

## Quantitative mineral analyses of planetary surfaces using reflectance spectroscopy

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**Abstract**—There are several uses of reflectance spectroscopy for remote compositional analyses: mapping of lithologic units, identifying minerals present on a surface, quantifying the abundance of minerals present, and characterizing the composition of minerals present. Three very different approaches currently used to identify and quantify mineralogy are summarized with examples. (1) Empirical approaches. These include comparing or 'matching' spectra with a library of spectra for natural and prepared materials with known physical and chemical properties, documenting trends of spectra for known materials and correlating with observations, developing statistical frameworks through which to evaluate spectra of unknown materials, developing spectral parameters which measure or are correlated with spectral trends that follow composition. (2) Spectral mixture analyses. These approaches are based on the premise that natural surfaces consist of mixtures of a small number of mineralogical or lithologic components (endmembers), and the reflectance spectrum of the surface is a systematic combination of the reflectance spectra of the endmembers. Models for both linear (spatially distinct) and non-linear (intimate) mixtures have been compared, evaluated, and applied to planetary science problems that require information on the relative proportion of materials in a naturally mixed surface. (3) Deconvolution of individual mineral absorption bands allowing quantitative assessment of the diagnostic properties of individual electronic transitions or groups of such diagnostic absorptions. Examples to date include quantification of properties of pyroxenes and their mixtures leading to abundance determination for mixtures and determination of olivine composition from spectral variations of deconvolved electronic transitions. Extrapolating from the rapid progress of the past, our ability to contribute to the exploration and understanding of various solar system bodies using reflectance spectroscopy will continue to expand productively as quantitative approaches mature.

### INTRODUCTION

REFLECTANCE SPECTROSCOPY, or spectrophotometry, is the quantitative measurement and study of light reflected from a surface as a function of wavelength. The use of reflectance spectroscopy to evaluate the mineralogy of planetary surfaces came of age in the 1970's with the fortunate convergence of several research activities. First was publication of a book that clearly describes the fundamental physics and crystal field theory that give rise to the diagnostic absorption bands of many rock forming minerals in the visible to near-infrared (BURNS, 1970a). Second was the development of detectors and telescopic instruments that could acquire high precision spectroscopic data for planetary objects (*e.g.*, ADAMS and McCORD, 1969; McCORD *et al.*, 1970, 1972, McCORD and JOHNSON, 1970). Third, was parallel efforts to identify and characterize diagnostic features in laboratory reflectance spectra of rocks and minerals in order to develop the interpretive base for the remote observations (HUNT and SALISBURY, 1970; ADAMS, 1974, 1975). Over the last few decades, each of these areas of research has matured, and with the publication of the revised and expanded second edition of Burns' book

(BURNS, 1993) it is appropriate to also assess the progress, accomplishments, and future challenges for the use of reflectance spectroscopy in remote compositional analysis. In the discussion below it is assumed the reader is familiar with crystal field theory and the origin and nature of diagnostic electronic transition absorptions that occur in minerals containing transition element ions (BURNS, 1993).

Before discussing recent advances in the use of reflectance spectroscopy, a clarification of important distinctions between several different types and scientific applications of remote spectroscopic measurements is warranted. There is no single approach to spectroscopic analysis of a planetary surfaces and the different objectives, as well as specific instruments and analytical tools available, can be confusing. In all cases, variations in the spectral properties of natural materials provide valuable compositional information. In general, however, increasing complexity of spectral measurement and sophistication of analytical capabilities provides increased understanding and thus increased utility for various scientific applications.

#### *Mapping lithologic units*

Color photography is the oldest form of remote spectral measurements. This naturally evolved to

multi-spectral imaging when digital detectors became available. When spectral information is obtained in two spatial dimensions (image format), spectral differences can be examined and their spatial relations mapped. An example of a digital image for a region on the Moon is shown in Fig. 1 along with a spectral ratio image (the reflectance at  $0.41 \mu\text{m}$  divided by the reflectance  $0.66 \mu\text{m}$ ) of the same area. Typically, geometrically co-registered images of the surface are obtained in a small number of spectral channels. Although such multispectral images cannot identify minerals, if the wavelengths of the spectral channels span parts of the spectrum containing absorption features and if the detectors achieve appropriate precision and accuracy, then different lithologies can usually be distinguished from each other and their spatial relations mapped. Obviously, a large the number of spectral channels usually increases the ability to distinguish between different lithologies. Most multispectral imaging systems contain between 3–12 bandpasses. Multispectral cameras have continued to improve along with development of efficient and accurate algorithms to distinguish and map surface materials. The relation between multispectral imaging and spectroscopy is largely complementary. As separate approaches, the former is principally a tool to *map* the spatial distribution of distinct materials, the latter a tool to *characterize* the composition of surface materials (*e.g.*, see concept discussion in HEAD *et al.*, 1978).

#### *Identifying minerals present*

When the number of spectral channels of an instrument is sufficiently high (often loosely referred to as high spectral resolution) and spectral coverage spans continuously across individual absorption bands to fully determine their properties (shape, strength, etc.), then the measurement approach is called spectroscopy, or hyperspectral, rather than multispectral. Reflectance spectra of several common materials of interest to planetary scientists are shown in Fig. 2. An up-to-date survey and review of the reflectance properties of most rock forming minerals can be found in GAFFEY *et al.* (1993c). Remote measurements with an appropriate spectrometer (high spectral resolution, spectral coverage, precision, accuracy) can measure the presence or absence of a particular diagnostic absorption band, which in turn usually indicates the presence or absence of a mineral. Such use of spectroscopy blossomed in the 1980's and has been highly successful with the advent of near infrared spectrometers used on earth-based telescopes. These instruments allowed spectra (hundreds of spectral channels) to be obtained for individual areas, or spots, on the surface (typically 5–15 km on the Moon, hundreds of km on Mars, and the whole body for asteroids). Most work has focused on mafic minerals (orthopyroxene, clinopyroxene, olivine), ferric oxides, hydrous minerals, and plagioclase. A variety of analyses have accumulated since

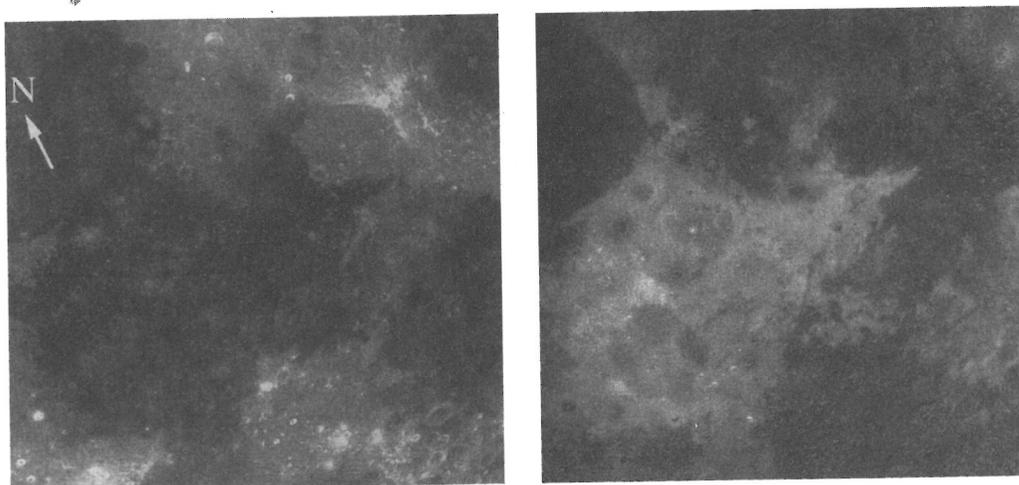


FIG. 1. Galileo digital image of the Mare Tranquillitatis to Mare Serenitatis region of the Moon. The image on the left is a reflectance image obtained at  $0.66 \mu\text{m}$  and the image on the right is a UV/VIS spectral ratio image ( $0.41/0.66 \mu\text{m}$ ) for the same area. This spectral ratio is particularly sensitive to variations in basalt type. The Galileo data are from the second Earth-Moon encounter (BELTON *et al.*, 1994).

