CONSTRAINED BAND ESTIMATION FOR ABSORPTION BAND MODELING AND SIMULATION (C-BEAMS) A. J. Brown[1], [1]Plancius Research, Severna Park, MD, 21146 (adrian.j.brown@nasa.gov).

Introduction: The Modified Gaussian Method (MGM) of Sunshine et al. [1-3] is currently the preferred method to provide a constrained fit to olivine and pyroxene compositions [4]. The olivine composition estimate is based on the ability of MGM to track the shift of the 1 μm band to longer wavelengths with increasing Fe content [3]. The 1 μm band in fact consists of three overlapping Gaussian shapes (called band I, II and III or M1-1, M2 and M1-2) that are individually tracked by MGM, and this indicator was reported to be relatively independent of grain size [3]. It has recently been shown that MGM does not have the ability to take grain sizes >250 microns into account [5].

In order to deal with this obstacle, and get closer to the underlying physics, we are developing an algorithm to fit the imaginary optical constants, which drives the absorption band observed in reflectance, and is therefore a more primitive article to investigate [6]. Our algorithm uses a model developed to simulate scattering by a pile of plates [7], also by Shkuratov et al. [8] to account for variations in albedo due to grain size. We call the resultant approach, which is still in development, Constrained-Band Estimation for Absorption Band Modeling and Simulation (C-BEAMS).

MGM method: The MGM approach [1-3] uses the following modified Gaussian formula to fit the crystal field absorptions of olivine and pyroxene:

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

The technique uses an iterative non linear least squares method [9] to constrain the three parameters in eqn (1) of three Gaussian bands to the olivine 1 μm band, along with a user-defined type of continuum line.

MGM examples: Figure 1 shows an example of a good MGM fit to Fo60 (KI3189) olivine of grain size 60-70 microns [3]. [3] recommends that band I be held at 0.55*band III is order to achieve the best results. We adopted this recommendation by using a filter/pass through in the "stocfit" function of the MGM code. This result is shown in Figure 1 for small grain sizes.

Grain size effects. [2] and [3] studied three grain sizes and reported that the MGM results were independent of the grain sizes tested. The grain sizes they used were <75nm, 75-125nm and 125-250nm. [2] reported observing some band saturation effects even at these small grain sizes.

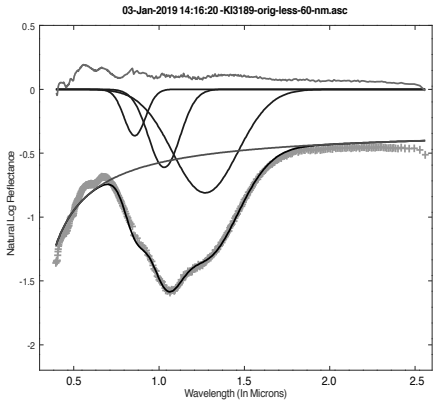

Fig. 1. Example of a good MGM fit of KI3189 Fo60 olivine with grain size <60nm.

We analysed a Fo60 250 microns grain size spectrum using the CBEAMS technique and MGM successfully performed a fit on it.

For olivine spectra of >250 microns, the MGM process becomes less satisfactory, as seen in Figure 2. In order to help the MGM process succeed, we tried:

a. Set elements of initial covariance matrix to 100
b. Removing all restrictions on parameters.
c. Placing 1 restriction that band I = 0.45*band III
d. Placing 1 restriction that band I = 0.55*band III

We found that the best fits were obtained with option b (no restrictions). The results of this fit are shown in Fig. 2, which shows the spectra and the three band centroids versus the inferred Fo#. This shows that the MGM results at 500nm provide unrealistic Fo# estimates, as reported in [5] which used Fo88-82 olivines. In fact, more Fe-rich and larger (500microns-1mm) grain sizes are relevant to Mars, as discussed elsewhere in this conference [10].

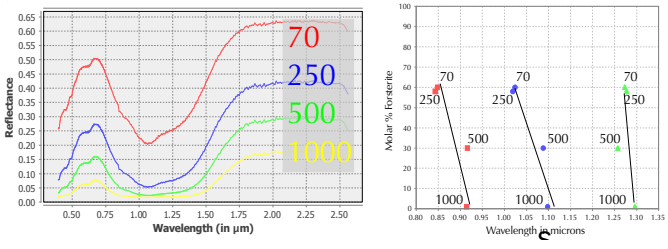

Fig. 2. Example of a less satisfactory MGM fit to KI3189 Fo60 olivine with four different grain sizes: 70, 250, 500 and 1000 microns. The figure shows that the MGM fit gives longer wavelength centroids indicative of a lower Fo#. For the 1mm grain size, the Fo# is negative based on the band I and II centroids.

