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RAMAN spectrometer: development of SPU FM based on enhanced qualification model for Exomars 2020

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ABSTRACT

The Raman Laser Spectrometer (RLS) is one of the Pasteur Payload instruments within the ESA's ExoMars mission. The RLS instrument scientific goal consists of perform in-situ Raman spectroscopy over different organic and mineral powder samples of the Mars subsoil. It consists of three main units: SPU (Spectrometer Unit), iOH (Internal Optical Head), ICEU (Instrument Control and Excitation Unit) which are interconnected by an optical and electrical harnesses (OH and EH).

The SPU is one of the most critical units of the RLS instrument. The Engineering Qualification Model (EQM) unit has been already delivered after a proper qualified campaign in a very demanding environment with very restrictive design constraints, including Planetary Protection requirements. Also, a complete set of functional tests had been carried out under representative environment, simulating not only Mars rover's laboratory conditions (thermal range and pressure), but also the cruise phase. Previously, an exhaustive qualification campaign was developed with two different purposes: to mitigate the risks associated to new optical elements included in the design and without space heritage; and to obtain a detailed comprehension of their behaviour under Mars conditions for facing the Flight Model (FM) optical design with guarantee of success.

EQM results were successful in terms of Engineering, and a SWaP-optimized system had been reached. The acquired knowledge of that model has been used to implement little improvements into SPU FM for acceptance. For operations, a big amelioration has been the reduction of the image ROI on the Charge-Coupled Device (CCD) after the improving of the alignment of the inclination degree of the image plane on CCD under the tightly integration constrains, letting to download the minimum necessary data bytes. These improvements achieved by a proper analysis of the image on the SPU CCD will allow to evaluate far better the Raman spectrum effects.

SPU FM Mechanical, Thermal-Vacuum campaign has been already finished in order to accept for flight the current unit which will be already completed and "flight qualified" at RLS system level before the congress. If everything continues on this way, the desired Technology Readiness level, TRL 8 maturity level, will be reported during the following text.

Keywords: Space optics, Exomars, Raman Spectrometry, Opto-mechanical design.

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1. INTRODUCTION

Space observation and exploration missions are very demanded in the aerospace industry nowadays. In this context, the program ExoMars (Exobiology on Mars) is bound to become one of the most important planetary missions in the upcoming years. ExoMars is a joint programme of the European and the Russian space agencies. The 2020 robotic planetary mission is being instrumentalized to drill down up to 2m and take Martian subsoil samples which will be crushed into a fine powder. Applying Raman Spectroscopy to those samples, RLS [1] pretends to characterize the mineral phases produced by water-related processes and to characterize water/geochemical environment as a function of depth in the shallow subsurface. Also, RLS will attempt to identify the mineral products, indicators of biologic activities; to detect organic compounds and search for signs of life.

Figure 1. RLS functional Flow.

1.1 How does it works?

The RLS instrument working flow is depicted in Fig. 1 and consists of three main units: the iOH, the SPU and the ICEU; which are interconnected by optical fibres and electrical harness.

The powdered sample will be illuminated by a 532nm laser light coming from the pump diode housed at the ICEU by means of the iOH excitation optical path. The obtained Raman reflected signal will be properly filtered by the iOH collection optical path and delivered (through the reception fibre) to the SPU. At the SPU, the Raman signal will be collimated to be dispersed through the transmission diffraction grating and focused by the collector onto the CCD. The generated image will be sent back to the ICEU FEE (Front End Electronics) and processed before routing to the Rover for downlink.

2. SPU OVERVIEW

One of the most critical Units of the RLS instrument is the SPU [2] that performs spectroscopy technique and operates in a very demanding Martian environment (radiation, temperature, dust, etc.) with very restrictive design constraints of schedule, Size, Weight and Power (SWaP). It is a small optical instrument capable to cope with 0.12–0.15nm/pixel of spectral resolution and withstand with the Martian environment (operative temperature conditions: from -40°C to 6.3°C). The design selected is based on a single transmissive holographic diffraction grating especially designed to actuate as the dispersion element.

The main goal of the design of the SPU is not only to reach the scientific requirements as spectral resolution and SNR; but also to reach them in a reduced lightweight (844.60g for the EQM vs 828.21g for FM) and maintaining performances in the operative thermal range with low power consumption.

Figure 2. SPU FM Design (main body transparent).

