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## A MODEL FOR ANALYSIS OF THE SPECTRAL REFLECTANCE OF MINERAL MIXTURES

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**Abstract:** We proposed a model to determine the spectral reflectance of mineral mixtures as a function of relative abundance of mineral components on the basis of both diffuse spectral reflectance and diffuse spectral transmittance of the components. In order to test the model, we measured spectral reflectances of sized olivine and pyroxene samples separated from Nuevo Mercurio ordinary chondrite and examined variations of spectral reflectances of the olivine-pyroxene mixtures as a function of relative mineral abundance. Spectral reflectances calculated for olivine-pyroxene mixtures based on our model agree well with measured spectra of the mixtures.

### 1. Introduction

Spectral reflectance spectroscopy is one of the most accessible approaches for remote sensing of planetary surfaces (*e.g.*, ADAMS, 1974). In order to determine the mineral assemblages of the surfaces, it is necessary to decompose the planetary spectra into contribution to the spectra of constituent minerals, because planetary surfaces are generally thought to be covered with regolith-like materials. However, the decomposition is often accompanied by the difficulty in getting a relative abundance of constituent minerals. Spectral changes in mineral mixtures are, therefore, usually examined by changing the amount of constituent minerals and the spectra are compared with the asteroidal reflectance spectra to help interpret the mineral assemblages of the surfaces (*e.g.*, HUNT and SALISBURY, 1970; NASH and CONEL, 1974; CHAPMAN, 1976; GAFFEY, 1976; GAFFEY and MCCORD, 1978; SINGER, 1981; PIETERS, 1983; MIYAMOTO *et al.*, 1983). CLOUTIS *et al.* (1986) carried out calibrations of end-member abundances, chemistries, and particle size for olivine-orthopyroxene mixtures from visible and near-IR spectral reflectances by deriving analytical techniques for deconvolving reflectance spectra of olivine-pyroxene assemblages. On the other hand, SASAKI *et al.* (1983) proposed a method for estimating the spectra of pure components from the spectra of unknown mixtures with various relative concentrations on the basis of principal component analysis and a constrained nonlinear optimization.

Some investigators have performed theoretical or semiempirical treatment for light scattering on the analysis of reflectance spectra. CLARK and ROUSH (1984) have compared several methods. HAPKE (1981) and LUMME and BOWELL (1981) have introduced some analytical expressions for the scattering of light applicable to remote sensing studies. JOHNSON *et al.* (1983) have presented a simple semiempirical method

for determination of the spectral reflectance of a powdered binary mineral mixture based on a two-stream radiative transfer solution on a semi-infinite medium of isotropic scatters after HAPKE's theory (HAPKE, 1981). MORRIS *et al.* (1982) have applied the Kubelka-Munk theory of diffuse reflectance to discussing light scattering in reflectance spectra. The Kubelka-Munk function (WENDLANDT and HECHT, 1966, p. 62) which contains two independent variables (scattering coefficient and absorption coefficient) has been often used for analyses of spectral reflectance. Analytical approaches based on the Kubelka-Munk function have, however, shown that it has limitations for interpreting spectral changes in reflectances of mineral mixtures (*e.g.*, CLARK and ROUSH, 1984).

We propose a model to semiempirically determine the spectral reflectance of a mineral mixture as a function of abundance of mineral components in the mixture on the basis of optical properties of each mineral component which are determined by diffuse spectral reflectance and transmittance of the component (KINOSHITA *et al.*, 1985a, b). We formulate a relation between the spectral reflectance of a mineral mixture and optical properties of the component minerals, and a relation between the spectral reflectance of the mixture and abundance of component minerals in the mixture. In order to test our model, we use olivine and pyroxene samples separated from an ordinary chondrite (MIYAMOTO *et al.*, 1983). One of the major purposes of our model is to easily obtain the spectra of mineral mixtures on the basis of both the reflectance and transmittance spectra of end-member minerals.

