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ABSTRACT

Remote Laser-Evaporative Molecular Absorption (R-LEMA) spectroscopy is a sensor concept for probing molecular composition of asteroids from an orbiting spacecraft. R-LEMA uses a high-power laser aboard the spacecraft which is used to melt and evaporate a spot on the surface of the target; the heated spot is then viewed by a spectrometer through the plume of ejected material. Research supported by the NASA Innovative Advanced Concepts (NIAC) program aims to adapt a laboratory R-LEMA system for operational tests in the space environment. A CubeSat mission is envisioned as a test of the R-LEMA concept in the space environment, with a laser and spectrometer aboard a main craft, and a target craft flying in formation. A systems analysis is presented for the spectrometer and optical subsystem. For typical targets, selected molecular species are deemed to be important resources, e.g. water, hydrocarbons, economic minerals, etc. Infrared spectra of important resources are reviewed for general characteristics, and operational specifications for the spectrometer and optical subsystem are derived from the spectra. Operational and engineering trade-offs for grating and FT-IR spectrometers are compared. Speed, resolution and wavenumber accuracy of FT-IR designs are preferable, but long-motion interferometers become unwieldy in a CubeSat design. Bruker’s patented two-beam interferometer with double pivot scanning mechanism provides a compact FT-IR compatible with CubeSat geometry. Simulation results are presented for detection of important resources under various operational scenarios using the CubeSat design. Even at low concentrations, detectability of water and hydrocarbons is expected.

Keywords: Asteroid Composition, FT-IR, Remote Source

1. INTRODUCTION

1.1. NIAC

The NIAC initiative is a program that stimulates, promotes and enhances innovative researches in the Astronautical sector, which may one day revolutionize the knowledge bases of the area through these new concepts developed. Participation in the program takes place in early stages of Technology Readiness Levels (TRLs), and this paper seeks to describe an experiment that could move the R-LEMA concept from TRL-2, which is the process of formulating the application of the proposed technology, advancing steps through TRL-3 and TRL-4. The remote probing system R-LEMA\textsuperscript{[1]} that analyses bulk molecular composition of solid targets from a distant vantage was proposed. But it requires an extensive viability testing before it is deployed.

What was suggested as proof-of-concept for evaluation of the R-LEMA system in a space environment is the use of a pair of attached CubeSats in LEO (Low Earth Orbit), one 4U named as ‘target’, carrying a sample material, and one 6U carrying the whole sensor system, consisting of a diode LASER, an spectrometer alongside with the Structural...
components, Power system, Command and Communication system, Attitude and Control system, Tracking and Telemetry system, and Heat Control system. When it reaches the stipulated altitude and enters orbit, the two spacecraft will fly in formation to carry out the mission. As the two spacecraft are flying at a specified stand-off distance, the main craft will fire the laser at the target. Light from the heated spot on the target will be viewed by the FT-IR spectrometer on board the main craft, providing a test of the sensor system function. The double system works as a space-environment laboratory testing the basic concepts and clearing doubts about any issues that were raised by the theoretical models (which will be discussed further on).

1.2. Composition analysis applications

The formation of the solar system, 4.6 billion years ago, left as traces a vast number of asteroids and comets wandering in stable orbit within the heliosphere. These celestial bodies, which are nothing more than a leftover from the formation process of telluric (asteroid) and Jovian (comet) planets, carry a very rich load of knowledge about the constitution of our solar system.

Scientific interest is then a great stimulant for the exploration of new horizons of space. And now, our next step is to reach the domain of control that touches the landmark of the asteroid belt. That is traditionally designated as being located between the orbits of Mars and Jupiter and is composed of an exorbitant amount of asteroids. Astronomical observations, until the present, have identified more than 600,000 of these bodies with varying sizes, which reach larger diameters up to 240 km. With the possibility of acquiring new information about these compositions, a wide range of studies, not only from the aerospace industry, could one day be favored. Representing then an important step progressing in the evolutionary process of our methods and technical resources in technological scope.

Figure 1. Schematic representation of the main-belt of asteroids, between the orbits of Mars and Jupiter.
In addition to the incalculable scientific value of this type of research, a more pragmatic issue comes into sight, which is the fact of bodies wandering in space and consequently the existence of many of them passing very close to our orbit. Asteroids with a near trajectory are called NEAs (Near Earth Asteroids) and a more general class of this group, which includes comets as well, is the NEOs (Near Earth Objects). The prevention of possible collisions of these bodies with Earth has increased since the moment we became more aware of the real chances of such catastrophes. According to the latest survey by the NEOWISE mission data from the NASA WISE probe, there are 1,885 PHAs\(^2\) (Potentially Hazardous Asteroids) known, and an estimated total of 4,700 ± 1,500\(^3\), with at least a 100 m diameter and closer than 8 × 10\(^6\) km to the Earth\(^4\).

