

CHARACTERIZATIONS OF MINERAL MIXTURES USING SPECTROSCOPY:

PHYSICAL AND STATISTICAL MODELS

TABLE OF CONTENTS

A. Scientific/Technical/Management Section	1
1.0. Background and Research Objectives	1
2.0. Understanding Reflectance Spectra	4
2.1. Spectral Characteristics of Mineral Mixtures	4
2.2. Physical Models for Interpreting Reflectance Spectra of Minerals and their Mixtures	5
2.3. Statistical Models for Interpreting Reflectance Spectra of Minerals and their Mixtures	7
3.0. Research Objectives.....	9
3.1 Task #1: Creation and Spectral Characteristics of Mineral Mixtures.....	9
3.2 Task #2: Test Physical Models for Interpreting Reflectance Spectra.....	11
3.3 Task #3: Test new statistical models as alternatives to current physical models	12
3.4 Timetable for proposal tasks	14
4.0. Relevance to NASA Goals.....	15
4.1. Goals of the Mars Planetary Geology and Geophysics Program.....	15
5.0. Data Distribution.....	15
6.0. Perceived Impact.....	15
7.0. Planetary Major Equipment Request	16
B. References	21
C. Biographical Sketch: Mario Parente	26
Biographical Sketch, Melinda Darby Dyar.....	28
Biographical Sketch, Jerry Marchand.....	29
D. Current and Pending Support.....	30
E. Budget Justification: Narrative and Details.....	34
Summary of Personnel, Commitments, and Cost	38
F. Facilities and Equipment	39
G. Instrument Quotes	41

CHARACTERIZATIONS OF MINERAL MIXTURES USING SPECTROSCOPY: PHYSICAL AND STATISTICAL MODELS

A. Scientific and Technical Management Section

SUMMARY OF RESEARCH OBJECTIVES

This proposal seeks to make fundamental advances in the interpretation of reflectance spectra of **mineral mixtures** in a more detailed and thorough fashion than has previously been attempted. This proposal has three goals:

1. Create a small spectral database of 10,000 well-characterized (with respect to complete chemical composition, purity, and very fine increments of grain size distribution) mineral mixtures.
2. Test the widely used Hapke's model, which encodes the light scattering properties of intimate mixtures.
3. Test new statistical models of reflectance spectra of mixtures as alternatives to existing physical models.

Through this research, we will produce an invaluable reference set of mineral mixtures for current and future spectroscopic measurements useful to planetary science. Our public spectral library will provide optimal data for testing and developing spectroscopic models of mineral mixtures on planetary surfaces. Both our spectra and our samples will be made available for future work. Results will improve our ability to detect and quantify minerals in mixtures and rocks through remote sensing, enhancing our understanding of geological processes on the surfaces of terrestrial planets.

1.0. BACKGROUND AND RESEARCH OBJECTIVES

Since the publication of Hunt and Salisbury's pioneering compilation of reflectance spectra of minerals (1970, 1971, Hunt et al. 1971a,b, 1972, 1973), the discipline of planetary science has come to rely upon spectral databases to interpret remote sensing data of terrestrial planetary surfaces. Several extraordinary databases are currently in use in the planetary community: the Advanced Spaceborne Thermal Emission and Reflectance Radiometer (ASTER) library at JPL (Abrams 2000, Yamaguchi et al. 1998; Abrams and Hook 1995; Baldridge et al. 2009, van der Meer 2012), the U.S.G.S. library (Clark et al. 1990, Clark 1999, Clark et al. 2007), RELAB at Brown University (Pieters 1993), and various small databases assembled by individual investigators. This massive investment of effort has created a robust assemblage of modern spectral libraries that provide broad representation of individual mineral spectra.

However, many variations and inconsistencies in the existing libraries remain. Reflectance geometries (biconical vs. bidirectional) are highly variable, depending on the facilities at the labs where spectra were acquired. Sample purity and phase identification are often problematic (Fan et al. 2012). Complete chemical compositions (e.g., including hydrogen and other light elements) are rarely known or recorded. Although grain size distributions are generally reported, the increments used vary and are often too broad, often complicating the analysis using physical models of reflectance. The existing databases focus primarily on characterizing spectral details of individual minerals, and spectra of mineral mixtures are poorly represented in any of the available spectral libraries.

The focus of this proposal is thus on the latter problem of understanding spectral signatures of mineral mixtures. Early empirical studies suggested that spectra of mineral mixtures are simply linear combinations of end-members for coarser size fractions (Singer and

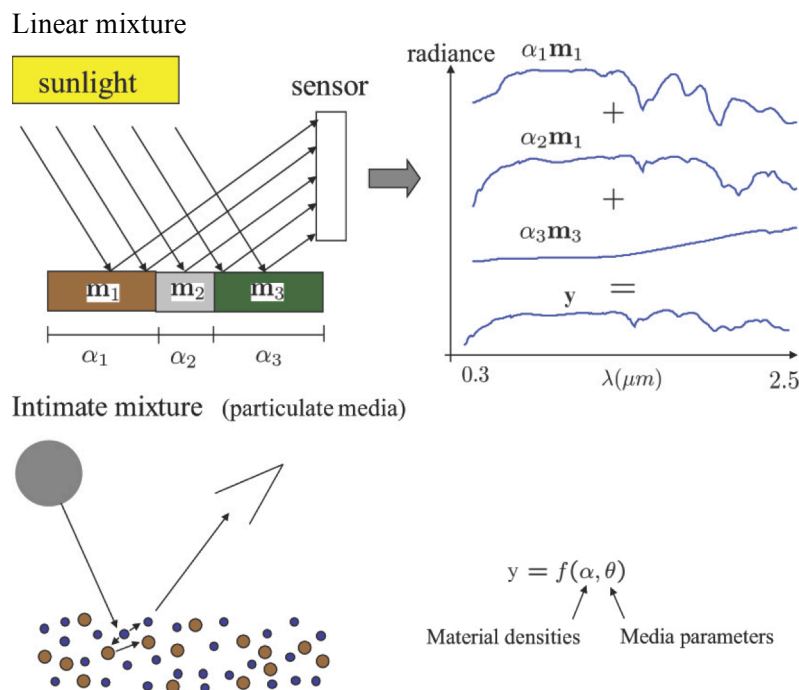


Figure 1: Pictorial comparison of linear and intimate mixing. If the end-member materials are spatially separated within the sensor field of view, the sensed spectrum is a linear combination of the end-member spectra. For intimate mixtures the light scatters multiple times off particles of several end-members before reaching the sensor. The resultant spectrum is a nonlinear function of end-member spectra, their densities and distributions.

proposal, and of our goal to provide new fundamental data on mineral mixtures, lies in the fact that spectral mixtures are not simply linear combinations (single scattering) of end-member phases. Light scatters off particles in mineral mixtures in a process defined as intimate mixing. This problem is prevalent at all scales on planetary surfaces. Multiple volume and surface scattering events from particles of different phases make the spectra of mixtures a complex nonlinear function of the end-member spectra (Figure 1). Such functions depend critically on the optical properties of the minerals themselves, the particles size distributions of each mineral in the mixture and the geometry of sensing.

Our understanding of theoretical models describing the interactions of light with these mixtures would be improved if there were multiple spectra in database libraries that contained mineral mixtures of well-characterized samples. Unfortunately, the vast majority of existing library spectra of mineral mixtures were created using weight proportions (e.g. 50 mg of olivine, 50 mg of pyroxene). If the compositions of those phases are known in detail, then the weight fractions can be converted to volume percentages (mineral modes), which are the units used by petrologists to quantify phase abundances in rocks. However, only rarely are complete chemical compositions of samples in mineral mixtures known well enough to make this conversion.

This raises the issue that creation of experimental samples suitable for understanding phenomena associated with spectra of intimate mixtures is non-trivial, for several reasons. 1) Large or multiple crystals of pure, un-zoned minerals must be available as starting materials in kilogram-weight quantities. These are rarely available in sufficient quantities from museums, so

McCord, 1979) and non-linear mixtures for microscopic and intimate mixtures (Nash and Conel 1974, Hapke 1981, Singer 1981, Lawrence and Lucey 2007, Shkuratov et al. 1999). Mustard and Pieters (1987) proposed a simplified approach to deconvoluting mineral mixtures with an estimated 5% accuracy. Subsequent improvements in modeling techniques for mineral mixtures (e.g., Sunshine and Pieters 1993) have been widely adopted within the planetary science community for spectral deconvolution and interpretation. Models of mineral mixing have been so broadly accepted that spectra of mineral mixtures are now only rarely acquired (c.f., McKeown et al. 2011; Bishop et al. 2013).

The importance of this

samples must be obtained directly from mines, private collections and mineral dealers, usually through personal contacts. 2) Minerals that grow as large single crystals may not be analogous to rock-forming minerals found on planetary surfaces. Care and attention to petrological relevance are needed to ensure the usefulness of database results. It may be better to use multiple crystals from the exact same locality than to use a single large crystal. 3) Analytical expertise is needed to accomplish complete chemical characterization of those starting minerals, particularly for hydrous phases and those containing elements that are difficult to analyze by electron microprobe (e.g., B, Li, C). 4) Size fractions must be created by hand grinding and sieving from each mineral end-member, in order to produce equivalent masses distributed over as many increments as possible, before physical mixtures are created. 5) Mixing mineral phases to ensure a random particle distribution of different phases is simply difficult, and requires many repetitions of measurements where mixtures are gently agitated to mix the components without altering their grain sizes. In short, providing the planetary community with adequate spectral data and models of mineral mixtures is thus a hands-on, time-consuming task requiring patience, persistence, and multiple expertises.

Accordingly, this proposal brings together two faculty members with the experience to make this happen. P.I. Parente has modeled spectra and worked on remote sensing of Mars since 2003 (Parente et al. 2009, 2010, 2011a,b). Co-I Dyar is a mineralogist who studies the chemical variation of minerals that are relevant to rock-forming parageneses. She has worked for more than 30 years with the international mineral collecting community and provided chemically-characterized standards for many analytical techniques including the ion microprobe, electron microprobe, and laser-induced breakdown spectroscopy. The P.I.s are joined in this work by Mount Holyoke SEM technician Jerry Marchand, who also owns the Rock and Bone Mineral Shop and has contacts with mines and collectors around the world. He will provide both the samples to be studied and the patience needed to prepare 10,000 mineral mixtures over three years. Finally, both P.I.s also employ modern machine learning techniques that implement state of the art statistical methods for geological applications (Parente et al. 2011b, Saranathan and Parente 2013, Rohani and Parente 2013, McKibben and Dyar 2011, Dyar et al. 2011, 2012, Parente and Duarte 2013). Together, this team brings to this project both an understanding of the needs of the planetary science community and the laboratory and machine learning expertise to obtain the necessary spectra and model them.

Thus, the objectives of this proposal are:

1. **We will create a small but unique spectral database of well-characterized (with respect to chemical composition, purity, and grain size distribution) mineral mixtures.** Dyar and Marchand will use their contacts in the mining and mineral collector's communities to obtain kg-weight samples of four minerals. They will purify the samples by handpicking, use various analytical techniques (electron microprobe, ion microprobe, LECO method for sulfur) to characterize them completely, and then employ x-ray diffraction to confirm phase purity. We will grind each sample into 10 increments of grain size and then create intimate mixtures of ca. 10,000 combinations of four phases and several grain sizes. Spectra of end-members and mixtures will be acquired at the University of Massachusetts in a new goniometric facility equipped with an ASD spectroradiometer and capable of fast and accurate multi-angle measurements (see Planetary Instrumentation request, pp, 16-20 of this proposal).
2. **We will use our data to test Hapke's model that encodes the spectral characteristics of mixtures.** Understanding of the current physical models of light scattering in mixtures

is made difficult by the fact that intimate mixtures with well-constrained characteristics (grain size distributions, chemical compositions, purity of phases, volumetric rather than weight proportions) are poorly represented in currently-available databases. Spectra of mixtures are available at very few grain size and abundance fraction combinations of the end-members. Reflectance measurements at different sensing geometries are even scarcer. We believe that some of the limitations observed in the application of theoretical models to reflectance measurements of mixtures can be ascribed to the fact that the currently available datasets scarcely sample the crucial parameters. We are confident that building a more detailed dataset will allow us to better characterize the biases of Hapke's model and to better constrain its parameters.

3. **We will develop and test new statistical models as alternatives to existing physical models.** Parente and Dyar benefit from their expertise in statistical learning and the proximity of and ongoing work with Collaborator Sridhar Mahadevan, an expert in transfer learning in the School of Computer Science at the University of Massachusetts. By extending statistical models developed by us for mineral identification (Parente and Duarte 2013) and building upon novel machine learning techniques implemented by Mahadevan and his students, we will use statistical models to characterize the subtle changes in the spectral features of measured samples. A first experiment will consider single end-members measured at different illumination and sensing geometries and a different grain sizes, in order to assess if the model can succinctly represent the spectral variability in a family of minerals. A second test will attempt at inferring mass fractions from spectra of intimate mixtures.

Through this research, we will produce an invaluable reference set of mineral mixtures for current and future spectroscopic measurements useful to planetary science. Our public spectral library will provide optimal data for testing and developing models of mineral mixtures on planetary surfaces. Both our spectra and our samples will be made available for future work. Our results will inform remote sensing studies of planetary surfaces and thus enhance our understanding of mineralogical and geological processes on the surfaces of terrestrial planets.

2.0 UNDERSTANDING REFLECTANCE SPECTRA

In this proposal, our goal is to create a broad suite of mineral mixtures, and then use them to test physical models of mineral mixing and to develop new alternative statistical models for the reflectance of intimate mixtures. To inform detailed discussion of our tasks, it is appropriate here to review briefly the existing background in this field and the current methodologies for dealing with their theoretical constraints.

2.1. Spectral Characteristics of Mineral Mixtures

Many investigators have proven that the reflectance spectra of most natural surfaces are modeled by intimate mixing. Examples are soil surfaces (Borel and Gerstl 1994) and mineral mixture surfaces (Nash and Conel 1974, Clark 1983). In an intimate mixture, each component is randomly distributed in a homogeneous way, within the field of view of the instrument (Mustard and Pieters 1989). The light interacts with multiple materials as it is scattered by the mixture before enters the sensor. As a result, the reflectance spectrum of the mixture is a nonlinear combination of the reflectance spectra of the individual components (Nash and Conel 1974, Clark 1999). These kinds of mixtures are treated as particulate media (Johnson 1983).

A large and growing body of research on the spectroscopy of naturally occurring particulate media has been conducted largely by the planetary geoscience community. The object of the studies has generally been the spectral signature systematics of extraterrestrial regoliths

composed of mixtures of naturally occurring mineral particulates such as plagioclase feldspar, olivine, pyroxene, and iron oxides; iron-rich glass agglutinates in the lunar regolith have also been studied (Pieters et al., 1993; James et al., 2001; Pieters and Taylor, 2003). Martian research has been focusing on clays and carbonates (e. g. Bishop et al. 2013, McKeown et al. 2011)

2.2. Physical Models for Interpreting Reflectance Spectra of minerals and their mixtures

Models to describe the interaction of light with particulate surfaces based on the theory of radiative transfer (Chandrasekhar 1960) have been developed by many investigators using different approaches such as Monte Carlo ray tracing (e.g. Govaerts and Verstraete 1998), the radiosity model (Borel and Gersti 1991) and the multi-stream method (Chandrasekhar 1960). These models can explain the light scattering properties of the particulate medium.