## 2. Multilayer Model

We assume that a mineral mixture is composed of plane parallel layers, where the thickness of each layer is equal to the mean dimension of the grains (WENDLANDT and HECHT, 1966), and assume that each layer is composed of unit cells whose size is equal to the thickness of the layer (Fig. 1a). We assume that the grain size of constituent minerals is the same. We can calculate reflectance and transmittance of each layer,

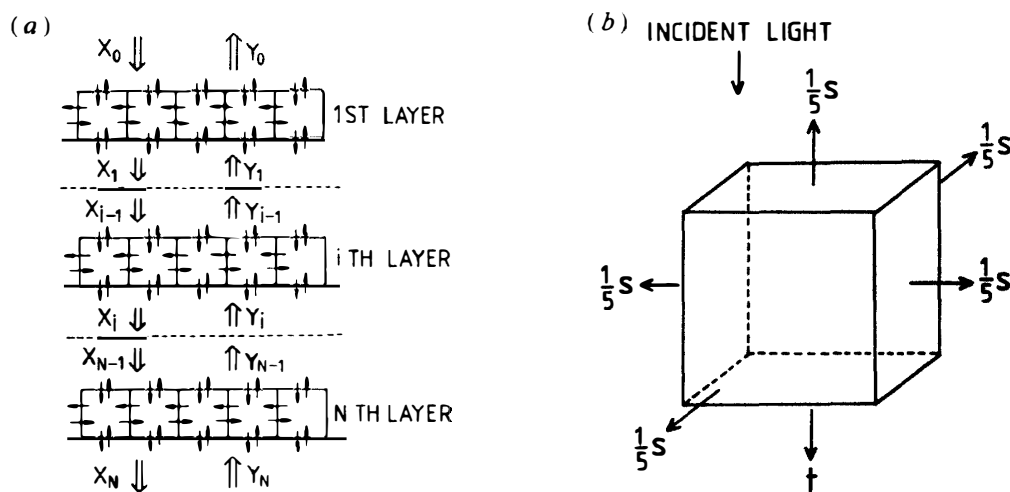


Fig. 1. Multilayer model. (a) Each layer consists of cubic unit cells. (b) Optical properties of a cubic unit cell

on the basis of the optical properties for unit cells.

We assume that a unit cell is cubic (Fig. 1b). Let scattering activity “ $s$ ”, transmitting activity “ $t$ ” and absorbing activity “ $a$ ” for the unit cell denote intensity of total scattered light, transmitted light and absorbed light for unit incident light, respectively, where we define  $a=1-s-t$ . The intensity of scattered light is assumed to be equivalent for each surface and the intensity of scattered light is  $0.2s$  at each surface (Fig. 1b).

The number of the layers is  $N$ , and the thickness of each layer is  $\Delta d$ .  $X_i$  is the light flux from the  $i$ -th to  $(i+1)$ -th layer.  $Y_i$  is the light flux in the opposite direction.  $R$  and  $T$  are reflectance and transmittance of a single layer, respectively (Fig. 1a). Reflectance  $R$  and transmittance  $T$  of each layer are calculated by summing up the multiple-scattering within the layer determined by the scattering activity ( $s$ ) and transmitting activity ( $t$ ) of a unit cell and we get the following formulae as the sum of infinite series:

$$\begin{aligned} R &= 0.2s + 0.2(1-0.2)s^2/[1-t-(1-2 \times 0.2)s] \\ T &= t + 0.2(1-0.2)s^2/[1-t-(1-2 \times 0.2)s] \end{aligned} \quad (1)$$

The relations among  $X_i$ ,  $Y_i$ ,  $X_{i-1}$ , and  $Y_{i-1}$  are

$$\begin{aligned} X_i &= T \cdot X_{i-1} + R \cdot Y_i \\ Y_{i-1} &= R \cdot X_{i-1} + T \cdot Y_i \end{aligned} \quad (2)$$