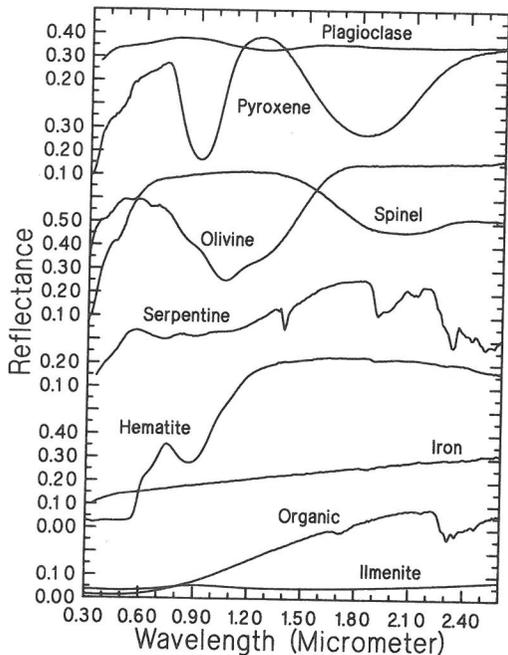


FIG. 2. Reflectance spectra of various rock forming minerals (after PIETERS and MCFADDEN, 1994)

the early observations and there are several recent reviews that summarize the type of minerals or mineral assemblages identified for solar system silicate bodies: Mars (ADAMS and MCCORD, 1969; SODERBLOM, 1992; ROUSH *et al.* 1993); Asteroids (MCCORD *et al.*, 1970; GAFFEY *et al.*, 1993a; PIETERS and MCFADDEN, 1994); and the Moon (MCCORD and JOHNSON, 1970; PIETERS, 1986; 1993).

#### *Quantifying the abundance of minerals present*

Identifying the presence of minerals requires accurate spectrometers, and sometimes a bit of luck. Nature tends to produce minerals in mixtures, sometimes simple, sometimes complex. In many applications, further complications arise due to alteration, both physical and chemical, by the local environment. The more interesting scientific issue, and more difficult task for spectroscopy, is to go beyond simply identifying the presence of a mineral, and to quantify the actual abundance of minerals present in a natural mixture. The ultimate goal is to describe the first order petrology of the material. As summarized below, several approaches to this problem have been developed for spectroscopy including empirical measurements of a range of

materials, theoretical modeling of spectra in a mixture, and separating the individual components of a composite spectrum.

#### *Characterizing the composition of minerals present*

Several important rock forming minerals are part of a solid solution series and can exist over a range of compositions (*e.g.*, olivine, pyroxene). The composition of the mineral is often as important scientifically as its presence on the surface of a silicate body. Various empirical approaches that document regular variations of absorption bands with composition have been used to obtain good approximations of mineral composition. More recently, deconvolution of individual absorptions in reflectance spectra has been successful in quantifying compositional trends for some observed absorptions and linking them directly with crystal field theory predictions.

The instrument technology available for remote mineralogical analyses has advanced considerably over the last two decades along with enormous expansion of computing capabilities and the development of very sophisticated analytical capabilities for information extraction. Although the technical capabilities will not be reviewed here, the concepts are simple. Spectroscopy and imaging have readily merged in new instruments called imaging spectrometers which produce an "image cube" of coregistered data: two dimensions of spatial information and one dimension of spectral information, with each dimension containing hundreds of elements. Such hyperspectral imaging data is the preferred type of data to address compositional issues in a geologic context and it is anticipated such data will gradually replace the more limited single-point spectroscopy and multi-spectral imaging.

The discussion below focuses in more detail on quantitative approaches to spectroscopic analysis. An excellent earlier discussion can be found in CLARK and ROUSH (1984) who describe appropriate methods for quantifying features observed in reflectance spectra. The discussion here concentrates on applications to electronic transition absorptions, although these more recent methods can be generalized to other forms of absorption as well. Results from three very different approaches currently used to identify and quantify mineralogy are summarized here. The first covers empirical approaches for which laboratory analogs of anticipated surface components are prepared and systematic variations of spectral properties are noted. The second relies heavily on theoretical frameworks

which describe the interaction of light with particulate media and specifically how the spectral properties of individual components combine together to form a spectrum of a mixture. The third approach models individual absorption features in a reflectance spectrum and provides a direct link to the physical understanding of absorptions provided by crystal field theory.

### EMPIRICAL APPROACH TO COMPOSITION AND MIXTURES

From the onset, empirical methods of comparing laboratory and remote reflectance spectra served as the primary tool for identifying the composition of planetary surfaces (*e.g.*, ADAMS and McCORD, 1968; McCORD *et al.*, 1970; McCORD and JOHNSON, 1970). This approach has been quite successful in providing an initial, but usually qualitative, assessment of the mineralogy of planetary surfaces. The assumptions are simple. If the spectral properties of minerals, rocks, and soil are well documented, a spectrum of an unknown material needs only be compared (or "matched") to the library of known materials. Since spectral properties are controlled by composition, when a good match is found in well known laboratory materials, the composition of the unknown material is thought to be comparable to the known material. Similarly, trends observed in a series of known materials are often extrapolated and applied to unknown surfaces. Many of the early applications relied on visual inspection and simple qualitative correlation. The basic analytical procedures have recently been implemented into more sophisticated and rigorous computer programs that use numerical algorithms to determine goodness of fit. These new methods are thus more objective and can often accommodate noisy data, while allowing rapid searches over large spectral libraries (*e.g.*, CLARK *et al.*, 1993).

The greatest utility of these approaches is in the identification of minerals present on a surface, which, through the use of computers and spectral libraries, can now be used to search through large data sets. There are, however, some fundamental limitations. The identification of minerals present is necessarily limited by the completeness of the spectral library upon which comparisons are made. Results are constrained to the presence or absence of comparable materials in the library, and though mineral assemblages may be identified if present in the library, modal abundance is not easily determined. A further complication is the frequent presence of overlapping absorptions, which require libraries to accommodate various combinations of

mixtures and their textures. In addition, this approach is generally unable to reproduce processes such as weathering and alteration, which are at the heart of some of the more important problems in studies of planetary surface composition.

In several commonly used forms, empirical approaches document systematic trends in spectral variation through a series of spectral measurements made for well defined material with a controlled variable such as particle size or proportion of mineral in a mixture. Although this procedure often provides numerical values (see examples below), it is important to continually recognize the basic assumptions and scope of the data inherent in empirical comparisons. In short, the *uniqueness* of a given interpretation or "match" in empirical approaches is often difficult to assess.

#### *Mineral mixtures*

Several laboratory studies have addressed spectral trends observed in carefully prepared mixtures of common rock forming minerals. Some of the earliest (NASH and CONEL, 1974; PIETERS, 1974) documented effects of particle size and opaques on diagnostic absorptions of mafic minerals in mixtures (*e.g.* Fe<sup>+2</sup> band near 1  $\mu$ m). It was noted that spectral properties of individual components in a reflectance spectrum combine in a very non-linear manner, with dark absorbing materials having a disproportionately large influence. The nonlinear effects of opaque components on a reflectance spectrum was later expanded substantially by CLARK (1983) who analyzed abundance and, more importantly, particle size of the absorbing species in a mixture with more translucent materials. Fine grained opaque particles (a few micrometers in size) dispersed in a translucent (or silicate) matrix are *exceptionally* efficient at absorbing radiation and darkening the mixture.

The properties of a variety of additional two component mixtures involving one or more mafic minerals were documented by SINGER (1981), PIETERS (1983), CLOUTIS (CLOUTIS *et al.*, 1986; 1990a,b), and CROWN and PIETERS (1987). These studies were principally used to evaluate trends in mixtures that might be useful in interpreting remotely acquired spectra. For example, Singer's data allowed bounds to be set on the relative abundance of orthopyroxene to clinopyroxene in a two pyroxene mixture based on the band center of the combined absorption near 1  $\mu$ m. Such a trend can easily be noted in the spectra of pyroxene mixtures shown in Fig. 3. Similarly, the detectability in a mixture of crystalline plagioclase and pyroxene by

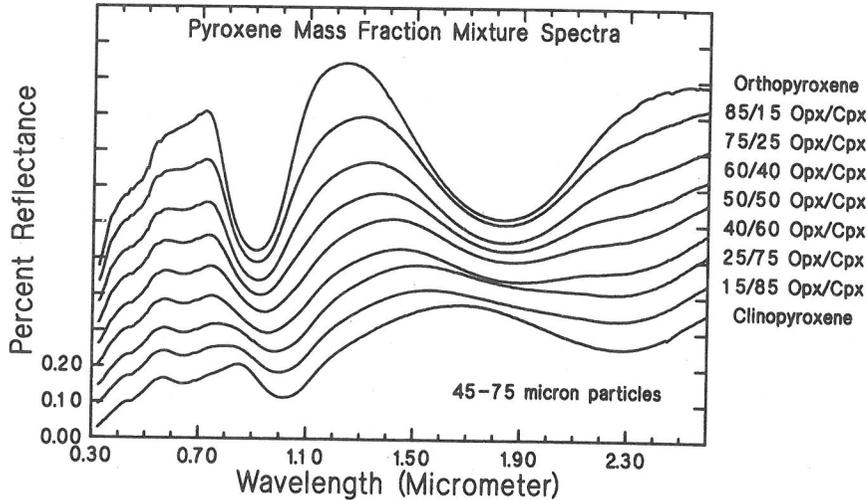


FIG. 3. Reflectance spectra for a sequence of prepared mineral mixtures of 45–75  $\mu\text{m}$  particles which contain various proportions of low-calcium orthopyroxene and high-calcium clinopyroxene (after SUNSHINE *et al.*, 1990). The spectra are displayed from bottom to top with increasing orthopyroxene fraction and a 5% offset in reflectance between each successive spectrum.

their ferrous absorptions (CROWN and PIETERS, 1987) was shown to be much easier for pyroxene ( $\geq 5\%$ ) than for plagioclase ( $\geq 50\%$ ). Parameters derived from the trends for mixtures of olivine and orthopyroxene observed by CLOUTIS *et al.* (1986) are some of the most widely used in asteroid studies and are discussed further below.