Hapke (1981) presented a solution of the radiative transfer problem for a particulate medium by deriving a first-order analytic expression relating parameters such as bidirectional reflectance and single-scattering albedo (Johnson 1983). Variables in Hapke's equation have physical significance. Equations are presented for computing the mass fractions of components in intimate mixtures (Mustard and Pieters 1989).

Hapke (1981) derived an expression for the bidirectional reflectance model of a semi-infinite medium surface filled with isotropic scatterers. The particle (grain) size is assumed to be

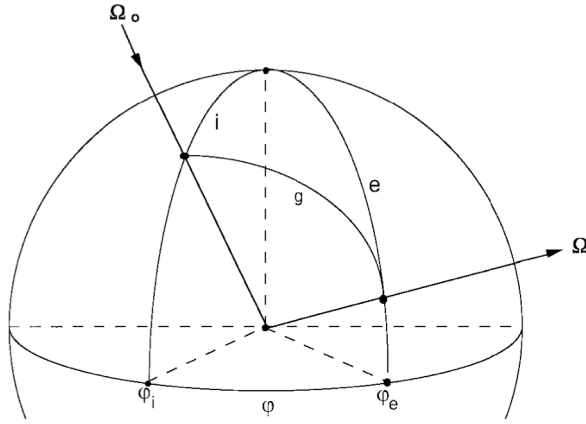


Figure 2. Illumination and sensing geometry for the measurements of bidirectional reflectance (adapted from Hapke (2002)).

much larger than the wavelength of light under consideration. Such expression is a non-linear relation of the scattering properties of the material and the geometry of illumination and detection. One of the scattering properties is the single-scattering albedo, which describes the interaction of light with a single particle within the surface. This interaction includes the reflection, absorption and scattering caused by the particle (Hapke 1981,1993)

This is of interest because the mixing model for an intimate mixture is linear if the reflectances are expressed as single-scattering albedos (Mustard and Pieters 1989). The average single-scattering

albedo of a mixture is a linear combination of the single-scattering albedos of each of the components in the mixture. Several researchers used this approach in nonlinear unmixing problems (e.g. Clark and Roush 1984, Mustard and Pieters 1989).

In our experiments, reflectance measurements will be obtained as ratios of the brightness of the sample at a specific viewing geometry to the brightness of a reference standard identically illuminated. This illumination and sensing geometry is depicted in **Figure 2**. Because the scattering behavior of our reference standard will be approximately assumed to be a Lambertian surface, the reflectance coefficient R (brightness relative to a Lambertian surface) is given by Hapke (1981, 1986, 1993, 2008) as:

$$R_{\lambda}(i, e, g) = K \frac{w}{4} \frac{1}{\mu_0 + \mu} \{ [1 + B(g)] p(g) + H(\mu_0) H(\mu) - 1 \}. \quad (1)$$

Here $R_{\lambda}(i, e, g)$ is the reflectance coefficient at wavelength λ , w is the average single-scattering albedo of the mixture, $\mu = \cos e$, $\mu_0 = \cos i$, i is the incident angle of the collimated light

source, e is the viewing angle of the detector with respect to the surface normal, g is the phase angle formed by the direction to the light source Ω_0 and the direction of the reflected light Ω , and $p(g)$ is the phase function (Hapke 1986, 1993), which expresses the dependence of the relative amount of light scattered by the particulate surface, on the angle formed by the incident and viewing direction. $B(g)$ is the backscatter function expressing a sharp surge in the brightness at near zero degrees of phase angle (Hapke 1986), and $H(x)$ is Chandrasekhar's H -function (Chandrasekhar 1960) for isotropic scatterers. We assume that we can prepare the samples in such a way that the effect of the macroscopic roughness on the reflectance can be neglected (Hapke 1984).

The parameter K is used to account for the effect of porosity and is calculated for equant particles as (Hapke 2008): $K = -\ln((1 - 1.209\phi^{2/3})/1.209\phi^{2/3})$ (2)

where ϕ is the filling factor. Hapke's approximation to the exact H -function, which results in an error of less than 4% from the exact values everywhere (Hapke 1993) is given by (Hapke 2008):

$$H(x) = \frac{1 + \frac{2x}{K}}{1 + \frac{2x\sqrt{1-w}}{K}} \quad (3)$$

The backscatter function, also known as the opposition effect in planetary observations, and the hot spot in remote sensing of plant canopies, is the relative amount of light scattered back along the preselected direction the incident ray came from. This effect is a general property of particulate media, such as vegetation and soil (Hapke 1993).

While deriving the solution for radiative transfer equation for an intimate mixture of minerals the effect of decreasing inter-particle spacing has to be taken into consideration. To account for such effects Hapke introduced another parameter in the reflectance equation, which is known as the backscatter function (Hapke 1986, 1993): $B(g) = \frac{B_0}{1 + (1/h) \tan(g/2)}$ (4).

The parameter h characterizes compaction of the regolith and size of the particle ranges. If the particle size distribution is narrow and the particles equant, then $h = -3\ln(1 - \phi/8)$ (5) where ϕ is the filling factor. The parameter B_0 defines amplitude of the opposition effect. For a low-albedo surface, the parameter $B_0 = 1$. The phase function $p(g)$ can be given using Legendre polynomial (Hapke 1981, 1993) as in:

$$p(g) = 1 + b \cos(g) + c \frac{(3\cos^2(g) - 1)}{2} \quad (6)$$

For realistic phase functions, coefficient b is constrained to lie between -1.732 and 1.732 while c may vary between -1.0 and 2.0 (Mustard and Pieters 1989). Admissible combinations of b and c that do not allow unrealistic scattering behavior (e.g., negative scattering) are slightly more limited than the above general limits indicate. The $\cos(g)$ can be evaluated using i , e , and ϕ (the differential azimuth angle): $\cos(g) = \cos(i) \cos(e) + \sin(i) \sin(e) \cos(\phi)$. (7)

From the variables that appear in equation (1), single-scattering albedo is used to predict the mixing model of intimate mixtures. The average single-scattering albedo of a mixture, considered a close-packed medium (powder or soil), is a linear combination of the single-scattering albedos of each pure class in the mixture (Hapke 1993). The relationship is given by:

$$\bar{w} = \frac{\sum_j \frac{M_j}{\rho_j D_j} w_j}{\sum_j \frac{M_j}{\rho_j D_j}} \quad (8)$$

where M_j , ρ_j , D_j , and w_j are the mass fraction, single-particle density, average effective particle size, and single-scattering albedo of the j -th component in the mixture. Components can be different minerals or different grain sizes of the same material or both. The phase function and

the opposition effect function for an intimate mixture also depend on the corresponding functions calculated for the end-members and such dependencies are expressed by equations similar to equation (4) (Hapke 1993) and involve the end-member mass fractions as unknowns.

The model expressed in equation (1) is defined as the “porosity correction” to the isotropic multiple scattering approximation (IMSA) by Hapke (1981, 1993, 2008). Many researchers over the years have attempted to quantitatively assess the validity of the model (e.g., Hiroi and Pieters 1994, Poulet and Erard 2004, Shepard and Helfenstein 2007) including Hapke himself (e.g., Hapke et al. 2009). Several considerations lead us to employ this model:

- 1) Hapke found good agreement of the IMSA model with the reflectance measurements of a well-characterized medium (Hapke et al. 2009) when compared to a complicated direct numerical solution of the radiative transfer equations by Mishchenko et al. (1999).
- 2) Many of the proposed models in the literature (e.g. Hapke 1981, 1993, 2002, 2008, Shkuratov et al. 1999, Mishchenko et al. 1999) introduce some systematic bias with respect to the observations due to the various assumptions and approximations. Our approach to the problem, instead of trying to minimize the bias in the IMSA model, attempts to completely characterize the bias using a very large number of measurements. Such information can be used in future applications of the IMSA model on other samples.
- 3) Although several improvements to the model have been proposed, including a more accurate multiple scattering term taking into account anisotropic scatterers and the coherent backscatter opposition effect (Hapke 2002), such models require more complicated integral equations and a proliferation of parameters. The IMSA model is widely utilized also because of its analytical formulation and the relatively low number of parameters, which allows a more direct interpretability of the fitting results. For example, it is not clear how to interpret the relationship between phase functions of end-members and mixtures if a more complicated model than the IMSA is used.

2.3. Statistical Models for Interpreting Reflectance Spectra and their Mixtures

There are some limitations of the Hapke’s model that are difficult to overcome. For example, the Hapke’s model and other models based on geometric optics assumptions (e.g. Shkuratov et al. 1999) require that the diameter of particles composing the medium under study be several times larger than the observed wavelength. The scattering behavior of small particles is not completely understood but recent studies (e.g. Piateck 2003) show that small particles do not tend to scatter independently. A related issue is that the model (and in particular equation (8)) does not take into account that the single scattering albedo of a distribution of grain sizes in a mineral is often dominated by smaller grain sizes. In general, we recognize that a physical model cannot explain away all the possible situations.

In addition to limitations on the theoretical formulation of Hapke’s model or other physically-based models, the variations in the model parameters are not directly interpretable as variations of spectral features, such as absorption band position and depth, which are the diagnostic information that spectroscopists use to identify mineral species. We will develop a flexible mathematical model that promises to capture all the subtle changes in reflectance spectral shapes that are due to changing measurement conditions, particle sizes, and (for mixtures) fractional abundances of end-members. In particular, we consider a model that can capture scientifically meaningful information from the spectral signatures of minerals under study and encode it in a succinct fashion for use in efficiently identifying mineral spectra.

While other researchers have constructed complicated ad-hoc rules to encode the diagnostic features of mineral spectra (e.g. Clark et al. 2003), our proposed model, based on

wavelet-domain representations, will be able to encode the same diagnostic information as physically-based models without relying on ad hoc rules, interpreting unknown spectra based on training data obtained automatically from a library of reference spectra.

2.3.1. Wavelet-based statistical model for mineral representation.

We will use a continuous wavelet transform (CWT) to provide a multi-scale analysis of a spectrum’s content, effectively encoding in a compact fashion the locations and scales at which diagnostic structure is present. The CWT of a spectrum $x(\lambda)$ is composed of wavelet coefficients $w_{s,u}$ labeled by a scale s and offset u , and defined as $z_{s,u} = \int x(\lambda)\psi_{s,u}(\lambda)d\lambda$, where $\psi_{s,u}$ denotes the mother wavelet ψ dilated to scale s and translated to offset u , i.e., $\psi_{s,u}(\lambda) = \psi((\lambda - u)/s)/\sqrt{s}$.

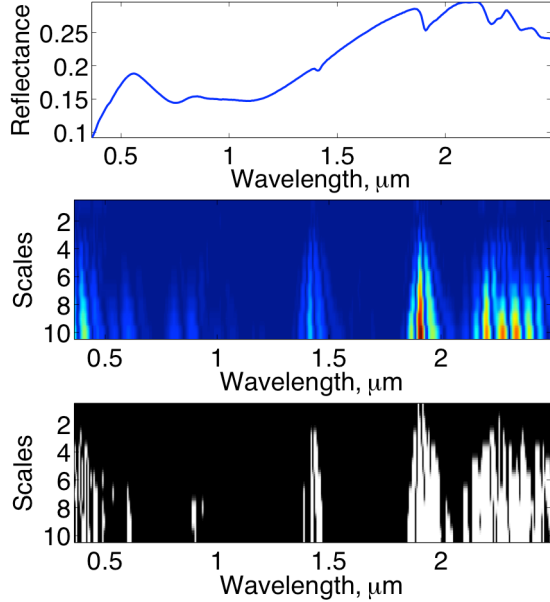


Figure 3. Top: Example spectral signature. Center: Corresponding CWT coefficient array (9 scales). Small/large coefficient magnitudes are shown in blue/red. Bottom: labels obtained for the example spectral signature using a NHMC model. White corresponds to large labels; black to small.

Each coefficient $z_{s,u}$ at scale s represents a discontinuity detector over a portion of the spectrum of size proportional to s around the offset u . A large wavelet coefficient (in magnitude) generally indicates the presence of a discontinuity inside its support; a small wavelet coefficient indicates a smooth region. The wavelet coefficients over a grid of scales s and offsets can be organized into a matrix Z , where each row represents a different scale and each column represents a different band (cf. Figure 3). A pair of coefficients $z_{s,u}$ and $z_{s+1,u}$ at the same offset and neighboring scales are referred to as a parent and child coefficient, respectively; the columns of coefficients in Figure 3b correspond to sequences of parent/child wavelet coefficients.

Discontinuities in general manifest themselves in the wavelet domain as chains of large coefficients propagating across scales, a phenomenon known as persistence. In Figure 3b, we see persistence causes absorption bands of each mineral to be represented by peaks of large wavelet coefficients.

To capture the correlation between parent and child wavelet coefficients, we will use a model based on Nonhomogeneous Hidden Markov Chains (NHMC) (Parente and Duarte 2013). In such a model, each wavelet coefficient $z_{s,u}$ is statistically modeled using a mixture of two Gaussians. The first component features a large variance, which models large nonzero coefficients and receives a small weight (to encourage few such coefficients). The second component features a small variance that models small and receives a large weight. The weights of wavelet coefficients are linked probabilistically because the weight of coefficient $z_{s+1,u}$ depends on the weight of the parent coefficient $z_{s,u}$. We separately train an NHMC on each of N wavelengths to capture the dynamics of observable spectral signatures for each wavelength individually. Details of the model can be found in Parente and Duarte (2013).

The model uses machine-learning approaches to learn a set of labels. Label $S_{s,u}$ is defined LARGE (SMALL) if the weight of coefficient $z_{s,u}$ is more likely to be large (small). The presence of a fluctuation in a spectral signature, such as an absorption band, is represented by

chains of LARGE labels $S_{s,u}$ appearing for the corresponding wavelengths (cf. [Figure 3](#)). The algorithm also returns the variances of wavelet coefficients as a byproduct.

The model is trained on a large number of available spectra. Ideally, the training library would be composed of a variety of minerals acquired at different geometries and grain sizes. This is a fundamental difference with more physically based approaches. The model learns diagnostic labels in a statistically significant way from a library of spectra, which represents as much as possible the full array of possible mineral signatures in nature. The labels will be able to represent a mineral in a really discriminative way without the need to define discriminative rules for any possible mineral family.

3.0. RESEARCH OBJECTIVES

3.1. Task #1: Creation and Spectral Characteristics of Mineral Mixtures

3.1.1. Selection of Minerals. For this project, we will focus on using samples found on airless bodies on terrestrial planets in our solar system. [Table 1](#) summarizes the major minerals found on the Moon, asteroids, and Mercury, from which we will make our selections. Our goal is to choose only four minerals to study thoroughly, though we will add additional samples as time and funding allow. It is impossible to represent the compositional variability in all airless bodies, but we will choose samples with maximum usefulness. From [Table 1](#), it is apparent that these four phases should be olivine (likely Fo_{70-90}), feldspar (An_{70-90}), orthopyroxene (pure or very low Fe enstatite), and a clinopyroxene (augite or diopside). Of course, we recognize that these four minerals will not encompass the breadth of geological diversity on airless bodies, and it will be very tempting to include additional phases in our measurements. However, we wish to use the tests of physical and statistical models in tasks 2 and 3 of this proposal to carefully investigate effects of both

mineralogical diversity and physical and statistical models. By simplifying one variable (mineralogy) to only four possibilities, we will obtain maximum insights from those models. So we choose to keep this study very focused, using only four different minerals.