Therefore, we obtain

$$\begin{bmatrix} X_{i-1} \\ Y_{i-1} \end{bmatrix} = \frac{1}{T} \begin{bmatrix} 1 & -R \\ R & T^2 - R^2 \end{bmatrix} \begin{bmatrix} X_i \\ Y_i \end{bmatrix} = A \begin{bmatrix} X_i \\ Y_i \end{bmatrix} \quad (3)$$

By using eq. (3) repeatedly

$$\begin{bmatrix} X_0 \\ Y_0 \end{bmatrix} = A^N \begin{bmatrix} X_N \\ Y_N \end{bmatrix} \quad (4)$$

A boundary condition is  $Y_N=0$ . Then the reflectance  $R_N$  and  $T_N$  of  $N$  layers (multi-layer) are

$$\begin{aligned} R_N &= Y_0/X_0 = [A^N]_{21}/[A^N]_{11} \\ T_N &= X_N/X_0 = 1/[A^N]_{11} \end{aligned} \quad (5)$$

When we let  $N$  approach infinity, that is,  $R_N$  is equal to  $R_{N+1}$ , then reflectance  $R_\infty$  becomes

$$R_\infty = 2 \cdot R / (1 + R^2 - T^2 + \sqrt{(1 + R^2 - T^2)^2 - 4 \cdot R^2}) \quad (6)$$

We define scattering activity  $s_{\text{mix}}$  and transmitting activity  $t_{\text{mix}}$  of a unit cell for mineral mixture as

$$\begin{aligned} s_{\text{mix}} &= \sum c_j \cdot s_j \\ t_{\text{mix}} &= \sum c_j \cdot t_j \end{aligned} \quad (7)$$

where  $c_j$  is the volume fraction of mineral component  $j$ , and  $s_j$  and  $t_j$  are scattering activity and transmitting activity of mineral component  $j$ .

The reflectance and transmittance of a single layer of the mixture is given by substituting  $s_{\text{mix}}$  and  $t_{\text{mix}}$  in eq. (7) for  $s$  and  $t$  in eq. (1).

We show the relation between our model and Kubelka-Munk theory in Appendix I (KINOSHITA *et al.*, 1983).

### 3. Instrumentation and Samples

Measurements of reflectance spectra and transmittance spectra were made with a Beckman UV 5240 UV-Visible and NIR spectrophotometer with an integrating sphere. Incident light is perpendicular to the surface of the sample plate and BaSO<sub>4</sub> reference plate. A PbS cell detector was used in the spectral range of 0.8–2.5  $\mu\text{m}$ , a photomultiplier was used in the range of 0.5–0.8  $\mu\text{m}$ , and the two detectors were located perpendicular to the incident beam. Scan speeds in 0.8–2.5  $\mu\text{m}$  and 0.5–0.8  $\mu\text{m}$  region were 0.5 nm/s and 0.125 nm/s, respectively. The spectral data were recorded every second on a floppy disk in digital form. Samples for measurements of reflectance spectra were placed in a holder blackened by acrylic plastic paint, 1.4 cm  $\times$  1.7 cm in area and 0.4 mm deep, and were covered with glass. Samples for measurements of transmittance spectra were placed into a glass-holder which was made of two parallel glass slides, where the interior of the glass-holder was 2.2 cm  $\times$  4.0 cm in area, 150  $\mu\text{m}$  thick. We corrected the effects of cover glasses theoretically by taking the multiple scattering by the glasses into account. A program system on a HITAC-M280H computer was used to process and display the spectral data on a graphics display terminal.

Nuevo Mercurio, an H5 ordinary chondrite was crushed with an agate mortar and pestle, and sieved with a stainless steel sieve to obtain 53–37  $\mu\text{m}$  size fractions. Olivine and pyroxene were separated from the 53–37  $\mu\text{m}$  sample by using an isodynamic magnetic separator (S. G. Frantz CO., Inc., L-1). Small amounts of chromite and troilite were contained in the olivine and pyroxene samples, and were separated by using Clerici's solution. About 100 crystal grains from each sample were embedded in araldite for chemical analysis, using a JEOL JXA-733 electron-probe X-ray micro-analyzer. For comparison, olivines and pyroxenes (74–37  $\mu\text{m}$  in size) were separated from olivine sand from Hanauma Bay, Oahu Island, Hawaii in the same manner as the Nuevo Mercurio sample.

