MODELLING RELATIONSHIP BETWEEN COLOR RATIO C(321 nm/ 415 nm) AND TiO_2 CONTENT.
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Introduction: A number of expressions for remote assessment of the TiO_2 abundance in the lunar regolith using spectral measurements have been proposed [e.g., 1-3]. All of them were established empirically from chemical and spectral data of lunar samples. The spectral slope or color ratio $C(\lambda_1/\lambda_2) = A(\lambda_1)/A(\lambda_2)$, where $A(\lambda)$ is the spectral albedo, is the simplest parameter that may characterize the TiO_2 abundance, where λ is the wavelength. An empirical expression has been suggested by Sato et al. [4]

$$\mathrm{TiO_2[wt.\%]} = 100\, C\left(321\,\mathrm{nm}/415\,\mathrm{nm}\right) - 68.9 . \qquad (1)$$

Equation (1) in combination with LRO WAC images allows one to built the TiO_2 lunar map that is available at http://wms.lroc.asu.edu/lroc/view_rdr/WAC_TIO2. The correlation coefficient corresponding to Eq. (1), which is calculated from the regolith samples returned by Apollo missions, is high, 0.98. However, physical mechanisms of the correlations are still rather vague as no distinctive spectral features like absorption bands are within the spectral range. We may observe only that the spectral slope tends to be neutral for high TiO_2 abundance. A possible explanation for this effect was given by Shkuratov [5]. It was supposed that the decrease of the spectral albedo slope is due to an increase in the relative contribution of light reflected by the particle surfaces when the TiO_2 content increases. The Fresnel reflection is neutral in the spectral regard, as not related to the passage of light through regolith particles. Instead of the Fresnel reflection there is another way to add dark and spectrally neutral components. These can be through inclusion of agglutinates and/or ilmenite.

To provide better understanding of the mechanisms of the correlation of C(321 nm/410 nm) with TiO_2, we apply 1D light-scattering modes to spectral mixtures [6,7]. We consider that the lunar regolith consists of three components: the relatively bright (low-Ti basalt), dark Ti-containing (ilmenite), and dark agglutinates. We take into consideration the agglutinates as their abundance in the lunar regolith is significant, up to 70% [8]. However, in the present modeling we assume the regolith does not contain Ti, despite this being highly improbable.

Source data: We choose the spectrum LRCMP216_70017 of light brown pyroxenes returned by Apollo 17 as the bright component, the spectrum LRCMP218_70017 of ilmenite (both were taken from http://www.planetary.brown.edu/LRMCC/ [9]), and the agglutinate spectrum LS-CMP-045 from RELAB (www.planetary.brown.edu/relabdocs/relab_disclaimer.htm). As the spectrum of the last sample was measured started from 350 nm we linearly extrapolate this spectrum to 320 nm. These three spectra are shown in Fig.1.

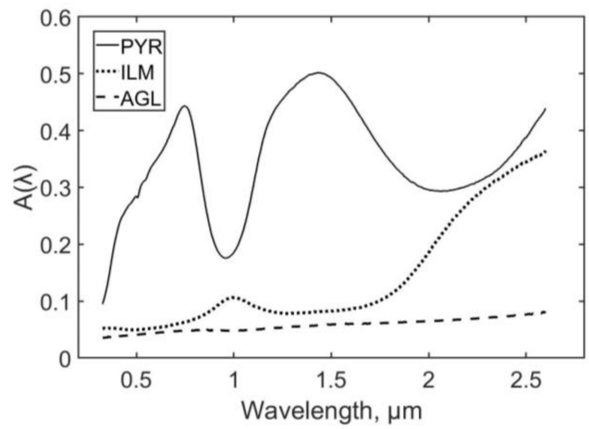

Fig. 1. The RELAB spectra of the main components of modeled media

1D nonlinear spectral mixture model: We use a 1D spectral model based on the geometrical optics approximation [5,6]. The model enables us to estimate reflectance A of a particulate surface as a function of λ, if the real and imagery parts of the refractive index $m(\lambda) = n(\lambda) + ik(\lambda)$ are known. The model exploits the parameter q that characterizes porosity of particulate surfaces. This parameter influences results weakly, and therefore, we may consider it as, e.g., q=0.5. The value $k(\lambda)$ characterizes the spectral dependence of the absorption coefficient: $\tau(\lambda) = 4\pi k(\lambda)/\lambda$, where l is the characteristic length of light propagation in particles. The function $n(\lambda)$ can be taken for each component from independent sources. The function $k(\lambda)$ can be calculated for each component from their spectra, like those shown in Fig. 1. The length l can be taken equal for all components or made to vary, depending on the task.

The model is invertible, i.e. starting from the spectral albedo and supposing the values of n and l are known, one can obtain an expression for the spectral absorption coefficient. This also allows one to model spectra of material mixtures using linear combinations of single-scattering albedo with suitable weight coefficients that are the volume fractions of the mixture components c_{ilm}, c_{pyr}, and c_{agg}. In addition, $c_{ilm} + c_{pyr} + c_{agg} = 1$.