Because we have been thinking about this project for several years, we already have in hand some materials appropriate for this project. We were fortunate to find a large quantity of gem-quality olivines (Sapat Mine in the Kohistan District, NWP, Pakistan) from an old collection that was de-accessioned by a

Table 1. Simplified Summary of Mineralogy on Airless Bodies

Body	Mineral	References
Moon	feldspar (Ca-rich, ca. An_{95}) ilmenite olivine (Fo_{61-89}) clinopyroxene (augite/pigeonite) e.g., $\text{Wo}_{28}\text{En}_{20}\text{Fs}_{52}$ orthopyroxene spinel	Papike (1996, 1998) Papike et al. (1998) Karner et al. (2003) Dhingra et al. (2011) Kaur et al. (2013)
Mercury	tridymite/quartz plagioclase (An_{85-100}) clinopyroxene (diopside/augite) olivine (Fo_{92-95}) corundum orthopyroxene (enstatite) Fs_{7-17} sulfide	Vilas (1988) Nittler et al. (2011) Weider et al. (2012) Stockstill-Cahill et al. (2012) Charlier et al. (2013)
Asteroids	Olivine, average Fo_{70-86} Pyroxene, average Fs_{14-25} augite or diopside, typically $\text{Fs}_{10}\text{Wo}_{45}$ Fe metal enstatite feldspar hydrated minerals	McSween et al. (1991) Brearley and Jones (1998) Middlefehldt et al. (1998) Gaffey et al. (2002) Burbine (2013) Dunn et al. (2013)

collector. We have identified a collector with large amounts of true anorthite from the Sterling Mine deposit in Ogdensburg, New Jersey, which is very difficult to find. Pure ilmenite from the Iron Hill locality in Gunnison Co., Colorado is commercially available. Enstatite occurs in blades up to 50 cm length in lamprophyre dikes at the Whatcom Co. localities (Twin Sisters Mountain) in northwestern Washington State, which is commercial production for its olivine; the host rock there also contains olivine and clinopyroxene (Onyeagocha, 1978). If we can obtain a large mass of unaltered samples from that locality, it may provide both pyroxenes (though it would require hand-picking on a massive scale). In all cases, we will carefully re-analyze all samples, checking for homogeneity, before we undertake preparation of samples.

3.1.2. Sample Preparation Methodology. In this task, we will undertake the formidable project of preparing ~10,000 mineral mixtures with varying grain sizes. Key to this endeavor are the skills of Mount Holyoke SEM technician and staff member Jerry Marchand, who will be supported by this grant half-time for its duration. Jerry also owns the Rock and Bone Mineral Shop, attends numerous mineral shows throughout the year, and has contacts around the world in both museums and the mining community. He has frequently been successful in obtaining both donated samples and wholesale pricing for Dyar's research group; for example, he has built up an excellent meteorite collection at the College for very little cost. Jerry will be charged with obtaining samples needed for this project through his sources, with help from Co-I Dyar; we have budgeted ~\$6,500 for their purchase, an amount that represents our best guess of the wholesale cost of what we will need. Once the samples have been obtained, Dyar will coordinate the analytical work that needs to be done, likely using the services of ACT-LABS (see Budget Explanation for Mount Holyoke College).

Jerry Marchand will also prepare the initial splits of mineral separates for this project, carefully grinding each sample into ten different size fractions from 10 μm to 500 μm . This step must be done by hand to ensure that roughly equal amounts of sample are produced in each desired grain size fraction. Mineral mixtures will then be calculated for our target of ~10,000 samples, working from volume percent to weight percent using the determined composition and tables of density for the minerals used.

We calculated that the total number of samples generated by mixing 4 minerals, each at any of m grain sizes and at any of $k+1$ abundance fractions (including 0% and 100%) is $S = m^4 (k+1)(k+2)(k+3)/3!$. The values of S closest to 10000 are obtained for $m=3$, $k=7$ ($S=9720$) and for $m=5$, $k=3$ ($S=12500$). We will then create a recipe sheet for creating the mixtures, 144 at a time (the number of vials in the box). In doing this, we can account for the fact that we will likely produce uneven quantities of mass for some bin sizes. Although this represents a massive effort, it is necessary to produce the first statistically-significant dataset to deal with different aspects of variability in scattering models.

We estimate that preparing the starting size fractions of four samples by hand will take roughly 80 hours of effort, while creating the 10,000 mineral mixtures in labeled vials will need roughly five minutes per sample, or roughly 833 hours (21 full-time weeks). So preparation of samples should require a full year of Marchand's time at 50% effort. We believe that this project is ambitious but manageable. Working in Dyar's lab, Jerry Marchand has recently prepared 3,000 pressed pellets of rock powders for ChemCam calibration on Mars Science Laboratory (requiring roughly 15 minutes per pellet!), so we know that he has patience and meticulous attention to detail to successfully make the required mineral mixtures. In the latter two years (or whatever time is left after creating the mixtures) of the proposal, Marchand will also work 50% time to acquire data on our spectrometer.

3.1.2. Measurement Methodology. For the bidirectional reflectance measurements, the sensor–target distance will be set at 15 cm. The IFOV of the ASD will be set at 1°. The area of ground from which spectra are recorded, or ground-field-of-view (GFOV) can be as small as 2 mm when the spectrometer is set at 10-15 cm from the sample. Measurements will be taken at a different discrete illumination zenith angles. Typical values are 30° or 45°.

Data are collected in radiance mode via the spectro-radiometer. The full measurement cycle is also performed for a Spectralon reference panel under the same geometrical configurations used for the samples. This process corrects for any asymmetry of the light source footprint on the target, ensuring that the amount of light incident to the sample holder is always the same for two corresponding measurements of sample and Spectralon. Consequently, errors resulting from the experimental setup such as illumination heterogeneity or detector footprint variations are likely to cancel because they occur for both the reference panel and target measurements in an equal way (Hapke 1993, Schönermark et al. 2004). The division of the two radiance cycles provides the reflectance of the target at each sensor-light angle combination.

The reflectance factor for the geometry (i, e) is given by

$$REFF_\lambda = \left(\frac{\frac{DN_\lambda(i,e) - DC_\lambda}{\frac{DN_{\lambda, \text{spectralon}}(i,e)}{C_{\lambda, \text{spectralon}}} - DC_\lambda}}{1} \right) \quad (9)$$

$DN_\lambda(i, e)$ and $DN_{\lambda, \text{spectralon}}(i, e)$ are the spectral digital number recorded by the ASD spectro-radiometer for the view zenith angle e and view azimuth angle from the target sample and the Spectralon respectively, DC_λ is the spectral dark current measurement and $C_{\lambda, \text{spectralon}}$ is the spectral calibration coefficient provided by the manufacturer that allows absolute reflectance measurements. Dark current is the digital number recorded by the ASD when the fore optic is completely occulted and represents the inherent instrument noise. The sample will be measured by selecting resolution values over the full azimuthal plane and over a range of zenith angles (e.g. from -60° to $+60^\circ$). Additional measurement can be performed over the principal plane to better characterize specular components and around the for the characterization of the backscatter. A resolution of 30° over the azimuthal plane and of 15° over the zenith range -60° to $+60^\circ$ will produce around 80 measurements.

3.2. Task #2: Test Physical Models for Interpreting Reflectance Spectra

3.2.1 Current unmixing approach.

The Hapke model can be summarized as:

$$R_p(\lambda_k) \approx R(i_p, e_p, \phi_p, w(\lambda_k), B_0, b, c, \phi), \quad (10)$$

where i_p , e_p , and ϕ_p form the vector \mathbf{x}_p of independent variables (i.e. the angles for the p -th geometrical arrangement) while $w(\lambda_k)$ and the $\vec{a} = (B_0, b, c, \phi)$ represent the (unknown) parameters of the problem, $R_p(\lambda_k)$ is the measured reflectance of a sample at the wavelength λ_k , w_k is the single scattering albedo at wavelength λ_k , and R is the function in equation (1).

According to several studies in the literature (e.g., Helfenstein 1986 and refined by Helfenstein and Veverka 1987), unmixing is performed by deriving the single-scattering albedo of the mixture using least square error fitting with equation (5). The single-scattering albedo w is chosen so that it minimizes χ^2 , which is here defined as:

$$\chi^2 = \sum_{p=1}^n \left[\frac{R_p - R(w, i_p, e_p)}{\sigma_p} \right]^2 \quad (11)$$

where σ_p , R_p , i_p and e_p are the measurement error, the measured reflectance value of a material, the incident angle of the light, and viewing angle of the p th experiment. $R(w, i_p, e_p)$ is the

theoretically predicted bidirectional reflectance by equation (1) for the p -th sensing geometrical arrangement. So this method requires the measurement of the reflectance of the mixture for several geometries (e.g., at several angles of (e_p, i_p)), to obtain a reliable value for its albedo.

We define w_{kj} to be the single-scattering albedo of component j th at spectral band k th. Therefore, the combined albedo is given by equation (4) (but for w_{kj}), where w_k is the average single-scattering albedo of the mixture in the k th spectral band. The end-member and mixture single-scattering albedos derived by (5) are then used to solve equation (4) in the least square error sense again to obtain the abundances M_j . We will apply this model and verify the discrepancy between the calculated and measured abundances.

A complication in the application of equation (5) is the strong coupling between the parameters. Several investigators (e.g., Helfenstein and Veverka 1987, Mustard and Pieters 1989) have noted that the parameters can be strongly coupled in a mathematical sense, which may result in solutions to the equation that are physically unrealistic. We will investigate the issue and establish the dependence of the problem on the number of measurements. A related issue is that the technique prescribes the solution of equation (5) independently for each end-member and mixed spectrum and for each wavelength. Because it operates independently on each wavelength it will produce wavelength dependent values for B_0 , b , c , and ϕ . We will explore such spectral dependencies and observe variations as a function of the number of measurements.

3.2.2 Alternative unmixing approach. The dependence of the α parameters on wavelength, which stems from the current fitting approach, is contrary to the Hapke formulation. An alternative approach will solve the problem simultaneously for all wavelengths. The N experimental design variables x_p , $p = 1, \dots, N$ are fixed and known, so we can form the $N \times M$ observation matrix \mathbf{R} with (p,k) -th element $R_p(\lambda_k)$, with M equal to the number of wavelengths and the $N \times M$ expected response matrix $H(\Omega)$ with (p,k) th element $R(i_p, e_p, \phi_p; w_k, B_0, b, c, \phi) = R(x_p; w(\lambda_k), \alpha)$. Also, Ω is the vector $(w_1, \dots, w_M, \alpha)$. From R and $H(\Omega)$, we create the residual matrix $Z(\Omega) = R - H(\Omega)$.

A simple least squares formulation is needed to find the parameter Ω that minimizes $Tr(Z^T Z) = \|Z\|_F^2$, subject to some constraints on the parameters. Trust region algorithms can be used to solve the least squares problem (reference). This approach has the advantage of finding wavelength independent values for the α parameters but it ignores the possible correlation between reflectance values at different wavelengths.

3.2.3 Improvement on the constraints on the abundances. The algorithm proposed in section 3.2.1 calculates the abundances of the end-members exclusively based on the single scattering albedo (equation (4)). Such approach ignores the dependence of the phase function and opposition effect function of the mixture from the corresponding functions calculated for the end-members. We will investigate the effect of using such equations together with equation (4) to constrain the abundance values.

3.3. Task #3: Test new statistical models as alternatives to existing physical models.

We will also use our new data set to innovate novel statistical methods that provide potentially-powerful alternatives to the physical models. We have undertaken considerable proof-of-concept work in this area. Parente and Duarte (2013) showed that a statistical model outperformed other automatic approaches in tasks where the goal was to identify the dominant mineral species in an observed spectrum by comparing it with a small library of reference signatures. The spectra to be identified were taken from the library itself or from a hyperspectral image. We believe that the discriminating nature of the state labels in this application allows for

efficient and simple classification algorithms such as nearest-neighbor search, in contrast with existing ad-hoc approaches that aim to capture these cues using custom similarity measures.

In this proposal, we will use the statistical models not as classifiers, but rather to characterize the subtle changes in the spectral features of measured samples. A first experiment will consider single end-members measured at different illumination and sensing geometries and a different grain sizes, in order to assess if the model can succinctly represent the spectral variability in a family of minerals. A second test will attempt at inferring mass fractions from spectra of intimate mixing.

3.3.1 Characterization of mineral spectral variability. Based on our experience with the Hapke physical model of reflectance, we hypothesize that geometry and particle size will tend to mostly affect the overall albedo and the contrast of absorption bands (e.g. Hapke 1993, Sunshine 1990, Mustard and Pieters 1989, etc.) whereas grain size has the potential to cause more complex effects. A complicating issue is that real samples contain a range of particle sizes, where each narrow range contributes to the spectrum, so it is important to accurately characterize the size fraction distribution of the measured samples. Thus we will compare the label maps of spectra of all the grain size separates in each mineral family acquired at different sensing geometries to identify patterns of variations that are independent of composition. While several trends are known in the literature (e.g., the invariance to grain size variations of position of the minimum of absorption bands), the combination of the effects of geometry and grain size has not been studied in detail. Furthermore, the NHMC model allows us to represent all possible spectral changes in the label maps. We will rely on our collaborator Dr. Mahadevan to suggest viable machine-learning approaches to establish a mineral independent functional of the spectral variations due to particle size and geometry.

3.3.2 Characterization of end-member fractions. In this experiment, we will consider mixture modeling through use of the NHMC model. This is a more complicated task than mineral identification because the model must correctly identify the presence of fluctuations in the spectra of reduced magnitudes that are characteristic of element mixtures. Strings of labels that are associated with spectral regions that are discriminative for each of the mixture elements would also be discriminative for the mixed spectra. In such a case, the label representations of the mixed spectra should only differ from those of the end-members in localized regions, while discrepancy between map values of mixed spectra and other spectra in the library (non end-members) should be more extensive.

To validate the hypothesis formulated in the previous section, we will set up a contrived experiment using the USGS mineral spectral library (Clark et al. 2007) to train the NHMC model. Two elements of the library are linearly mixed (out of 480 mineral spectra, sample 226, a montmorillonite and sample 304, a nontronite) with abundances of montmorillonite varying between 10 % and 90%. **Figure 4a** depicts the spectra of montmorillonite, the brighter spectrum, nontronite, the darker spectrum and the progression of mixed spectra in between them. We used linear mathematical mixing of intimate mixtures make the results more easily interpretable. After training the model on the USGS mineral spectra we extract labels for each mixed spectrum. **Figure 4(b--d)** shows the similarity between element mixtures, mixture component end-members, and next closest minerals in the USGS library, using different similarity metrics. Metrics generated from NHMC labels clearly provide higher discriminability between end-members in the mixture and the rest of the end-member library than the original spectra. Note that for a large fraction of the mixtures, one of the component end-members is closer than the rest of end-members in the library in **Figure 4(b--c)**. In contrast, **Figure 4 (d)** shows the potential for

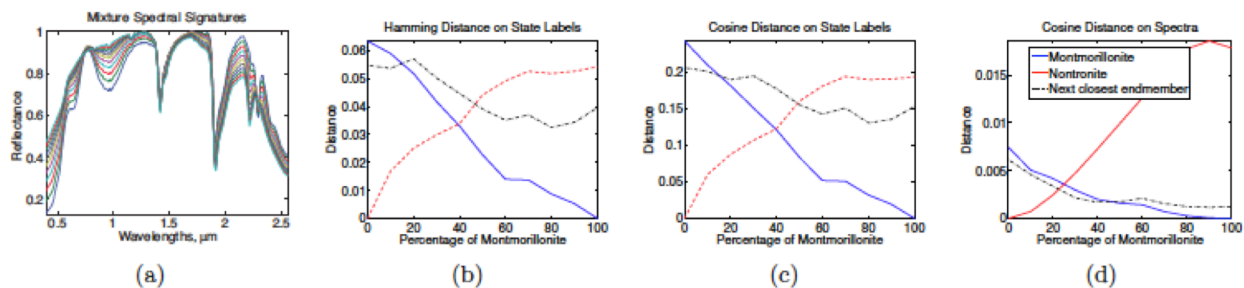


Figure 4. Performance of HMM labels for spectral unmixing. An HMM is trained using 480 end-members from a USGS database. (a) Spectral signatures for varying mixtures of montmorillonite and nontronite end-members. (b){d} distances between each mixture spectra and the nontronite and montmorillonite end-member spectra, as well as to the next closest end-member spectrum in the database; distances used are (b) Hamming distance on HMM labels, (c) cosine distance on HMM labels, (d) cosine distance on spectra.

mislabeling mixture elements: the distance between the mixture and montmorillonite is close (or larger) to that of the closest end-member not present in the mixture for all abundance values. The experiment shows that labels carry discriminative information. We can use the same set-up to identify end-members in unknown mixtures because the model needs no prior information.

