

Multi Kubelka Analysis of Vis-Nir Reflectance Spectra

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To obtain a mineral mixing ratio from diffuse reflectance spectra, a modified Kubelka equation is applied, named the multi Kubelka analysis (*MKA*)^(1,2). Four various grain size groups of spectral measurements with consisting of ten different mixing ratio are prepared for examining the *MKA*⁽³⁾.

The Kubelka equation is related diffuse reflectance $R(\lambda)$ of powdered surface to coefficients of absorption $K(\lambda)$ and scattering $S(\lambda)$, introducing a Kubelka function $Q(\lambda)$, as

$$Q(\lambda) = \frac{K(\lambda)}{S(\lambda)} = \frac{(1 - R(\lambda))^2}{2R(\lambda)}. \quad [1]$$

The coefficients of $K_m(\lambda)$ and $S_m(\lambda)$ for mineral mixture are linear combination of those of individual minerals, $K_i(\lambda)$, $S_i(\lambda)$, and weighted variable $A_i(\lambda)$ is an area portion of cross section of i mineral with $A_i(\lambda) = 1$,

$$K_m(\lambda) = \sum_{i,\lambda} A_i(\lambda) \cdot K_i(\lambda), \quad [2]$$

$$S_m(\lambda) = \sum_{i,\lambda} A_i(\lambda) \cdot S_i(\lambda), \quad [3]$$

Introducing and a new function $L_{ij}(\lambda) = K_i(\lambda)/K_j(\lambda)$ ($L_{ii}(\lambda) = 1$), so that we get

$$Q_m(\lambda) = \sum_{i,\lambda} \frac{A_i(\lambda)L_{ij}(\lambda)}{A_i(\lambda)L_{ij}(\lambda)/Q_i(\lambda)}. \quad [4]$$

The value of $Q_m(\lambda)$ can be converted to the value of diffuse reflectance spectrum $R_m(\lambda)$ by using equation [1]. To estimate the mixing ratio $A_i(\lambda)$ of mineral mixtures from the observed reflectance spectrum $R_m^{meas}(\lambda)$, we calculate the residual between $R_m^{meas}(\lambda)$ and $R_m^{pred}(\lambda)$, and find out the point of residual minimum.

$$\sum_{\lambda} (R_m^{meas}(\lambda) - R_m^{pred}(\lambda))^2 \rightarrow \min. \quad [5]$$

The ratios $A_i(\lambda)$ of mineral mixtures for $R_m^{pred}(\lambda)$ satisfying the equation [5] is considered to be the most provable one. Twenty eight data of mineral mixtures of these spectra are used for observed spectrum $R_m^{meas}(\lambda)$, while twelve spectra consisting four different grain sizes for three end member minerals are used to calculate the mineral mixing ratio from diffuse spectrum of multi mineral mixtures (table 1).

Figure 1 shows the example of the *MKA* (predicted) and the *LIA* (calculated) spectra for A101 sample. The value of *LIA* (linear interpolated analysis) spectrum is much larger than that of measured spectrum at infrared and 250–800nm regions. Absorptions of clinopyroxene near 600nm, affected by Cr^{3+} and 2300nm by Fe^{2+} are contributed to decrease the albedo and suppress other spectral features of mineral mixture reflectance spectra. In *MKA* method, the relation of $R(\lambda)$ and $Q(\lambda)$ represents this effect well. Because the value of $Q_m(\lambda)$ is affected by the lowest value of $Q_i(\lambda)$.

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The C011D of MKA spectrum in Figure 2 means that C indicates the grain size of $R_m(\lambda)$ is 105 to 250 μm grain size, 011 is the mixing ratio of composing minerals and D is the grain size of composing minerals $R_i(\lambda)$. Similarly C011A, C011B and C011C are the same as C011D. The most probable value as MKA for measured spectrum C011 is C011C, the residuals of others are slightly greater than C011C. The value of MKA spectrum is affected seriously by the grain size of composing minerals.

Several methods have still been developed to obtain mineralogical information from the visible and near-infrared diffused reflectance spectra⁽⁴⁾. Also the multi Kubelka analysis yields a consistent result which estimates fairly well the mixing ratio of mineral mixtures from diffuse reflectance spectrum $R_m^{meas}(\lambda)$ as far as grain size and composing minerals are known.

REFERENCES

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Table 1. Residuals minimum between MKA and measured spectra

grain size	A	B	C	D
ol:opx:cpx	(%)	(%)	(%)	(%)
110	3.26	3.23	4.09	3.47
101	1.89	1.74	3.68	2.00
011	2.97	3.57	3.81	4.43
111	2.56	3.68	3.87	2.88
211	2.19	2.51	4.09	2.74
121	2.61	3.76	2.83	3.36
112	2.15	3.09	3.65	3.07

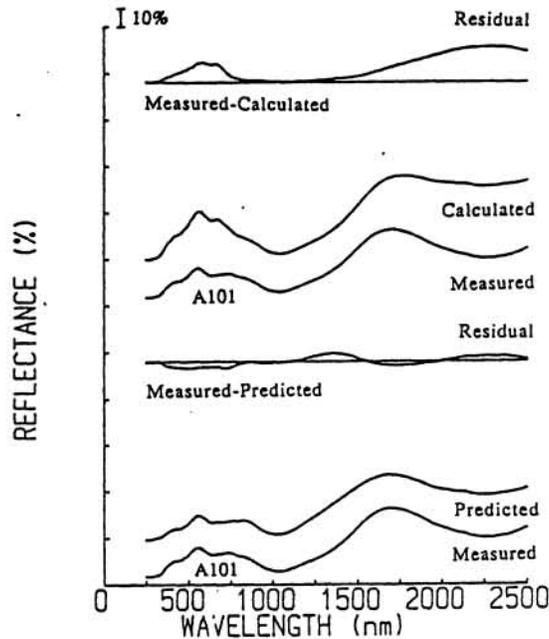


Figure 1. Predicted(MKA), calculated(LIA) and measured spectra of A101 and residuals

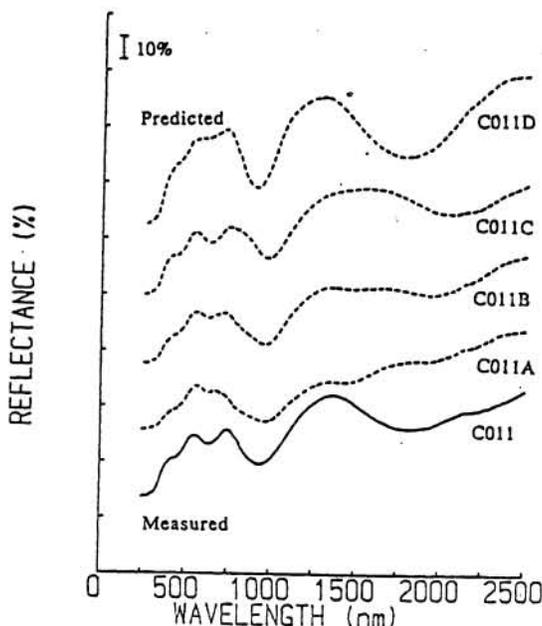


Figure 2. Measured spectrum of C011 and MKA spectra of C011A to C011D