The SPU represented above is mainly composed by:

- Optical Fibre Entrance Assembly: with a 50 microns core multimode fibre is housed on a MiniAVIM connector through a receptacle to rout the reception signal from the iOH to the SPU.
- Collimator: This optical subsystem collects the light supplied by the fibre and collimates it to reach the diffraction Grating Assembly (GA) element.
- Main body. It is the main structural housing and holds inside the GA, composed by a transmission grating that disperses spectrally the flux produced by the collimator subsystem. The grating is the key element of the SPU and the GA has been re-designed from the EQM to FM in order to avoid the risk of get some micro-cracks observed near the Titanium-glass contact areas after the qualification mechanical tests [3].
- Collector: This optical subsystem collects the energy dispersed through the grating and focuses it onto the detector located inside the FPA.
- SPU Focal Plane Assembly (FPA): contains the Detector Assembly (DA). The DA has a thermally controlled two-dimensional CCD array. The CCD detector provided from e2v technologies was previously fully qualified at SPU unit level by Leicester University.

3. SPU DESIGN

3.1 Optical Design

The SPU EQM and FM have the same optical concept design (Figure 3) and it was performed by INTA Optical Space Engineering Lab [4].

Figure 3. SPU optical ray trace and 3D-design

SPU collimator brings the light collimated from the MiniAVIM (multimode fibre with 50 microns core) receptacle to the Volume Phase Holographic Grating (VPHG) which disperses the incoming light with an efficiency up to 70% in the whole spectral range (533-676nm). Finally, the collector focus the light onto the 2-dimension array CCD. The VPHGs work at angles of incidence and diffraction of 32.84° and are recorded on dichromated gelatine.

Other optical performances and characteristics are displayed with more detail in the Results Section (Sec. 5).

3.2 Thermomechanical Design

SPU is composed by an external Ti6Al4V structure (receptacle, collimator barrel, main body, cover, collector barrel, and FPA) and by internal subunits as the GA, retaining rings and spacers to fix optical lenses, manufactured with the same titanium. This Ti blocks (see Fig. 4) have a relative low thermal conductivity and a Coefficient of Thermal Expansion (CTE) very similar to the SPU optical components so it is the ideal material to maintain a controlled and uniform temperature along the SPU optical components due to the absence of dissipative components.

Figure 4. FM Spectrometer Sub-units and whole Unit Titanium structures detailed.

SPU is sensitive both to operating thermal range and to the thermal stability along the whole Raman operation. To get these thermal requirements in these items, several thermal analyses had been performed to guarantee that different components are within their allowable range of temperatures and they reach optimum temperatures to assure best performances. Also, it allows to verify that the required interface heat fluxes and electrical heat power do not exceed the specified values for SPU operating conditions. Thermal design concept assures the good performance of some critical components by means of a thermal active control in operation mode and in non-operational temperatures. Two items are hosted within the SPU with special thermal caution:

1. The optical elements are sensitive to alignment mismatching due to temperature variations and gradients (or both of them). For hence, the selection of glass was done to assure the behaviour of the instrument in the operative thermal range. Optical materials for the lenses were selected taking into account the impact on the chromatization and thermalization of the Unit. So, the ideal selection case would be pairs of glass (doublets) that compensate for both aberrations, chromaticity and sensitivity of temperature changes. In a first approximation, the change in the focal length of the doublets was calculated with the wavelength and the temperature following the classical procedure [5] to carry out this compensation, using the equation (1):

$$V_A \cdot \varepsilon_A = V_B \cdot \varepsilon_B \quad (1)$$

where V is the Abbe number for each doublet lens and ε is given by

$$\varepsilon = \left(\frac{1}{(n-1)} \cdot \frac{dn}{dT} \right) - \alpha \quad (2)$$

where α is the thermal coefficient of a single lens.

2. The CCD requires a specific cold condition (-10°C) to provide the optimal performance. An internal temperature control of the CCD is carried out by a Thermo-Electrical Cooler (TEC) in both models. The temperature stability is assured by conduction through the SPU stands and the thermal strap interfaces with the Rover. Current SPU design foresees the use of a thermal strap to exchange the heat dissipated in the hot side of the TEC during CCD operation.

It was included heaters for the active thermal regulation for EQM model but in FM all those heaters were removed due to the impossibility of controlling them by the ICEU.

A set of Pt-1000 sensor thermistors were fixed in different representative spots to monitored all this thermal control and thus to maintain the required thermal environment for proper operations of SPU taking into account different Mars environment conditions.

3.3 Optomechanical Design

As explained before, the design of the SPU that withstands with the Martian environment is a very demanding optical effort to get an adequate strength and ensure high dimensional stability to maintain optical alignment. This is another reason to compose SPU by titanium Ti6Al4V for the external structure material of the main assemblies: collimator barrel, main body, cover, collector barrel and FPA. Its low density lets to support tight overall mass budget (< 900g) and high stiffness to meet minimum launch frequency.

