Progress Report on “Penn State Activities in the NASA GSFC Transmissive Microshutter Array Technology Development Program” (NASA NAG5-10617, 04/01/01-03/31/02)

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1. Project Description
This is a one year contract starting on April 1, 2001 to design the Rapid Infrared and Visible Multiple Object Spectrometer (RIVMOS) and its auxiliary dispersing elements, design and fabricate silicon grisms, and reduce testing data with silicon grisms. Here I report our progress made during the funding period.

2. Research and Development (4/01/01 – 03/31/02)

2.1 Design of RIVMOS
A wide field (6x6 arcmin²) Rapid Infrared-Visible Multi-Object Spectrometer (RIVMOS) has been designed as part of the Next Generation Space Telescope (NGST) development and new technology demonstration. The primary goal is to demonstrate that the microshutter arrays, currently being designed for the NGST Near Infrared Spectrometer (NIRSpec) as programmable 2D selection masks, can achieve the optical performance required for faint object imaging and spectroscopy. The optical design includes both reflective and refractive optics. The required optical performance is achieved for both multi-object spectroscopy and camera imaging over the entire field-of-view. The optical design consists of six optical subsystems including (1) an image relay consisting of a three-mirror anastigmat (TMA), (2) the microshutter assembly, (3) a triplet collimating optic, (4) a grism/filter assembly, (5) a pupil imaging optic, and (6) a five element telecentric camera design.

Figure 1. (Left) the layout of the optical design of RIVMOS imaging mode, it a three-mirror anastigmat (TMA), collimator, camera and detector. (Right) RMS spot diagrams within the 6x6 arcmin² FOV. The square box represents 2x2 InSb detector pixels (or 54x54 μm²).
The all-spherical optical design reduces construction costs and facilitates fabrication of the optical assembly while maintaining an encircled energy of 2 pixels within the FOV for wavelengths between 0.6 and 5.0 microns. The 512x512 microshutter array is located at the cold focal plane formed by the TMA, which provides the required spatial sampling on the microshutter array. The TMA relay also forms a cold pupil on its secondary where a cold pupil mask is located to reject extraneous thermal emissions from the telescope structure, such as the central obscuration. This design of the TMA is a novel variation on the classical Offner relay. The vertices are constrained in a fashion that gives diffraction-limited imagery at the microshutter, while using only spherical surfaces. Not only does this eliminate the need for aspherical surfaces, but also induced astigmatism is corrected which ultimately results in a simpler camera design.

Figure 1 shows the optical layout of the imaging mode in RIVMOS and its spot diagrams within the 6 arcmin FOV. More than 80% encircled energy is within 2×2 pixels. The spectroscopy will be conducted by inserting a grism on a filter wheel at the last pupil location. Figure 2 shows the optical layout of the spectroscopy mode with R = 1000 and its spot diagrams within the 1k×1k detector. More than 80% encircled energy is within 2×2 pixels. Therefore, our design for imaging and spectroscopy meets the requirement for demonstrating the capability of the microshutter array for scientific observations.

2.2 Development of New Processes for Making High Quality Silicon Gratings:

(a). TMAH +AP process
Late in 2001, we developed a new etching process with Tetramethyl ammonium hydroxide (TMAH), ammonium persulfate (AP) and a thin silicon dioxide mask (~ 100 nm thickness) and
post-processing process, which helps us to significantly reduce grating surface roughness. By the end of the year, we were able to reach ~15 nm rms roughness for the silicon wafer gratings with

10×10 mm² etched area and 66 μm grooves. This roughness is a factor of 2 times lower than that in November 2001. Scanning electron micrograph (SEM) pictures of etched gratings with and without AP processes are shown in Figure 3. The grating with the AP process has much smoother grating facet surfaces and less defects. The grating with the AP process represents our first significant improvement in grating surface quality with the NASA support. For a direct comparison, we have also shown a commercially made grating surface under a 100x optical microscope. Visually, there are many uneven grooves which are caused by the replication process and also transfer of defects in the master grating made through mechanical ruling, the traditional grating fabrication technique. Our grating made by the TMAH and AP chemical etching process shows very organized groove structures and also smoother grating surfaces.