Such collisions are usually devastating if they occur in densely populated places, as it is unworkable a total evacuation and recovery of the damages caused. And besides, there are still one of the biggest challenges to overcome: planning. That involves determining the exact date and location of the crash, but it turns out to be very difficult, even to the best simulation integrators, because it is a chaotic dynamic system with a lot of interference from externalities.

An example of a constantly controlled PHA is the Apophis\(^5\) asteroid, which has a 270 m diameter and a speed of 6 km/s. It has the potential to destroy a third of the planet\(^6\), and the greatest danger prediction is for 2036, but it has unstable collision probabilities, which vary by each measurement. Events in recent years have alerted us to PHAs, such as that which occurred in Chelyabinsk\(^7\) in 2013 in Russia, which left 1,200 injured and damages in the cost of 50 million dollars. And another case in Tunguska\(^8\) in 1908 that had an explosive energy a thousand times greater than the bomb of Hiroshima\(^9\) (4.2 - 6.3 × 10\(^6\) J).

Another factor that demands notice when it comes to the exploration of asteroids is the vast amount of metallic resources that composes it and that can mean for us as a reserve of raw material necessary for the colonization of space on a large scale. Some asteroids have a value around tens of trillions of dollars\(^10\) in iron, nickel and cobalt, basically. This, apart from allowing the extraction of resources to be used on Earth, would be an essential step for interplanetary colonization.

But firstly, an analysis of the logistics of obtaining and mainly a more precise idea of the composition of these bodies is needed. And it is precisely in the intention of determining the NEO structure composition that the idea of the R-LEMA project enters, seeking to do this analysis without the costs of landing and takeoff of the probes in the NEOs, such as TGL (touch-and-go landing), that are taken as the largest expenses of the operations. The objective is to reduce costs to facilitate the collection of data, which until now have been difficult to obtain due to the discouragement generated by the high value needed for landing missions.

2. SPECTROMETER SPECIFICATIONS

2.1. Material aiming analysis

The intention is to focus efforts to recognize essential molecules to the scientific analysis field, such as water, hydrocarbons and organic compounds in general (which would help in understanding the origin of life in the solar system), methane or other types of fuel (for interplanetary supply), titanium or other building metals (which would benefit the in-situ extraction of manufacturing resources), precious metals (such as gold, silver, platinum, nickel and cobalt) and rare-earth metals (that are applied in most cutting-edge technology nowadays).

It took then, at this stage, an optimization in the choice of materials that would pass through this process of tests in spectrometer, since there is in this situation a considerable restriction in the bands of operation of the spectrometer. And since the size of the target component in the test is very limited, restricting the diversity of elements to be analyzed, we have to choose one that fits the scope of the study and conformities of spectral range.

2.2. Infrared Spectroscopy

As there were many variables to be considered in the process, some data had to be fixed. Considering the power required to melt rocky materials (10 MW/m\(^2\)) and operating-time of the system’s LASER, the final sample is meant to heat until it hits the temperature of ~2500K and emits a blackbody radiation. This established information was taken as the one to be worked with. What it means is that the thermal energy emitted by the heated spot would be maximum at approximately 1.07 eV, as given by the Wien’s law:
\[ f_{\text{max}} = \frac{T \cdot c}{b} \quad (1) \]

and

\[ E = h \cdot f \quad (2) \]

Where \( b \) is the Wien's displacement constant, equals to \( 2.8977685 \cdot 10^{-3} \) (in m \cdot K), \( c \) is the speed of light (in m\cdot s\(^{-1}\)) and \( T \) is the temperature reached in the sample (in K). Thenceforward, there is a wide range of wavelengths that can be read, but the highest reading will be made around wavelength 1.16 \( \mu \text{m} \), which means that the operation will be mainly in near-infrared (0.7 to 2.5 \( \mu \text{m} \)), but for a matter of pragmatic way, it may also consider it acts a bit in mid-infrared (2.5 to 25 \( \mu \text{m} \)) and far-infrared (25 to 1000 \( \mu \text{m} \)). That is an important premise since this already decreases the variety of choices for spectroscopy method and already being clear the advantages of some methods over others in this case. And as it has been defined in what spectrum it operates, one needs to understand how infrared spectroscopy works.