Titanium turned out to be also the best choice for fix the internal optical structures (See shadow elements of Fig 5) as the diffraction GA, optical fibre receptacle, internal lens retaining rings and spacers.

Figure 5. SPU optomechanical layout and "building block"

In addition, the internal parts of SPU contain surfaces with high emissivity in order to reduce straylight levels. This high emissivity will increase the radiative coupling between the components, helping to homogenize the temperature of unit.

There are several glass to metal contacts in the SPU design. Those contacts appear in collimator, grating and collector subsystems, with different implemented solutions:

- For the collimator, the design used consists in encasing the two lens doublets in the barrel, leaned on one internal face of the barrel and separated by a spacer. In the other side, the assembly is blocked by an internal low pitch nut designed specifically for this joint. This nut also allows a right centring of the optical assembly. The lenses are positioned inside the barrel using an H7- g6 tolerance. Additionally, they have been glued using MAPSIL® QS1123 silicone with the appropriate glass and metal primers.

Figure 6. SPU collimator and collector subsystems internal layout

- In the collector, the glass to metal contacts are similar to those used in the collimator but in this case three nuts and one spacer are used. The lenses lean in one internal Titanium flat face (or in the flat side of the spacer) and are

blocked by a nut in the external side. A 0.6Nm torque is used when mounting the nuts, which have rounded edges in the area with direct contact with the lenses.

- Concerning the diffraction grating (Fig. 7), it is a VPHG recorded on dichromatic gelatin and embedded between two fused silica glasses covered by an antireflective layer and glued with a NOA61 space compatible adhesive. It has 1800 l/mm and has been manufactured for the wavelength of 603nm. Due to the limited information provided by the supplier it was required a prior characterization of the device to get the optical behavior in space environment.

For EQM it was initially fixed in its plane by three cylindrical BeCu springs and three lobes in the titanium GA support. Out of plane it was fixed by three thin titanium clamps (holders). The tightening of the diffraction grating was controlled using peelable shims. Those shims also absorbed the variations in dimensions of the diffraction gratings due to manufacturing processes

Figure 7. Grating assembly (initial design) and the Volume Phase Holographic Grating (VPHG).

For FM, the novel introduction of Vespel® SP1 shims as intermediate ad-hoc material to avoid direct contact between metal and fused silica not only let us to get an improving of the grating housing but also to mitigate the crush risk. This material has a low outgassing rate (Tab. 1) and despite the rates were slightly higher than the recommended for optical instruments, it fits with the optical and bioburden [6] [7] [8] requirements of the mission and due to the reduced exposed surface of the introduced parts.

Table 1. Margins of the molecular contamination.

	%RML	%TML	%CVCMM
Optical requirement	<0.1		<0.01
ESA requirement	<1		<0.1
Vespel® SP1	0.36	1.09/0.858	0

4. EXPERIMENTAL EQM QUALIFICATION AND FM ACCEPTANCE CAMPAIGNS

RLS EQM passed a tight qualification test campaign allowing to verify the opto-thermo-mechanical designs within a very demanding environment (vacuum and partially simulated Martian atmosphere). These tests have the aim to check critical aspects of its functionalities not only at room conditions but also at relevant environmental conditions. This campaign took place at the end of 2016 and the first half of 2017 and proved the functionality and good performances of the instrument in terms of spectra acquisition. The process has also proved the qualification of the different optical subsystems and their main optics performances.

After the qualification test campaign, the Critical Design Review (CDR) performed in July 2017 was successfully passed. The FM production, AIV activities and the acceptance test campaign have been concluded at the beginning of this year with the results exposed in the next section.

All SPU EQM functional objectives were reached before, during and after tests campaigns.

5. SPU FM RESULTS

The SPU EQM and FM have been designed, manufactured controlled, integrated, optically characterized and tested by INTA engineering with the support of Leicester University engineering in all the issues related with the CCD integration, adjustment, calibration and test.

A very restrictive opto and thermo-mechanical designs have been demonstrated as proper for the AIV on-ground process and its further working conditions, in compliance with the stringent planetary protection (PP) [6], Cleanliness and Contamination Control (C&CC), and performance requirements [7] according to the Committee for Outer Space Research (COSPAR) category IV recommendations to prevent the contamination of Mars in terms of molecular, particular and especially in bioburden contamination.

After the in-lab conditions integration and attending to the optical performance checks carried out before, during and after AIT campaign can be concluded to be successfully passed as reported on the table 2 of this manuscript.

Table 2. Comparison between EQM and FM test campaign.