Most of these mineral mixture studies also examined the effects of particle size with ideal size separates. Since it is radiation transmitted through grains that produces the observed diagnostic absorption bands, the spectrum of a sample of large particles generally has stronger absorption bands than spectra of smaller particles. This is true until the band is so strong or the particles so large that the band saturates. The effects of well defined particle size can be modeled for reflectance, but most natural soils have a range of particle sizes leading to a non-unique solution (see next section). As an example, three particle size separates for an orthopyroxene are shown in Fig. 4 along with synthetic soils prepared with various particle size distributions. The small particles of a soil dominate the optical properties, even when present at only 10%.

#### Correlation and monotonic trends

More commonly, an empirical relation is observed between a particular type of reflectance measurement and composition, although the details of what causes the relation may not be well known.

Once established, this relation can nevertheless be used to estimate the composition of unknown surfaces. The Moon has been a principal beneficiary of this approach since ground truth information is available to define compositional relationships with measured spectra.

One of the most widely used empirical relations for lunar spectra is that between the red-sloped

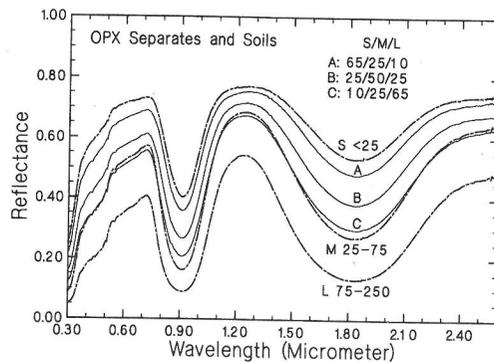


FIG. 4. Reflectance spectra of prepared size separates for an orthopyroxene. Individual size separates ( $< 25 \mu\text{m}$ ,  $25-75 \mu\text{m}$ , and  $75-250 \mu\text{m}$ ) are shown in dashed lines. Synthetic monomineralic soils are shown in solid lines prepared with the following proportions of the small, medium and large particles: 65/25/10, 25/50/25, and 10/25/65. Note that the smaller particles tend to dominate the soil spectra and that the spectral contrast is reduced.

lunar visible continuum, often referred to as the UV/VIS ratio, and the TiO<sub>2</sub> content of mature mare soils, in which flatter (or bluer) spectra are associated with higher abundances of TiO<sub>2</sub> (CHARETTE *et al.*, 1974; PIETERS, 1978). It was originally suspected the observed relation may have something to do with an electronic transition of Ti<sup>+3</sup> since lunar materials are very reduced. No appropriate carrier has yet been found, however, and reduced Ti-rich glass exhibits an effect opposite to that observed (BELL *et al.*, 1976). After much debate within the community, this relation between TiO<sub>2</sub> content and the UV/VIS continuum slope of basaltic soils is now believed to be due largely to spectral contrast issues rather than any specific absorption feature. It is important to note that although the precision of reflectance data can readily be measured to better than 1% (JOHNSON *et al.*, 1991; MELENDREZ *et al.*, 1994), the accuracy of the compositional estimation is nevertheless limited to several percent because the uniqueness issues cannot be resolved (see discussion in PIETERS, 1993 and PIETERS *et al.*, 1993).

A more comprehensive empirical approach uses sophisticated statistical analyses, such as principal components, to identify the primary spectral variations of a collection of spectra. These statistically derived principal components of spectral variation can then be associated with quantified information on compositional variations. Such an approach to compositional analyses has been developed using a suite of lunar sample spectra to define compositional associations of spectral variations within the suite (JAUMANN, 1991). As would be expected, some compositions are highly correlated with spectral variations, particularly those associated with albedo. Spectral variations of rock types with abundant minerals exhibiting diagnostic absorptions are also correlated with compositional trends. This type of probability analysis can be very useful for estimating expected bulk compositions when there is some assurance that the original data suite used to define the correlation are representative of the materials being studied remotely or in the laboratory. It is, however, not suitable for evaluating complex mineral assemblages or for assessing the importance of subtle spectral variations.

#### Paramaterization

Bridging pure empirical approaches and approaches that are solidly based on a physical and chemical understanding of cause and effect are a variety of paramaterized approaches that contain elements of a physical basis but fall short of being

able to quantify the detailed interaction of radiation with specific solid surfaces. These approaches nevertheless have been and will continue to be enormously useful, some more so than others, depending on the closeness of their link with physical reality.

One of the most solidly based relations is that between composition and the band center of pyroxene absorptions established by ADAMS (1974) using reflectance spectra. This was carried further by HAZEN *et al.* (1978) using transmission spectra and expanded with additional reflectance spectra by CLOUTIS and GAFFEY (1991). In these studies, the band centers observed for pyroxene samples were selected as a simple minimum relative to a general continuum. Adams showed that the band centers of pyroxene, both those near 1  $\mu\text{m}$  and those near 2  $\mu\text{m}$ , move to longer wavelengths as Fe and Ca substitute for Mg in the pyroxene structure. He also noted that additional ions (such as Al or Ti) in the pyroxene structure disrupt the smooth trend. Nevertheless, if the band center of an unknown pyroxene can be accurately measured, then its composition can typically be estimated to about 10%. Due to the abundance of pyroxene across many solar system bodies, this has proven to be one of the most widely used relationship in remote mineralogical analyses.

Because the spectral properties of olivine and low-Ca pyroxene are very different from each other (see Fig. 2), mixtures of the two follow very systematic trends that are well suited to parameter measurement. Low-Ca pyroxenes have two very well defined absorptions centered near 0.9 and 1.8  $\mu\text{m}$ ; olivines have a broad composite feature near 1.05  $\mu\text{m}$  but no feature at 2.0  $\mu\text{m}$ . The relative strength of the feature near 2  $\mu\text{m}$  in a mixture should thus indicate the relative proportion of low-Ca pyroxene present. CLOUTIS *et al.* (1986) devised a parameter to approximately cancel the effect of particle size on band strength measurements by measuring the relative strength of absorptions through a band area ratio. For olivine and low-Ca pyroxene mixtures, the ratio (BII/BI) of the absorption observed near 2  $\mu\text{m}$  to the combined absorption observed near 1  $\mu\text{m}$  (both measured by the band area) varied systematically with the relative abundance of the two minerals. This band area parameter was shown to be able to estimate olivine/low-Ca pyroxene abundances of mixtures to about a 10% accuracy (CLOUTIS *et al.*, 1986). It should be noted, of course, that this band area parameter is only suitable for mixtures of these two specific minerals and is demonstrably inappropriate if other

minerals are present with absorptions in this part of the spectrum (*e.g.*, clinopyroxene, spinel, etc.).

Olivine and low-Ca pyroxene are some of the most common mafic minerals found in stony meteorites and mixtures of these two minerals are thus expected to also be common on asteroid surfaces. GAFFEY *et al.* (1993b) later used the band area ratio of CLOUTIS *et al.* (1986) and a measure of the center of the composite band near 1  $\mu\text{m}$  (BI) to derive a taxonomy for S-type asteroids based on near-infrared spectra. A comparison of these two spectral parameters derived for the S-type asteroids and for several meteorite groups is shown in Fig. 5. GAFFEY *et al.* (1993b) concluded from such relationships that only their SIV subset of the S-asteroids might be consistent with ordinary chondritic mineral assemblages. It was later shown that the proposed zones in Fig. 5 are certainly diffuse, that different sides of the same asteroid stretch the limits of the SIV boundaries (MURCHIE and PIETERS, 1996), and that alteration effects can move an ordinary chondrite out of the SIV zone completely (MOROZ *et al.*, 1996).

