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Laboratory spectroscopic ellipsometer for bidirectional reflectance of planetary surfaces

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ABSTRACT

Reflectance spectroscopy is a technique widely used to investigate the composition and physical properties of a surface. The spectro-polarimetry adds the investigation of the polarimetric state of the light, while keeping the spectroscopy dependency. This technique is currently limited for the characterization of the surface, but can bring another clue on the composition and physical properties of the studied surface. We present here the design of a novel ellipsometer, optimized for the investigation of the polarization state of the light reflected by a granular surface. This instrument is able to measure the linear and circular components of the polarization over a wide spectral range from the ultraviolet to near-infrared and at a wide choice of geometrical configuration. The wide spectral range is achieved with the use of a photoelastic modulator acting like a retardance waveplate over the whole working range. Spectro-polarimetric investigations of terrestrial and extra-terrestrial samples will have application to mineralogical investigations, planetary surface explorations, and improve our understanding of the Solar System.

Keywords: Spectro-polarimetry, Ellipsometer, Bidirectional reflectance, Planetary surfaces

1. INTRODUCTION

Reflectance spectroscopy is widely used to characterize the composition and physical properties of a surface and remote sensing spectroscopic instruments are onboard a majority of planetary-targeting spacecrafts. The amount of reflectance, the spectral slope, as well as the detection of absorption features are traces of the various endmembers, the granular state and porosity of the surface, as well as clues on the temperature and alteration history of the surface. However, data retrieved from spacecrafts need to be coupled to laboratory investigations to assess the precise composition and properties by finding a configuration generating data matching the spacecraft's observations. Spectro-polarimetry proposes to couple the spectroscopic characterization of the surface with the measurement of the polarimetric state of the reflected light. Such techniques can add further information about the target, improving our current characterization capabilities.

Spectro-polarimetry applied to surface characterization is currently in its early-state and requires a full exploration of the capabilities of such techniques. This requires instruments capable of investigating the polarimetric state over a spectral range matching these of the planetary missions, assessing the effect of the directions of illumination and observation on the polarization of the reflected light, and presenting a spectral resolution fine enough to characterize the polarimetric behavior in absorption features. We present here the design of a home-made bidirectional reflectance spectro-gonio ellipsometer, optimized for the spectro-polarimetric studies of the light reflected off mineralogical samples, with applications to planetary research.

2. SCIENTIFIC GOALS

2.1 Characterization of the polarimetric state

Visible spectro-polarimetric observations of primitive asteroids demonstrated the variety of polarimetric signals due to the heterogeneous composition of the target^{1,2}, emphasizing the link between the surface properties and the excess of polarization of the reflected light. Previous laboratory experimentations showed the dependence of the reflected polarization of icy samples on the grain size distribution³. However, observational spectro-polarimetric studies are still limited to the investigation of the linear component of the polarization and in the visible spectral range. Recent

experimental studies focus on the circular polarization induced by life biosignatures^{4,5}. Spectro-polarimetric observations of vegetation scenes present, in addition to the spectroscopic absorption, an excess in linear polarization due to the reflectance on the surface and to the atmospheric constituents such as O₂, plus an amount of circular polarization tracing the presence of homochiral biotic molecules⁴. These studies also point out the small amount of circular polarization to be detected compared to the linear polarization for surface analysis. In the visible range, the amount of circular polarization measured in biosignatures can be lower than 0.5%, while the linear branch can be of several percent. This placed a major constraint on the detection and measurement capabilities of laboratory instruments, strengthening the difficulty of the full characterization of the polarization of the reflected light for surface analysis. Moreover, additional laboratory investigations are necessary to characterize the contributions of gases and subtract them to spectro-polarimetric observations of the surface of a planetary body presenting an atmosphere.