Figure 3. The etched silicon wafer gratings with the TMAH process and without AP (left) and with AP dose (middle). On the right, a fused-silica transmission grating with 10 μm grooves, commercially made by Richardson grating company, is shown for comparison. Irregularity and surface roughness can be clearly seen in this commercial grating.

Figure 4. Progression of reduced roughness with increased amounts of ammonium persulfate.
Quantitative measurements of these etched gratings with and without AP processes shown in Figure 4 indicate roughness reduction depends on the dose of the AP in the TMAH etchant. The total improvement in surface roughness can reach ~ 32%, which is being reported in a paper (McDavitt, Ge et al. 2002 in preparation). In addition, as shown in Figure 3, defects on the grating surfaces are significantly reduced with the AP process. Our examination under a 10x optical microscope shows that visible defects with typical dimension of ~ a few microns or larger have been reduced to less than 1 per cm² from originally more than 100 per cm² a year ago.

(b). Post-processing
Further improvement in surface roughness has also been observed in our post-processing. This process involves application of a thin oxide layer, usually ~ 20 nm to finished grating surfaces and etching away of the oxide layer with buffled HF (BHF). This takes advantage of different oxide growth rate at different location of an uneven silicon surface. As illustrated in Figure 5, the rms surface roughness has been further reduced by ~ 25% after a single post-processing run (Bernecker, Ge et al. 2002 in preparation). The lowest rms toughness we achieved with a combination of the AP and the post processing is about 15 nm. We have also found that the average surface roughness increased slightly after two runs. In addition, grating surface becomes much rougher after three post-processing runs. Upon investigation, it was discovered that pits had formed in the three run gratings. The pits on the Czechralski (CZ) wafers three run samples ranged in size from 0.2-0.3µm and 2.5-3µm. Those on the float zone (FZ) wafers three run samples ranged in size from 0.5-1µm. Our conclusion is the single run of post-processing run gives the smoothest grating surface.

2.3 Optical Performance of the Etched Silicon Gratings

(a). Precise surface roughness measurements by the Atomic Force Microscope (AFM)
The RMS surface roughness reported values above were from the measurements with a profilometer at the Penn State Nanofab. Since the stylus of the profilometer has a resolution of ~ 10 µm, the measurements is a convolution of the stylus sensitivity and grating surface roughness. These results can only represent estimated surface quality over a large scale (typically a few hundreds of microns). A much better way to evaluate the surface roughness, especially on the scale of ~ µm is through an atomic force microscope (AFM). Figure 6 shows comparison of AFM surface roughness among etched gratings over a period of 8 months. These measurements were conducted at the Penn State Material Research Institute. It is very clear that the grating surface gets much smoother in June 2002. In November 2001, the typical RMS surface roughness for the best etched silicon gratings with the TMAH and AP process over ~ 1 µm scale
is 9 nm. In March 2002, the RMS surface roughness for the best etched gratings is down to 3 nm. In June 2002, the rms roughness is reduced to 0.9 nm. The surface roughness for these gratings is lower than that for the HST mirror, 12 nm.

![November 2001](image1) ![March 2002](image2) ![June 2002](image3)

Figure 6. Atomic Force Microscope scanning of the best etched silicon gratings in November 2001, March 2002 and June 2002. The RMS surface roughness over 2 μm in randomly chosen grating surfaces are 9 nm, 3 nm and 0.9 nm from the right to the left, respectively.

(b). Integrated scattered light measurements
An etched grating with ~ 15 nm rms roughness has been evaluated with our optical spectrograph. The total measured integrated scatter at 0.633 μm is less than 1% scatter as shown in Figure 7. This level of scatter is already a factor of three times better than that of a commercial 23.2 l/mm echelle grating measured Kuzmenko & Ciarlo in 1998. It is also a factor of ~ 10 times better than previous results by other groups (Kuzmenko et al. 1998; Keller et al. 2000).