Recently, several approaches have been developed to estimate the abundance of iron for the surface of the Moon using optical parameters. Each approach must separate optical effects due to composition from those due to surface exposure or maturity (space weathering). The first method, derived by FISCHER and PIETERS (1994), uses a spectral ratio parameter (950/750 nm) to identify mature soils and the measured strength of the ferrous ab-

sorption band near 1  $\mu\text{m}$  to estimate the abundance of iron. The 950/750 nm ratio is a composite measure of both continuum slope and band strength; it is empirically related to the soil maturity parameter  $I_s/\text{FeO}$  of MORRIS (1978) through measurements of lunar samples. Similarly, band strength of a mature soil is empirically related to FeO content of lunar highland soil samples. This empirical relation between FeO and band strength essentially mirrors the abundance of Fe-bearing minerals in lunar anorthositic soils. The second and third optical method for estimating iron abundance use the 950/750 nm ratio and a measure of albedo (*e.g.*, reflectance at 750 nm). LUCEY *et al.* (1995) uses measurements of these two parameters for lunar samples to empirically derive a coordinate transformation from which a parameter  $\Theta$  is derived and FeO estimated. FISCHER and PIETERS (1996) start with the 950/750 nm spectral parameter to derive soil  $I_s/\text{FeO}$  and then use this soil maturity index and the albedo (750 nm reflectance) to estimate iron and titanium abundance, again using lunar samples for calibration. These latter two methods are essentially measuring the correlation of composition with the abundance of optically bright, but iron-poor, anorthosite. Since all three approaches use limited empirical data for calibration, the accuracy of the extrapolated composition estimates is difficult to determine. Results from the LUCEY *et al.* (1995) method suggest that large regions of the northern lunar farside may contain vast areas of extremely low abundance of iron, an observation with very important implications for the early crustal evolution of the Moon.

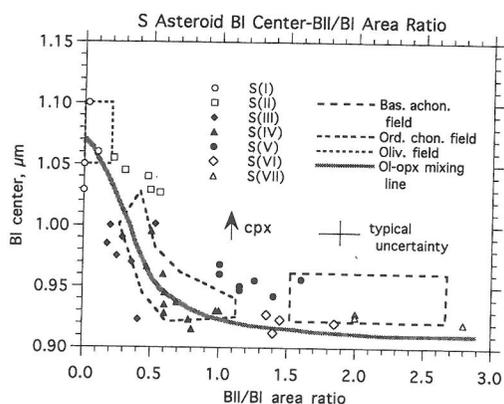


FIG. 5. Wavelength of the Band I band center versus the Band II/Band I area ratio for S-type asteroids, selected meteorite types, and laboratory mixtures of olivine and orthopyroxene (after GAFFEY *et al.*, 1993b; modified by MURCHIE and PIETERS, 1996). Band I refers to the 1  $\mu\text{m}$  band of pyroxenes and olivines; Band II refers to the 2  $\mu\text{m}$  band of pyroxenes.

## SPECTRAL MIXTURE ANALYSIS

The empirical approaches discussed above are based on specific absorption features or broad scale trends in spectral properties that are readily characterized by simple parameters or statistical techniques. A suite of parallel approaches have been pursued that are based on physical modeling from first principles, using fundamental properties such as spatial relation of components in a mixture, optical constants, particle size and shape, internal and external scattering efficiencies, and physical properties of a surface (*e.g.*, HAPKE, 1981; 1993; HIROI and PIETERS, 1992a,b). These models, particularly the radiative transfer model of Hapke, have been used widely in studies ranging from photometric studies of planetary bodies and the determination of modal abundances from reflectance spectra of mineral mixtures to the mapping of relative abundances across the surface.

The empirical trends in the spectral properties of mineral mixtures noted in the previous section are explicitly accommodated in reflectance models for particulate surfaces. Over the last two decades, there has been much activity in the testing and application of models that derive surface mineral or lithologic abundance. The basic premise of mixture modeling is that natural surfaces consist of mixtures of a small number of mineralogical or lithologic components (endmembers), and the reflectance spectrum of the surface is a systematic combination of the reflectance spectra of the endmembers. Thus if the spectral properties of the endmembers can be defined, either locally from within a remotely sensed data set, or globally through a library of reflectance spectra or optical properties, then the endmember abundances within the surface mixture can be derived through an appropriate model that combines them to form the spectrum of a mixture. Endmember spectra are usually treated as a whole (all wavelengths) and some statistical measure of goodness of fit is used to assess the degree to which the spectrum computed from endmember spectra models the actual or natural spectrum. Numerical values are provided for the fractional abundances of each endmember required for the best fit.

The basic equation for spectral mixture analysis is:

$$r_b = \sum_{i=1}^N F_i R_{ib} + E_b \quad \text{and} \quad \sum_{i=1}^N F_i = 1.0$$

where  $r_b$  is the reflectance of the observed spectrum in band  $b$ ,  $N$  is the number of endmembers,  $F_i$  is the fractional abundance of endmember  $i$ ,  $R_{ib}$  is the reflectance of endmember  $i$  in band  $b$ , and  $E_b$  is the error of the fit of the spectrum calculated from endmembers to the observed spectrum in band  $b$ . The second equation constrains the sum of the fractions to be unity. If  $M$  is the number of bands, then there will be  $M$  equations in  $N$  unknowns. As long as the number of bands is equal to or greater than the number of endmembers, a solution can be found and the fractional abundance derived.

#### *Linear mixing (spatial mixtures)*

The theoretical development and application of mixing models fall into two broad categories: linear and nonlinear mixing. Linear mixing models are the simple case where it is assumed that the components of interest are located in physically discrete areas on the surface (i.e. a checkerboard). In this case, the reflectance of the mixture is a linear combination of the reflectance of the endmembers, and

the abundance is the aerial fraction of each endmember within the field of view. A basic assumption of the linear spectral mixture model is that reflected radiation encounters only one component of the mixture, and thus there is no multiple scattering of radiation between components. This approach was initially developed for planetary applications by SINGER and McCORD (1979), but has since evolved to an increased level of sophistication largely through the efforts of Adams and co-workers (e.g. ADAMS *et al.*, 1986; SMITH *et al.*, 1990; ADAMS *et al.*, 1993). The approach has been developed and tested on multispectral and hyperspectral data using lithologic and mineralogic endmembers derived from spectra acquired remotely as well as from library spectra.

This model has enjoyed wide application in recent years, fueled to some extent by the ease of use and versatility, by the recognition that it is based on a physically realistic model of many surfaces, and, more importantly, by the new insights into surface composition and processes it can provide. A linear mixing approach is particularly appropriate when distinguishing and mapping different lithologies in a spatial context when the size of individual components is below the measurement spatial resolution (e.g., trees in a field). It is especially useful for data with low spatial resolution when the measured signal is a combination of signals from different neighboring lithologies. This approach was used, for example, with telescopic spectra of asteroids (effectively a point source of radiation) which were assumed to contain spatially coherent different lithologies (HIROI *et al.*, 1993). In this case, the spectra of a few (but not all) S-type asteroids were successfully fit with various proportions of different laboratory spectra obtained from primitive achondrites and iron meteorites. If the assumption of spatially coherent lithologies is correct, and if the laboratory meteorite spectra accurately represent these lithologies, then the proportion of each meteorite spectrum used to produce the best fit is an indication of the spatial extent of that material on the asteroid.

A more common approach is to model spectral variations in image data, where the result of the mixture model is maps (fraction images) of the abundance of the spectral endmembers on the surface (ADAMS *et al.*, 1993). Fraction images then become fundamental new tools for understanding surface and physical processes. Strictly speaking, linear spectral mixture models treat each endmember as a spatially coherent material (see below). An example of such a spectral mixture analysis performed with Galileo multi-spectral images

(six channels from 0.41 to 1.00  $\mu\text{m}$ ) is shown in Fig. 6. This particular example (from STAID *et al.*, 1996) uses a linear mixture analysis with four endmembers chosen to represent the properties of two types of basalt, one relatively blue (a) and one relatively red (b), freshly excavated mare crater (c), and highland soil (d). These endmember fraction images separate highland contamination from the basalt units, allow the spatial and stratigraphic relations between several mare units to be distinguished, and provide the basis for a more direct link between the basalt units of Mare Tranquillitatis and samples returned from Apollo 11 (STAID *et al.*, 1996).

Given the high quality data often provided by CCD multispectral imaging, the Moon has been a common target for scientific investigations using

image mixture analysis. Additional recent examples include an examination of mixing relationships between mare and highland lithologies in order to investigate modes of emplacement of basin ejecta and to explore for evidence of buried mare deposits in highland terrain (MUSTARD *et al.*, 1992; 1994; HEAD *et al.*, 1993; MUSTARD and HEAD, 1995; BLEWETT *et al.*, 1995), an evaluation of the spatial extent of feldspathic surface units across the crater Copernicus (PINET *et al.*, 1993), and an evaluation of the distribution and maturity of basaltic units in the region between Mare Serenitatis and Mare Tranquillitatis (BELL and HAWKE, 1995).