2.2 Polarimetric behavior around absorption features

Spectro-polarimetric investigations are now enabled beyond 1 μ m thanks to developments in optics and electro-optics. For instance, a newly published study used polarized spectroscopy around the hydroxide absorption band around 2.7 μ m to discriminate between surface absorbed and internal water molecules⁶. This study uses the polarizability differences between specular reflectance and internal diffusion to identify the position of the water molecules on or between the grains. With current applications to the lunar surface, this investigation is of interest for and to be applied to all planetary airless planetary surfaces. This study can also be extended to all components of the hydration band to possibly detect various polarimetric behaviours depending on the metal-OH component host-cation⁷. Moreover, the spectro-polarimetric investigation centred on the absorption features can be beneficial for the identification of molecules and minerals of interest, and can provide complementary information when linked to spectroscopy alone.

2.3 Evolution with varying phase angle and incidence direction

Polarimetric phase curves are used as a new classification method for the Solar System's small bodies and comparison with the reflectance spectra start to highlight a link between the observed polarization and the mineralogical composition of the target⁸⁻¹². Polarimetric phase curves are currently used as a classification method for asteroids². Finally, as the bidirectional aspect of the reflected light showed great impacts on the spectroscopy¹³, one can expect a dependency on the illumination direction on the spectro-polarimetry.

2.4 Rationale for the development of the instrument

Instrumentation developments are currently required to highlight the application of spectro-polarimetry to planetary sciences. Laboratory instruments are necessary to investigate the dependence of the polarization on the chemical, mineralogical and physical compositions around planetary spectroscopic features of interest, as well as to simulate the results of potential futures space-borne spectro-polarimeters orbiting their targets. Current polarimeters and ellipsometers do not offer such flexibility, either on the spectral range reachable or on the variety of geometrical configurations available. Most ellipsometers stay at the specular configuration where the direction of observation is symmetric to the direction of illumination with respect to the normal to the surface. In this scope, the complete development of a new type of laboratory instrument is required, the first step toward the implementation of spectro-polarimeters onboard space missions.

3. INSTRUMENTAL REQUIREMENTS

The measurement of the polarization state of the reflected light can be applied to various types of surfaces. The requirements for the laboratory setups have been fixed based on planetary sciences applications as they apply the most constraints to the system.

3.1 Features of interest

The instrument should be able to measure the polarization state, linear and circular, of the reflected light around the mineralogical and chemical features of interests from the ultraviolet to the near-infrared without intervention by the operator and in a single run. The optimal targeted spectral range spans from 300 nm to 4500nm in order to investigate from the Fe²⁺-Fe³⁺ charge transfer up to the CO₂ absorption bands, including the olivine, pyroxene, water and CO₂ ices, hydration, carbonates and organics absorption features. One of the scientific goals of the instrument is to investigate the

polarimetric behavior inside the mineralogical absorption features of interest as a precursor to space-borne instruments. The targeted spectral resolution should be fine enough to observe fine features while ensuring a signal-to-noise ratio high enough over the whole spectral range. In this scope, the targeted spectral resolution has been set to less than 20nm over the whole spectral range.

3.2 Surface textures

The instrument should be able to hold samples representative of the surfaces of the Solar System rocky planetary bodies. Such could be either rocks representative of boulders, or fine-grained powders similar to regolith. In this scope, this constrains the position of the surface to horizontal to avoid the grains falling from the sample holder. A nadir illumination of the sample will thus be represented by a vertical incident beam on arriving on a surface.

In the case of a powdered sample, the instrument should perform the measurement on a number of grains high enough to be statistically relevant. Grains can be considered as a groups of facets that are randomly oriented, and the observation of a small number of these facets can result in a false interpretation of the reflected light, not representative to the whole sample. In this scope, the instrument should illuminate and observe at least 100 grains in order to perform a statistically relevant measurement. This poses a constraint on the illumination and observation spot size, as well as fixes the maximum grain size observable.

3.3 Temperature control

The instrument should be able to investigate the polarization state of the light reflected by icy surface or ice-rich samples. This capacity is of interest for the study of the surfaces of the Jovian and Saturnian icy moons, comets, and Trans-Neptunian Objects (TNOs). In this scope, the instrument should be able to at least maintain the sample at a cold and fixed temperature during the duration of the measurement to avoid physical changes of the surface.