Spectral reflectance and transmittance of each sample were measured. The thickness of each sample used for measurements of transmittance spectra was measured by using a micrometer; the thickness of olivine and pyroxene samples from Nuevo Mercurio was 143  $\mu\text{m}$  and 133  $\mu\text{m}$ , respectively, and the thickness of olivine and pyroxene samples from Hawaii was 133  $\mu\text{m}$ . Then the olivine and pyroxene sample were mixed, spectral reflectance of the mixture was measured to compare with reflectances calculated by our model.

### 4. Procedure

We calculated matrix  $A$  for each mineral component by using eqs. (5) and (6) on

the basis of observed spectral reflectance data and transmittance data of each sample (olivine or pyroxene sample for Nuevo Mercurio or Hawaii). The thickness of a layer in our model for Nuevo Mercurio samples and Hawaii samples was 45  $\mu\text{m}$  and 55  $\mu\text{m}$ , respectively. We describe the detailed procedure in Appendix II. We calculated spectral reflectance and spectral transmittance for a layer using eq. (3). We determined the scattering activity, “*s*” and transmitting activity, “*t*” of the mineral component using eq. (1). Then we calculated spectral reflectances for olivine-pyroxene mixtures using eqs. (7), (1), and (6).

The olivine (or pyroxene) sample from Nuevo Mercurio contained small amounts of pyroxene (or olivine) grains. The effects of impurities were reduced by the following procedure: Let suffix OL and PX denote the pure olivine and pure pyroxene, respectively. OLE and PXE denote olivine and pyroxene samples which contained impurities, respectively;  $c_{\text{PX}}$  and  $c_{\text{OL}}$  designate the volume fraction of the impurities estimated by chemical analyses of olivine and pyroxene samples, respectively. By writing eq. (7) explicitly we obtain

$$\begin{aligned} s_{\text{OLE}} &= (1 - c_{\text{PX}})s_{\text{OL}} + c_{\text{PX}}s_{\text{PX}} \\ t_{\text{OLE}} &= (1 - c_{\text{PX}})t_{\text{OL}} + c_{\text{PX}}t_{\text{PX}} \\ s_{\text{PXE}} &= c_{\text{OL}}s_{\text{OL}} + (1 - c_{\text{OL}})s_{\text{PX}} \\ t_{\text{PXE}} &= c_{\text{OL}}t_{\text{OL}} + (1 - c_{\text{OL}})t_{\text{PX}} \end{aligned} \quad (8)$$

By solving eq. (8) for  $s_{\text{OL}}$ ,  $s_{\text{PX}}$ ,  $t_{\text{OL}}$  and  $t_{\text{PX}}$ , we obtained the scattering activity and transmitting activity of pure mineral components.

## 5. Results and Discussion

Table 1 shows the results of chemical analyses of olivine and pyroxene from Nuevo Mercurio. Deviations of the chemical compositions of the grains are fairly small. About 10% of the grains in the pyroxene sample were olivine grains, and about 20% of the grains in the olivine sample were pyroxene grains. Olivine sand from Hawaii was almost entirely separated into olivine and pyroxene (MIYAMOTO *et al.*, 1983).

Figure 2 shows observed spectral reflectances of the olivine and pyroxene samples from Nuevo Mercurio. The wavelength positions of the absorption bands are consistent with the previous studies (*e.g.*, BURNS, 1970; ADAMS, 1974). Figure 3 and Table 2 compare the spectral reflectances of the olivine-pyroxene mixtures calculated by the model with the observed ones. Reflectance and wavelength positions of the band minimum near 1  $\mu\text{m}$  agree well with those observed. This result shows that eqs. (1) and (7) are a good approximation of the reflectance and transmittance of a layer for binary mixtures of particulate minerals.

