

EFFECTS OF GRAIN SIZE AND SHAPE IN MODELING REFLECTANCE SPECTRA OF MINERAL MIXTURES; T. Hiroi and C. M. Pieters, Department of Geological Sciences, Brown University, Providence, RI 02912, U.S.A.

The effects of grain size and shape on reflectance spectra of mineral mixtures are investigated to improve a reflectance model called "isograin model" [1], whose prototype [2] was proposed by M. Kinoshita in 1985. The sample powder is assumed to consist of infinite number of layers, each of which has the same thickness with the grain size d .

Fig. 1 (a) shows the mixing of two components which have scattering activities s_1 and s_2 , transmitting activities t_1 and t_2 , and mixing ratios c_1 and c_2 ($c_1 + c_2 = 1$), respectively. Unit incident light from the upper layer to a grain is transmitted by t to the lower layer and scattered by s to the upper layer (ω_1 portion) and within the layer ($1 - \omega_1$ portion). An incident light x from within the layer is transmitted by t and scattered by s to the upper and lower layers (ω_2 portion, respectively) and within the layer ($1 - 2\omega_2$ portion).

If x is homogeneous within the interstices of grains of one layer, total light flux from grains to interstices should be equal to the opposite one. Then we can obtain x as:

$$x = (1 - \omega_1)s_M / [1 - t_M - (1 - 2\omega_2)s_M]$$

$$s_M = c_1s_1 + c_2s_2, t_M = c_1t_1 + c_2t_2$$

Therefore in a mixture, s and t combine linearly. Reflectance R and transmittance T of one layer become

$$R = \omega_1s_M + \omega_2s_Mx, T = t_M + \omega_2s_Mx$$

where R and T have no more linearity. Reflectance of the whole sample (infinite number of layers) R_∞ is

$$R_\infty = 2R / (B + \sqrt{B^2 - 4R^2}), B = 1 + R^2 - T^2$$

Here, s and t are assumed to be expressed in the same way as a flat crystal. Fig. 1 (b) shows the light scattering process of a flat isotropic crystal, whose thickness is d , absorption coefficient is α , and boundary reflectivities from outside and inside are r_E and r_I , respectively. This gives

$$t = (1 - r_E)(1 - r_I)p / (1 - r_I^2p^2), s = r_E + ptr_I, p = e^{-\alpha d}$$

By assuming isotropic light and Fresnel's law, r_E and r_I are deduced from refraction index n [3] as is shown in Fig. 2. Because it was difficult to deduce n from reflectance of powders, a function $n = 1.2286 + 0.2214/\lambda$ (λ : wavelength / μm) was adopted for all the transparent minerals here, and ω_1 and ω_2 were assumed to be 0.3 and 0.1, respectively.

Fig. 3 shows reflectance spectra of eight grain-size fractions of blue glass powder. Calculated spectra agree well with observed ones except for the smallest size fraction

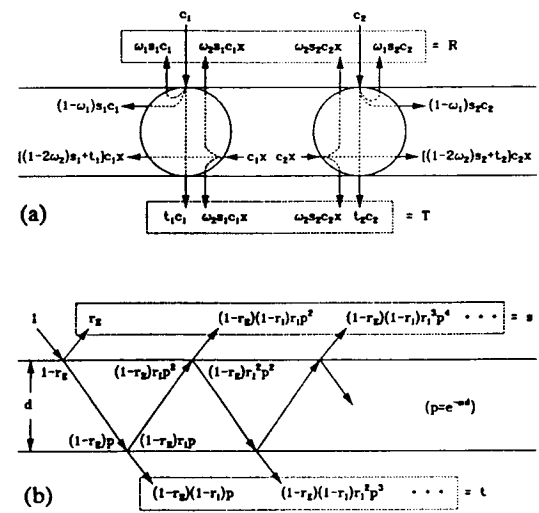


Fig. 1. Isograin model.

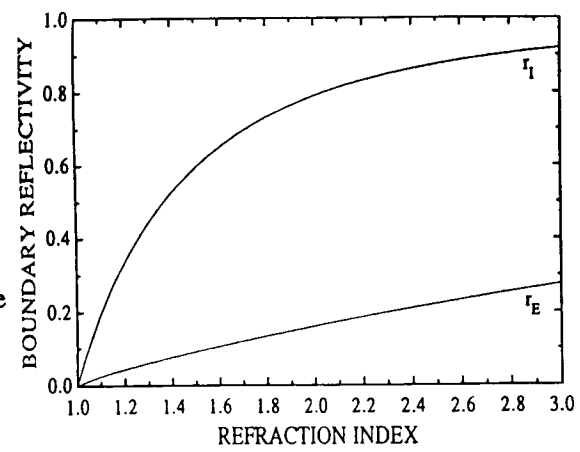


Fig. 2. Refraction index v.s. boundary reflectivities.

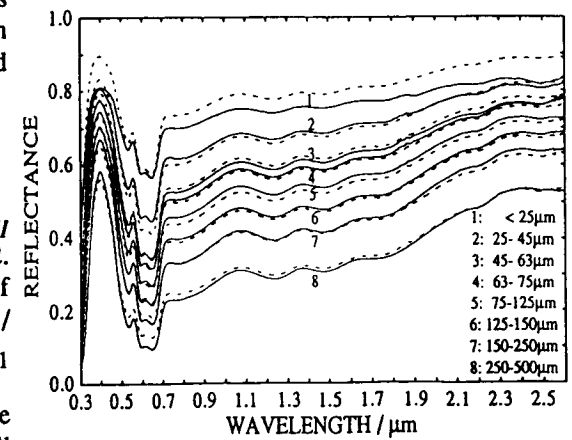


Fig. 3. Reflectance spectra of grain-size fractions of blue glass (solid: observed, broken: calculated).