3.4 Acquisition time

The instrument was originally developed to investigate granular surfaces, with a stable composition and structure in time. However, the temperature and humidity environment around the instrument may change during the acquisition and modify the registered data, for example with the appearance of CO₂ and water vapor absorption bands, unrepresentative of the sample but of the air the light goes through. While the acquisition time has no specific limitation, it would be beneficial to maintain it as short as possible, while maintaining the temperature and humidity conditions around the instruments.

Finally, it is planned that the instrument should be able to analyze icy samples. For these specific targets, a cold cell will be developed to maintain the sample at low temperature to ensure its stability during the acquisition.

Considering the possible long acquisition time, it is mandatory that the illumination source should be stabilized in intensity, with maximum variations of less than 1% peak-to-peak over 24 hours.

3.5 Geometrical flexibility

Polarimetry is currently investigated through the dependence with the phase angle, i.e. difference between the directions of illumination and observation. However, the dependence of the reflected spectroscopy on both the incidence and emergence angles independently has been proven by previous studies¹³. In this scope, the instrument should be able to independently change the direction of illumination and phase angle, outside of the specular configuration. With independent directions, the same phase angle can be achieved under different illumination directions. Finally, the instrument is a proof of concept for the use of spectro-polarimetry in planetary sciences and thus should be able to reach various geometrical configurations achievable by an orbiting spacecraft. The direction of the illumination should be changeable from nadir to grazing direction (0° to 80° with respect to the normal to the surface), and the observation direction should run from the direction of illumination to the grazing direction (minimum phase angle to 160° of phase angle). Figure 1 presents a common geometric nomenclature for reflectance experiments, which the presented instrument will follow.

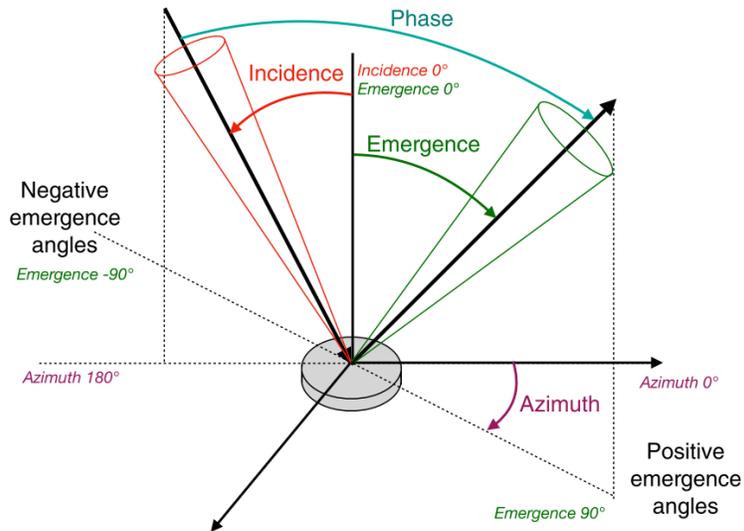


Figure 1: Illustration of the definition of the incidence (illumination), emergence (observation) and azimuth angles, in the case of a bidirectional reflectance experiment. Note that this instrument will not investigate the azimuth angles. Figure taken from ¹⁴.

Considering the fact that, for a flat surface of homogeneous composition over the studied area, the reflectance is symmetrical with respect to the incidence plane, it is possible now to investigate both sides of the incidence direction. However, this also requires the sample to be horizontal through the use of a tip-tilt correction stage under the sample holder.

The instrument should be able to investigate the polarimetric phase curves of the samples, with a focus on the minimum polarization value and inversion angle. In this scope, the minimum phase angle reachable with the system should be small enough for this investigation, and has been set to 5° . The value of the angular resolution should be a compromise between the angular polarimetric variations to observe and the signal-to-noise ratio. A nominal angular resolution value has been set to 8.0° , with the possibility to lower it for finer angular investigation while keeping in mind the induced reduction of the SNR.

4. DESIGN OF THE SPECTRO-ELLIPSOMETER

The Polarimetric Goniometer (PoGo) is currently under development at the Faculty of Aerospace Engineering. The scheme of the instrument is presented in Figure 2.