Infrared spectroscopy is based on the fact that photon energies associated with this spectrum range are not enough to excite electrons, but the absorptions may induce vibrational excitation. Molecules absorb frequencies that are characteristic of their bond structure and these absorptions occur at resonant frequencies, i.e. the frequency of the absorbed radiation matches the vibrational frequency. That is, it sweeps a frequency spectrum and records at each point information about the rate of absorption of the emitted beam used to increase the amplitude of the vibrations in the bonds within the molecule. There are 6 types of vibration: symmetric and antisymmetric stretching, scissoring and rocking latitudinal and wagging and twisting longitudinal. Each one of these in any compound is activated by different frequencies in the spectrum graph.

For didactical purposes the connections between atoms are considered as springs that vibrates only at specific frequencies. The equation that estimates this frequency is derived from Hooke's spring law, and says:

\[ \bar{\nu} = \frac{1}{2 \pi c} \left( \frac{f}{M_x + M_y} \right)^{\frac{1}{2}} \quad (3) \]

Where \( \bar{\nu} \) is the vibrational frequency (in cm\(^{-1}\)), \( c \) is the light speed (in m\cdot s\(^{-1}\)), \( f \) is the bond strength constant (in dinas\cdot cm\(^{-1}\)) and, \( M_x \) and \( M_y \) are masses of atoms X and Y (in g).

2.3. Dimensional limitation

Besides those requirements, there is the dimensional limitation. As the spectrometer will be placed on a 6U CubeSat, it would not have too much space available. Therefore leads to a necessary precise choice of the spectrometer, which reaches a good range but fits in a small space. The dimensions firstly estimated by the structure department were 45 \( \times \) 50 \( \times \) 80mm, so that it fits. This represents another specification to be fulfilled by spectrometer department.

3. SPECTROMETER SELECTION

3.1. Diffraction grating and FT-IR spectrometers

The spectrometer is an instrument used to study properties of light in a particular range of the electromagnetic spectrum. For a chemical analysis of the surface from a plume obtained by the laser, two types of spectrometer were studied: diffraction grating and FT-IR (Fourier Transform Infrared).

The diffraction grating theory is an extension of the theory made to observe the interference pattern due to double-slit (Young's experiment) in the case of many slits. The analysis of the interference pattern produced by a diffraction allows determination of the spectrum of the radiation emitted by a light source. Thus, a diffraction grating is capable of dispersing a beam of several wavelengths in a spectrum of associated lines. A simple scheme of how this type of spectrometer works is in Figure 2.

The diffraction grating of a spectrometer has an impact on optical resolution and maximum efficiency for a wavelength range, which is inversely proportional to the grid dispersion due to its fixed geometry. However, the higher the dispersion, the higher the resolution power of the spectrometer. On the other hand, decreasing the frequency of the groove decreases dispersion and increases wavelength coverage at the cost of spectral resolution. Thus, sacrificing the optical resolution increases the wavelength coverage.
Due to the limit on the longest wavelength to be diffracted by a grid, there is an upper limit on the grid spectral range. This can restrict the maximum slot density allowed in a spectrometer, for near infrared applications.

Using Linear Variable Filter (LVF) technology as solid-state dispersion gratings is possible to take near, mid or far IR spectral readings.

Figure 2. Simple diffraction grating spectrometer.

The Fourier Transform Infrared (FT-IR) spectroscopy was developed to overcome the limitations encountered with dispersive instruments. One solution was the use of a very simple optical device called interferometer, to measure all infrared frequencies simultaneously, rather than individually.

Most interferometers employ a beamsplitter that takes the incoming infrared beam and divides it into two optical beams. One beam reflects on a flat mirror that is fixed. The other beam is reflected in a movable flat mirror. The two beams are recombined when they meet back in the beam cutter. The resulting signal (interferogram) is the interference of both. As the interferogram is measured, all frequencies are measured simultaneously. Thus, the use of the interferometer results in extremely fast measurements (most FT-IR measurements are made in a matter of seconds instead of several minutes – Felgett Advantage). For a frequency spectrum (a graph of the intensity at each individual frequency), a mathematical technique called Fourier transform is used, which is performed by the computer. A diagram of this system can be analyzed in Figure 3.