We further propose to use labels to infer abundances of end-members in mixtures, possibly by comparing the label maps of end-members and their intimate mixtures and analyzing the number and positions of labels that change state. For binary mixture, we should be able to extract a trend should be proportional to the abundance of each end-member in the mixtures similar to the trend we observed in [Figure 4](#). For mixtures of three or more minerals, the relationship is multidimensional and we need more experiments to hypothesize a solution.

3.4. Timetable for Proposal Tasks

Work on our proposal objectives will proceed in parallel during the three years of the grant; though the tasks will all complement and feed into one another. A summary of tasks, timing and personnel is presented in [Table 2](#) below.

Parente and his graduate student will purchase, install, and operate the new ASD spectrometer. Meanwhile Dyar and Marchand will assemble the mineral mixtures. The team will work together to acquire spectral data on all samples and post them on a web site. Parente's graduate student on this project will then use the mineral mixture spectra to test existing physical and statistical models for mineral mixing and develop new innovative techniques, with advice from Collaborator Mahadevan. Members of the team will make presentations and write publications to disseminate this work. Finally, Dyar will curate the mineral mixtures and make them available to the community for other types of non-destructive spectroscopic measurements.

Table 2. Proposed Work and Timetable (Details)

Tasks	Personnel	Yr 1	Yr 2	Yr 3
1A. Acquire samples for mineral mixtures	Dyar, Marchand	X		
1.B. Obtain chemical analyses of minerals	Dyar	X		
1.C. Prepare mineral mixtures	Marchand, Dyar	X	X	
1.D. Acquire reflectance spectra	Marchand, Parente, graduate student	X	X	X
2.A. Test Hapke model	Parente, graduate student	X	X	
2.B. Test alternative unmixing approaches	Parente, graduate student	X	X	X
2.C. Improve constraints on abundances	Parente, graduate student	X	X	
3.A. Characterize mineral spectral variability	Parente, Dyar, graduate student, Mahadevan	X	X	X
3.B. Characterize end-member fractions		X	X	X
4. Purchase and install ASD spectrometer	Parente, graduate student	X		
All. Prepare and submit publications	Parente, Dyar, graduate student	X	X	X

4.0. RELEVANCE TO PLANETARY GEOLOGY AND GEOPHYSICS GOALS

The goals of the PGG (Planetary Geology and Geophysics) program are to foster the synthesis, analysis, and comparative study of data that will improve the understanding of the extent and influence of planetary geological and geophysical processes on the bodies of the Solar System. This investigation requests support of a fundamental scientific investigation of the spectral characteristics of mineral mixtures, in direct service of the PG&G goal to further our understanding of planetary surfaces through enhanced analysis of mineralogy. Our work will support several types of research solicited by this program, including “Mineralogical, lithological, and geologic mapping of planetary surfaces” and “Generation of new data in a laboratory or field environment.”

5.0. PRODUCTS AND DATA DISTRIBUTION

All software written for this package will be in the “R” language, which is freely distributed. We will post our packages for implementation of different models on Comprehensive R Archive Network (CRAN) at <http://cran.r-project.org/>. CRAN is a network of ftp and web servers around the world that store identical, up-to-date, versions of code and documentation for R. Thus our software products will be widely available for other users.

Moreover, all spectral data collected for this project will be posted on the Dyar lab website at www.mtholyoke.edu/go/mars. This effort will be supported by a web programmer who will build the site for Dyar that is analogous to existing sites for Mössbauer and laser-induced breakdown spectroscopy data. We have requested funds in our budget for an undergraduate researcher in each summer to build and maintain our data on this web site for public distribution.

The other resource created by this project will be our physical library of mineral mixtures (contained in 10,000 glass vials). These samples will be curated by Dyar in her collections (which also include numerous other international standards) until she retires. At that time, they will be turned over to Parente. This will ensure that the mixtures will be available to other researchers for other types of non-destructive spectroscopic measurements in the future.

6.0. PERCEIVED IMPACT

Because both the spectra and the physical samples (mineral mixtures in vials) from this study will be made available to the planetary community for future work. Advances in statistical and physical models by many workers will be made possible by the availability of our data. Other analytical techniques (Raman, mid-IR, high- and low-temperature reflectance, etc.) will benefit from measurements of these mixtures. As technology advances, it will also be possible to re-measure the reflectance spectra of these samples, ensuring the long-term impact of the initial investment in creating this suite of mixtures.

The immediate impact of this project will be improvements in our ability to accurately estimate mineral abundances on terrestrial planetary surfaces (including Earth). Our suite of improved and novel models will support gaining new insights into the mineralogy and geochemistry of their surfaces. Geological questions that will be informed by the work in this proposal include significant issues such as planetary formation and evolution, the composition and parageneses of crustal materials, and links between surface deposits and climate. *Every improvement in the accuracy of models that recognize and quantify mineral signatures in reflectance spectra will improve our ability to address those critical questions*, and this is our motivation for and the primary impact of the proposed work.

7.0. PLANETARY MAJOR EQUIPMENT REQUEST

7.1. The Need for more precise BDRF measurements

In order to fit a physical or mathematical model of the reflectance coefficient, often called Bidirectional Reflectance Factor (or BRF), accurate bidirectional measurements at different illumination, view and phase angle have to be acquired. Traditionally such measurements have been performed in a laboratory setting using a gonio-reflectometer. The device has a lamp attached to a motorized carriage that moves along a hoop, which is used to

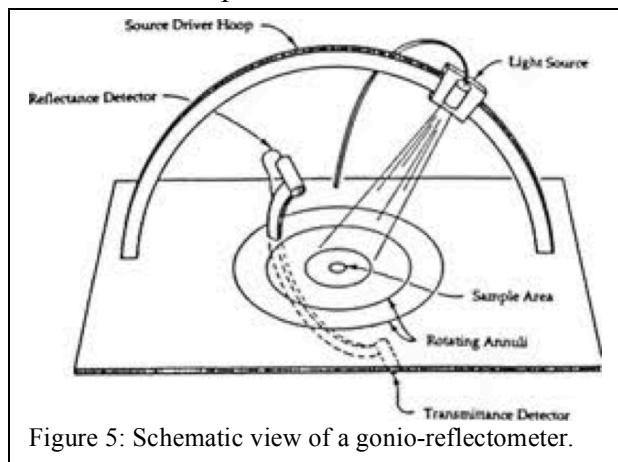


Figure 5: Schematic view of a gonio-reflectometer.

control the incident illumination angles. The light source can be an incandescent lamp. It also has a detector that is mounted to a ring-like structure called an annulus, which control the reflection azimuthal angle for measurement. The sensor zenith angle can be also adjusted. The optical arrangement of the lens and aperture restricts the field of view of the detector to the sample and nearby area only. The detector is usually a spectro-radiometer that measures the entire light spectrum reflected from the sample.

Examples of facilities with this capability

include the Cornell light measurement laboratory

<http://www.graphics.cornell.edu/research/measure>, the European Goniometric Facility (EGO) of the Joint Research Centre (Sandmeier et al. 1998), the Sandmeier Field Goniometer (SFG) of NASA Ames (Sandmeier 2000), the Israeli Goniometric Facility (IGF) of the University of Tel-Aviv (Feingersh et al. 2010), the University of Lethbridge Goniometer System (ULGS) (Coburn and Peddle 2006) and the Compact Laboratory Spectro-Goniometer (CLabSpeG) of the Catholic University Leuven (Biliouris et al. 2007).

The gonio-reflectometers above are systems that are limited in flexibility of hemisphere size and measurement positions, and take a long time for sampling a full hemisphere, which causes problems when many measurements of the same sample are required or when samples are susceptible to changes in spectral characteristics (an example could be rehydration of dry sulfate samples in the laboratory environment).

Following a recently proposed approach (Roosjen et al. 2012) we intend to create a gonio-reflectometer set up that replaces the annulus with a robotic arm. The use of a programmable robotic arm allows fast, highly repeatable positioning of the spectrometer at different azimuthal and zenithal angles and at different distances from the sample. This new facility is required in order to accommodate in a reasonable amount of time the overwhelming number of measurements involved in this project. Even 100 measurements for each of the ~10000 samples, would completely monopolize any other facility. The flexibility of the robotic arm even allows the positioning of the sensor below the horizontal plane, thus allowing measurement of the amount of light passing through an object. The facility can therefore be used for transmission measurements in the future.

Another reason for constructing our own goniometric facility is the fact that we will optimize the set-up to use small masses of sample. The smaller the sample size, the larger the number of mineral mixtures we will be able to make out of the 1-2 kg of material we plan to purchase for each mineral end-member. We will modify the original design proposed by (reference) by including the hoop mounting for the light source from the traditional gonio-

reflectometer design.

Table 3. Itemized List of Components and Costs

Instrument	Component	Cost
Spectrometer	*FieldSpec® 4 Hi-Res Spectroradiometer	\$65,950.00
	*Radiom. Calibrated Fore optic lenses	\$ 2,748.00
	*Spectralon White Reference panel + case	\$ 2,054.00
	*Illuminator: Quartz-Tungsten-Halogen Lamp	\$ 846.00
	Optics for Collimation	\$ 1,000.00
	SUBTOTAL	\$72,598.00
Robotic arm	*Kawasaki RS10N industrial robot + E Controller unit	\$38,000.00
	SUBTOTAL	\$38,000.00
Other parts	Machined Parts and Assembly	\$ 4,000.00
	TOTAL	\$114,598.00

*quotations for these items are included as attachments to the proposal.

7.2. Elements of Proposed Laboratory Gonio-reflectometer facility

The core of the goniometer system is an industrial robot arm, on which an ASD FieldSpec 4 spectroradiometer is mounted. In the following subsections, the components of the system will be described.

7.2.1. Kawasaki Robot. The robotic system will consist of a Kawasaki RS10N industrial robot. The robotic system consists of the arm itself and a controller. The controller can be programmed to command the arm to reach every point within a space at 1.450 mm horizontal reach and a vertical reach of 2.582 mm due to the presence of six movement axes. The robotic arm will have a lifting capacity of 10 kg, enough to support the mounting of the ASD spectrometer. Position repeatability is ± 0.04 mm, as is necessary to obtain reliable repetitive measurements. On average, making a measurement and moving to the next position would take about 6 seconds. As a result, the spectral characteristics of the target can be assumed to be constant while sampling a full hemisphere.

For use as a goniometer, the robotic system will be fully programmed in “hemisphere mode” for hemispherical measurements. In hemispherical mode, there are a number of options, where the most common set-up is to measure view zenith angles from -90° to $+90^\circ$ off nadir. In this set-up, the radius of the hemisphere can be varied from 25 to 100 cm, although some positions cannot be reached at larger hemisphere sizes. Theoretically, an unlimited number of positions of the hemisphere can be measured. Positions will be programmed in such a way that we also can take additional measurements of the opposition surge point, the position where illumination and observation direction coincide precisely, while avoiding shadow casting by the detector.

7.2.2. Illumination and Collimation. A Quartz Tungsten Halogen (QTH) lamp will be used as artificial light source. QTH lamps are used as visible and near-infrared light sources in reflectance spectroscopy because of their smooth spectral curve and stable output. The light has a separate regulated power supply used in conjunction with a light intensity controller to reduce the effects of electronic fluctuations and lamp aging. We are exploring several options to obtain collimated rays. One solution is to use a focusing mirror and an off-axis parabolic mirror. With such a set-up, the STARR facility at the National Institute of Standards and Technology has successfully obtained collimated light fluxes with less than 1° of divergence over the whole

optical path (Barnes et al. 1998). The light source remains fixed throughout the measurements. Light rays incident on the sample are approximately parallel and illuminate it uniformly.

7.2.3. ASD FieldSpec. Spectral reflectance and radiance measurements in the range of 350–2,500 nm measurements will be performed with an ASD Fieldspec 4 spectroradiometer. The spectral sampling interval is 1.4 nm at 350–1,000 nm, and 2 nm at 1,000–2,500 nm. The field of view (FOV) of the instrument can be selected as 1°, 8° or 25° using fore-optics. The hemisphere can be sampled continuously up to a few degrees from the opposition surge position. One configuration of the measurement allows the illumination to be used without collimating optics. Because both the spectroradiometer and the illumination source have conical fields of view/illumination, we can measure biconical reflectance (Schaepman-Strub et al. 2006) instead of bidirectional reflectance. For bidirectional reflectance measurements, the collimating optics are used and the 1° field of view fore-optic will be attached to the spectrometer fiber optic. The steering of the robotic arm and the reading of the spectro-radiometer are fully automated in such a way that reflectance measurements are obtained at a fixed, predefined distance from the target and at predefined positions (viewing angles).

7.2.4. Machined parts. We will need to custom build a few parts. A sample holder capable of holding several samples will be machined out of aluminum. The holder will have a stepper motor that will allow the holder to be rotated at small angle increments in order to position each sample precisely at the center of the spectrometer field of view. One of the sample cups will hold the spectralon material. For each measurement, the motor will put the reference and the current sample in position to be measured.

We will also machine an adaptor to attach the fiber optic cable to the extremity of the robot arm together with a semicircular mounting to change the azimuthal angle for the illumination source.

7.2.5. Software. The total set-up will be controlled by the “Control PC” We will use a Desktop computer connected with the Robot Controller via Ethernet cable and with the ASD spectrometer via Wifi. We will use the robot proprietary programming language to automatically select the positioning of the arm and LabView software to coordinate the activity of all the system. The sequence of operations to be performed in order to successfully acquire a measurement are: 1) rotation of the sample holder to put the reference in place, 2) movement of the arm to a predefined distance and angular position, 3) acquisition by the ASD spectrometer in radiance mode, 4) storage of the raw reference measurement, 5) rotation of the sample holder to put the current sample in place, 6) ASD radiance measurement of the sample, 7) storage of the raw sample measurement, 8) calculation of reflectance of sample, 9) storage of reflectance spectrum.

We will create a project directory where all information about the measurement is stored, including configuration settings, calibration parameters and the measurement results. The exact time and position of each individual measurement will be stored in the file name, while the raw data will be stored in separate text files. These text files contain the wavelength, digital number, radiance and reflectance for the spectral measurements.

