Laboratory Studies in Support of Planetary Surface Composition Investigations

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1.0 Introduction

One of the most fundamental questions that can be asked about any planetary object is: What is its composition? Except for the four gas giant planets, the remaining planets in the solar system and a multitude of moons, asteroids, and icy dwarf planets all have a solid surface to which we can direct investigations regarding their composition. The mineralogy and chemistry at the surface of these objects records the history of their formation and subsequent alteration over time. This knowledge then contributes to other investigations ranging from planetary interiors to habitability. Telescopic, spacecraft, and in situ data are available to address surface composition, most commonly in the form of spectroscopic measurements. In most cases, laboratory measurements are required to translate those data into knowledge about the surface from which they were obtained. Without laboratory measurements, most of the planetary data are inscrutable squiggly lines.

Decades of laboratory studies of a range of materials under various environmental conditions have been used to develop spectral libraries, analytical models, and databases. These have yielded remarkable discoveries throughout the solar system. But as planetary observations and instrumentation become more diverse and sophisticated, so too must the laboratory studies needed to support the interpretation of the ever-expanding data sets. Across many disciplines, there is a growing need for laboratory measurements relevant to the materials and environmental conditions of a given planetary surface. Such measurements are often challenging. But the time and expense associated with these efforts is expected to yield significant improvements in the state of knowledge of surface composition of solar system objects. We outline below a range of representative laboratory studies applied to this topic and build a case for why additional efforts are worthy of funding and necessary for the success of the next decade of planetary exploration. We strongly recommend that existing NASA research programs supporting laboratory studies be retained and perhaps augmented.

2.0 Surface Mineralogy

Remote determination of surface mineralogy currently is the exclusive domain of spectroscopy. Here we include ices and the amorphous phases of ices and minerals because their composition also can be probed via spectroscopy. With the advent of the Mars Science Laboratory (MSL) rover, X-ray diffraction measurements will be the first departure from spectroscopic mineral determination. Current remote spectral observations of planetary surfaces span the wavelength range from ultraviolet (UV) to thermal infrared (TIR). Interpretation of these spectral data is entirely dependent upon laboratory spectral measurements because there is not yet a theory-based approach that can model all the parameters that affect spectral character. The same is true of Mössbauer spectroscopy, which also is an in situ technique. Other types of spectroscopy-based in situ techniques are in development or have been proposed, including microscopic thermal emission, various forms of Raman, and attenuated total reflectance (ATR) experiments. Thus, the vast majority of laboratory studies applied to planetary surface mineralogy rely upon spectral measurements. A partial survey of these studies, their associated challenges, and areas for improvement are given below.

2.1 Icy Bodies

Volatile compounds in the form of ice dominate the surface and/or bulk composition of numerous outer solar system objects including the icy satellites of the giant planets (e.g., Europa, Ganymede, Enceladus), comets, icy dwarf planets like Pluto, and smaller Kuiper belt objects. There are many tens of candidate compositions for outer solar system ices including H_2O, CO_2, NH_3, CH_4, alcohols, carbonyls, oxides, and many other volatile compounds. A sample listing of over 125 candidate compounds is available at http://mos.seti.org. Temperature, pressure, contaminants, mixtures, particle size, and viewing geometry all affect the spectral characteristics of these compounds. Laboratory studies must address this range of variables in order to properly and completely interpret the spectral measurements from telescopes and spacecraft instruments that already exist or are planned.

Analytical methods: The bulk of our knowledge regarding the surface composition of icy bodies is derived from visible to near-infrared (VNIR) reflectance spectra from spacecraft and telescopes. Individual compounds can be identified by their absorptions, but this process is inefficient compared to modeling the entire spectrum. Spectra can be modeled either as linear (areal) mixtures, or as nonlinear (intimate) mixtures, to yield estimates of relative abundance of surface compounds. Nonlinear mixture analysis requires the real and imaginary indices of refraction (optical constants), which can be calculated from laboratory spectra. Linear mixture analysis can be done with optical constants or laboratory reflectance measurements of pure compounds. It is the need for reflectance spectra and optical constants of appropriate compounds that drives many of the laboratory studies in this field. As shown by other studies, Raman spectroscopy applied in situ also holds promise as a companion technique for future in situ missions.

Current state of the art: To date, most candidate compounds proposed as surface constituents of icy bodies have not been characterized sufficiently for use in the analysis of planetary spectra. For example, most infrared spectra of candidate compounds published to date were measured in the TIR for purposes of understanding the interstellar medium. There are many absorption features in observed planetary spectra that remain unidentified because of spectral gaps in the laboratory data and incomplete or insufficient libraries. In order to make proper identifications and constrain abundances of surface materials from spectral observations of icy bodies, cryogenic laboratory measurements for all candidate compounds are needed.