Figures 4 and 5 show the scattering activity, transmitting activity and absorbing activity of the unit cell for each sample from Nuevo Mercurio. Values of scattering activity of each sample in a high reflectance region is roughly equal to 0.56. Wavelength position of the absorption band shown in the absorbing activity spectra is almost equal to that shown in the reflectance curve. Both olivine and pyroxene show a low value of absorbing activity and higher values of transmitting and scattering activities. This indicates that the olivine and pyroxene grains used in this study are transparent.

Table 1. Chemical compositions (wt %) of olivine and pyroxene (opx) from Nuevo Mercurio.

	Olivine		Pyroxene (opx)	
	Mean (N=13)	Range	Mean(N=13)	Range
SiO <sub>2</sub>	39.4	38.7 - 39.8	56.1	54.4 - 56.6
TiO <sub>2</sub>	0.16	0.00 - 0.86	0.15	0.07 - 0.21
Al <sub>2</sub> O <sub>3</sub>	0.02	0.01 - 0.04	0.22	0.12 - 0.39
Cr <sub>2</sub> O <sub>3</sub>	0.01	0.00 - 0.04	0.13	0.05 - 0.21
FeO	16.5	15.9 - 17.0	10.3	10.2 - 10.6
MnO	0.47	0.39 - 0.55	0.50	0.42 - 0.60
MgO	44.1	43.0 - 45.3	30.9	30.3 - 31.3
NiO	0.01	0.00 - 0.05	0.00	0.00 - 0.01
CaO	0.00	0.00 - 0.01	0.87	0.71 - 1.41
Na <sub>2</sub> O	0.00	0.00 - 0.00	0.01	0.00 - 0.05
K <sub>2</sub> O	0.00	0.00 - 0.01	0.01	0.00 - 0.02
V <sub>2</sub> O <sub>3</sub>	0.00	0.00 - 0.00	0.00	0.00 - 0.00
Total	100.4	99.1 - 101.7	99.20	97.1 - 99.80
Si	0.991	0.981 - 1.002	1.992	1.978 - 2.000
Ti	0.000	0.000 - 0.002	0.004	0.002 - 0.006
Al	0.001	0.000 - 0.001	0.009	0.005 - 0.010
Cr	0.000	0.000 - 0.001	0.004	0.001 - 0.006
Fe	0.347	0.338 - 0.359	0.307	0.301 - 0.315
Mn	0.010	0.008 - 0.012	0.015	0.013 - 0.018
Mg	1.658	1.636 - 1.684	1.634	1.612 - 1.676
Ni	0.000	0.000 - 0.001	0.000	0.000 - 0.001
Ca	0.000	0.000 - 0.000	0.033	0.027 - 0.053
Na	0.000	0.000 - 0.000	0.001	0.000 - 0.001
K	0.000	0.000 - 0.000	0.000	0.000 - 0.001
V	0.000	0.000 - 0.000	0.000	0.000 - 0.000
Total*	3.008	2.998 - 3.017	Total**	4.000
			Ca***	1.68
Mg***	82.69	82.10 - 83.29		1.37 - 2.70
Fe***	17.31	16.71 - 17.90		82.77
				15.55
				15.28 - 15.97

\* Cations per 4 oxygens.

\*\* Cations per 6 oxygens.

\*\*\* Atomic %.

Figure 6 shows the spectral reflectance calculated for the purified olivine and pyroxene samples from Nuevo Mercurio. Figures 7 and 8 show the spectral reflectance curves of different amounts of pyroxene in the olivine sample. Figure 9 compares the wavelength positions of the band minimum of the spectral reflectance curve of the olivine-pyroxene mixture from Nuevo Mercurio with those from ALH-769 ordinary chondrite (L6) reported by MIYAMOTO *et al.* (1983).

Our model rests on the assumption that the incident flux density to a layer is uniform. This requires that the thickness of a layer is approximately equal to the mean size of grains in the layer. When we apply our model to interpreting asteroidal surface materials, we have to assume that the thickness of a layer is the mean size of regolith-like grains. In the future we need to consider a more precise theory which exactly includes the effects of the grain size.