By assuming that ilmenite has the idealized chemical formula $FeTiO_3$, we can assess the TiO_2 abundance and derive the wt.% of ilmenite in the mixture with the following equation.

$$Ilm[wt.\%] = \frac{c_{ilm}\rho_{ilm}}{c_{ilm}\rho_{ilm} + c_{pyr}\rho_{pyr} + c_{agg}\rho_{agg}}$$

For the calculations of weighted per cents of TiO_2 abundance in the mixture, we use the following densities of the principle components: ρ_{pyr} = 3.35 g/cm^3, ρ_{ilm} = 4.72 g/cm^3, and ρ_{agg} = 3.35 g/cm^3. Note, that the density of agglutinates varies significantly.

Results and discussion: To show the relation of the color ratio C(321 nm / 410 nm) on the TiO_2 abundance we produce the set of 40 reflectance spectra of three-component modeled mixtures with different volume fractions of ilmenite. We took the following values of model parameters: q = 0.5, l = 30 μm, n_{pyr} = 1.6, n_{ilm} = 2.1, n_{agg} = 1.6. The volume fraction of agglutinates (c_{agg}) was constant and taken equal to 0.5. The volume fractions of the ilmenite and bright pyroxene component varied with the condition $c_{ilm} + c_{pyr} = 0.5$. The modeled spectra reveal the prominent dependence of spectral slope on the TiO_2 content (see Fig. 2): the greater the TiO_2 content, the less the steep of the spectral slope over the whole range of UV-Vis.

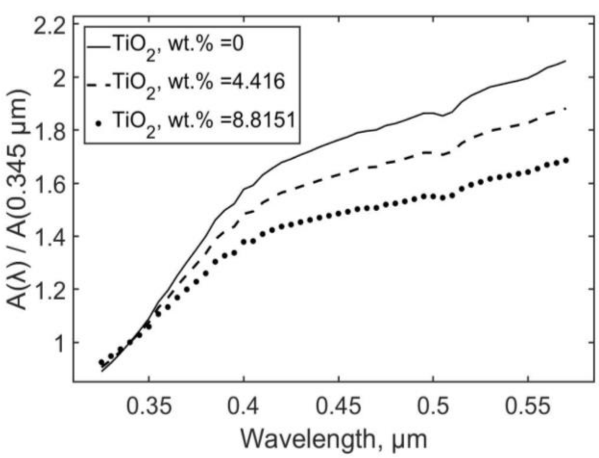

Fig. 2. Normalized reflectance spectra of the mixtures with different TiO_2 (ilmenite) content. They were obtained using a 1D light-scattering model.

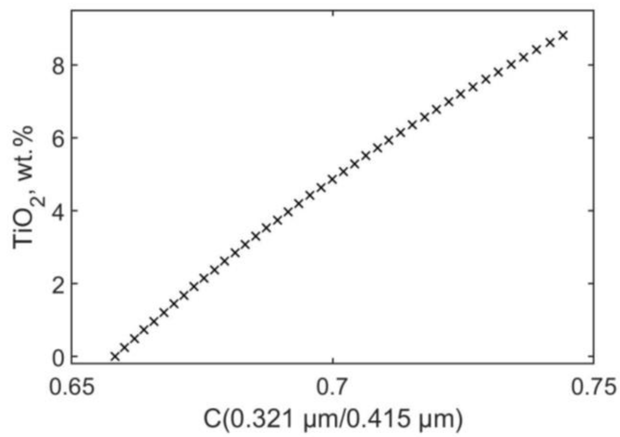

Fig. 3. The modeled relation between the color ratio proposed by Sato et al. [4] and the TiO_2 abundance.

We calculate the color ratio C(321 nm / 410 nm) for each spectrum. The dependence of the color ratio on TiO_2 abundance is shown on Fig. 3. It is slightly nonlinear over this range of TiO_2 content. The key result of our study is the approximation of this dependence by the following equation:

$$\mathrm{TiO_2[wt.\%]} = 102.7\ C\left(321\ \mathrm{nm}/415\ \mathrm{nm}\right) - 67.2 \quad (2)$$

We note that this is very similar to the empirical Eq. (1). This result shows numerically that the correlation between the color ratio in UV-Vis and Ti-abundance in the lunar regolith can be explained by the fact that the spectral slope in this range is governed by the dark Ti-bearing minerals like ilmenite.

Another important result is obtained from Fig. 2 that any color ratio $C(\lambda_1/\lambda_2)$, where $\lambda_1 < \lambda_2$ in UV-Vis, directly correlates with TiO_2 abundance if the non-linear dependence is monotonic, as shown in Fig. 3.

References: [1] Charette M.P. et al. (1974) *JGR* 79(11), 1605-1613. [2] Pieters C.M. and McCord T.B. (1976) *Proc. Lunar Sci. Conf. 7th*, 2677-2690. [3] Blewett D.T. (1997). *JGR* 102, 16,319-16,325.. [4] Sato et al. (2017) *Icarus* 296, 216-238. [5] Shkuratov Y. (1982) Solar Syst. Res. 16(2), 51-56. [6] Shkuratov et al. (1999) *Icarus* 137, 235-245. [7] Shkuratov et al. (2011) *PSS* 59, 1326-1371. [8] McKay D., et al. (1991) The Lunar Regolith. Lunar Sourcebook / Heiken G.H., et al., Eds., New York: Cambridge Univ. Press, 1991, Chap. 7, pp. 285–356. [9] Isaacson P.J., et al. (2011) *Meteorit. Planet. Sci.* 46, 228-251.