C-BEAMS examples: Figure 3 shows an example of C-BEAMS fits to KI3189 (Fo60) olivine. The fit in the visible region and at 2 µm has not been optimized, due to the requirement for a further Gaussian absorption in that region as discussed in [11].

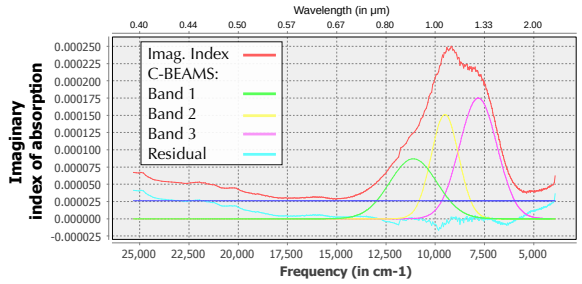

Fig. 3. C-BEAMS example fit to 70 micron grain sizes of KI3189 Fo60 olivine, note the fit and plot is in energy space so that the Gaussian shapes are symmetrical.

C-BEAMS approach. C-BEAMS uses a Kramers-Kronig approach to derive the absorption index of a spectrum, given an assigned average grain size. It then uses the "pile of plates" ansatz pioneered by [7] and used by Shkuratov et al. [8] to derive the spectrum of a given average grain size in order to verify the K-K derivation was correct. For olivine analysis, the absorption index is then iteratively fitted using 3 Gaussian shapes in energy space (Fig. 3).

Similarities between C-BEAMS and MGM. C-BEAMS and MGM both carry out a least squares fit in energy space (see Fig. 3). In this space, the width of band M1-1 and M1-2 are both of similar, and M2 is around half the width of the M1 bands. Band M1-1 is around half the height of band M1-2.

In Fig. 4, we show the variation in wavelength centroid of the three olivine bands, which has been used as a basis to successfully to derive the Fo# of olivine in previous laboratory and lunar studies [1-4]. The Fo41 sample is problematic, however this behaviour was already reported in [3]. While the values of the actual centroid fits are somewhat different (e.g. to those in Fig 4. of [3]), the strength of the M2 band grows with Fo# and the trends of increasing band centroid with Fo# remain, and therefore so does the predictive capability. However, C-BEAMS is able to cope with large grain sizes and using to the imaginary index moves the fitting process closer to the underlying physics.

Differences between C-BEAMS and MGM. The optical constants of a material are traditionally viewed as positive when a substance is absorbing (Fig. 3). This means that C-BEAMS Gaussian shapes are positive, in contrast to MGM negative Gaussian features (Fig. 1).

Because C-BEAMS operates on the imaginary index of the optical constants, a feature which is narrower than the reflectance bands it causes, the widths of the C-BEAMS features are around half the widths reported for MGM studies [1-3, 11]. As mentioned above however, the relative widths are similar. This gives confidence that the C-BEAMS approach is able to build upon the heritage of the MGM, which is based upon the pioneering work of Roger Burns [12].

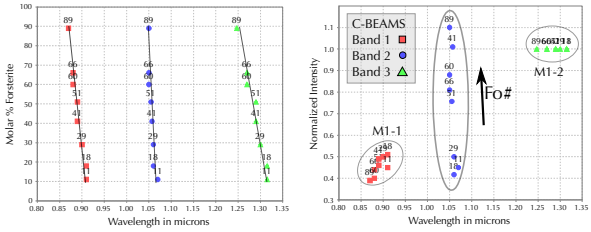

Fig. 4. Variations in centroid wavelength for olivine band M1-1, M2 and M1-2 with olivine composition.

Take away message: We have developed an initial enhancement of the MGM process which moves the fit into the optical constants space. In this manner, we have increased the admissible range of grain sizes to larger than 250 microns. These large grain sizes have been reported to corrupt MGM results [5], however they are relevant to current Martian hyperspectral observations and investigations, particularly of olivine-carbonate in the Nili Fossae region [10]. Future enhancements will include a public version of the code for testing and use in other projects.

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