7.1.1. Wall and ceiling coatings. To avoid unwanted scattering, the walls of the laboratory will be covered with wall panels that are painted with black latex. The robot, the floor and the ceiling will be covered with black PVC foil. Both the latex and the foil have a reflectance of less than 3% in the visible and NIR. The cost of the coated panels is included in the budget line regarding general supplies and it is not considered as an equipment cost in Table 3.

7.3. Facility Management and User Access

The requested instrument will be classified as an Investigator Facility Instrument as defined in the AO for the PME program. An investigator facility instrument is defined as an instrument acquired or developed by an investigator to support the P.I.'s research where an identified portion of its time is to be reserved for use by the P.I., but where an additional specified portion of its time will be made available to other knowledgeable NASA-supported planetary program investigators, and where all details of access, method of use, charging, and data rights are determined by the P.I. in negotiation with potential users. Co-I Dyar has operated her Mössbauer spectrometer in this fashion for more than 25 years (with up to 30 outside users per year), so she has the experience to set up a smoothly-operating facility.

We plan to encourage collective use of the goniometric facility by other members of the scientific community. Management of the proposed new equipment is simple and straightforward. The lab will be run by the P.I. and Co-I themselves, who have extensive experience in many types of spectroscopy. The P.I. was trained at Stanford University, the SETI Institute and the Department of Geological Sciences at Brown University. The co-I has over 35 years of experience developed at M.I.T., Caltech, the University of Oregon, West Chester University, and Mount Holyoke College. The P.I. will decide priorities as to which samples must be run when and in what order, based upon the needs of this research program, students, colleagues, and outside users.

We expect that 10-50% of the instrument's time would be available to other users. Because of the safety training needed to operate the equipment, most outside users would be supervised by Parente, Dyar, Marchand, or graduate students and other staff members, except for heavy users, who could do safety training at the University of Massachusetts or Mount Holyoke. Access would be provided during business hours or beyond, depending on needs of the users, and users would apply to Parente in writing for access.

Maintenance of the equipment will be the responsibility of the P.I., and he will be aided by his graduate students. Day to day operation of the lab will be the direct responsibility of the P.I. and his staff and students. Title to this equipment will vest with the proposing institution in accordance with the provisions of §1260.74 of NASA's *Grants and Cooperative Agreement Handbook* found online at <http://ec.msfc.nasa.gov/hq/grcover.htm>.

The goniometric facility will be housed in the Knowles Engineering Building at the University of Massachusetts in a designated lab space, which will be prepared specifically to house high fidelity reflectance measurements. The room already has an adequate power supply, internet access, and relevant security. It is an ideal space for the equipment.

7.4. Dissemination

Once acquired, all the data acquired at the University of Massachusetts by this project will be made available to institutional and academic users. This project will develop and abide by a data release policy. Data will remain within the project for 6 months or until publication (whichever is first), at which point it will be available to the broader community for academic use. Any changes in this policy will be widely announced, and will not be retroactively applied to data already collected.

We will setup and maintain a project specific web page that will provide data access, data usage policies and general information about the measurement facility and instruments. The website will host a database of all the measurements and ancillary data. The database will be linked with the one posted at <http://www.mtholyoke.edu/courses/mdyar/database/>, a website

where all data acquired in the Mineral Spectroscopy Laboratory at Mount Holyoke College are posted. The site has received >280,000 hits since going live in 2005. The site currently provides an easily-accessible data set of (mostly) Mössbauer and some FTIR, and TES spectra of minerals collected over a range of temperatures. Data are posted in both graphical format (as JPG files) and as raw data in the form of ascii text files. The web site also has an Education link to provide information for those wishing to learn about how Mössbauer and other types of spectroscopy work.

B. REFERENCES

- Abrams, M. (2000) The Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER): data products for the high spatial resolution imager on NASA's Terra platform. *Intl. J. Remote Sensing*, 21, 846-859.
- Abrams, M., and Hook, S.J. (1995) Simulated ASTER data for geologic studied. *IEEE Trans. Geosci. Remote Sensing*, 33, 692-699.
- Baldrige, A.M., Hook, S.J., Grove, C.J., and Rivera, G. (2009) The ASTER spectral library version 2.0. *Remote Sensing Environment*, 113, 711-715.
- Barnes, P.Y, Early, E.A. and Parr, A.C. NIST MEASUREMENT SERVICES:Spectral Reflectance , National Institute of Standards and Technology (NIST) Special Publication 250-48. March 1998.
- Biliouris D., Verstraeten W.W., Dutré P., Van Aardt J.A. N., Muys B., Coppin P. (2007) A compact laboratory spectro-goniometer (CLabSpeG) to assess the BRDF of materials. Presentation, calibration and implementation on *Fagus sylvatica* leaves. *Sensors*, 7, 1846–1870
- Bishop, J.L., Perry, K.A., Dyar, M.D., Bristow, T.F., Blake, D.M., Brown, A.J., and Peel, S.E. (2013) Coordinated spectral and XRD analyses of magnesite-nontronite-forsterite mixtures and implication for carbonates on Mars. *J. Geophys. Res.*, doi:10.1002/jgre.20066.
- Borel, C.C. and Gerstl, A.W. (1991) The radiosity method in optical remote sensing of structured 3-D surfaces," *Remote Sens. Environ.* 36, pp. 13-44.
- Borel , C.C. and Gerstl, A. W. (1994) Nonlinear spectral mixing models for vegetation and soil surfaces, *Remote Sens. Environ.* 47, pp. 403-416.
- Brearley, A.J., and Jones, R.H. (1998) Chondritic meteorites. *Revs. Mineral.*, 36, 3-100-3-398.
- Burbine, T.H. (2013) Asteroids. *Treatise on Geochemistry*, 2nd ed., Elsevier.
- Chandrasekhar, S. (1960) Radiative transfer, Dover Publication.
- Charlier, B., Grove, T.L., and Zuber, M.T. (2013) Phase equilibria of ultramafic compositions on Mercury and the origin of the compositional dichotomy. *EPSL*, 363, 50-60.
- Clark, R.N. (1983) Spectral properties of mixtures of montmorillonite and dark carbon grains: Implications for remote sensing minerals containing chemically and physically adsorbed water, *J. Geophys. Res.* 88, pp. 10,635-10,644.
- Clark, R.N. (1999) Spectroscopy of rocks and minerals and principles of spectroscopy. *Manual of Remote Sensing*, A.N. Rencz, eds., John Wiley and Sons.
- Clark, R.N. and Roush, T.L. (1984) Reflectance spectroscopy: quantitative analysis techniques for remote sensing applications, *J. Geophys. Res.* 89, pp. 6,329-6,340.
- Clark, R.N., King, T.W., Klejwa, M., Swayze, G.A., and Vergo, N. (1990) High spectral resolution reflectance spectroscopy of minerals. *J. Geophys. Res.*, 95, B8, 12653-12680.
- Clark, R.N., Swayze, G.A., Livo, K., Sutley, S. Dalton, J., McDougal, R. Gent, C., (2003) Imaging spectroscopy: Earth and planetary remote sensing with the USGS Tetracorder and expert systems, *J. Geophys. Res.*, 108, E12.
- Clark, R.N., Swayze, G.A., Wise, R., Livo, E., Hoefen, T., Kokaly, R., Sutley, S.J., (2007), USGS digital spectral library splib06a: U.S. Geological Survey, Digital Data Series 231, <http://speclab.cr.usgs.gov/spectral.lib06>.
- Coburn C.A., and Peddle D.R. (2006) A low-cost field and laboratory goniometer system for estimating hyperspectral bidirectional reflectance. *Can. J. Remote Sens.* 32, 244–253.

- Dhingra, D., Pieters, C.M., Boardman, J.W., Head, J.W., Isaacson, P.J., and Taylor, L.A. (2011) Compositional diversity at Theophilus Crater: Understanding the geological context of Mg-spinel bearing central peaks. *Geophys. Res. Letts.*, 38, L11201 DOI: 10.1029/2011GL047314.
- Dunn, T.L., Burbine, T.H., Bottke, W.F. Jr., and Clark, J.P. (2013) Mineralogies and source regions of near-Earth asteroids. *Icarus*, 222, 273-282.
- Dyar, M.D., Carmosino, M.L., Tucker, J.M., Speicher, E.A., Brown, E.B., Clegg, S.M., Wiens, R.C., Barefield, J.E., Delaney, J.S., Ashley, G.M., and Driese, S.G. (2011) Error analysis for remote laser-induced breakdown spectroscopy analysis using combinations of igneous, sedimentary, and phyllosilicate samples. *Lunar Planet. Sci. XLII*, Lunar Planet. Inst., Houston, CD-ROM #1258 (abstr.).
- Dyar, M.D., Carmosino, M.L., Speicher, E.A., Ozanne, M.V., Clegg, S.M., and Wiens, R.C. (2012) Comparison of partial least squares and lasso regression techniques for laser-induced breakdown spectroscopy of geological samples. *Spectrochim. Acta B*, 70, 51-67.
- Fan, C., Xie, H., Wu, H.J., Wu, J., and Birnbaum, S. (2012) Analysis of United States Geological Survey spectral library of silicate minerals: implication for remote sensing applications. *J. Applied Remote Sensing*, 6, 063514 DOI: 10.1117/1.JRS.6.063514.
- Feingersh T., Ben-Dor E., Filin S. (2010) Correction of reflectance anisotropy: A multi-sensor approach. *Int. J. Remote Sens.* 31, 49–74.
- Gaffey, M.J., Cloutis, E.A., Kelley, M.S., and Reed, K.L. (2002) Mineralogy of asteroids. In *Asteroids III*, eds. Bottke, W.F., Cellino, A., Paolicchi, P., and Binzel, R.P. University of Arizona Press, Tucson., pp. 183-204.
- Govaerts, Y. M., and Verstraete, M. M. (1998). Raytran: A Monte Carlo ray-tracing model to compute light scattering in three-dimensional heterogeneous media. *Geoscience and Remote Sensing, IEEE Transactions on*, 36(2), 493-505.
- Hapke, B. (1981) Bidirectional reflectance spectroscopy. 1. Theory. *Journ. Geophys. Res.*, 86, 4571–4586.
- Hapke, B. (1984) Bidirectional reflectance spectroscopy: 3. Correction for macroscopic roughness, *Icarus*, vol. 59, no. 1, pp. 41–59, 1984.
- Hapke, B. (1986) Bidirectional reflectance spectroscopy, 4, extinction and the opposition effect," *Icarus* 67, pp. 264-280.
- Hapke, B. (1993) *Theory of reflectance and emittance spectroscopy*, Cambridge University Press.
- Hapke, B. (2002) Bidirectional reflectance spectroscopy: 5. The coherent backscatter opposition effect and anisotropic scattering, *Icarus*, vol. 157, pp. 523–534.
- Hapke, B., (2008) Bidirectional reflectance spectroscopy. 6. Effects of porosity. *Icarus* 195, 918–926.
- Hapke, B, Shepard, M.K., Nelson, R.M., Smythe, W.D., Piatek, J.L. (2009) A quantitative test of the ability of models based on the equation of radiative transfer to predict the bidirectional reflectance of a well-characterized medium, *Icarus*, 199, 210–218.
- Helfenstein, P., (1986) Derivation and analysis of geological constraints on the emplacement and evolution of terrains on Ganymede from applied differential photometry, Ph.D. thesis, 414 pp., Brown Univ., Providence, R.I.
- Helfenstein, P., and Veverka, J. (1987) Photometric properties of lunar terrains from Hapke's equations, *Icarus*, 72,343-357, 1987.

- Hiroi, T., and Pieters, C. M. (1994) Estimation of grain sizes and mixing ratios of fine powder mixtures of common geologic minerals. *Journ. of Geophys. Research Planets*, 99(E5), 10867-10879.
- Hunt, G.R., and Salisbury, J.W. (1970) Visible and near infrared spectra of minerals and rocks, I, Silicate minerals. *Mod. Geol.*, 1, 283-300.
- Hunt, G.R., and Salisbury, J.W. (1971) Visible and near infrared spectra of minerals and rocks, II, Carbonates. *Mod. Geol.*, 2, 23-3.
- Hunt, G.R., Salisbury, J.W., and Lenhoff, C.J. (1972) Visible and near infrared spectra of minerals and rocks, V, Halides, arsenates, vanadates and borates. *Mod. Geol.*, 3, 121-132.
- Hunt, G.R., Salisbury, J.W., and Lenhoff, C.J. (1971a) Visible and near infrared spectra of minerals and rocks, III, Oxides and hydroxides. *Mod. Geol.*, 2, 195-205.
- Hunt, G.R., Salisbury, J.W., and Lenhoff, C.J. (1971b) Visible and near infrared spectra of minerals and rocks, IV, Sulphides and sulphates. *Mod. Geol.*, 3, 1-14.
- Hunt, G.R., Salisbury, J.W., and Lenhoff, C.J. (1973) Visible and near infrared spectra of minerals and rocks, VI, Additional silicates, *Mod. Geol.*, 4, 85-106.
- James, C. L., Basu, A., Wentworth, S. J., and McKay, D. S., (2001) Grain Size Distribution of FeO Globules in Lunar Agglutinitic Glass: First Results from Apollo 17 Soil,” *GSA Annual Meeting, 2001* **78241**(Abstract 24733).
- Johnson, P.E. (1983) A semi-empirical method for analysis of the reflectance spectra of binary mineral mixtures, *J. Geophys. Res.* 88, pp. 3,557-3,561.
- Karner, J., Papike, J.J., and Shearer, C.K. (2003) Olivine from planetary basalts: Chemical signatures that indicate planetary parentage and those that record igneous setting and process. *Amer. Mineral.*, 88, 806-816.
- Kaur, P., Bhattacharya, S., Chauhan, P., Ajai, A.S., and Kumar, K. (2013) Mineralogy of Mare Serenitatis on the near side of the Moon based on Chandrayaan-1 Moon Mineralogy Mapper (M³) observations. *Icarus*, 222, 137-148.
- Lawrence, S.J. and Lucey, P.G. (2007) Radiative transfer mixing models of meteoritic assemblages. *J. Geophys. Res.*, 112, E07005.
- McKeown, N.K., Bishop, J.L., Cuadros, J., Hillier, S., Amador, E., Makarewicz, H.D., Parente, M., and Silver, E.A. (2011) Interpretation of reflectance spectra of clay mineral-silica mixtures: Implications for martian clay mineralogy at Mawrth Vallis. *Clays Clay Mins.*, 59, 400-415.
- McSween, H.Y. Jr., Bennett, M.S. III., and Jarosewich, E. (1991) The mineralogy of ordinary chondrites and implications for asteroid spectrophotometry. *Icarus*, 90, 107-116.
- Mishchenko, M., Dlugach, J., Yanovitskij, E., Zakharova, N., (1999). Bidirectional reflectance of flat, optically thick particulate layers: An efficient radiative transfer solution and applications to snow and soil surfaces. *J. Quant. Spectrosc. Radiat. Trans.* 63, 409–432. May be downloaded at <http://www.giss.nasa.gov/~crmim/publications/>
- Mittlefehldt, D.W., McCoy, T.J., Goodrich, C.A., and Kracher, A. (1998) Non-chondritic meteorites from asteroidal bodies. *Revs. Mineral.*, 36, 4-1001-4-196.
- Mustard, J.F., and Pieters, C.M. (1987) Quantitative abundance estimates from bidirectional reflectance measurements. *J. Geophys. Res.*, 92, B4, E617-R626.
- Mustard, J. F. and Pieters, C.M. (1989) Photometric phase functions of common geologic minerals and applications to quantitative analysis of mineral mixture reflectance spectra, *J. Geophys. Res.* 94, pp. 13,619-13,634, 1989