(<25μm) and around the strong absorption band. We used a simple average of two mesh sizes for each grain size *d*. Glass was chosen for this test so that *n* could also be measured directly (in progress).

Fig. 4 shows the optimization of mixing ratios for quartz-alunite mixtures of the same grain sizes. Calculated spectra fit observed ones well, and errors of mixing ratios are within 3%.

Not all grains in a mixture, however, are equidimensional. In general, scattering and transmitting activities should be mixed in proportion to the total scattering area *a* of each component, which is not proportional to its total volume *v* in a mixture of different size or shape grains.

For a spherical grain, volume and scattering area of one grain are $(4\pi/3)(d/2)^3$ and $\pi(d/2)^2$, respectively. Therefore,

$$a(\text{sphere}) \propto \frac{v(\text{sphere})}{(4\pi/3)(d/2)^3} \pi(d/2)^2 = \frac{v(\text{sphere})}{(2/3)d}$$

For a thin disk-shaped grain, the effective scattering area is reduced to a half of its surface area after averaged for all the directions of incident lights. Therefore,

$$a(\text{disk}) \propto \frac{v(\text{disk})}{\pi(d/2)^2\delta} \pi(d/2)^2/2 = \frac{v(\text{disk})}{2\delta}$$

where δ indicates the thickness of the disk. By comparing the above two results,

$$a(\text{sphere}) : a(\text{disk}) = \frac{v(\text{sphere})}{d} : \frac{v(\text{disk})}{d_e}, d_e = 3\delta,$$

where *d_e* indicates effective grain size of a disk-shaped grain, which can be used for any nonspherical grains for convenience.

We provide two examples of reflectance spectra of mixtures that require this grain shape consideration.

Fig. 5 shows reflectance spectra of olivine-metal mixtures prepared by E. A. Cloutis [4] and measured at RELAB at Brown University. For opaque minerals as metals, transmitting activity *t* should be 0 and only its scattering activity *s* must be determined. Because each metal grain had a flat shape (average thickness about 10μm measured by a scattering electron microscope), an effective grain size *d_e* should be used in the mixing formula. Thus obtained *d_e* value 39μm corresponds to the disk thickness of 13μm, which agrees well with the observed one.

Fig. 6 shows reflectance spectra of calcite-chlorite mixtures also measured at RELAB. Chlorite is a member of phyllosilicates that have a perfect cleavage, and each grain has a flat shape. The optimized thickness 31μm is reasonably thin compared with its average diameter 191μm.

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References: [1] Hiroi T. and Takeda H. (1990) *Icarus* 88, 205-227. [2] Kinoshita M. and Miyamoto M. (1990) Proc. NIPR Symp. Antarct. Meteorites 3, 230-239. [3] Hapke B. (1981) *J. Geophys. Res.* 86, 3039-3054. [4] Cloutis E. A., Gaffey M. J., Smith D. G. W., and Lambert R. St J. (1990) *J. Geophys. Res.* 95, 8323-8338.

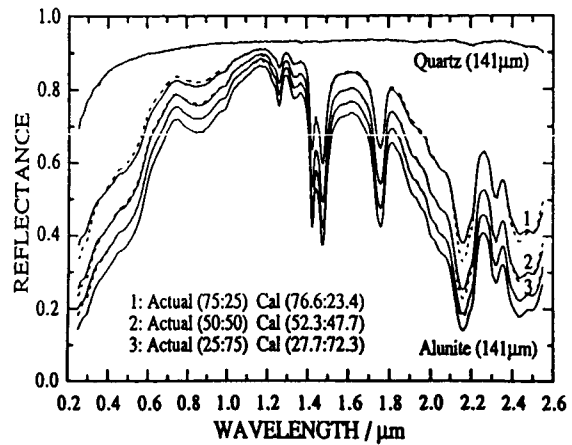


Fig. 4. Mixing ratio optimization for quartz-alunite mixtures.

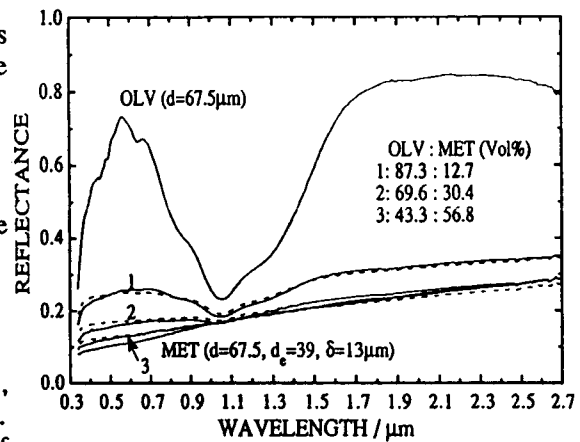


Fig. 5. Olivine-metal mixtures.

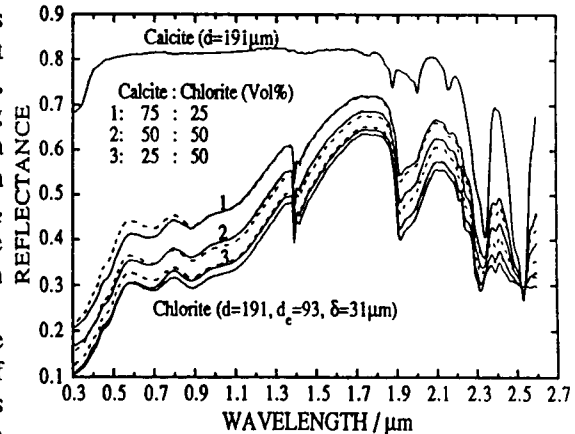


Fig. 6. Calcite-chlorite mixtures.