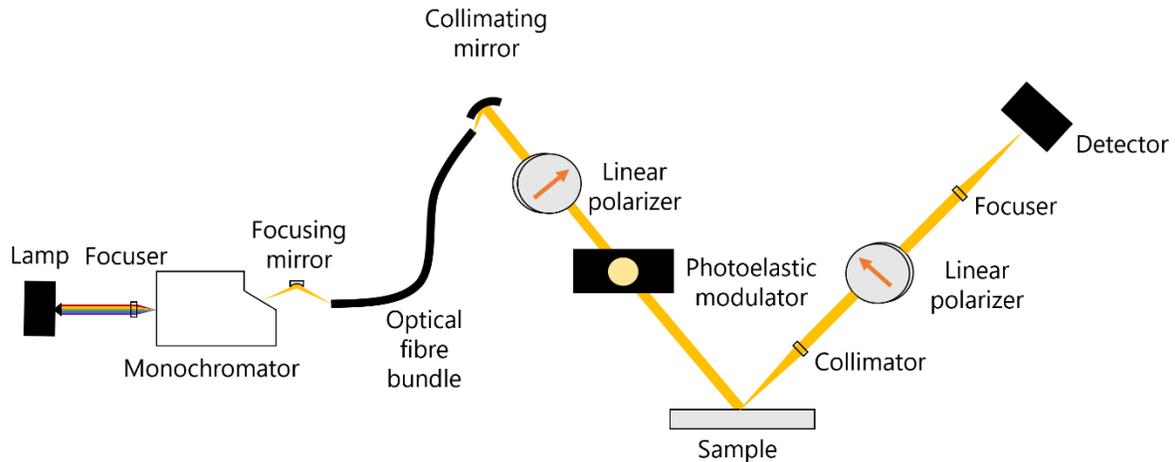


Figure 2: Schematic view of the ellipsometer.

The incident light is generated by a 250W QTH (Newport), focused on the entrance slit of a monochromator (Oriel Cornerstone CS260B). This monochromator contains 4 gratings on a turret, covering from 250nm to 6000nm. The secondary orders are suppressed from the exiting beam by 4 long-pass filters. The output beam is focused on the entrance of a ZrF₄ fibre bundle, guiding the light to the goniometer. The light exiting the fibers is collimated to form the incidence beam. The polarization of this incident light is controlled by a wire-grid linear polarizer, installed in a motorized rotation mount. The rotating wave plate is replaced here by a photoelastic modulator (Hinds Instruments). This component induces a retardance of the passing light by applying stress to a crystal via an incident electric signal at 42kHz. The voltage of the signal needs to be adjusted to the current wavelength. The incident beam then illuminates the surface sample, mounted on a tip-tilt stage to correct a possible deviation from horizontality. The light reflected from the surface is collimated, sent into a wire-grid polarizer, and focused onto the active cells of the detector. To cover the whole spectral range, the detector is a double-stage Si-InSb detector (Hamamatsu K1713-003). The signal from both cells is amplified by a pre-amplifier, and measured with a lock-in amplifier synchronized to the photo-elastic modulator's input frequency.

The incidence and emergence optics are held onto two arms, installed on off-the-shelf motorized rotation mounts (Newport). It is thus possible to adjust independently the direction of illumination and observation, from nadir (vertical to the surface) to the grazing direction.

5. EXPECTED PERFORMANCES

Table 1 presents the current configuration of the instrument and achieved accuracy and performances.

Table 1: Characteristics and performance of the system.