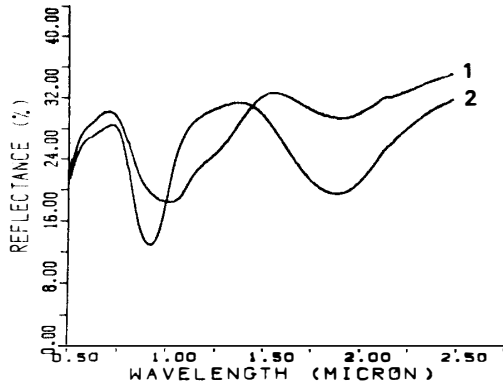


Fig. 2. Observed spectral reflectance curve for samples from Nuevo Mercurio. (1) olivine, (2) pyroxene.

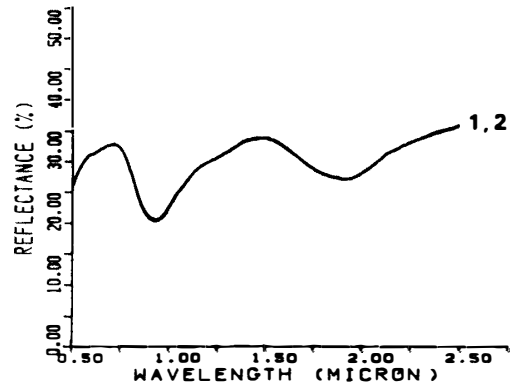


Fig. 3. Spectral reflectances of a mixture from Nuevo Mercurio (olivine 50% + pyroxene 50%). (1) calculated, (2) observed.

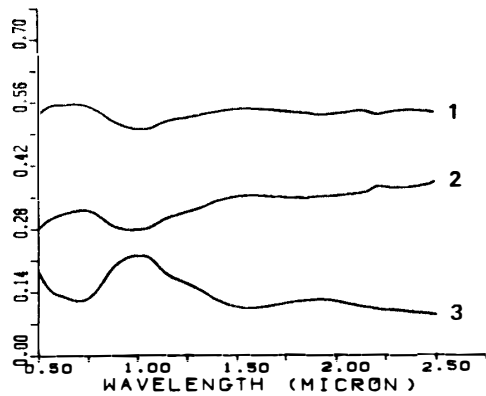


Fig. 4. Optical properties of a unit cell (45  $\mu\text{m}$  in size) for olivine from Nuevo Mercurio. (1) scattering activity, (2) transmitting activity, (3) absorbing activity.

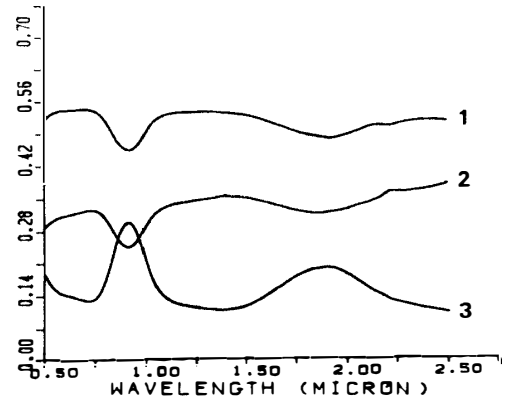


Fig. 5. Optical properties of a unit cell (45  $\mu\text{m}$  in size) for pyroxene from Nuevo Mercurio. (1) scattering activity, (2) transmitting activity, (3) absorbing activity.

Table 2. Wavelength positions of band minimum near 1  $\mu\text{m}$  of olivine-pyroxene mixtures from (a) Nuevo Mercurio, (b) Hawaii.

