BAND QUANTIFICATION IN REFLECTANCE SPECTROSCOPY. W. W. Mendell and R. V. Morris NASA-Johnson Space Center, Houston, TX 77058

Recent publications from planetary science groups working in reflectance spectroscopy have employed a Gaussian band-fitting technique to quantify absorption features in reflectance spectra (1,2,3,4). As part of the procedure a continuum is estimated for the absorption features. McCord et al. (4), argue that continuum approximation by a straight line across the wings of the band is adequate because the nature of the continuum is not well known. However, other workers (2,3) have described the continuum with a polynomial. A normalized spectrum is formed by ratioing the full spectrum to the estimated continuum. Gaussians, representing the assumed bands, then are fitted in energy space either to the normalized spectrum (1,4) or to the natural logarithm of the normalized spectrum (2,3).

McCord et al. (4), characterize the procedure as purely empirical and advocate Gaussians as the "simplest available functions" which "fit this class of absorptions" adequately. The cited papers derive the number of bands and their positions from the least squares fit, but extract no other physical parameters.

We will propose here an alternate quantification procedure in which the derived parameters have physical significance. In addition, the new procedure does not produce false multiple Gaussians for deep bands in dark materials or for shallow bands in bright materials. We begin with the radiative transfer equation for plane parallel geometry (5).

$$\mu \frac{dI}{dz} = -(\kappa + s) I(z,\mu) + \frac{1}{2} s \int_{-1}^{+1} P(\mu,\mu') I(z,\mu') \, d\mu' \qquad (1)$$

The solution is the radiant intensity I at depth z along direction cosine μ. The medium is characterized by a scattering function P, a bulk scattering coefficient s, and a bulk absorption coefficient κ. If the medium is a slab of thickness d with no scattering (s = 0), then the transmitted intensity is given by the familiar Bouger-Lambert Law,

$$I = I_0 \exp(-\kappa d) \qquad (2)$$

A transmission spectrum, plotted as absorbance (d^{-1} ln (Io/I)), vs. cm^{-1}, thus gives the bulk absorption coefficient. Transmission spectroscopists fit Gaussians to the bands and interpret the area under the curves in terms of concentration, molar extinction, or oscillator strength (6,7).

For diffuse reflectance the radiative transfer equation must be solved using both absorption and scattering. The result from Kubelka-Munk (K-M) theory for reflectance from an infinitely thick scattering medium is the equation (5,6,9).

$$\kappa/s = (1 - R_\infty)^2 / 2R_\infty \qquad (3)$$

The quantity on the right-hand side of the equation is called the remission function, $F(R_\infty)$. Morris et al. (8), have shown that the general behavior of a suite of grain-size separates of an orthopyroxene is described adequately by K-M theory. Since the absorption coefficient is represented theoretically by a Gaussian (or Lorentzian) line-shape function in energy space it is ap-

© Lunar and Planetary Institute • Provided by the NASA Astrophysics Data System

parent from Equation (3) that the fit should be made to $F(R_\infty)$ plotted against an energy parameter such as wave number. That is, there is a basis in theory for converting experimental reflectance data to remission data and then performing the band fits in $F(R_\infty)$ - wave number space. This procedure will be valid within the range of validity of K-M theory.

Morris et al. (8) have shown that bands can develop flat bottoms in the reflectance domain (e.g., at low reflectance). A Gaussian curve cannot represent such a band adequately, and a least squares fitting procedure will yield spurious multiple bands. The band shape remains undistorted in the remittance representation where the spectral characteristics of the absorption coefficient are reproduced directly.

The two figures illustrate a second class of problem which arises from analysis in the reflectance domain. In Fig. 1, curve 1 is a strong ultraviolet absorption. Curve 2 shows a weak infrared absorption superimposed on the wing of the UV absorption. An analogous situation obtains for hematite, where the ligand field absorption is ~3 orders of magnitude weaker than the charge transfer band. The weak band is very prominent in the reflectance spectrum containing both bands (curve 2, Fig. 2). For analysis of the IR band, curve 1 of Fig. 2 should be taken as the continuum. The dotted line is the approximation to the continuum given by the currently used quantification procedure. Clearly, the approximation is poor; and the normalized band will be a distortion of the actual band shape. We believe these examples demonstrate the importance of revising band quantification procedures in reflectance spectroscopy of planetary surface materials.

References:

1. Farr, T. G. et al. (1980) Proc. Lunar Planet. Sci. Conf. 11th, p. 719-729.
2. Singer, Robert B. (1981) JGR, 86, 7967-7982.
3. Clark, Roger N. (1981) JGR, 86, 3087-3096.
4. McCord, Thomas et al. (1981) JGR, 86, 10883-10892.
5. Kottler, Frederich (1969) in Prog. in Opt., Vol. III, ed. E. Wolf, p.1-28.
6. Marfunin, A. S. (1979) Physics of Minerals and Inorganic Materials, Springer-Verlag, 340pp.
7. Smith, G. and Strens, R. G. J. (1976) in Physics and Chemistry of Minerals and Rocks, ed. R. G. J. Strens, p. 583-612.
8. Morris, R. V. et al. (1982) GRL, in press.
9. Kortüm, G. (1969) Reflectance Spectroscopy, Springer-Verlag, 366pp.

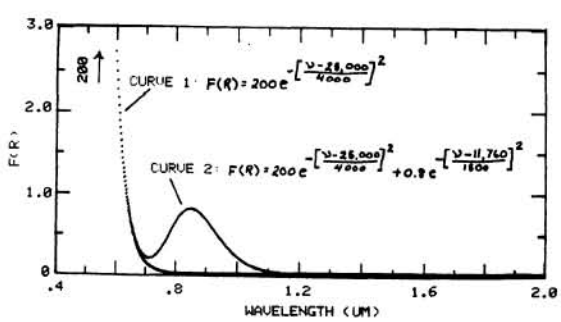

Figure 1

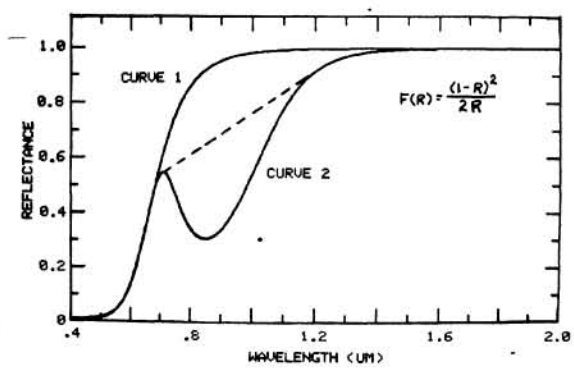

Figure 2

© Lunar and Planetary Institute • Provided by the NASA Astrophysics Data System