CHARACTERISTIC	SPECIFICATION
SPECTROSCOPY	
Spectral Range	300 – 3500 nm
Gratings	G1: 250 – 900 nm (1200 lines/mm) G2: 800 – 2300 nm (600 lines/mm) G3: 1600 – 3000 nm (200 lines/mm) G4: 2400 – 6000 nm (150 lines/mm)
Spectral Resolution	G1: 2.32 – 2.43 nm G2: 4.63 – 4.86 nm G3: 14.15 – 14.38 nm G4: 18.84 – 19.17 nm
POLARIMETRY	

Extinction Ratio	300 – 600 nm: > 100:1 600 – 2250 nm: > 1000:1 2250 – 4000 nm: > 10000:1
Retardance Precision	< 1% across spectral range
GONIOMETRY	
Incidence Angle Range	0° - 80°
Emergence Angle Range	-80° - 80°
Phase Angle Range	4.4 - 160°
Angular Resolution	8°
DIMENSIONS	
Minimum Sample Size	2.6 cm x 2.6 cm
Illumination Spot Major Diameter	25.4 – 146.3 mm
Observation Spot Major Diameter	4.4 – 25.34 mm

5.1 Spectral range and resolution

The configuration presented on Figure 2 will enable the investigation of the spectro-polarimetry from 300nm to 3500nm. The transmission of the PEM decreases strongly around 3500nm and falls to less than 20% beyond this value. It is used as a retardance waveplate, so the investigation of the circular polarization will be limited at the end of the instrument's spectral range. It will be still possible to investigate the linear component of the spectro-polarimetry of the light beyond 3500nm, by removing the PEM from the setup and performing the analysis with a polarizer/analyser configuration. The investigation of the CO₂ bands around 4200nm will be possible with such a modification.

The monochromaticity of the incident light is ensured by a monochromator, based on 4 reflection gratings of parameters, working range and resulting spectral resolution are presented in Table 1. The spectral resolution is kept under 20nm over the whole spectral range, which agrees with the initial requirements. It is important to note here that these resolutions are achieved with the nominal opening of the monochromator entrance and output slit of 0.7mm. The lower values of spectral resolutions can be achieved by reducing the width of the slits, while impacting the amount of light entering and exiting the monochromator, so lowering the signal to noise ratio.

5.2 Signal-to-noise ratio

The most critical aspect of the instrument is the amount of light passing through all optical elements and reaching the detector. In addition to the global absorption of the optics, polarizing elements reject at least half of the incident intensity, due to the selection of the polarization direction. In addition, because of the bidirectional aspect of the measurement, a small portion of the light is caught by the observation arm, depending on the reflectance of the sample at this specific direction, the size of the collimating optics and its distance from the surface. Figure 3 presents the decrease of the light intensity through the instrument, considering a Lambertian surface with a reflectance of 10% at the selected wavelength of 3μm.

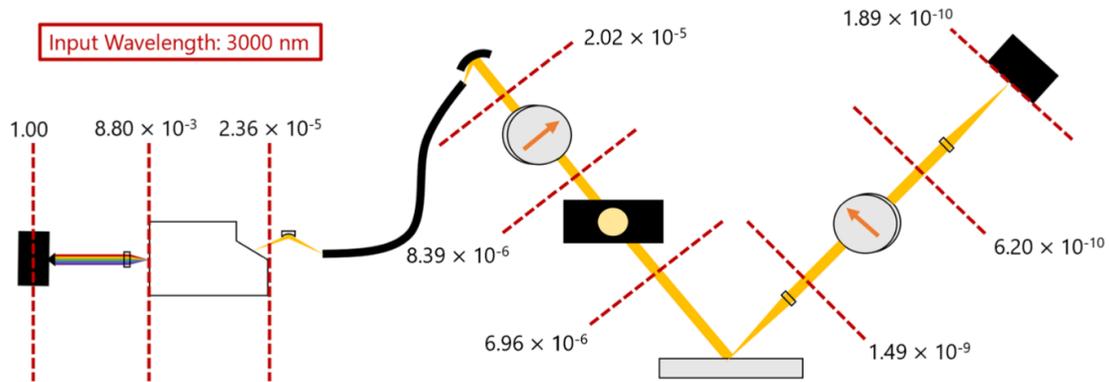


Figure 3: Simulated normalized light intensity through the instrument considering a Lambertian surface with a reflectance of 10% at 3 μ m.