#### *Nonlinear mixing (intimate mixtures)*

A fundamental limitation of the linear model is that it is only strictly valid for the situation where

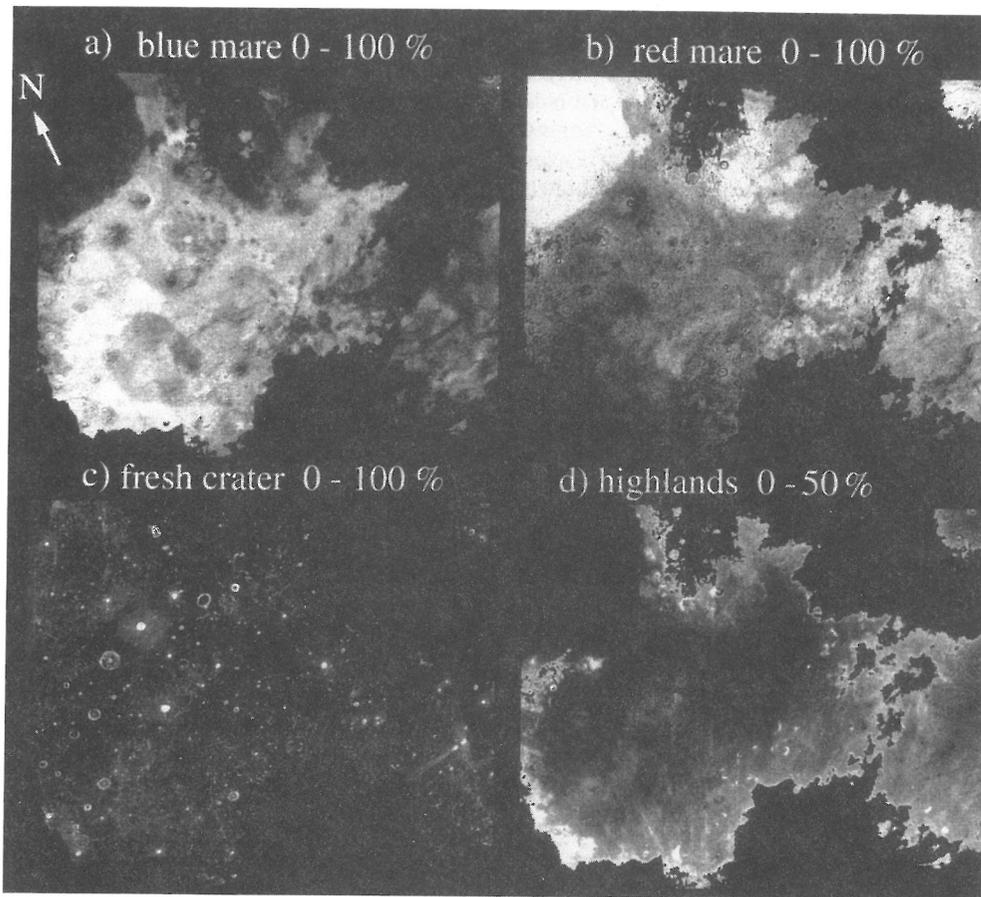


FIG. 6. Spectral mixture analysis for the same lunar area as in Fig. 1 centered on Mare Tranquillitatis (after STAID *et al.*, 1996). The Galileo data contain six spectral bands from 0.41 to 1.00  $\mu\text{m}$  (BELTON *et al.*, 1994). Shown are fractional abundance images for the four endmembers used in the linear mixing analysis: blue mare, red mare, fresh mare crater, and highlands.

the endmembers are arranged in discrete patches on the surface. The scale of components can be from centimeters up to several kilometers. Many science issues of interest in planetary settings, however, are associated with particulate regoliths, where the endmember minerals that make up the soil are intimately mixed on spatial scales smaller than the path length of photons through the medium (typically—1 mm). In these settings, light usually interacts with more than one component, and the measured spectrum is a complex convolution of the endmember spectra rather than a simple additive (linear) mixture.

The nonlinear effects in spectra of particulate mixtures has been recognized for many years (*e.g.*, NASH and CONEL, 1974; PIETERS, 1974) and a variety of methods have been developed to treat this situation. The photometric model of HAPKE (1981; 1993) has been shown to be a powerful and useful model for application to nonlinear spectral mixing. The validity of the model for linearizing the mixture systematics has been demonstrated in laboratory studies of directional-hemispherical reflectance (JOHNSON *et al.*, 1983; 1992) and bidirectional reflectance (MUSTARD and PIETERS, 1987a; 1989). For controlled laboratory samples, the Hapke model has been shown to accurately predict mineral abundance to approximately 5% absolute abundance. The technique has also been successfully applied to imaging spectrometer data for desert soils in Utah (MUSTARD and PIETERS,

1987b) allowing the spatial extent and abundance of serpentinized ultramafic microbreccia to be mapped. Reflectance spectra of the icy satellites of Jupiter have also been successfully modeled using a nonlinear mixing model (CALVIN and CLARK, 1991; ROUSH *et al.*, 1990) that includes methods to model grain sizes. A second model for nonlinear intimate mixing using different assumptions for bidirectional reflectance is that of Hiroi. In modified form, both the Hapke and Hiroi models can model reflectance spectra of mixtures within 4% accuracy (HIROI and PIETERS, 1992a,b).

#### Comparison of linear and nonlinear mixing

The effects of nonlinear mixing on reflectance spectra can be quite dramatic, as illustrated in Fig. 7. This 2-dimensional figure presents a reflectance data cloud generated using five endmembers, labeled A to E, in a mixing scenario. Reflectance in TM band 3 is plotted against the reflectance in TM band 4. In Fig. 7a, the 75 mixture points that constitute the cloud were calculated using a linear mixing model with prescribed fractions of the endmembers. Along the planes joining the endmembers (*e.g.* line A-C), the mixtures are in 25% increments. Visually, one recognizes this instantly as a linear relationship, with the points spread equidistant along the lines joining the endmembers in this reflectance space. The systematics are very different in Fig. 7b where the same 5

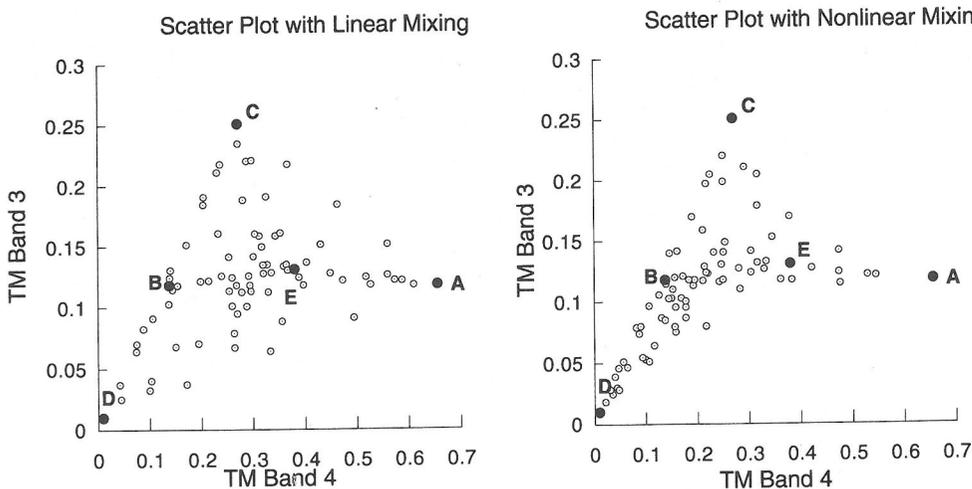


FIG. 7. Data clouds modeled for mixtures of five endmembers (A, B, C, D, and E). Individual points are reflectance values of each sample for TM bands 3 and 4 (near  $0.68 \mu\text{m}$  and  $0.88 \mu\text{m}$ , respectively). (a) Mixtures modeled with a linear mixing model. (b) Mixtures modeled with a nonlinear (Hapke) mixing model.

endmembers and the 75 mixture points with the same fractional abundances are shown, but here the mixture spectra were calculated using the nonlinear mixing model of MUSTARD and PIETERS (1989) adapted from HAPKE (1981). The nonlinear effects on reflectance values for mixtures are clearly indicated by the curvilinear segments joining endmembers (*e.g.* A-C, A-D). In addition, the entire data cloud is shifted to the left against the segment C-D, and towards the low albedo endmember (D). What drives this shift is the predominance of low albedo endmembers in nonlinear mixing situations.

There are some important implications of these differences for spectral mixture analysis. If a linear mixing model is used on data where the relation between components are nonlinear, the calculated fractions will be significantly in error. In tests of linear vs. nonlinear mixing on laboratory data, the calculated fractions can show differences by as much as 30% (MUSTARD, unpublished data). A linear model can cause considerable ambiguity and incorrect fractions when used on intimate mixtures. For example, a least square fitting approach will minimize errors using any of the endmembers in the equations. Thus in the fitting process endmembers not present in a mixture may be calculated to be present simply to minimize the error. This is illustrated in Figs. 8 and 9. In Fig. 8 are shown reflectance spectra of intimate mineral mixtures prepared in the laboratory with known abundances of particulate samples of three minerals, an anorthite, an olivine, and an enstatite. In Fig. 9, the abundances used to prepare the mixtures (open circles) are shown on a ternary diagram together with the best fit calculated abundances using a nonlinear

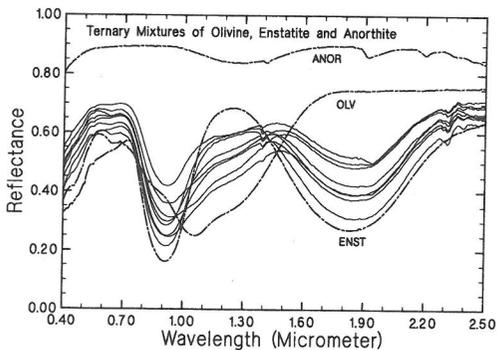


FIG. 8. Reflectance spectra of particulate samples of three mineral separates (Anorthite, Olivine, and Enstatite) shown in dashed lines, and intimate mixtures of these minerals with known abundances shown in solid lines (samples discussed in MUSTARD and PIETERS, 1989).