- Nittler, L.R., Starr, R.D., Weider, S.Z., McCoy, T.J., Boynton, W.V., Ebel, D.S., Ernst, C.M., Evans, L.G., Goldstein, J.O., Hamara, D.K., Lawrence, D.J., McNutt, R.L., Schlemm, C.E., Solomon, S.C., and Sprague, A.L. (2011) the major-element composition of Mercury's surface from MESSENGER x-ray spectrometry. *Science*, 6051, 1847-1850.
- Onyeagocha, A.C. (1978) Twin Sisters dunite: Petrology and mineral chemistry. *GSA Bull.*, 89, 1459-1471.
- Papike, J.J. (1996) Pyroxene as a recorder of cumulate formational processes in asteroids, Moon, Mars, Earth: Reading the record with the ion microprobe. *Amer. Mineral.*, 81, 525-544.
- Papike, J.J. (1998) Comparative planetary mineralogy: Chemistry of melt-derived pyroxene, feldspar, and olivine. *Revs. Mineral.*, 36, 7-01 – 7-12.
- Papike, J.J., Ryder, G., and Shearer, C.K., (1998) Lunar samples. *Revs. Mineral.*, 36, 5001-5234.
- Parente, M. and Duarte, M. (2013). A new semantic wavelet-based spectral representation. 4th IEEE WHISPERS (Workshop on hyperspectral image and signal processing: evolution of remote sensing) Conference. Accepted for publication, abstr. # 164.
- Parente, M., Bishop, J.L., and Bell, J.F. III (2009) Spectral unmixing for mineral identification in pancam images of soils in Gusev crater, Mars. *Icarus*, 203, 421-436.
- Parente, M., Clark, J.T., Brown, A.J., and Bishop, J.L. (2010) End-to-end simulation and analytical model of remote-sensing systems: Application to CRISM. *IEEE Trans. Geosci. Remote Sensing*, 48, 3877-3888.
- Parente, M., Makarewicz, H.D., and Bishop, J.L. (2011a) Decomposition of mineral absorption bands using nonlinear least squares curve fitting: Application to Martian meteorites and CRISM data. *Planet. Space Sci.*, 59, 423-442.
- Parente, M., Mustard, J.F., Murchie, S., and Seelos, F. (2011b) Robust unmixing of hyperspectral images: Application to Mars. *IEEE Intl. Symp. Geosci. Remote Sensing*, 2011, 1291-1294.
- Piatek, J. L. (2003) *Size-Dependent Scattering Properties of Planetary Regolith Analogs*. Doctoral Dissertation, University of Pittsburgh.
- Pieters, C.M. (1983) Strength of mineral absorption features in the transmitted component of near-infrared reflected light – 1st results from RELAB. *J. Geophys. Res.*, 88, 9534-9544.
- Pieters, C. M., Fischer, E. M., Rode, O., and Basu, A. (1993) Optical effects of space weathering: The role of the finest fraction,” *Journal of Geophysical Research* **98**(E11), 20, 817–20, 824.
- Pieters, C. M. and Taylor, L. A., (2003) Systematic global mixing and melting in lunar soil evolution,” *Geophysical Research Letters* **30**(20), 2048 (2003).
- Poulet, F., and Erard, S. (2004). Nonlinear spectral mixing: Quantitative analysis of laboratory mineral mixtures. *Journal of geophysical research*, 109(E2), E02009.
- Rivard, B., Feng, J., Gallie, A., and Sanchez-Azofeifa, A. (2008) Continuous wavelets for the improves use of spectral libraries and hyperspectral data. *Remote Sensing Environ.*, 112, 2850-2862.
- Rodricks, N., and Kirkland, L.E. (2004) Drawbacks of using linear mixing modeling on hyperspectral images. *Imaging Spectrometry X, Proc., Soc. Photo-Optical Instrum. Engineers*, 5546, 416-426.
- Rohani, N., and Parente, M. (2013) End-member detection in CRISM images using GRAPHs. *LPSC 44*, Abstract 2894.

- Roosjen, P.P.J. , Clevers, J.G.P.W. , Bartholomeus, H.M. , Schaepman, M.E. , Schaepman-Strub, G. , Jalink, H. , Schoor, R. van der , Jong, A. de (2012) A laboratory goniometer system for measuring reflectance and emittance anisotropy *Sensors* 12 (12), 17358 - 17371.
- Sandmeier S., Müller C., Hosgood B., Andreoli G. (1998). Physical mechanisms in hyperspectral BRDF data of grass and watercress. *Remote Sens. Environ.* 66, 222–233.
- Sandmeier S.R. (2000). Acquisition of bidirectional reflectance factor data with field goniometers. *Remote Sens. Environ.* 73, 257–269.
- Saranath, A., and Parente, M. (2013) Automatic extraction of unique spectra signatures from the M³ database. LPSC 44, Abstract 3056.
- Schaepman-Strub, G.; Schaepman, M.E.; Painter, T.H.; Dangel, S.; Martonchik, J.V. Reflectance quantities in optical remote sensing-definitions and case studies. *Remote Sens. Environ.* 2006, 103, 27–42
- Shkuratov, Y., Starukhina, L., Hoffmann, H., and Arnold, G. (1999) A model of spectral albedo of particulate surfaces: Implications for optical properties of the Moon. *Icarus*, 137, 235–246.
- Shepard, M.K., and Helfenstein, P. (2007) A test of the Hapke photometric model, *Journal of Geophysical Research: Planets*, 112, E3, 2156-2202.
- Schönermark, M.; Geiger, B. and Röser, H.P. Reflection Properties of Vegetation and Soil with a BRDF Data base. Wissenschaft und Technik Verlag: Berlin 2004, pp 352
- Stockstill-Cahill, K.R., McCoy, T.J., Nittler, L.R., Weider, S.Z., and Hauck, S.A. (2012) Magnesium-rich crustal compositions on Mercury: Implications for magmatism from petrologic modeling. *J. Geophys. Res.*, 117, E00L15, doi:10.1029/2012JE004140.
- Sunshine, J.M., and Pieters, C.M. (1993) Estimating modal abundances from the spectra of natural and laboratory pyroxene mixtures using the Modified Gaussian Model. *J. Geophys. Res.*, E5, 98, 9075-9087.
- Tamaguchi, Y., Kahle, A.B., Tsu, H., Kawakami, T., and Pniel, M. (1998) Overview of Advances Spaceborne Thermal Emission and Reflection Radiometer (ASTER). *IEEE Trans., Geosci. Remote Sensing*, 36, 1062-1071.
- Van der Meer, F.D., van der Werff, H.M.A., van Ruitenbeek, F.J.A., Hecker, C.A., Bakker, W.H., Noomen, M.F., van der Meijde, M., Carranza, J.M., Boudewijn de Smeth, J., and Woldai, T. (2012) Multi- and hyperspectral geological remote sensing: A review. *Intl. J. Applied Earth Observ.*, 14, 112-128.
- Vilas, F. (1988) Surface composition of Mercury from reflectance spectrophotometry. *Mercury*, (F. Vilas, Ed.), University of Arizona Press.
- Weider, S.Z., Nittler, L.R., Starr, R.D., McCoy, T.J., Stockstill-Cahill, K.R., Byrne, P.K., Denevi, B.W., Head, J.W., and Solomon, S.C. (2012) Chemical heterogeneity on Mercury's surface revealed by the MESSENGER x-ray spectrometer. *J. Geophys. Res.*, 117, E00L05, DOI: 10.1029/2012JE004153.

C. BIOGRAPHICAL SKETCH

MARIO PARENTE

Department of Electrical and Computer Engineering
University of Massachusetts Amherst,
151 Holdsworth Way, Amherst, MA 01003
phone: (413) 5456860, fax: (413) 5454652

11 Overlook drive
Amherst, MA 01002
(413) 8350351
email: mparente@ecs.umass.edu

EDUCATION

2010 STANFORD UNIVERSITY: PhD in Electrical Engineering
2005 STANFORD UNIVERSITY: M.S. in Electrical Engineering and Statistics
2003 UNIVERSITY FEDERICO II, Naples, IT: M.S. Telecomm. Engineering, (Magna Cum Laude)
2001 UNIVERSITY FEDERICO II, Naples, IT: B.Sc. Telecomm. Engineering, (Magna Cum Laude)

AWARDS

2001– 2003 EUROPEAN COMMUNITY: Scholarship for information technology
2009 BEST PAPER AWARD IEEE Geoscience and Remote Sensing (WHISPERS)

PROFESSIONAL POSITIONS

2011 – present UMASS AMHERST, Dept. of Electr. & Comp. Eng., Assistant Professor
2010 – 2011 BROWN UNIVERSITY, Dept. of Planetary Geosc., Post-doctoral Research Associate
2003 – 2010 SETI INSTITUTE: Graduate Research Associate
2008 – present APPLIED PHYSICS LAB, Johns Hopkins University. Consultant
2010 – 2013 JET PROPULSION LAB, Pasadena, CA, machine learning group. Consultant

RESEARCH ACTIVITIES

- Remote sensing image processing of Mars and lunar data
- Integration of robotics and hyperspectral sensing for terrestrial and planetary missions
- Algorithm development for spectral data analysis
- Correlation of textural and spectral properties of Martian and lunar outcrops.
- Instrument calibration and data reduction for spectrometer data
- Produced software packages officially used in CRISM and M3 Data Processing Pipeline

COMMUNITY ACTIVITIES

2013 – present ASSOCIATE EDITOR IEEE Geoscience and Remote Sensing Letters
2010 – present PANEL REVIEWER for NASA programs
2009 – present TECHNICAL COMMITTEE MEMBER IEEE WHISPERS and IGARSS
2009 – present REVIEWER for the IEEE Transactions on Geoscience and Remote Sensing
2012 – present REVIEWER for the IEEE Transactions on Image Processing
2011 – present REVIEWER for the IEEE Geoscience and Remote Sensing Letters
2010 – present REVIEWER for the AGU Journal of Geophysical research

TECHNICAL / SCIENTIFIC AFFILIATIONS

2006 – present MEMBER OF IEEE Signal Processing Society
2006 – present MEMBER OF IEEE Geoscience and Remote Sensing Society
2006 – present MEMBER of SPIE International Society for Optical Engineering
2004 – present MEMBER of the NASA Astrobiology Institute
2005 – present MEMBER of the Mars Reconnaissance Orbiter (CRISM) Science Team
2010 – present MEMBER of the Moon Mineralogy Mapper (M3) Science Team

SELECTED PUBLICATIONS

Parente is the author or co-author of than 16 papers published in refereed journals, from topics dealing with spectroscopic study of rocks and minerals, statistical analysis of spectra and machine learning of hyperspectral images. He was also author or co-author of more than 100 conference abstracts. Selected publications include:

- M. Parente and M. Duarte (2013). A new semantic wavelet-based spectral representation. 4th IEEE WHISPERS (Workshop on hyperspectral image and signal processing: evolution of remote sensing) Conf Accepted for publication, abstr. # 164.
- N.Rohani and M. Parente (2013). Graph-Based Identification of Boundary Points for Unmixing and Anomaly Detection 4th IEEE WHISPERS (Workshop on hyperspectral image and signal processing: evolution of remote sensing) Conf. Accepted for publication, abstr. # 158.
- J.L. Bishop, D. Loizeau, N.K. McKeown, L. Saper, M.D. Dyar, N. Tosca, D. DesMarais, M. Parente, S.L. Murchie (2013). What the Ancient Phyllosilicates at Mawrth Vallis can tell us about Possible Habitability on Early Mars, Planetary and Space Science, in press.
- A.M. Saranathan, M. Parente (2013). Automatic Extraction of Unique Spectral Signatures from the M³ Database, *Lunar Planet Science Conf*, XLIV, abstr. # 3056
- J.M. Bioucas-Dias, A. Plaza, N. Dobigeon, M. Parente, Q. Du and P. Gader (2012). Hyperspectral Unmixing Overview: Geometrical, Statistical and Sparse Regression-Based Approaches, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, Volume 5, Issue 2, 354-379, doi:10.1109/JSTARS.2012.2194696.
- J.L. Bishop, D. Tirsch, L. Tornabene, R. Jaumann, A.S. McEwen, P. McGuire, A. Ody, F. Poulet, R. Clark, M Parente and 11 others (2012). Characterizing the mineralogy and morphology of geologic units at Libya Montes, Mars: Ancient aqueous outcrops, mafic flows, fluvial features and impacts, *Journal of Geophysical Research CRISM Special Issue*, in press.
- JL Bishop, M Parente, VE Hamilton, (2011) Spectral Signatures of Martian Meteorites and What They Can Tell Us About Rocks on Mars, *Meteoritics and Planetary Science Supplement* 74, 5393.
- J. R. Michalski, J.-P. Bibring, F. Poulet, D. Loizeau, N. Mangold, E. Noe Dobrea, J. L. Bishop, J. J. Wray, N. K. McKeown, M. Parente, E. Hauber, F. Altieri, F. G. Carrozzo and P. B. Niles, (2010). The Mawrth Vallis region of Mars: a potential landing site for the Mars Science Laboratory (MSL) mission, *Astrobiology*, 10 (7), 687-703.
- M. Parente , J.T. Clark, A. Brown and J.L. Bishop (2010) End-to-end simulation and analytical of remote sensing systems: application to CRISM, *IEEE Transactions on Geoscience and Remote Sensing* , vol. PP, issue 99, DOI: 10.1109/TGRS.2010.2050000, p. 1-12.
- M. Parente, H. Mackarevicz and J. L. Bishop. (2010) Decomposition of mineral absorption bands using nonlinear least squares curve fitting: application to Martian meteorite and CRISM data, *Planetary and Space Science*, 59, pp. 423-442, doi:10.1016/j.pss.2011.01.009.
- M. Parente, J. L. Bishop and J. F. Bell III, (2009), Spectral unmixing and anomaly detection for mineral identification in Pancam images of Gusev soils, *Icarus*, Vol 203, N. 2, p. 421-436.
- N.K. McKeown, J. L. Bishop, E. Z. Noe Dobrea, M. Parente, B. L. Ehlmann, J. F. Mustard, S. L. Murchie, J-P. Bibring, E. Silver (2009). Characterization of phyllosilicates observed in the central Mawrth Vallis region, Mars, their potential formational processes, and implications for past climate.. *J. Geophys. Res.*, 114, E00D10, doi:10.1029/2008JE003301.
- J. L. Bishop, M. Parente, C. M. Weitz, E. Z. Noe Dobrea, L. H. Roach, S. L. Murchie, P. C. McGuire, N. K. McKeown, C. M. Rossi, A. J. Brown, W. M. Calvin, R. Milliken, J. F. Mustard, (2009) Mineralogy of Juventae Chasma: Sulfates in the Light-toned Mounds, Mafic Minerals in the Bedrock, and Hydrated Silica and Hydroxylated Ferric Sulfate on the Plateau. *J. Geophys. Res.*, 114, E00D09, doi:10.1029/2009JE003352.
- Bishop J. L., Noe Dobrea E. Z., McKeown N. K., Parente M., Ehlmann B. L., Michalski J. R., Milliken R. E., Poulet F., Swayze G. A., Mustard J. F., Murchie S. L., and Bibring J.-., P. (2008) Phyllosilicate diversity and past aqueous activity revealed at Mawrth Vallis, Mars. *Science* 321, DOI: 10.1126/science.1159699, pp. 830-833.