This intensity loss will drastically affect the measurement quality. We consider the signal to noise (SNR) ratio as the following formula

$$SNR = 10 \log \left(\frac{S_D}{N_T} \right)$$

with S_D the detected scientific signal and N_T the amount of noise. The signal to noise ratio can be increased by either increasing the integration time, reducing the spectral resolution or increasing the lamp intensity for specific samples with a low reflectance. Figure 4 presents the signal to noise ratio of the instrument through its working spectral range, considering the nominal spectral resolution and an integration time of 1 second, on a Lambertian surface with a reflectance of 10%.

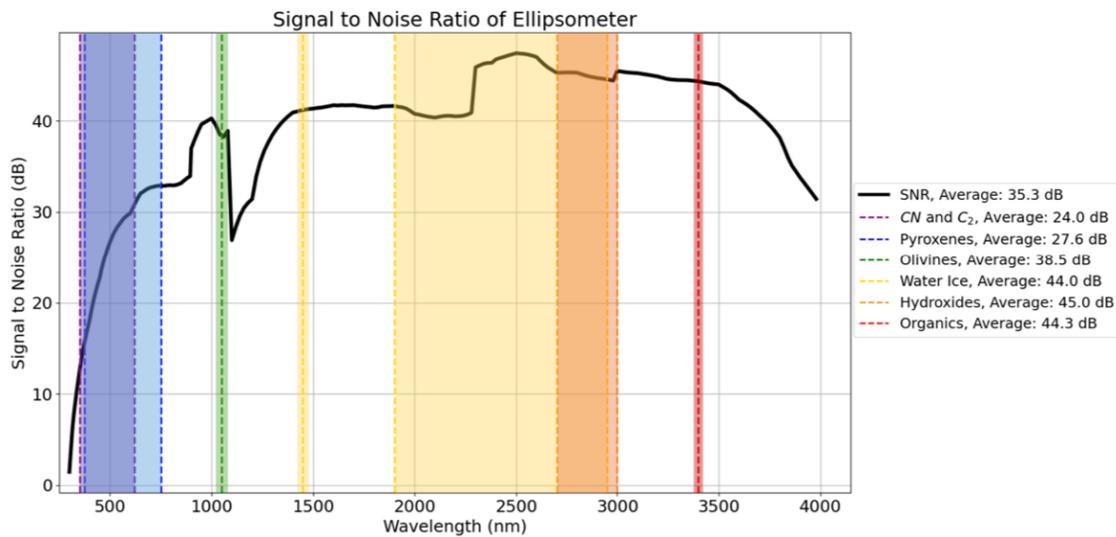


Figure 4: Estimated signal to noise ratio of the instrument through the working spectral range considering an integration time of 1s. The colored regions mark the position of the absorption features of interest.

Though this figure highlights the worst case scenario with a reflectance of 10%, hence the minimum set by the requirement, low signal to noise ratio can be met in deep absorption bands with localized low reflectance values.

5.3 Illuminated and observed areas

The PEM requires a collimated light in order to ensure a proper retardance, and has a clear aperture of 1". Thus this also fixes the width of the illumination beam, and so the size of the illuminated area on the surface. The observed area should be contained in this illuminated area in all geometrical configurations achieved. The observed spot has thus been set to 4.4mm in diameter under nadir observation, and forming an ellipse of 1" in major axis at the widest angle achievable. This configuration requires the illumination to be homogeneous over the sample to avoid generating false spectro-polarimetric variations over different geometries. The homogeneity of the beam will be assessed during the calibration phase and possible inhomogeneities will be thus corrected during the scientific acquisitions.

6. CONCLUSION

We present here the design of the future spectro-gonio ellipsometer, for bidirectional reflectance spectro-polarimetry of granular surfaces. The selected configuration enables the investigation over the requested spectral range from the ultraviolet to the near-infrared, with a full characterization of the polarimetric state. The expected performance matches the initial requirements, while the real performance will be assessed after the calibration phase.

Coupling spectroscopy with polarimetry can bring new information to improve our detection and surface characterization capabilities and would be of interest for planetary exploration. The instrument PoGo is the first step toward the implementation of spectro-polarimetry for surface investigation and the development of new types of instruments, being laboratory-based, ground-based or spaceborne.

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