

SPECTRAL MODELLING OF THE UNKNOWN: AN EXAMPLE USING TALC AND ACTINOLITE

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Introduction: Derivation of mineralogic information from visible to near-infrared reflectance spectra is one of the primary goals of geologic remote sensing. If there is only one mineral causing the observed absorptions, or several minerals with widely separated and well resolved bands, unique interpretations are possible. If however, there are several minerals with overlapping, superimposed or poorly resolved absorptions, the task is more difficult. Presented here is a quantitative application of the Modified Gaussian Model (MGM) [1] to extract the spectral properties of an unknown mineral from an intimate mixture of two minerals. In this analysis, the first overtone of the hydroxyl stretch modes are considered, but the approach is general and can be applied to any absorptions which can be modelled by this approach [2].

Problem: Reflectance spectra in this analysis are from the RELAB spectrometer, measured with a 2 Angstrom sampling resolution. In the spectrum from a natural rock containing an intimate mixture of talc and actinolite shown in Figure 1 (bottom), four well resolved and distinct band minima are observed. Both actinolite and talc exhibit overtone absorptions of fundamental hydroxyl stretching modes in this wavelength region. The wavelengths of the band minima depend on the coordinating ions, which in a typical Fe-Mg solid solution series are, from shorter to longer wavelengths, 3Mg, 2MgFe, Mg₂Fe, and 3Fe [3,4]. A small sample of pure actinolite was isolated from the whole rock, the spectrum of which is shown in Figure 1(top). The actinolite absorptions are symmetric and of different relative strength than the whole rock spectrum which shows an asymmetry in the band shapes and a shift in the band minima towards shorter wavelengths. There is quite clearly an additional component in the whole rock spectrum which we know to be mostly talc. The objective is to model the spectrum of the unknown component.

Spectral Modelling: Mustard [5] performed extensive modelling of the 1.4 μm overtone absorptions for a suite of 19 well characterized actinolite samples using the MGM model. This work indicated that the MGM model is a reasonable and accurate tool for the analysis of these overtone absorptions. In addition, the band centers and widths were constant to within 1 nanometer across a large range of compositions. Using constraints on band centers and widths determined in that study, the actinolite spectrum in Figure 1 was modelled with the MGM and the result is presented in Figure 2. Each absorption is modelled by a distribution defined by a center, strength and width. The top line in this and the following MGM plots is the error in the fits between the model and the spectrum, the distributions are shown below which are superimposed on a continuum (dashed line) to show the absolute quality of the fit. The actinolite model spectrum is then used as an input to the analysis of the whole rock spectrum. Continuum parameters (slope and intercept) are adjusted to bring the model actinolite into the approximate albedo space of the rock spectrum. This result is shown in Figure 3. The difference between the model actinolite and the whole rock spectrum, labelled Error in Figure 3, gives a first approximation to the spectral properties of the unknown components. The error spectrum is extracted and modelled with the MGM to determine the center and widths of absorptions for the unknown component, shown in Figure 4. The error is much higher in this solution than for the pure actinolite because of the reduced signal to noise in the derivative spectrum and the band widths were tightly constrained. The sinusoidal shape of the error spectrum near 1.3875 μm suggests an additional band is required. Band parameters determined from the analysis of the pure actinolite (Fig. 2) were combined with band parameters for the unknown component (Fig. 4) and used to model the whole rock spectrum. This result is shown in Figure 5. Note a small band centered near 1.3875 is included in this analysis. Finally, the individual absorptions associated with each component required to model the whole rock can be extracted and used to predict the spectra of the individual components. This is shown in Figure 6 where the top spectrum is a model actinolite, the second spectrum is measured from the extracted actinolite, the third spectrum is from the whole sample, and the last spectrum is the modelled additional component interpreted as talc.

Summary: This simple exercise illustrates a powerful application of the MGM model in the derivation of the spectral properties of components in sample containing minerals with very similar

spectral properties. In addition this allows the identification of components that are not evident in combined spectra.

References: [1] Sunshine, J.M., C. M. Pieters, and S. F. Pratt, *JGR* 95, 6955-6966, 1990 [2] Sunshine, J. M. and C. M. Pieters, (*this volume*) 1991 [3] Burns, R. G., and R. G. J. Strens, *Science*, 153, 890-892, 1966 [4] Farmer, V. C. ed., *The Infrared Spectra of Minerals*, pp. 539, 1974. [5] Mustard, J. F., Chemical analysis of actinolite from reflectance spectra (*submitted*) *Am. Mineral.* 1991.