In addition to speed, the FT-IR technique has other advantages. The detectors used are much more sensitive, the optical throughput is much higher (Jacquinot Advantage), which results in much lower noise levels and fast scans allow the coaddition of several scans to reduce random measurement noise at any desired level. There is mechanical simplicity; the moving mirror in the interferometer is the only part that continuously moves on the instrument, so there is little possibility of mechanical breakage. Another feature is the internal calibration (Connes Advantage), since they never need to be calibrated by the user\textsuperscript{11}. However, a higher resolution is a result of a greater distance of movement of the moving mirror, for example a distance of 4 cm results in a resolution of 0.25 cm\textsuperscript{-1}. 

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3.2. Two-beam interferometer with double pivot scanning mechanism

As the design is of a CubeSat 6U, which has small dimensions and the FT-IR spectrometer with an adequate resolution has inappropriate proportions, it was found a patent US7480055B2 assigned to ABB, Inc. which is two-beam interferometer for Fourier Transform spectroscopy with double pivot scanning mechanism.

This system has a first-reflector, a second-reflector, a central body, the first pendulum rotatable, the first retro-reflector, a second rigid pendulum rotatable, the second retroreflector, a beamsplitter fixed in the central body and a linkage. It is in the beamsplitter where one of the beams is directed to the first-reflector and the other is to the second-reflector, there is also the recombination of the beams from the retroreflectors to form an interference pattern.

Therefore, the first and the second rigid pendulum rotatable about a first and a second axis of rotation respectively, which are linked by the linkage to each other to constrain the rotation of the first pendulum relative to the rotation of the second pendulum.

In this design, the beamsplitter divides the incoming radiation to be measured in two partial radiations. A partial radiation reaches the retroreflector and leaves in a parallel. This partial radiation is reflected back through the stationary mirror of the optical system and exits at the original entry point to achieve the beamsplitter. In Figure 4, this function can be observed with the beamsplitter S, a partial beam S1, retroreflector 3, mirror 4. For the second partial radiation S2, the same occurs but with retro-reflector 12, stationary mirror 13. The two reflected partial radiations S1 and S2 reach the divisor of beam 1 in interference with each other and the detector 5 arrives as radiation S1-2. While the two rigid pendulum arms (8 and 10) are fixed at the bearing (7), the two retroreflectors spin around bearing 7 within the tolerance provided by the drive magnets (9 a, 9 b). The figure 5 shows another design for a scanning interferometer without the retro-mirrors (ABB Bomem Inc.). However, the design in accordance with the invention US7480055B2 is in Figure 6.

In this interferometer, the beamsplitter is the object represented by “60”. The two cube corners 52 and 54 are associated on two pendulums 56 and 58 of a double pivot double pendulum set (66). When the pendulums 56 and 58 are rotated around their respective axes 56 b and 58 b, the arms 56 a, 56 d and 58 a, 58 d spin together. These pendulums 56 and 58 are connected by a coupling linkage 62 and bearings 56 c and 58 c. In addition, there is counterweight (64).

The optical compensation is related to the position of pivots 56 b and 58 b, which define the circles described by the movement of the cube corners 52, 54[12].
Figure 4. Design for a double pendulum scanning Michelson interferometer.

Figure 5. Design for a scanning interferometer of without the retro-mirrors on the left, and its condition for the mechanical shear compensation on the right.

Figure 6. Top view of a double pendulum type scanning Michelson interferometer at rest on the left, and with the necessary condition for optical/mechanical shear compensation on the right.
For a more compact FT-IR spectrometer design than a linear FT-IR spectrometer, Bruker Optics Inc. has a product of dimension 208 x 310 x 140 mm. This incorporates dual retroreflecting gold coated cube corner mirrors in an inverted double pendulum arrangement for maximum efficiency and sensitivity. Besides, the temperature-stabilized detector makes the system very robust against variations of the ambient temperature.

4. CONCLUSION

During the process of choosing the spectrometer, a FT-IR model was chosen for several reasons. Such as the required spectral region is in the infrared; the data obtained quickly; need for a high spectral resolution because we may be dealing with weak signals due to oscillations caused by CubeSat or target uncontrolled attitude; need for accuracy caused by a possible unplanned high-density plume.

It has been argued that the main issue that influences the resolution amplitude performance of the FT-IR type spectrometer is its freedom of movement for the moving mirror. But as the dimensions of a CubeSat does not allow this freedom necessary to achieve a high reading performance, this was main challenge of the project. It was necessary to reconcile the necessary power for the satisfactory execution with the small space available.
However, this 'resolution vs. size' dilemma will most likely not persist until more advanced stages of TRL. And it will not be a problem for the R-LEMA system, as it will have a sufficiently good volume for a great and effective spectrometer, that will have a wider range of bands. But for now we need to deal with issues like this to keep advancing the project.

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