MELINDA DARBY DYAR

Department of Astronomy
Mount Holyoke College
South Hadley, MA 01075
(413) 538-3073

161 Chestnut St.
Amherst, MA 01002
(413) 230-3553
mdyar@mtholyoke.edu

Education:

Ph.D., Geochemistry, M.I.T., Cambridge, Mass. Advisor: R.G. Burns.

B.A., Geology and Art History, Wellesley College, Wellesley, Mass.

Employment:

Full (2008-present), Associate (2002-2008) and Assistant (1998-2002) Professor, Mount Holyoke College and Five College Astronomy Dept., University of Massachusetts.

Assistant Professor, Dept of Geology and Astronomy, West Chester University, 1993-1998.

Assistant Professor, Dept. of Geological Sciences, University of Oregon, 1986-1993.

Research Fellow, Division of Geological and Planetary Sciences, California Institute of Technology, 1985-1986 (G.R. Rossman, supervisor).

Post-Doctoral Fellow, Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, 1985 (R.G. Burns, supervisor).

Scientific and Technical Performance on Research Efforts:

Dyar has 32 years of experience in the field of mineral spectroscopy, including optical, FTIR, LIBS, Mössbauer, and many other types of spectroscopy. Her research includes study of both extraterrestrial (lunar and meteoritical) and terrestrial rock types. Her work has been continuously supported since 1986. She is currently funded by several NASA grants in support of Mössbauer and LIBS spectroscopy; NSF grants support her XANES and education research.

Books and Electronic Media:

McKillop, S. and Dyar, M.D. (2010) *Geostatistics Explained, An Introductory Guide for Earth Scientists*. Textbook. Cambridge University Press.

Dyar, M.D., and Gunter, M.C. (2008) *Mineralogy and Optical Mineralogy: A Three-Dimensional Approach*. Textbook. Mineralogical Society of America.

Dyar, M.D. (1999) *Hands-On Mineral Identification*. CD-ROM. Tasa Graphic Arts, Albuquerque, N.M.

Dyar, M.D., McCammon, C.A., and Schaefer, M.W., Eds. (1996) *Mineral Spectroscopy: A Tribute to Roger G. Burns*. Special Publication #5, The Geochemical Society, Washington, D.C., 400 pp.

Peer-Reviewed Publications:

Dyar is the author or co-author of more than 160 papers published in refereed journals, all dealing with spectroscopic study of rocks and minerals, and more than 350 abstracts. Her analytical expertise includes use of Mössbauer, optical, FTIR, LIBS, TES, NMR, PIGE, XRD/SREF, SIMS, XANES, XRF, and EPMA. Selected relevant publications (underlines indicate undergraduate coauthors) include:

Dyar, M.D., Klima, R.E., Fleagle, A., and Peel, S.E. (in press) Fundamental Mössbauer parameters of synthetic Ca-Fe-Mg pyroxenes. *Amer. Mineral.*

Bishop, J.L., Perry, K.A., Dyar, M.D., Bristow, T.F., Blake, D.F., Brown, A.J. and Peel, S.E. (2013) Coordinated spectral and XRD analyses of magnesite-nontronite-forsterite mixtures and implications for carbonates on Mars. *JGR*, 118, doi:10.1002/jgre.20066.

Dyar, M.D., Carmosino, M.L., Speicher, E.A., Ozanne, M.V., Clegg, S.M., and Wiens, R.C. (2012) Comparison of partial least squares and lasso regression techniques for laser-induced breakdown spectroscopy of geological samples. *Spectrochim. Acta B*, 70, 51-67.

Dyar, M.D., Breves, E.A., Emerson, E., Bell, S.M., Nelms, M., Ozanne, M.V., Peel, S.E., Carmosino, M.L., Tucker, J.M., Gunter, M.E., Delaney, J.S., Lanzirotti, A., and Woodland, A.B. (2012) Accurate determination of ferric iron in garnets in bulk Mössbauer spectroscopy and synchrotron micro-XANES. *Amer. Mineral.*, 97, 1726-1740.

Klima, R.L., Dyar, M. D., and Pieters, C. M. (2010) Near-infrared spectra of clinopyroxenes: effects of calcium content and crystal structure. *Meteor. Planet. Sci.*, doi: 10.1111/j.1945-5100.2010.01158.x.

GERARD J MARCHAND

Department of Astronomy
Mount Holyoke College
South Hadley, MA 01075
(413) 538-3173

47 Lyman Rd.
Westhampton, MA 01027-9522
(413) 527-5158
jmarchan@mtholyoke.edu

Education:

A.S. (Associates Degree) with Honors, Electronic Technology, Holyoke Community College, 1973.
A.S. (Associates Degree) with Honors, Biology, Holyoke Community College, 1978.
B.A. (Bachelor of Science) with Honors, Computer Science, Westfield State College, 1983.
B.A. (Bachelor of Science) with Honors, Biology, Westfield State College, 1989.

Employment:

Owner, Rock and Bone Mineral Shop, Westhampton, Massachusetts, 1990-present.
SEM Technician, Mount Holyoke College, South Hadley, Massachusetts, 2000-present.
Engineering Electronic Technician, New Venture Technology, Enfield, Connecticut, 1995-2000.
Design Engineering Technician, Quantum Corporation, Shrewsbury, Massachusetts, 1990-1995.
Electronic and Engineering Technician, Digital Equipment Corporation, Westfield, Massachusetts, 1972-1990.

Scientific and Technical Performance on Research Efforts:

Marchand has worked for the Departments of Geology and Geography and Astronomy at Mount Holyoke for 12 years. His job responsibilities include thin section preparation, rock cutting and polishing, equipment maintenance, curation of rock and mineral collections, sample preparation for reflectance, transmission, LIBS, and Mössbauer spectroscopy, and operation and maintenance of spectrometers. He works with students and faculty on projects involving use of SEM. His professional expertise also includes meteorites and mineral identification and curation. He currently works with Dyar roughly 8 hours/week during the academic year and full-time in the summers, maintaining her lab and equipment.

Publications:

Marchand's professional responsibilities do not include a need for publications. However, he has been a coauthor on the following projects, and an invaluable, if too often unsung, contributor to nearly every paper written by Dyar in the last decade.

Dyar, M.D., Glotch, T.D., Lane, M.D., Wopenka, B., Tucker, J.M., Seaman, S.J., Marchand, G.K., Klima, R., Hiroi, T., Bishop, J.L., Pieters, C., and Sunshine, J. (2011) Spectroscopy of Yamato 984028. *Polar Res.*, 4, 530-540.

Jawin, E.R., Dyar, M.D., Lane, M.D., Bishop, J.L., and Marchand, G.J. (2011) Inter-relationships among Mössbauer parameters of phosphate minerals and crystal structures. *Lunar Planet. Sci. XLII*, Lunar Planet. Inst., Houston, CD-ROM #1259 (abstr.).

Dyar, M.D., Lane, M.D., Glotch, T., Hiroi, T., Wopenka, B., Klima, R., Bishop, J.L., Pieters, C., Sunshine, J., Marchand, G.J., and Seaman, S.J. (2010) Spectroscopy of Yamato 984028. *Lunar Planet. Sci. XXXXI*, Lunar Planet. Inst., Houston, CD-ROM #1831 (abstr.).

Dyar M. D., Hiroi T., Glotch T., Lane M. D., Wopenka B., Klima R., Bishop J. L., Pieters C., Sunshine J., Marchand G. J. and Seaman S. J. (2009) Reflectance, transmission, emission, raman, and Mössbauer spectroscopy of Yamato 984028. *32nd Symposium on Antarctic Meteorites*.

Dyar, M.D., McCanta, M.C., Treiman, A.H., Sklute, E.C., and Marchand, G.J. (2007) Mössbauer spectroscopy and oxygen fugacity of amphibole-bearing R-chondrite LAP04840. *Lunar Planet. Sci. XXXVIII*, Lunar Planet. Inst., Houston, CD-ROM #2047 (abstr.).

Dyar, M.D., Pieters, C.M., Hiroi, T., Lane, M.D., and Marchand, G.J. (2005) Integrated spectroscopic studies of MIL 03346. *36th Ann. Lunar Planet. Sci. Conf.*, #1261.

Dyar, M.D., Mackwell, S.J., Seaman, S.J., and Marchand, G.J. (2004) Evidence for a wet, reduced martian interior. *35th Ann. Lunar Planet. Sci. Conf.*, #1348.

D. CURRENT AND PENDING SUPPORT

Current Support Mario Parente				
Title of Award or Project	Sponsoring Institution	Point of Contact & Phone & Email	Period of Performance	Budget (\$K) & %Commitment (WY)
None	N/A	N/A	N/A	N/A

Pending Support Mario Parente				
Title of Award or Project	Sponsoring Institution	Point of Contact & Phone & Email	Period of Performance	Budget (\$K) & %Commitment (WY)
Wavelet-Based Representations for Hyperspectral Data Processing and Interpretation Mario Parente Marco Duarte P.I.'s	NSF CIF III Program	Ms Dawn R. Patterson (703) 292-8910 dpatters@nsf.gov	9/1/13-31/8/16	\$492,651 total award 0.08* WY for Parente
Development of Northeast Terrain and Water Resource Mapper Mi-Hyun Park , P.I.	NSF MRI Program	Kathleen McCloud (703) 292-8236, kmcccloud@nsf.gov	8/1/13 – 7/31/16	\$2,487,684 total award 0.08* WY for Parente
SSERVI Regolith Physics Team Pascal Lee, P.I.	NASA Solar System Exploration Research Virtual Institute Cooperative Agreement	Dr. Robert A. Fogel (202) 358-228 rfogel@nasa.gov	2/1/14 – 1/31/18	0.00* WY for Parente
Mineralogical signatures of lunar basins: Insights into the compositional stratigraphy of the lunar crust Peter Isaacson, P.I.	NASA Lunar Advanced Science and Exploration Research	Dr. Robert A. Fogel (202) 358-228 HQ-LASER@mail.nasa.gov	3/1/14 - 2/28/17	\$ 157,927 to UMass 0.08* WY for Parente

Current Support M. Darby Dyar				
Title of Award or Project	Sponsoring Institution	Point of Contact & Phone & Email	Period of Performance	Budget (\$K) & %Commitment (WY)
<i>Proposals in gray shading will end before the current grant would begin.</i>				
Pyroxene Spectroscopy as a Tool to Probe the Composition and Thermal History of the Lunar Surface Rachel Klima, P.I.	NASA Lunar Advanced Science and Exploration Research	Dr. Paul Hertz (202) 358-0985 Paul.hertz@nasa.gov	5/1/10-10/31/13	\$104,914 for MHC 0.08* WY for Dyar
Technique Development for Laser-Induced Breakdown Spectroscopy: Calibration, Classification, and Light Element Analysis M.D. Dyar, P.I.	NASA Mars Fundamental Research Program	Dr. Mitchell Schulte (202) 358-0780 HQ-MFRP@mail.nasa.gov	6/1/09 to 5/30/14	\$519,392 total 0.08* WY for Dyar
The Moon as Cornerstone to the Terrestrial Planets: The Formative Years Carle M. Pieters, P.I.	NASA Lunar Science Institute Program	Dr. David Morrison (650) 604-1850 David.Morrison@nasa.gov	4/9/09-4/8/14	\$135,000 for MHC 0.08* WY for Dyar
Effects of Shock Metamorphism on Phyllosilicate Spectroscopy Joseph Michalski, P.I.	NASA Mars Fundamental Research Program	Dr. Mitchell Schulte (202) 358-0780 HQ-MFRP@mail.nasa.gov	6/1/10 – 5/31/14	\$68,976 to MHC 0.08 WY for Dyar
The State of Sulfur on Mars: Understanding the Interrelationships Among the Crystal Structure, Chemistry, and Spectroscopy of Sulfates and Sulfides M.D. Lane, P.I.	NASA Mars Fundamental Research Program	Dr. Mitchell Schulte (202) 358-0780 HQ-MFRP@mail.nasa.gov	4/1/11 – 3/31/14	\$97,754 total award 0.08* WY for Dyar
The Stability and Transport of Water on the Moon Karl Hibbitts, P.I.	NASA Lunar Advanced Science and Exploration Research	Dr. Robert A. Fogel (202) 358-228 HQ-LASER@mail.nasa.gov	9/1/11-6/30/14	\$106,614 to MHC 0.00* WY for Dyar
Integrated Spectroscopy of Pyroxenes: Composition, Structure and Thermal History Rachel Klima, P.I.	NASA Planetary Geology and Geophysics Program	Dr. Michael S. Kelley (202) 358-0607 HQ-PGG@mail.nasa.gov	8/5/11-8/4/14	\$32,711 total 0.08* WY for Dyar
Enhancing Science Return from ChemCam through Laboratory and Statistical Analyses and Integration with APXS** M. Darby Dyar, P.I.	NASA Mars Science Laboratory Participating Scientist Program	Dr. Max Bernstein 202-358-0879 sara@nasa.gov	2/1/12-12/31/14	\$476,885 total 0.16/ 0.59/0.44/ 0.19 WY for Dyar

Building Analytical Competence for Geoscience Students through use of Spectroscopic Tools John B. Brady M. Darby Dyar Eileen McGowan, P.I.s	NSF DUE - TUES-Type 1 Project	Dr. David Matty (703)292-5323 dmatty@nsf.gov	8/15/12-7/31/15	\$78,484 to MHC 0.04/0.04/0.0 WY for Dyar
Effects of Composition and Cooling Rate on Fe XANES Glass Calibrations Molly McCanta M. Darby Dyar, P.I.s	NSF Division of Earth Sciences	Dr. William Leeman 703-292-7411 wleeman@nsf.gov	8/1/12-7/31/15	\$115,363 to MHC 0.08 Y for Dyar
Pyroxene Spectroscopy, Composition, Structure, and Thermal History Rachel Klima, P.I.	NASA Planetary Geology and Geophysics Program	Dr. Michael S. Kelley (202) 358-0607 HQ-PGG@mail.nasa.gov	6/1/13-5/31/16	\$91,313 to MHC 0.08 WY for Dyar

*Effort has been reduced from original funded shown in current and future years with approval from program directors

**Note: this proposal received only 50% of requested funding, and all support for laboratory and statistical analyses was cut.

Pending Support M. Darby Dyar				
Title of Award or Project	Sponsoring Institution	Point of Contact & Phone & Email	Period of Performance	Budget (\$K) & %Commitment (WY)
Collaborative Research: Transfer Learning for Chemical Analyses from Laser-Induced Breakdown Spectroscopy M. Darby Dyar, P.I.	NSF Computational and Data-Enabled Science and Engineering	Dr. Sharon Neal (703) 292-4952 shneal@nsf.gov	9/1/13-8/31/16	\$269,319 to MHC 0.003/0.08/0.08 WY for Dyar
Remote, In Situ, and Synchrotron Studies for Science and Exploration Timothy Glotch, P.I.	NASA Solar System Exploration Research Virtual Institute	Dr. Robert Fogel (703) 292-4952 rfogel@nasa.gov	1/1/14-12/31/18	\$777,256 to MHC 0.01/0.01/0.08/ 0.08/0.08 WY for Dyar
Environment and Evolution of Exploration Destinations: Science and Engineering Synergism Carle Pieters, P.I.	NASA Solar System Exploration Research Virtual Institute	Dr. Robert Fogel (202) 358-2289 rfogel@nasa.gov	1/1/14-12/31/18	\$150,000 to MHC 0.01 WY for Dyar
Volatiles, Regolith and Thermal Investigations Consortium for Exploration and Science (VORTICES) Ben Bussey, P.I.	NASA Solar System Exploration Research Virtual Institute	Dr. Robert Fogel (202) 358-2289 rfogel@nasa.gov	1/1/14-12/31/18	\$51,998 to MHC 0.01 WY for Dyar
Biogenic Iron Oxide Transformations by Thermophilic and Mesophilic Iron-Reducing Microbes James Holden, P.I.	NASA Astrobiology: Exobiology and Evolutionary Biology	Dr. Michael H. New 9202) 358-1766 HQ-EXO@mail.nasa.gov	6/1/14-5/31/17	\$208,316 to MHC 0.01/0.08/0.08 WY for Dyar

Note: Current and Pending Support is not applicable for Marchand, who is a staff member.