Needed laboratory measurements and their challenges: Reflectance spectra and/or optical constants of candidate compounds and mixtures are needed. Ideally these should span at least the spectral range of existing observations like those from Galileo and Cassini cameras and spectrometers (298 to 5500 nm). Given the sensitivity to temperature of various spectral features, measurements must be obtained at appropriate temperatures, ideally covering the range from 20 to 150 K. Ices grown in the laboratory must be sufficiently thick to yield useful absorption features for the weak overtone and combination vibrational modes that make up most of the VNIR spectral signatures, without saturating the strong TIR fundamental absorptions. This usually requires repetition of the measurements over a range of thicknesses. Also, infrared absorptions of a compound can change shape, strength, or central wavelength when mixed with other materials. Therefore, measurements of ice mixtures are also necessary.

Improvements expected from lab studies: Scientific return from spacecraft and telescopic observations of icy bodies will be significantly enhanced by the proper application of cryogenic laboratory spectroscopy. With these measurements in hand, investigators can identify materials, derive their abundances, map their distributions, and infer their roles in the formation and evolution of these enigmatic bodies.

2.2 Rocky Bodies

Non-volatile compounds dominate the surfaces of rocky (terrestrial) bodies of the inner solar system, the asteroid belt, and many of the satellites of the outer solar system. Many of the Earth's major rock-forming minerals and alteration phases have been identified at the surfaces of the solar system's rocky bodies. Here we include meteorites and their constituent mineral phases because of their link to these bodies. Silicates (e.g., plagioclase, pyroxene, olivine, phyllosilicates, and amorphous phases), metal oxides, sulfates, and minor carbonate phases all have been recognized. But as is the case with the study of icy bodies, major gaps exist in our state of knowledge due to insufficient spectral libraries.

Analytical methods: A broader range of spectral measurements is or will be available for the investigation of the mineralogy of rocky bodies compared with icy bodies. The inner solar system bodies including the asteroids radiate with sufficient energy that TIR measurements are feasible in addition to VNIR. TIR spectra of surfaces with sufficiently coarse particles (>~60 μm) can yield both mineral identification and abundance via linear spectral deconvolution analysis. In situ exploration of Mars has allowed Mössbauer spectroscopy to be used to investigate Fe-bearing phases via the Mars Exploration Rovers. Raman spectroscopy also is envisioned for in situ measurements of rocky bodies, allowing for the investigation of organic compounds in addition to mineral phases.

Current state of the art: The spectral libraries required to interpret spectra from rocky bodies are more mature than those used for icy bodies. Thousands of geologic materials including minerals, rocks, and meteorites have been measured over the past few decades using the techniques described above. Measurements of synthetic and analogue materials have extended this diversity as have measurements obtained in the field and from airborne and Earth-orbiting platforms. Efforts to understand the spectral effects of temperature, thermal gradients/heterogeneities, pressure, dust accumulation, hydration state, surface texture, and impact shock pressure have been undertaken for various materials. The resulting spectra have had the greatest impact in the investigation of Martian mineralogy, consistent with the fact that Mars was the target for most of these measurements. But no other rocky bodies share the environmental conditions of Mars, leaving open significant deficiencies in the analysis of their spectra. And despite the range of studies and spectra applicable to the analysis of spectra from Mars, deficiencies remain.

Needed laboratory measurements and their challenges: Environment-appropriate spectral measurements are a major concern for the proper analysis of spectra from rocky bodies. The TIR spectra from airless bodies can be significantly different than those with an atmosphere due to thermal gradients in the spectrally active surface layer. High temperatures like those at the surface of Venus and the sunlit hemisphere of Mercury induce changes in TIR spectra. In the presence of an atmosphere, minerals are chemically reactive and in some cases, their spectral properties change depending on the temperature, atmospheric pressure, and atmospheric components. Environment chambers are thus a necessary addition to produce relevant laboratory spectra.

Another area that is underdeveloped is the understanding of spectral effects of particle size and mixing. A comprehensive knowledge of linear and nonlinear mixing effects requires a large number of mixture studies with multiple particle sizes, as well as modeling with optical constants. Ideally, optical constants would be determined and used in scattering models.

Despite the abundance of materials already measured, spectra from more minerals, rocks, soils, extraterrestrial materials, and shocked phases would allow more thorough characterization of planetary surfaces. It is vital to stress that complete chemical and mineralogical characterizations of these materials are needed before they become integrated into spectral libraries.

Improvements expected from laboratory studies: The mineralogy of most rocky bodies throughout the solar system is poorly constrained despite the growing set of spectral observations. The state of knowledge is strongly dependent on the available spectral libraries, which clearly are insufficient to accurately determine mineralogy. We expect that attention to the environmental conditions of the measurements, to particle size effects, and to more complete inventories of measured materials will significantly improve our ability to interpret existing and future spectral data.

3.0 Chemistry

Here we focus on laboratory studies that apply geochemical modeling and experimental petrology to better understand existing planetary data and those studies that are needed to support planned and future chemical and mineralogical sensors. This focus is distinct from that of another topical paper in this series dealing with surface chemistry. In that paper, the focus is on processing effects due to factors such as radiation and photolysis that impact surface chemistry.

