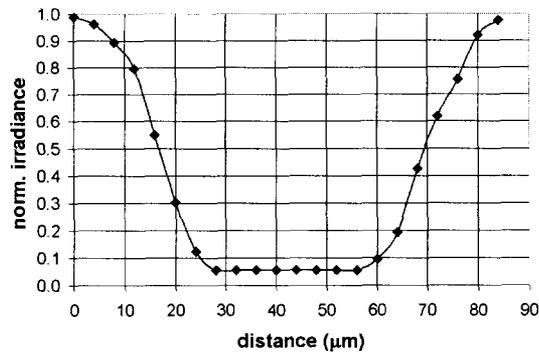
Wavelength (nm)	Encircled energy in $20 \text{ }\mu\text{m}$ radius	Diffraction limit for encircled energy
400	0.991	0.996
800	0.959	0.963
1200	0.930	0.942
2500	0.830	0.876

### 3. PRELIMINARY EXPERIMENTAL RESULTS

#### 3.1 Confocal fiber microscope

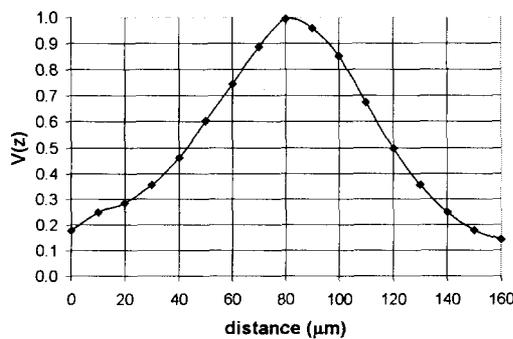
Preliminary experiments were performed with commercial refractive microscope objectives. Light from the illuminating fiber was collimated through a 5x or 10x objective, and focused onto the target through a 10x, 20x, or 40x objective. This arrangement was more convenient for inserting a beamsplitter in the collimated path and directing the light to a separate receiving fiber for comparison.

Figure 8 shows the lateral resolution of the multimode confocal microscope, obtained by scanning a commercial 50  $\mu\text{m}$  wide slit.



**Figure 8:** Image of a 50  $\mu\text{m}$  wide slit through the multimode confocal fiber microscope. The residual signal at the bottom is due to the reflectivity of the slit glass substrate. 4x (de)magnification. A  $\sim 16 \mu\text{m}$  edge spread is observed at the 10-90% points

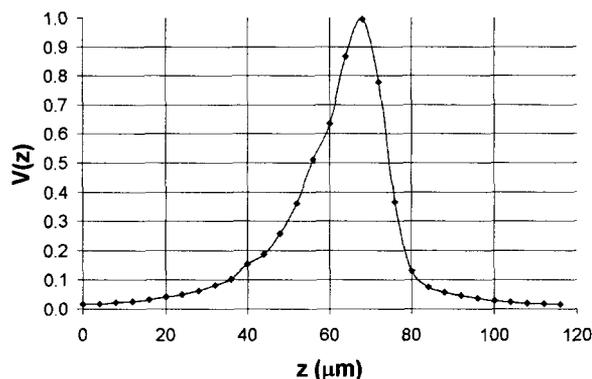
The vertical resolution is characteristic of the ability to acquire focus automatically and to perform 3-dimensional sectioning. It is shown in Fig. 9.



**Figure 9:** Light intensity through a receiving fiber of 50  $\mu\text{m}$  diameter as a function of focus. 4x (de)magnification, 0.35 objective NA. The vertical FWHM resolution shown is  $\sim 75 \mu\text{m}$ .

Using the single mode fiber, a much tighter vertical response can be obtained, as well as obviously better lateral resolution. This was tested using a 2x demagnification and an objective of 0.2 NA. The lateral resolution was as expected, approximately 4  $\mu\text{m}$  at the 90% and 10% points of an edge scan (the fiber modal field diameter is

approximately  $8 \mu\text{m}$  at  $830 \text{ nm}$ ). The vertical resolution, shown in Fig. 10, is also close to the theoretically expected for this numerical aperture. Vertical resolution is strongly dependent on the numerical aperture, and a significant improvement would be expected for a NA of 0.35. However, a more realistic demonstration would have to await fabrication of the Schwarzschild objective in order to account for the obscuration as well as reduce spherical aberration.



**Figure 10:** Light collected from a single mode fiber in a confocal arrangement, at  $830 \text{ nm}$ . A FWHM resolution of about  $20 \mu\text{m}$  is demonstrated for 0.2 NA. The asymmetry in the curve is likely due to spherical aberration in the commercial objectives, which were not corrected for the infinite conjugate arrangement used.