(solid circles) and linear (crosses) mixture model. It is evident that the nonlinear model most accurately predicts the modal abundances of the mixtures from the reflectance spectra. In general, the accuracy for such intimate mixtures is about 5%. The linear model fractions, on the other hand, are significantly in error, and for the enstatite-anorthite mixture series a component of olivine is predicted which is not present in the actual mixtures. Although a nonlinear model is clearly most appropriate for intimate mixtures, it is nevertheless important to note that for any given endmember, the abundances predicted using the linear model increase with an increase in that endmember. That is, if a linear model is used for intimate mixtures, the predicted fractional abundances *do* increase monotonically with the abundance of the real component, but the *rate* of increase is not accurate.

Despite the obvious advantages of using a nonlinear approach for intimate mixtures, this has not been widely applied to remotely acquired data of particulate planetary surfaces principally because such models are much more complex to implement than a linear model and are thus impractical. In their complete formulation nonlinear mixing models require detailed information on viewing geometry (incidence and emergence) and physical properties such as particle size and scattering properties of each endmember. One comparison of the two models undertaken by ADAMS and co-workers in which the mixing of primary material with local material was followed along a crater ray (PIETERS *et al.*, 1985) showed that the surface material was indeed better modeled with an intimate mixture than a linear mixture and the observed relative abundances of local to foreign material using the intimate mixing model was quite comparable to that predicted by crater experiments. Similarly, more thorough consideration of the nature of the remote measurements may allow many parameters in the nonlinear models to be reasonably approximated, and as spectral libraries become more well endowed with data, many of the obstacles may be sufficiently removed for nonlinear modeling to replace linear modeling as the approach of choice in remote sensing applications.

Spectral mixture analysis nevertheless is, of course, a tool and not a panacea. As described above, it is highly productive for some applications. A critical issue in the use of spectral mixture analysis is the accuracy of the choice of endmembers and the degree to which they characterize a scene uniquely (*e.g.*, ADAMS *et al.*, 1993; TOMPKINS *et al.*, 1995). There can be scientific issues, however, where neither linear nor non-linear mix-

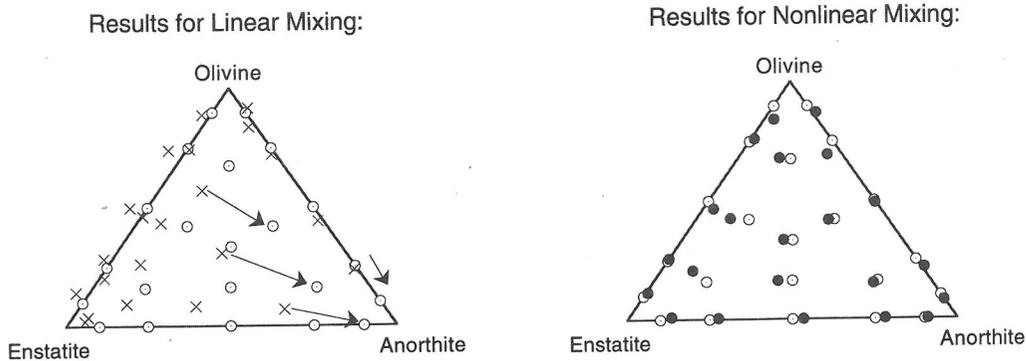


FIG. 9. Ternary diagrams of mineral abundances. Spectra of the endmember minerals were used to model the mixture spectra of Fig. 8. The open circles indicate the known abundances of the prepared mixture. The filled circles represent abundances predicted from a fit to the mixture spectra using a nonlinear mixing model. The crosses indicate the predicted abundances derived using a linear mixing model of the same mixture spectra.

ing approaches appear to converge on a viable solution, and assumptions about endmember characteristics and/or physical and compositional processes active on a surface need to be reassessed. A classic example is the continuing discussion about the character of S-type asteroids and the relation, if any, to ordinary chondrites. Although spectral mixture analyses as applied to this issue certainly accommodate a range of hypotheses (cited in several above sections), the approach can also be used to demonstrate that some endmembers logically assumed to be present on the asteroid as we currently understand them (such as various forms of Fe, Ni), simply cannot be modeled as a component for a large fraction of these asteroids using any current mixing model (CLARK, 1995).

#### DECONVOLUTION OF INDIVIDUAL ABSORPTION BANDS (MGM)

It is the individual absorption bands, such as the diagnostic crystal field electronic transitions (BURNS, 1993), that contain the most compositional information in reflectance spectra. However, in many, if not most spectra of natural surfaces, absorptions occur not as single isolated bands, but instead superimposed on other spectral features. The modified Gaussian model (MGM) of SUNSHINE *et al.* (1990) was specifically developed to address this problem and to provide a method to isolate individual electronic transition absorption bands in reflectance spectra. At the core of the MGM is a physically based mathematical expression, a modified Gaussian distribution, which (in sharp contrast to the often used Gaussian model) has been demon-

strated to accurately describe the shape of electronic transition absorptions. As an example, a comparison of modeling a single electronic absorption with a MGM distribution and with a Gaussian distribution is shown in Fig. 10. Having successfully described the shape of isolated bands, it is now possible to use the MGM to deconvolve reflectance spectra into their constituent absorptions. To facilitate this goal, the original development of the MGM includes implementation of fast, reliable, and flexible inversion techniques which together provide a powerful tool for quantitative mineralogic analysis (see SUNSHINE and PIETERS, 1993a,b and SUNSHINE *et al.*, 1993).

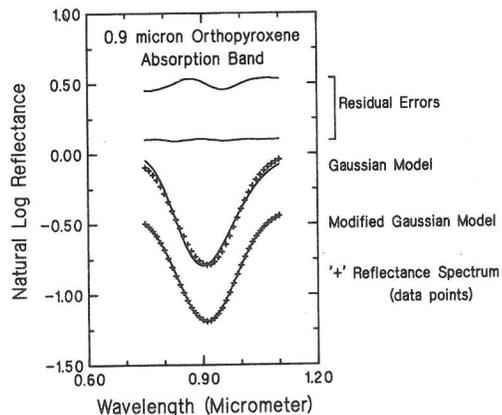


FIG. 10. Comparison of a Gaussian and a Modified Gaussian fit to an electronic transition absorption band of  $\text{Fe}^{+2}$  in an orthopyroxene. The reflectance spectrum of orthopyroxene is for a  $<45 \mu\text{m}$  particulate sample.

In the MGM, spectra are modeled simultaneously as a sum of overlapping absorption bands superimposed on a continuum (see SUNSHINE *et al.*, 1990 for model details). Each absorption is represented by a modified Gaussian distribution,  $m(x)$ , and described by three model parameters: a band center ( $\mu$ ), a band width ( $s$ ), and a band strength ( $\sigma$ ) where the MGM distribution is expressed as

$$m(x) = s \cdot \exp\left\{\frac{-(x^{-1} - \mu^{-1})^2}{2\sigma^2}\right\}$$

The continuum is normally characterized by a slope (straight line in energy) and an offset. Modeling is carried out in natural log reflectance and energy. Examples of MGM fits for particulate samples of two pyroxenes and their mixtures are shown in Fig. 11. It should be noted that in contrast to

other methods described above, the MGM neither relies on a library of spectra that may or may not reproduce all permutations and combinations of absorption bands, nor requires knowledge of endmember spectra, as is needed for both linear and non-linear mixing. Instead, the MGM derives compositional information directly from a measured spectrum. This is particularly useful in planetary remote sensing applications, where the exact petrology, major and minor element chemistry, and physical state (particle size, alteration state, etc.) of materials is unknown and often irreproducible from either spectra of terrestrial samples or samples that have been simulated in the laboratory.