3.1 Geochemical modeling and experimental petrology

Laboratory studies involving geochemical modeling and experimental petrology provide a framework for understanding the geologic conditions that led to the various mineral assemblages observed on planetary surfaces and in their proxies, meteorites. Experimental studies and synthesis experiments can be used to answer fundamental questions regarding the origin and evolution of mineral assemblages on a variety of planetary bodies. Through such experiments we can go beyond observation and evaluate the effects of process. For example, processes that record climate evolution in ancient sedimentary rocks on Mars, namely chemical weathering, chemical sedimentation and diagenesis, can be investigated in the laboratory. Similarly, laboratory experiments on the stability fields, phase boundaries, reaction paths, and kinetics of key mineral phases (e.g., hydrated sulfates) are crucial for deciphering environmental conditions.

Analytical methods: Piston-cylinder apparatuses, hydrothermal pressure vessels, and high temperature furnaces (for phase equilibrium studies under vacuum) permit synthetic or natural samples to be subjected to a variety of controlled conditions of pressure, temperature, and redox state, in order to assess changes in mineral assemblages induced by cooling, and/or interaction with fluids. Multi-anvil devices and diamond anvil cells have allowed for ultra-high pressure experimentation of petrologic systems in planetary science. Such experiments investigate a variety of processes, from impact processes that affect the highly reduced lunar regolith, to the formation of oxidized hydrothermal alteration assemblages on Mars, to the effects of deep fractionation of magmas on the development of crustal stratigraphy on planetary bodies. The equipment also is used to synthesize a variety of minerals for spectroscopic studies to expand the various databases used to interpret orbiter and lander data.

Other work has included experiments designed to focus on aspects of chemical weathering (for example using martian basalt synthesized with experimental petrology facilities). Experimental investigations of fluid evaporation and specific diagenetic reactions have been conducted in the laboratory to better understand mineral stability in response to changing aqueous chemistry and paleo-environmental parameters.

Current state of the art: Current research involves investigating relevant chemical systems that have been bounded as much as possible by telescopic, orbital, and in situ mission constraints. New developments in experimental and analytical techniques (e.g., hydrothermal diamond anvil cell provide for direct characterization of experiments at the relevant conditions of formation, allowing for more relevant systems to be constructed and investigations to be conducted in greater detail. The field of experimental petrology is at a stage where we are capable of synthesizing materials under a great variety of conditions relevant to many different planetary bodies, and with available analytical techniques, thoroughly characterizing the materials produced.

Needed laboratory measurements and their challenges: One of the deficiencies in this field remains an incomplete understanding of mineral stability on planetary surfaces under unique chemical conditions. Laboratory work contributes significantly to this goal and offers a level of detail and control that natural studies cannot afford. The challenges right now are not so much from an experimental point of view as from the need for more funding to be dedicated to such endeavors in order to train the next generation of planetary scientists in the development of experimentally testable questions and the techniques used to answer them.

Improvements expected from laboratory studies: Continued laboratory work on mineral stability at planetary surfaces over time will build a database with which to interpret future and existing data obtained from exploration missions. By constraining paleo-environmental parameters from laboratory studies of mineral stability, a clear record of climate evolution over time and its impact on the chances for life is the most important priority and expected result.

3.2 Laboratory studies in support of chemical/mineralogical sensors

Here we present a brief example of the need for laboratory studies to support the development and implementation of promising technologies that serve the objective of chemical and mineralogical investigations. Laser-Induced Breakdown Spectroscopy (LIBS) is a non-contact method for elemental (H up to Pb) identification and quantification in rock and soil samples either in-situ or at near distances (meters to tens of meters) from the instrument. LIBS provides primarily elemental compositions, but recent work has also exploited its capabilities in identifying organic materials through use of molecular as well as elemental emission lines. LIBS is of particular interest for volatile light elements such as hydrogen and carbon, which cannot be assayed by typical elemental analysis techniques such as XRF. For that reason, LIBS will be particularly useful in lunar polar exploration, cometary and volatile-rich investigations, as well as understanding the compositions of Mars' sedimentary regions. A LIBS system is currently planned to fly on the MSL rover under the name ChemCam.

Laboratory work is integral to understanding the data from ChemCam and the rest of the MSL instrument payload. All pioneering spacecraft instruments inevitably require extensive laboratory measurements to make sense of the data they obtain. Funding sources must be available not only for the instrument teams, but also for outside investigators to bring in additional areas of expertise to maximize the value of the returned data.

4.0 Summary and recommendations

Our ability to characterize surface composition of planetary bodies is critically dependent on laboratory studies that support telescopic and spacecraft data. Much of the focus of the Decadal Survey is necessarily directed at planning for future missions. But equally important is the recognition that data obtained from existing and future missions will not be fully utilized without the benefit of supporting laboratory studies.

Among the community of researchers dedicated to compositional studies, there is an emerging recognition that environment-appropriate measurements, materials, and models are necessary to properly interpret planetary data. We recommend that such studies be encouraged and properly funded. Current NASA research and analysis programs that allow laboratory studies must be maintained.

As laboratory studies become more sophisticated, often the costs associated with them rise. Hardware and computing needs must be supported through NASA's programs. Although the Planetary Major Equipment program in tandem with other programs addresses these needs, we suggest evaluating whether an additional standalone program would better serve the communities' needs.