(a) Pyroxene content (%)	0	25	50	75	100
Wavelength position (nm)					
calc.	—	944	929	921	—
obs.	1019	942	928	922	919
* $\sigma \cdot 10^3$	—	2.2	0.9	0.9	—
(b) Pyroxene content (%)	0	20	50	80	100
Wavelength position (nm)					
calc.	—	1051	1041	1028	—
obs.	1057	1048	1041	1029	1019
* $\sigma \cdot 10^3$	—	3.1	3.1	3.8	—

$$* \sigma = \left( \sum_i (R_{\text{calc},i} - R_{\text{obs},i})^2 / N \right)^{1/2}$$

$R_{\text{calc},i}$ : calculated reflectance at wavelength position  $i$ .

$R_{\text{obs},i}$ : observed reflectance at wavelength position  $i$ .

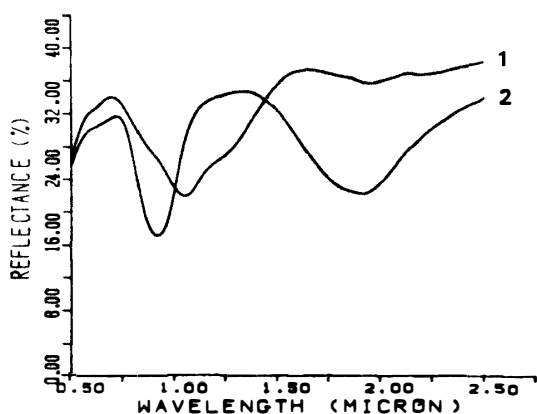


Fig. 6. Calculated spectral reflectance of pure olivine and pure pyroxene from Nuevo Mercurio. (1) olivine, (2) pyroxene.

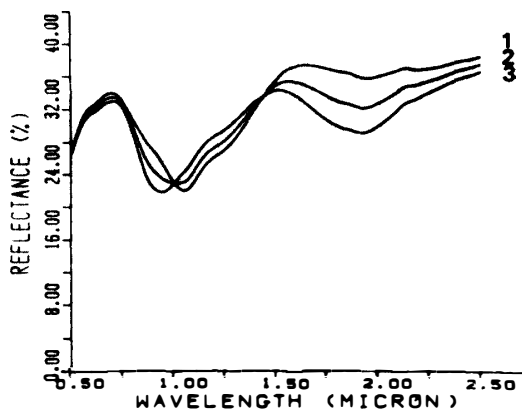


Fig. 7. Calculated spectral reflectance curves of volume percentage mixtures from Nuevo Mercurio. (1) olivine 100%, (2) olivine 80% + pyroxene 20%, (3) olivine 60% + pyroxene 40%.

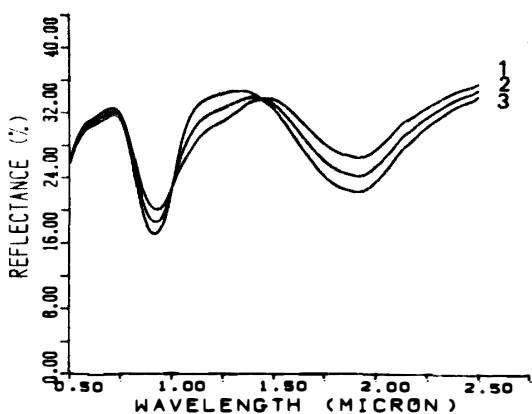


Fig. 8. Calculated spectral reflectance curves of volume percentage mixtures from Nuevo Mercurio. (1) olivine 40% + pyroxene 60%, (2) olivine 20% + pyroxene 80%, (3) pyroxene 100%.

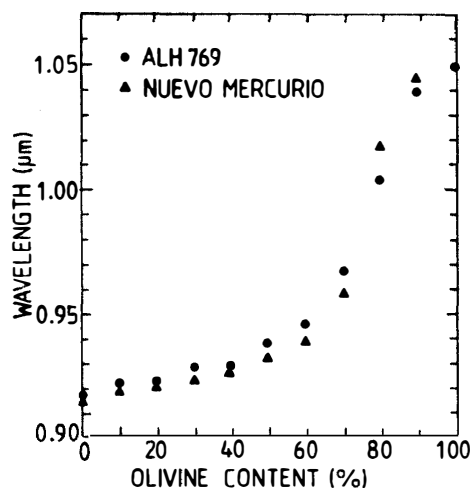


Fig. 9. Variations of wavelength position of absorption band near 1  $\mu\text{m}$  shown in reflectance curve of olivine-pyroxene mixture from Nuevo Mercurio and ALH-769.