The successful validation of the MGM approach for reflectance spectroscopy opens the way for quantitative assessment of the diagnostic properties of individual electronic transitions or groups of

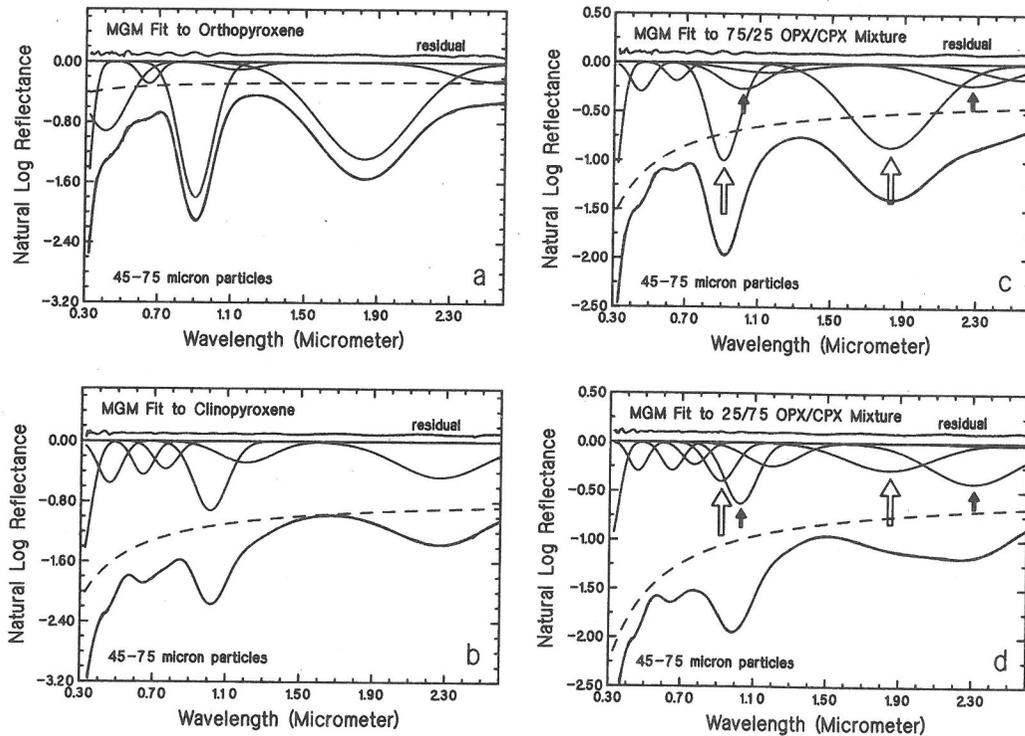


FIG. 11. Modified Gaussian model fits of reflectance spectra. Each figure includes (top to bottom): the residual error between log of the modeled spectrum and log of the actual spectrum (offset 10%), the individual modified Gaussian distributions representing absorption bands, the continuum (dashed line), and the modeled spectrum superimposed on the actual spectrum. a) MGM fit to orthopyroxene size separate. The symmetric non-random residual error near  $0.9 \mu\text{m}$  is a characteristic of minor band saturation (Sunshine and Pieters, 1993). b) MGM fit to clinopyroxene size separate. c) MGM fit to 75% orthopyroxene-25% clinopyroxene mass fraction mixture. d) MGM fit to 25% orthopyroxene-75% clinopyroxene mixture. In (c) and (d) open arrows correspond to absorptions from the low-Ca orthopyroxene phase. Filled arrows correspond to absorptions from the high-Ca clinopyroxene phase.

such diagnostic absorptions. The process of building a solid understanding of the properties of individual minerals and mixtures of minerals is in its early stages. While the MGM is a powerful tool which holds great promise, it currently needs to be used cautiously, particularly with remote data that have substantial noise and often lower spectral resolution, while the foundation of experience with well controlled laboratory samples is properly expanded. Discussed below are some of the benchmark results and a taste of the applications that have emerged in the last few years since the MGM was developed.

### Pyroxenes and their mixtures

A thorough analysis of two different types of pyroxene and their mixtures (a low-calcium orthopyroxene [OPX] and a high-calcium clinopyroxene [CPX]) was undertaken to determine whether discrete absorptions retained their well defined properties when mixed with similar materials (SUNSHINE and PIETERS, 1993a). MGM analyses were performed on three different particle sizes (<45  $\mu\text{m}$ , 45–75  $\mu\text{m}$ , and 75–125  $\mu\text{m}$ ) of the pure minerals and seven mass fraction mixtures. Mass fraction spectra for one particle size are shown in Fig. 3 and example MGM analyses are shown in Fig. 11. The results are remarkably consistent: the band centers and band widths are invariant for the primary diagnostic bands near 1 and 2  $\mu\text{m}$  which are due to ferrous iron in the M2 site. That is, the MGM fitting routine always converged on the same value for the orthopyroxene component and a separate value for the clinopyroxene component, regardless of the particle size or mass fraction. Such a task is virtually impossible with visual inspection. Furthermore, the absorptions bands determined from the mixture spectra were found to occur at the same wavelength as those of the endmember OPX and CPX pure mineral spectra. Thus for the first time, with the MGM, it is now possible to determine endmember absorption bands directly from a mixture spectra.

What is equally important for remote sensing applications is that the relative strengths of the diagnostic pyroxene absorptions in a mixture (the strength of the primary OPX band relative to the CPX band) were seen to vary in a very systematic manner with modal abundance. Such a band strength ratio is shown in Fig. 12 as a function of the clinopyroxene mass fraction in the mixture. The same relationship is seen for the absorptions near 1  $\mu\text{m}$  and for the absorptions near 2  $\mu\text{m}$ , consistent with the crystal field theory that shows the absorp-

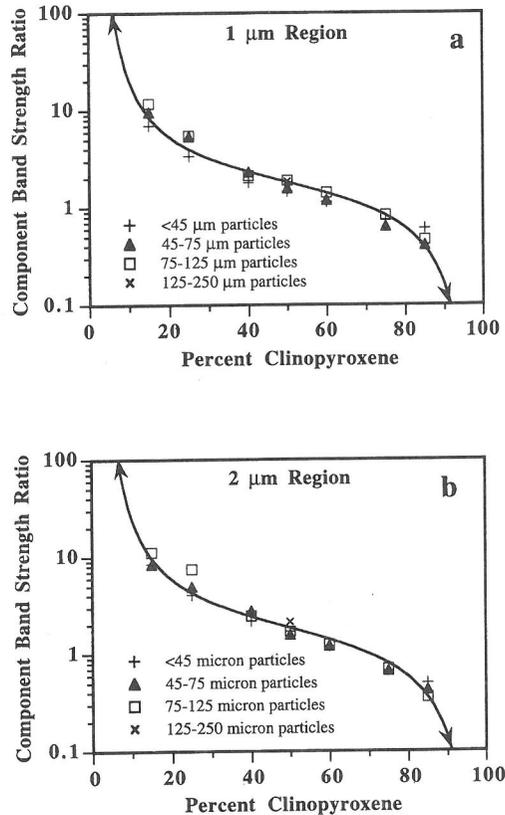


FIG. 12. Relation between modal abundance (wt %) in a mixture of pyroxenes and the 1 and 2  $\mu\text{m}$  band strength ratios for the primary orthopyroxene and clinopyroxene absorption bands (after SUNSHINE and PIETERS, 1993). a) ratio of OPX/CPX absorptions in the 1  $\mu\text{m}$  region, b) ratio of OPX/CPX absorptions in the 2  $\mu\text{m}$  region. The curves are the best fits to the data from all particle sizes. Note the particle size independence and the consistency between the 1 and 2  $\mu\text{m}$  regions.

tion in both regions arise from asymmetries in the M2 site. It is readily apparent that this relation is independent of particle size, making it an extremely valuable tool for estimating relative mineral abundances. Requirements for use are currently that pyroxenes be a dominant mafic component in a spectrum and that whatever the particle size is, it is more or less comparable for all components in the mixture. For further detail see discussion in SUNSHINE and PIETERS (1993a).

One of the first applications of the MGM pyroxene systematics was an evaluation of the two different basaltic lithologies that occurs in a shergottite meteorite, EETA 79001 (SUNSHINE *et al.*, 1993), believed to have come from Mars. MGM analyses of reflectance spectra of the two lithologies present

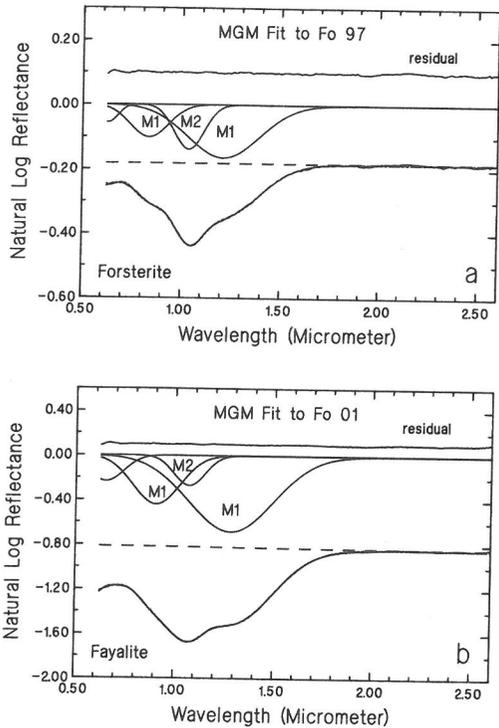


FIG. 13. MGM fit for two compositions of olivine. Note the difference in relative band strengths (M2 vs M1 bands) between the Mg-rich forsterite and the Fe-rich fayalite.

in this meteorite were used to determine that two pyroxenes are present in each of the lithologies, to estimate the composition of the two pyroxenes (based on band center), and to estimate the relative abundances of the two pyroxenes using the relationship of Fig. 12. These results compare very favorably (5–10%) to those of more traditional geochemical and petrographic methods to determine mineral abundance and composition. This first application not only provides a quantitative comparison of compositional information derived from spectroscopy with actual “ground truth”, but also serves as a model for how the MGM could be used in remote planetary applications.