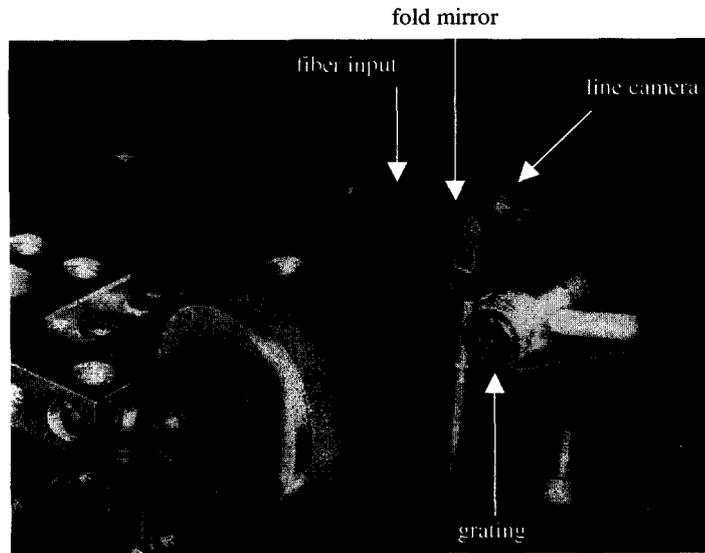
### 3.2 Raman spectrometer

The Raman spectrometer was assembled out of stock parts, with the grating being written on the convex face of a small planoconvex lens, using electron-beam lithography techniques outlined in ref. 5. A full report on the properties of this and similar designs will be published separately. A quick interferometric alignment method was developed consisting of the following steps: First, all three components are placed in their approximate locations within a few mm. The center of curvature of the concave mirror is then located interferometrically. The entire assembly is small enough to be seated on standard translation stages, which are used to move the focus of the interferometer beam to the location of the 3<sup>rd</sup> order of diffraction for the  $632.8 \text{ nm}$  wavelength (the second order is also potentially useable). A concave mirror placed on the input side of the spectrometer returns the beam to the interferometer. The wavefront error produced at that location is known from the optical design software, and the grating is adjusted in three directions until the desired wavefront error is achieved. The return mirror is then removed and replaced with a single mode fiber. Maximization of the light coupled into the fiber ensures that it is at the proper input location. At that point, the entire assembly can be removed from the interferometer. With this method, the spectrometer was aligned within approximately 1 hr.

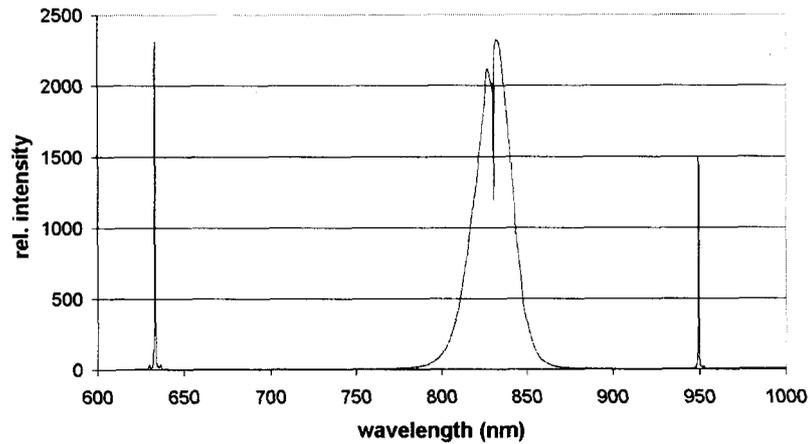
A picture of the spectrometer is shown in Fig. 11. Diffraction from the grating is discernible even in gray scale. Finally, figure 12 shows a sample spectrum. The two sharp lines shown arise from a HeNe laser, which is displayed in 2<sup>nd</sup> and 3<sup>rd</sup> order and is used to calibrate the wavelength scale. The broad curve is the spectrum of a superluminescent diode, and the notch near the middle is the reflection from a fiber Bragg grating.

## 4. CONCLUSIONS

This work has demonstrated the feasibility of several critical components of a combined fiber reflectance/Raman microspectrometer for in-situ planetary materials characterization. Miniature spectrometer modules have been designed and demonstrated. The instrument can serve as a platform for multiple imaging and spectroscopy modalities, necessary for complete and unambiguous characterization of materials.



**Figure 11:** Photograph of assembled spectrometer



**Figure 12 :** Sample spectra from the Raman spectrometer, showing HeNe laser in two orders (for calibration), as well as the superluminescent diode filtered by a fiber Bragg grating.

### ACKNOWLEDGMENTS

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