SPU Linear dispersion (nm/mm)					
<u>Spectral Zone</u>		<u>EQM</u>	<u>FM Tamb(23°C)</u>	<u>Relevant (-20°C)</u>	<u>(Theoretical)</u>
Large wavelengths	670 nm	7.9±0.8	10.3±1.0	8±1	(7.6±0.8)
Mid wavelengths	600 nm	9.1±0.8	8.3±1.0	10±1	(9.6±0.8)
Short wavelengths	530 nm	9.9±0.8	8.3±1.0	11±2	(9.9±0.8)
SPU Image size (spectral; spatial) (pixel ±1)					
<u>Spectral Zone</u>		<u>EQM</u>	<u>FM Tamb(23°C)</u>	<u>Relevant (-20°C)</u>	<u>(Theoretical)</u>
Large wavelengths	670 nm	10;3	8;3	7;3	10;3
Mid wavelengths	600 nm	9;3	7;3	6;3	8;3
Short wavelengths	530 nm	8;3	6;3	6;3	8;3

SPU EQM and FM functional tests consist of verifying these optical and electro-optics performances by means of spectral resolution and signal to noise ratio (SNR) in room conditions and relevant ambient (Mars conditions) and through the optical fibre image (Image size) on the focal plane it is determined those performances.

The digital SNR measurement is calculated through the relation of the photons coming from a monochromatic light and the photons of CCD noise. The signal depends on the number of pixels occupied by the image of the optical fibre. The SPU SNR provides the knowledge about how good is a Raman spectrum.

The spectral resolution is calculated through the linear dispersion measured between two wavelengths separate less than 0.2nm depending on the spectral range zone.

The CCD position and image size of the optical fibre always fit before and after environmental campaign. Thanks to a better performances of the EGSE used in EQM, a proper analysis of the image on the CCD could be done for FM, so the SPU FM lineal dispersion and the variations of the optical fibre image size and position in relevant environmental (vacuum and -20°C) improved the EQM values inside uncertainty of measurement margins. It allowed to evaluate far better the Raman spectrum effects. The grating assembly modification allows to improve the inclination degree of the image plane on CCD reducing the number of rows occupied by it (from 13 to 4) letting to get the minimum possible ROI which will let to download the least necessary data bytes for the operators in the future.

The SPU has a 0.7x magnification which translates the optical fibre to the image plane of the detector, reaching the resolution necessary to resolve the Raman peaks separated by 0.17-0.37nm, depending on the area of the visible spectral range. The quality of the instrument was evaluated and verified in terms of MTF (Figure 8) and impact diagram (Figure 9) [9].

Figure 8. MTF curves for the extreme and central wavelengths in the spectral working range of the spectrometer.

Figure 9. Spot diagram for the extreme and central wavelengths in the spectral working range of the SPU. The central box represents the size of a pixel, 15µm.

So, the materials selection ensure the performance of the instrument in terms of resolution and SNR in the mission's space environment.

The following figure shows the image in the CCD of the entire spectral working range of the spectrometer and the spectrum of a Ne calibration lamp, both images taken with the SPU FM.

Figure 10. SPU FM images with white light (left) and Ne calibration (right) lamps .

All the spectral and spatial performances are verified and confirm the adequacy of the design. SPU FM has reached the main optical performances predictions from EQM results made in [10] as Table 3 shows:

Table 3: FM and Current EQM main SPU Optical performances and characteristics.

	SPU FM	SPU EQM
Collimator Focal length	69.53mm	67.8mm
Collector Focal length	48.77mm	47.2mm
Magnification	1:07	1:07
Numerical Aperture	0.22	0.22
Optical Fibre Diameter	50 μm	50 μm
Image Optical Fibre	35 μm	35 μm
Pixel size	15 μm	15 μm
Spectral Range	Should be (533-676)nm Shall be (535-675)nm	(533-676)nm
Extension CCD (pixels)	~1200	~1170
Spectral Resolution	0.12-0.15 nm/pixel	0.12-0.15 nm/pixel
Lineal Dispersion	8-10 nm/mm	8-10 nm/mm
Throughput	>0.35 (required)	>0.50

6. CONCLUSIONS

SPU is a very demanding and challenge Unit which has been successfully qualified for ExoMars2020 under tight environmental conditions (ambient, cruise phase and operation in Mars). After the EQM campaign at Unit level and at Instrument level results have been used as feedback for enhancement of SPU FM with minor changes of the design. So, the FM of the SPU has been re-designed, manufactured, tested and delivered to the Instrument for RLS FM test and further delivery to ESA to achieving a TRL of 8.

Although these plans have been developed for a mission to Mars, the protocol and procedure applied are valid for any planetary exploration mission.

It should be also remarked that this SPU has demonstrated to be as flexible as needed due to several changes in the mission along the last years.

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