**ANALYSIS OF VISIBLE AND NEAR INFRARED REFLECTANCE SPECTRA OF PLANETARY MATERIALS USING A BAYESIAN ESTIMATION APPROACH.** [1]Seiji Sugita, [1]Kenji Nagata, [1,2]Nobuko Tsuboi, [3]Takahiro Hiroi, [1]Masato Okada, [1]Dept. of Complexity Sci. and Eng, Univ. of Tokyo, [2]Hewlett Packard Japan, Ltd., [3]Dept. of Geological Sci., Brown University

**Introduction:** Optical reflectance spectroscopy is a very powerful tool to observe the planetary surfaces remotely from both ground-based telescopes and spacecrafts. Because many silicate minerals have many absorption bands diagnostic to both crystalline structure and elemental composition in this wavelengths range, VNIR spectroscopic observations can reveal a wide variety of information on planetary surfaces [e.g., 1].

The reflectance spectra observed on the planetary surfaces are compared with those of minerals observed in laboratories to infer the mineralogical and elemental compositions of the surfaces. Because silicate minerals often exhibit complex absorption bands in the UV to NIR wavelengths range, such a complex absorption band is often deconvoluted into multiple simple (i.e., mathematically well-defined forms, such as Gaussian and Lorentzian) absorption bands is often used for quantitative comparisons and analyses. One simple approach would be to search for the optimum combination of simple absorption bands that minimized the difference with an observed spectrum by trying every possible parameter set. Such direct search is rather effective when only a small number of free parameters are involved. However, a direct search is not practical for reflectance spectroscopy of planetary surfaces because many simple absorption bands are required to describe their complex absorption band patterns. When Gaussian or Lorentzian is used, each simple band requires three model parameters: strength, central wavelength, and breadth. Thus, the number of parameter sets to try in searching for the best-fit synthetic spectrum becomes extremely large. For four Gaussians, for example, we need to try $10^{12}$ parameter sets if we choose ten different values for each parameter. It would require $10^{24}$ sets if we examine 100 different values for each parameters to attain a high accuracy.

Consequently, a more efficient mathematical method is necessary. In previous studies, the steepest descent method has been used frequently to resolve this problem. In particular, *Sunshine et al*. [2] propose an analytical approach using the steepest descent method to deconvoluted reflectance spectra of silicate minerals with a number of Gaussians and a continuum as a function of wavelength. Their approach, called modified Gaussian model (MGM), has been shown capable of decomvolving olivines [e.g., 3] and Mg-Fe pyroxenes [e.g., 4,5] very successfully and obtain clear correlations between the central wavelengths of deconvoluted Gaussian bands and chemical composition of minerals.

Although the steepest descent method is a very powerful mathematical method to find a minimum of a continuous function but is not necessarily good at finding the global minimum of a complex function with many local minima. Depending on the initial choice of parameters, an obtained result may be just a local minimum of the function. Furthermore, this mathematical procedure needs to be given how many model parameters (e.g., the number of Gaussians in this study) should be used before analysis. Generally, a model with more Gaussians will lead to a smaller $E$, but the complexity of the model also increases. Our recent analysis indicates that the use of different numbers of Gaussians for MGM analysis may dramatically change the result of the MGM analysis [6], underscoring the importance of the choice of the number of Gaussians.

In reflectance spectroscopy of silicate minerals, the choice of the number of Gaussians is very important for accurate description of their complex absorption bands. A numerical validation discussed in our companion paper by [7] indicates that a Bayesian estimation method using the exchange Monte Carlo (EMC) algorithm can estimate the optimum number of Gaussians much more accurately than other algorithms, such as cross validation, WAIC, and RJMCMC. Thus, our spectroscopic analysis of planetary surfaces, the newly developed Bayesian MGM algorithm is better suited for reflectance spectroscopy of silicate materials on planetary surfaces.

In this study, we derive a new MGM algorithm using a Bayesian estimation approaches namely exchange Monte Carlo (EMC) method and the annealing method. Both pure olivine samples with different Fe/Mg ratios and olivine-pyroxene mixture samples are used for analysis to examine the effectiveness of our new algorithm. Based on the results, we discuss the applicability of our new MGM method.

**Spectral Analysis:** The mathematical details and numerical validation of the algorithm used in this study are given in our companion papers by [7,8].

In order to examine the validity of the Bayesian MGM algorithm proposed in this study, we conduct actual spectral deconvolution analyses using a series of reflectance spectra, olivine powder samples with different Mg/(Mg+Fe) ratios (mg#) ranging from zero to one.

The reflectance spectra of olivine samples were obtained the web site of NASA's RELAB. Here, it is noted that the olivine samples whose reflectance spectra were used in this study are

different from those used by [4]. As shown in the following, nevertheless, the result of the analyses of this study and [4] exhibit very good agreement. This strongly suggests the robustness of the results of MGM results.