E. BUDGET JUSTIFICATION: NARRATIVE AND DETAILS

UNIVERSITY OF MASSACHUSETTS budget justification

Period	3/1/14 – 2/28/15	3/1/15 – 2/29/16	3/1/16/2/2 8/17	Totals
Salary Parente, Mario (0.11 AY per year)	10,528	10,896	11,278	32,702
Grad student salary (1 CY per year)	24,035	24,876	25,746	74,657
<i>Total Salaries & Wages</i>	<i>34,563</i>	<i>35,772</i>	<i>37,024</i>	<i>107,359</i>
PI & Sr. Personnel Fringe benefits	3,064	3,171	3,282	9,517
OT Fringe benefits	6,613	6,844	7,081	20,538
<i>Total Wages & Fringe Benefits</i>	<i>44,240</i>	<i>45,787</i>	<i>47,387</i>	<i>137,414</i>
Permanent Equipment	114,598	0	0	114,598
Travel - Domestic	1,500	1,500	1,500	4,500
Materials and Supplies	2,500	500	500	2,500
Subcontracts	74,955	84,524	86,842	246,321
Publishing	1,500	1,500	1,500	4,500
Misc - No Overhead (curriculum fees)	8,912	9,358	9,826	28,096
<i>Total Direct Costs:</i>	<i>248,205</i>	<i>143,169</i>	<i>147,555</i>	<i>538,929</i>
<i>Total Indirect Costs:</i>	<i>44,097</i>	<i>29,080</i>	<i>30,024</i>	<i>103,201</i>
Total Project Cost:	292,302	172,249	177,579	642,130

Salaries: Funding is requested by the University of Massachusetts for 3 months of P.I. Parente's academic time (1 academic month is 0.11 of Academic year (AY)) and 36 months of graduate student time over the 3 years of the project (1 calendar year (CY) per year). The salaries are calculated with a 3.5% standard Federal Prime rate yearly increase. The UMass senior personnel fringe for Dr. Parente is 29.10% and the "OT fringe" represents UMass student benefits. The UMass student curriculum fee is listed as "Misc.- No Overhead" and it is not included in the overhead calculations.

The University of Massachusetts benefits rates are based on actual costs calculated currently for UMass staff. UMass overhead rate is for research on campus is 59%. All information on University approved rates on fringes and indirect costs is obtained by the Office of Grant and Contract Administration (OGCA) University of Massachusetts, Amherst Campus Fact Sheet (rev. 01/02/13) downloadable at <http://www.umass.edu/research/training/ogcafact-sheet-htm>.

Equipment: This proposal requests funding for the creation of a goniometric spectroscopy facility at UMass. The request is consistent with the guidelines for a NASA Request for Planetary Major Instrumentation. Detailed costs are illustrated in Table 3 of section 7 of the narrative.

Travel: Travel support is requested for Dr. Parente and his graduate student to present results at the Lunar and Planetary Science Conference each year of the project. Detailed travel cost estimates are provided below.

Travel Detail

	2015	2016	2017
LPSC, March, 2015-17, BDL to HOU, 2 Travelers for 5 days			
Airfare	\$ 800	800	800
Per diem	\$ 300	300	300
Conference fees	\$ 300	300	300
Transportation	\$ 100	100	100
Total Domestic Travel	\$1,500	1,500	1,500

Other costs: We request \$3,500 for materials and supplies costs in support of building the new goniometric facility and for computer and office supplies. We estimated \$ 1,000 for the purchasing, painting and installation of coated panels in the goniometric facility. We request \$1,500/year for publication page charges, based on our average page charges for our group. The UMass budget also contains a subcontract detailed on the following page.

Indirect costs: Indirect costs are charged 59% of total budget except curriculum fee, permanent equipment and subcontract costs beyond \$25,000.

For UMass Amherst, the cognizant government audit agent is:

Michael Stanco, HHS Rep
26 Federal Plaza, Rm 41-122
New York, NY 01278
Phone: 212-264-0920

Mount Holyoke Subcontract, Budget Summary

	FY14	FY15	FY16	SUM
Faculty Salary for Dyar, 0.01/0.08/0.08	\$1,137.25	\$13,015	\$13,406	\$27,558
Marchand, 6 months	\$26,000	\$26,780	\$27,583	\$80,363
Undergraduate student @\$10/hour	\$2,000	\$2,000	\$2,000	\$6,000
Total	\$29,137	\$41,795	\$42,989	\$113,921
Benefits Faculty @30%	\$341	\$3,905	\$4,022	\$8,268
Benefits Staff / year @30%	\$7,800	\$8,034	\$8,275	\$24,109
Benefits student/ year @0%	\$0	\$0	\$0	\$0
Total benefits	\$8,141	\$11,939	\$12,297	\$32,377
Total Salary+fringes	\$37,278	\$53,734	\$55,286	\$146,298
Travel	\$1,500	\$1,500	\$1,500	\$4,500
Materials and supplies	\$16,500	\$500	\$500	\$17,500
Page charges	\$1,000	\$2,000	\$2,000	\$5,000
Total direct costs	\$56,278	\$57,734	\$59,286	\$173,298
ICC @64.1 on salaries only	\$18,677	\$26,791	\$27,556	\$73,024
Total	\$74,955	\$84,524	\$86,842	\$246,321

Salaries: Salary support is requested for Dyar at 1% effort in the first year and 0.08 FTE (1 month) during the last two years. Dyar will use the funds either during the academic year toward buying herself out of teaching a class, during a sabbatical year, or during the summer. If the salary is used in the summer, then the small difference in benefits rate between the academic year (30%) and the summer (9%) will be reapportioned back into salary. In the unlikely event that her time is overcommitted, we will use those funds to give additional funding to her lab manager or Jerry Marchand on this project, who will do the work under her direction. We also request \$25K (with inflation) to support 50% of Marchand's time for three years. Finally, we request \$2K/year to pay an undergraduate student work in Dyar's lab to assist Marchand with labeling, bookkeeping, posting on the web site, and organization of the mineral mixtures and reflectance spectra as they are created.

Travel: We request \$1,500/year (adjusted up for inflation in subsequent years) for travel, to be used by the post-doc and/or the students. At least one of these will be the LPSC March meeting, with a typical budget of airfare = \$400; per diem = \$800; shared rental car = \$300; registration = \$300). Dyar's travel to LPSC will be covered by other NASA grants.

Other Expenses. For the Mount Holyoke portion of this project, we request \$500 per year for materials and supplies for the post-doc in support of data acquisition and synthesis of mixtures of purchased oxides and rock powders. In year one only, we request an additional \$6,475 for the purchase of large gem-quality minerals, \$2,825 for the purchase of 10,000 1 dram glass sample vials (<http://www.discountvials.com/ProductDetails.asp?ProductCode=CT131545-144>)¹, \$600 for a set of 10 sieves, with a bottom pan and top cap², \$1,100 for a 4.8 × 3.9 × 2 in.

¹ <http://www.discountvials.com/ProductDetails.asp?ProductCode=CT131545-144>

² <http://www.dualmfg.com/products/16/4-diameter-sieves.html>

diamonite mortar and pestle³ exclusively for this project, \$5,000 (roughly \$300 per analysis, 4 aliquots of each) for complete chemical characterization of all samples at ACT Labs⁴. The cost of minerals is estimated based on prices we have paid in the past decade for large, museum-quality gemmy crystals, scaled up for the purchase of kg-sized specimens. The mortar and pestle will be needed to grind the large amounts of sample for this project in an Fe-free mortar. We further request a total of \$5,000, distributed over the three years of the grants, for page charges, in support of papers from both Mount Holyoke and the University of Massachusetts. This price represents the average cost of peer-reviewed publications from this group over the past two years.

Indirect costs are budgets at 64.1% of salaries only.

For Mount Holyoke College, the **cognizant government audit agency** is the Office of Naval Research. The administrative contracting office is:

Gregory J. Valenti
ONR Boston
495 Summer St. Room 221
Boston, MA 02210-2109
gregory.valenti@navy.mil
617-753-400

¹ <http://www.discountvials.com/ProductDetails.asp?ProductCode=CT131545-144>

² <http://www.dualmfg.com/products/16/4-diameter-sieves.html>

³ <http://www.fishersci.com/ecommm/servlet/itemdetail?productId=2671998&storeId=10652&langId=-1>

⁴ Analytical packages WRA + trace lithoresearch, code 4B-INAA, code 4F for SO₄, C, S, Cl, and B

³ <http://www.fishersci.com/ecommm/servlet/itemdetail?productId=2671998&storeId=10652&langId=-1>

⁴ Analytical packages WRA + trace lithoresearch, code 4B-INAA, code 4F for SO₄, C, S, Cl, and B

SUMMARY OF PERSONNEL, COMMITMENTS, AND COSTS:

Investigator:	Duration	Academic Year FTE (out of 9 months)**	Work Year or Equivalent FTE
P.I. Mario Parente	3/1/14-2/28/15	0.12	0.08
	3/1/15-2/29/16	0.12	0.08
	3/1/16-2/29/17	0.12	0.08
P.I. Darby Dyar	6/1/13-5/31/14	0.01	0.01
	6/1/14-5/31/15	0.12	0.08
	6/1/15-5/31/16	0.12	0.08
Staff: Jerry Marchand	6/1/13-5/31/14	n.a.	0.5
	6/1/14-5/31/15	n.a.	0.5
	6/1/15-5/31/16	n.a.	0.5
Graduate student (as yet unnamed)	6/1/13-5/31/14	n.a.	1.0
	6/1/14-5/31/15	n.a.	1.0
	6/1/15-5/31/16	n.a.	1.0

*These numbers reflect whole year FTE for a 12-month salary based on the sum of faculty's nine-month academic appointment plus three summer months.

**Academic year FTE is not applicable to staff members.

Statement of Work for Mario Parente:

P.I. Parente will purchase, install, and operate the new gonio-reflectometer facility requested in this proposal. Working with Co-I Dyar, he will oversee acquisition of spectral data on all samples and posting of those data on a web site. He will supervise the graduate student on this project, whose task will be performing the measurements and using the mineral mixture spectra to test existing physical and statistical models for mineral mixing. Dr. Parente will tutor the student on the correct application of the Hapke model and the development of new statistical technique. The student will be responsible for developing all the code for the project.

Dr. Parente will also work with Dyar and the graduate student to make presentations and write publications to disseminate this work. He will lead the publication effort on the technical aspects of the project.

Statement of Work for M. Darby Dyar:

Dyar will lead the effort to obtain mineral samples for mixtures, characterize their chemistry and purity, and prepare mineral mixtures. With Parente, she will oversee acquisition of spectral data on all samples and posting of those data on a web site. She will also work with Parente to make presentations and write publications to disseminate this work. Finally, she will curate the mineral mixtures and make them available to the community for other types of non-destructive spectroscopic measurements.

Statement of Work for Jerry Marchand:

Marchand will be responsible for obtaining four pure minerals in kg quantities for this study. He will also prepare both the size fractions and mineral mixtures for this work, and then do the daily work of acquiring all their spectra,

Statement of Work for Sridhar Mahadevan:

Mahadevan will be responsible for consulting the P-I and student on the development of new machine learning algorithms for the representation of reflectance spectra of minerals and their mixtures.

F. FACILITIES AND EQUIPMENT

FACILITIES AT THE UNIVERSITY OF MASSACHUSETTS

Dr. Parente and his graduate student use office, image processing and laboratory facilities in the Department of Electrical and Computer Engineering at UMass.

Dr. Parente has access to a laboratory space specifically designed for this project. The facility is completely enclosed, has no windows and will be outfitted with absorbing dark coatings so to allow accurate reflectance measurements with negligible stray light effects. The room is furnished with custom shelving for the storage and cataloguing of samples. The requested gonio-reflectometer system will be housed in this space.

Dr. Parente's group has built a state-of-the-art data processing and storing facility, which will allow timely and accurate manipulation and maintenance of the spectral database and the ancillary data products produced by this project.

The data storage and data processing system includes a server "rhogroup" connected to a mirrored RAID system:

- "rhogroup" Dell Red Hat server description:
 - 2 x 3.3 Ghz Quad-Core Intel Xeon processor
 - 64 GB DDR3 RAM
 - 1GB NVIDIA Tesla graphic processor
 - 20 TB ISCSI Dell Storage Array
- "rhogroup" software:
 - Red Hat 6.3 server Operative System
 - Matlab 2012a
 - ENVI 5.0
 - R software
 - LabView software

All data collected for this project will be posted on a custom website, which will interface with the database hosted on Parente's group server.

FACILITIES AT MOUNT HOLYOKE COLLEGE AND WITHIN THE FIVE COLLEGE DEPARTMENT

A back up of all the data collected will be posted on the Mars Mineral Spectroscopy web site, which is permanently maintained by the P.I. at Mount Holyoke College:

<http://www.mtholyoke.edu/courses/mdyar/database/>.

This web site contains spectroscopic data on more than 500 mineral samples representing >150 mineral species (organized by mineral group), and includes Mössbauer, reflectance, emittance, and Raman spectra (including both graphics of the spectra and source data), as well as chemical analyses. Its focus is on providing multiple spectroscopic analyses of the *exact same mineral samples*, to facilitate direct comparisons among analytical techniques. As LIBS spectra are acquired, they will be routinely posted on this site. The site is already extensively used by the scientific and educational communities as a source of reference data on various mineral groups, and receives roughly 10,000 hits per year.

Mount Holyoke College has a new laser-induced breakdown spectrometer analogous to the ChemCam instrument on Mars Science Lab (“*Curiosity*”). This instrument is a slightly modified version of the LIBS Soil Scanning (LIBS-SS) instrument that was designed, built and employed in the LIBS User Facility at LANL. The LIBS-SS instrument was designed to be operated by students and untrained laser workers. The MHC LIBS instrument uses a Big Sky laser operating at 1064nm and 10Hz. A laser power meter is permanently integrated into the instrument, allowing the user to reduce the power to that used by ChemCam, 15-20mJ/pulse. The laser focuses onto samples through a relatively long focusing lens (10 – 20cm). The long focal length reduces the fluctuations in the LIBS plasma intensity that can result from samples with uneven surfaces. The instrument is equipped with three Ocean Optics HR2000+ user-configured spectrometers and a Quantel Ultra 100 GRM laser system that can operate at 100 mJ @ 1064 nm with 20 Hz operation, 7 ns pulse duration, <1.5 mrad beam divergence, and a 4 mm beam diameter.

Because of Five College cooperative funding arrangements (and the fact that Dyar is on the Graduate Faculty at U Mass), the analytical facilities at U Mass are available to us for basically no charge, although small, lump sum donations are usually requested for grant-based research projects. If needed, we can use the X-ray fluorescence laboratory under the direction of Dr. Michael Rhodes in the Dept. of Geosciences at U Mass for some whole rock analyses or the electron microprobe under the direction of Dr. Michael Jercinovic.