Our model uses transmittance data of a mineral component as well as reflectance data and includes both scattering activity ( $s$ ) and transmitting activity ( $t$ ). This is one of the characteristics of our model different from the previous studies. We can easily measure transmittance spectra of minerals in the laboratory in the same manner as reflectance measurements. Another characteristic of our model is that it is a six-stream model considering cubic unit cells in a layer, although we assume that scattering for five directions is equal (Fig. 1b). The calculations based on our model are simple to obtain the spectral reflectance of a mineral mixture.



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### Appendix I

We use a multilayer model and assume that the thickness of the sample is infinite. Let  $R$  and  $T$  indicate reflectance and transmittance for a layer, respectively. We can express  $R$  and  $T$  by using of the thickness of the layer ( $\Delta d$ )

$$\begin{aligned} R &= \sigma \Delta d \\ T &= 1 - (\sigma + \kappa) \Delta d \end{aligned} \quad (9)$$

where  $\sigma$  and  $\kappa$  are scattering coefficient and absorption coefficient, respectively. Substituting eq. (9) in eq. (6) and letting  $\Delta d$  approach zero, we obtain

$$\lim_{\Delta d \rightarrow 0} R_{\infty} = 1 + \kappa/\sigma - \sqrt{(2 + \kappa/\sigma)\kappa/\sigma} \quad (10)$$

which yields the Kubelka-Munk function (KÖRTUM, 1969)

$$\kappa/\sigma = (1 - R_{\infty})^2 / 2R_{\infty} \quad (11)$$

Equations (6) and (9) are equivalent to the Kubelka-Munk differential equation when  $\Delta d$  approaches zero (WENDLANDT and HECHT, 1966). Kubelka-Munk theory is, however, a two-stream model. We note that the number of layer ( $N$ ) approaches infinity keeping the thickness of the layer ( $\Delta d$ ) unchanged in our model, although  $\Delta d$  approaches zero in the Kubelka-Munk theory.

### Appendix II

Let  $d$  denote the thickness of the sample for measurements of transmittance,  $\Delta d$  denote thickness of one layer. We assume that  $d$  and  $\Delta d$  are much greater than  $1 \mu\text{m}$ , and assume that  $d(\mu\text{m})$  and  $\Delta d(\mu\text{m})$  are integers. We define  $N$  as  $N = d/\Delta d$ , where  $N$  is not always an integer. In order to calculate matrix  $A$  in eq. (5) for a layer whose thickness is  $\Delta d$ , we calculated matrix  $A^*$  for a layer ( $1 \mu\text{m}$  in thickness) by the following procedure.

From eqs. (5) and (6) assuming  $R_{\text{obs}} = R_{\infty}$  and  $T_{\text{obs}} = T_{\infty}$ , we obtain

$$\begin{aligned} R_{\text{obs}} &= 2R^* / [1 + R^{*2} - T^{*2} + \sqrt{(1 + R^{*2} - T^{*2})^2 - 4R^{*2}}] \\ T_{\text{obs}} &= 1 / ((A^*)^d)_{11} \end{aligned} \quad (12)$$

where  $R_{\text{obs}}$  and  $T_{\text{obs}}$  denote observed reflectance and transmittance, respectively, and  $R^*$  and  $T^*$  denote reflectance and transmittance for the layer ( $1 \mu\text{m}$  in thickness). We can solve eq. (12) for  $R^*$  and  $T^*$ . Then we obtained matrix  $A$  by

$$A = (A^*)^{\Delta d} . \quad (13)$$