(c). Wavefront quality of etched gratings
Wavefront quality of the etched gratings has been evaluated by a Zygo interferometer at Lawrence Livermore National Lab through collaborating with Dr. P. Kuzmenko. Figure 8 shows the wavefront over 10×10 mm² etched grating area at 0.6328 μm in reflection. The RMS wavefront distortion is 0.035 waves, indicating diffraction-limited performance once the grating is operated in both immersed reflection and transmission. The high wavefront quality was achieved through using very thin oxide grating mask layer with typical thickness of 1000 Å. Our previous study shows that sharp mask pattern is the critical step for maintaining wavefront quality (Ge et al. 2002). This is why etched gratings with a plasma etching have better quality than those with wet etching. However, it is challenging to make masks on thick silicon substrates in the plasma chamber. Our thin mask layer made through a wet processing can maintain the grating pattern as sharp as those plasma-etched
grating mask, resulting in high wavefront quality. Maintaining high wavefront quality is critical for achieving the highest dispersion power provided by silicon immersion gratings.

2.4 Silicon Grisms Made through New Processes
The new etching technique, TMAH + AP process, has been applied in fabricating new generation silicon grisms. Figure 9 shows etched gratings on two silicon substrates with 100 mm in diameter and 20 mm thickness. One has 16 gratings. Each grating has 10×10 mm$^2$ etched area, a 54.7 deg blaze angle and 66 μm period grating grooves. The other has 4 gratings. Each has 25×25 mm$^2$ etched area, a 54.7 blaze angle, and 13 μm grating grooves. The surface roughness of one of the gratings with 66 μm grooves has been measured by the profilometer and shows ~15 nm rms roughness. These gratings have been cut and polished by SPEC Precision Optics Inc. in Tennessee. Figure 10 shows 4 finished grisms installed in mechanical mounts. The three smaller grisms are for testing and observing with our Penn State near IR Imager and Spectrograph (PIRIS). The larger one is for testing and observing at the Arizona Imager and Echelle Spectrograph (ARIES) at the MMT 6.5-m telescope. Recent lab testing shows that the integrated light levels from silicon grisms has the total integrated scattered light level of about 1% in the entire near-IR, 10 times better than our prototype made at LLNL in 2000.

2.5 Grating Performance Modeling
In addition to developing new grating fabrication processes, we have also conducted grating efficiency modeling using commercially available G-solver software in 2002. Figure 11 shows design of a silicon grism with 7.3 μm grooves and 22 deg
blaze in the J, H, K, L and M bands for RIVMOS. The grating efficiency is also shown in the Figure. The grism is operated in the first order at the M band, the 2nd order for the L band, the 3rd order for the K band, the 4th order for the H band and 5th order for the J band. This modeling has assumed that no scattered light loss. Without anti-reflection coating, the peak efficiency is about 60% for all these bands. With a single layer silicon nitride coating, the peak efficiency can reach 80%, which is beyond any of commercially available low resolution grisms (Rayner 1998; about 45% efficiency for the KRS-5 grisms in the Gemini NIRI camera, Simons 2001, private communications). This grism will provide \( R = 2000 \) in 1.2 – 5.5 \( \mu \)m with RIVMOS (Ge et al. 2002). We are about to purchase thick silicon substrates and make these grisms in 2003.

2.6 Silicon Grism Spectral Data Reduction

The cross-dispersed echelle spectra taken with our second-generation silicon grisms at the Lick Observatory were reduced and analyzed by my team in the Spring 2002. Data analysis shows that \( \text{Br}^\gamma \) emission lines are associated with both T Tauri N and S components (Figure 12), similar to what have been found by the Keck AO IR spectroscopy (Duchene et al. 2002; Ge et al. 2002). The spectrum of BD+65 1638 shows an enormous broad \( \text{Br}^\gamma \) absorption with a FWHM of 550 ± 50 km/s (~ 90% of stellar brake-up velocity) (Figure 13), indicating this star is perhaps undergoing an early phase of slowing the stellar rotation down to become a normal Be star (Ge et al. 2002; Chakraborty et al. 2002). These observations demonstrate the scientific capabilities of silicon grisms. Two scientific papers are being written to report the new scientific discoveries with the silicon grisms.
2.7 Technical and Scientific Publications

The following list is the papers or presentation published in the scientific journals and proceedings which are related to this project:

Published:
- McDavitt, D., Ge, J., Bernecker, J., & Miller, S., 2001, “Improved Results in the Development of Large Silicon Grisms using New Techniques,” BAAS, 199, 10207

In press:

Drafts to be submitted:
- Bernecker, J., Ge, J., Miller, S., & McDavitt, D., 2002, “A Post-processing Technique for Improving Si {111} Surface Roughness on Silicon Gratings,” to be submitted to Sensor and Actuator