**Analysis Results:** First of all, the results of our Bayesian MGM analysis indicate that the optimum number of Gaussian bands to reproduce the complex absorption band around 1 mm predicted is three for the reflectance spectra of all the olivine samples (Fig. 1). This optimum number is the same as the number estimated empirically by [4]. This coincidence is very important because the number of Gaussians is very difficult to determine objectively but highly influential to the model parameters to characterize individual Gaussian bands. This agreement between this study and previous fitting results by [4] strongly supports the validity of our Bayesian MGM algorithm

Furthermore, all the model parameters of individual Gaussian bands obtained in this study were practically the same as those obtained by [4]. The parameters include the central wavelengths, breadths, and strengths of the individual Gaussian absorption bands.

The central wavelengths of individual bands of 1-mm olivine increases gradually as mg# decreases; more iron leads to longer wavelengths (Fig. 2). The band widths and the relative intensities of the three individual bands are relatively constant regardless of mg# (Fig. 2). Here, note that the data sets of olivine spectra used in this study and those used by [4] are different. This supports that the results of these MGM analyses are not specific to some particular data sets but reflect the intrinsic properties of olivine.

Here, it is noted that the results of the preliminary analysis by [6] suggests that four Gaussians is more appropriate to fit the 1-mm absorption band of olivine than three as used by previous studies [2,4]. However, a detailed comparison of different algorithms using artificially generated data sets by [7] indicates that MGM analysis using Bayesian approach is significantly more accurate than that with cross-validation method, which is used by [7]. Thus, we conclude in this study that the optimum number of Gaussians for the 1-mm absorption band of olivine is three.

**References:** [1] Pieters, C.M. and P.A.J. Englert (1993), Remote geochemical analysis: Elemental and mineralogical composition; [2] Sunshine, J. M., et al. (1990), *J. Geophys. Res.*, *95*, 6955; [3] Sunshine, J. M. and C. M. Pieters (1993), *J. Geophys. Res.*, *98*, 9075; [4] Sunshine, J. M. and C. M. Pieters (1998), *J. Geophys. Res.*, *103*, 13,675; [5] Klima, R. L. et al., (2007), *Meteoritics and Planet. Sci.*, *42*, 235. [6] Tsuboi, N. et al. (2009), *Proc. of 42th Lunar and Planet. Symp.*, 118; [7] Nagata, K. et al. (2010) *Neural Networks*, to be submitted; [8] Sugita, S. et al., (2010) *J. Geophys. Res.* to be submitted.

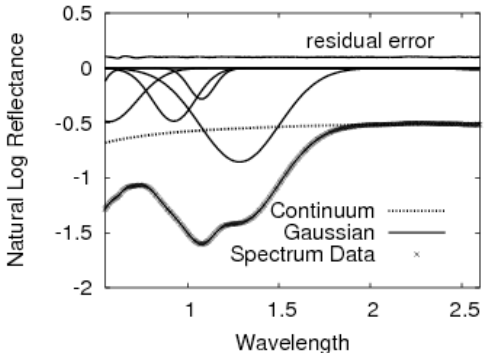


Fig. 1. MGM deconvolution result of an olivine spectrum using our Bayesian algorithm.

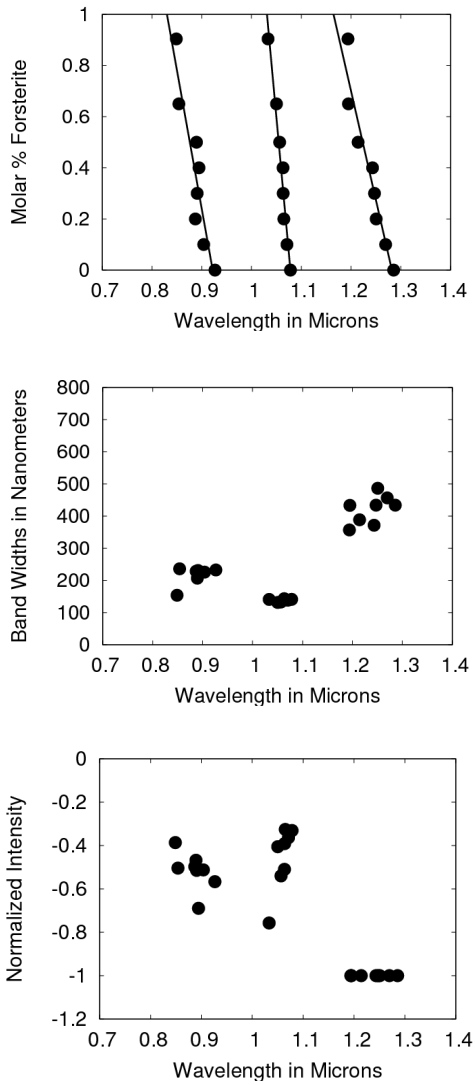


Fig. 2. The trend of central wavelength, width, and normalized intensities of deconvolved absorption bands of olivine with a variety of mg#.