One of the significant results of the MGM pyroxene analysis was that it also clearly documented an absorption band near 1.2  $\mu\text{m}$  in both pyroxenes (more prominent in clinopyroxenes) attributed to ferrous iron in the M1 site (e.g., BURNS, 1993). Since such a feature can easily be confused with a similar band in plagioclase (see Fig. 2), its identification is of great importance to remote mineral identification (see discussion in SUNSHINE *et al.*, 1993).

*Olivine*

Olivine exhibits a composite absorption band near 1.05  $\mu\text{m}$  consisting of three electronic transition absorptions. Transmission spectra have documented systematic trends with composition for the band centers of individual absorption bands in oriented olivine crystals (BURNS, 1970b). Previous work with olivine reflectance spectra (e.g., KING and RIDLEY, 1987) was able to document small shifts of the composite band minimum. Because the olivine absorption distributions overlap so much, almost any mathematical model can produce a “good” fit to a measured spectrum. However, since the MGM has been demonstrated to be an accurate characterization of electronic transitions, the MGM parameters derived for each of the three bands of olivine can be used with some confidence in compositional analyses across the olivine solid solution series.

Reflectance spectra for a suite of olivines of different compositions were obtained and analyzed with the MGM, examples of which are shown in Fig. 13 (from SUNSHINE, 1994). As might be expected from crystal field theory, the relative band strengths (probability) of the two absorptions derived from iron in the M1 site remained the same as iron composition varies. In contrast, the relative strengths of the M2 and M1 bands vary with composition. The widths of the olivine absorptions are also seen to be controlled by absorption site and to be largely compositionally invariant (SUNSHINE, 1994).

Results for the full suite of reflectance spectra for olivine samples are shown in Fig. 14 (SUNSHINE

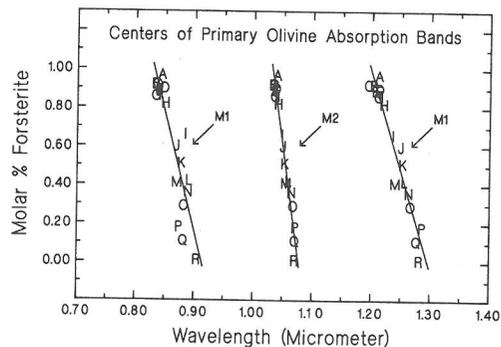


FIG. 14. MGM derived band centers for a suite of olivines of different compositions. Although all absorptions move to longer wavelengths with increasing iron content, both absorptions associated with the M1 site show a stronger change of energy with composition than the absorption from the M2 site.

and PIETERS, 1990, revised by SUNSHINE, 1994). The MGM derived band center for the three overlapping absorptions are seen to vary systematically with composition. This duplication of equivalent compositional results as those observed for transmission spectra of oriented crystals (BURNS, 1970b) is a substantial breakthrough for reflectance spectroscopy which effectively measures the combined signatures of randomly oriented crystals. The relations shown in Fig. 14 can now be used to estimate the composition of an unknown olivine from reflectance spectra.

#### *Remote sensing applications*

Given high quality remote spectra, MGM analysis can be straightforward. More commonly, however, remotely acquired data have lower signal to noise and/or lower spectral resolution than laboratory data. With such uncertainties, simple application of the MGM to produce to best mathematical model can result in physically unrealistic and uninterpretable solutions. Under these circumstances, additional constraints or assumptions may need to be imposed on the modeling approach. Constraints such as restricting solutions to be consistent with laboratory trends (*e.g.*, coupling of the relative strengths of the 1 and 2  $\mu\text{m}$  pyroxene bands or the M1 olivine bands) and only allowing parameters to range within natural compositions (*e.g.*, olivine band center that lie within 0–100% forsterite) are quite reasonable. The mathematical framework of the MGM explicitly allows for such constraints to be included in modeling (see SUNSHINE and PIETERS, 1993a,b; SUNSHINE, 1994).

The importance of applying physically reasonable constraints was demonstrated by MGM analysis of the telescopic spectrum of the surface of the asteroid 243 Asporina, an "olivine-rich" asteroid (SUNSHINE, 1994; SUNSHINE and PIETERS, 1993b). When the mathematically best fit for all parameters was determined with somewhat noisy data, the resulting absorption bands parameters (centers, widths, and relative strengths) were found to be inconsistent with those derived for any olivines in the laboratory. However, when a series of model variations were tested, which were partially constrained by band parameter coupling (*e.g.*, coupling of the relative strength of the M1 bands observed for olivine compositions), the results were quite dramatic. The surface of Asporina was shown to be totally inconsistent with fayalitic (Fe-rich) olivine, yet was successfully characterized to be distinctly forsteritic (Mg-rich).

Another elegant application of the MGM ap-

proach used high spatial resolution ISM imaging spectrometer data for Mars (MUSTARD and SUNSHINE, 1995) to make important compositional distinctions between different volcanic terrain. In this case, pyroxene mixtures and ferric alteration were considered as possible components contributing to the remotely acquired spectra. Solutions were sought which satisfied a set of criteria based on laboratory experience with pyroxene mixtures. These included such constraints as the band centers and band widths must be consistent with known properties of pyroxenes and the relative strengths of absorptions for two pyroxenes must be comparable for the 1 and the 2  $\mu\text{m}$  regions. Using this constrained MGM it was possible to model varying amounts of ferrous components in the martian spectra and to place compositional bounds on the ferric constituents. Successful solutions showed that volcanic terrain on Mars included two pyroxenes, that low-Ca pyroxene dominated the abundances, that the relative proportions of pyroxenes varied on the order of 20%, and that various amounts of a ferric component was present. This inferred basaltic composition is relatively uncommon on Earth, but is typical of the SNC meteorites which are believed to come from Mars. Through this combination of ISM data and MGM analysis it is now possible to conclude that the basaltic compositions present in the SNC meteorites are in fact representative of large regions of Mars.

#### EXPECTATIONS AND HOPES FOR THE FUTURE

Imaging spectrometers are high on the list of desirable instruments for most planetary exploration missions that are under consideration. There is no question that abundant information currently exists to clearly specify the type of spectroscopic measurements desired for quantitative remote compositional analysis. The above review of techniques and recent progress in quantitative approaches to remote spectral analysis has emphasized applications that involve electronic transitions of transition element ions, which typically occur in mafic rock forming minerals. However many of the same approaches have been or can be used for almost any type of diagnostic absorptions, including absorptions due to charge transfer electronic transitions and vibrational, bending, and stretching modes of molecular excitation that occur in spectra of minerals important to solar system bodies.

Many of the approaches described here, although highly productive, are still in the developmental stage. Due to the newness of these research efforts,

it is not surprising that little work has been done to combine these various methods. However, given that many approaches are complimentary, a natural direction would be to combine or link several in an integrated fashion to enhance interpretive capabilities and strengthen confidence in results. Technology and instrumentation is clearly heading in that direction with the implementation of imaging spectrometers. It can be envisioned that future analytical approaches may, for example, utilize MGM deconvolution methods to identify and couple critical diagnostic absorptions and then synthesize appropriate spectra to be used in various mixing models which will derive abundance information. Fortunately, computing capabilities appear to be keeping ahead of, or at least in line with, instrumentation and analytical approaches.

The last few decades of activity in spectroscopic applications for remote sensing have been very exciting. The future of remote reflectance spectroscopy is likely to include larger and more complex data sets with full spectral resolution that cover large, perhaps global, areas of planetary surfaces at higher spatial resolution. This expansion in data alone will provide significant new breakthroughs. Extrapolating from the past, parallel advances in advanced analysis techniques and computing capabilities should similarly add new dimensions to our ability to contribute to the exploration and understanding of various solar system bodies. As we progress to new horizons, the small but vigorous spectroscopy community is expected to continually expand upon the solid foundation of theoretical understanding provided by Roger Burns and as such provide a living legacy to his life's work.

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