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New frontiers in the Solar System: trans-Neptunian objects/Les nouvelles frontières du système solaire : les objects transneptuniens

Quantitative modeling of the spectral reflectance of Kuiper Belt objects and Centaurs

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Abstract

Reflectance spectroscopy of Solar System bodies provides a rich source of information on their compositions (minerals, ices, metals, and macromolecular carbon-bearing materials). Models calculated with radiative transfer theories for the spectral distribution of diffusely scattered sunlight from planetary surfaces yield information on the compositions, abundances, physical states, layering, and particle microstructure of those surfaces. We discuss and evaluate the scattering theories of Hapke and Shkuratov that are widely used for modeling the reflectance spectra and color data for Kuiper Belt objects, Centaur objects, and other airless bodies in the Solar System. Both theories yield good models of the reflectance spectrum of Centaur 5145 Pholus using five components (ices, carbon, a silicate mineral, and a complex organic material), although the derived abundances differ widely. ***To cite this article: D.P. Cruikshank et al., C. R. Physique 4 (2003).***

Résumé

Modélisation quantitative des spectres de réflectance des objets de la ceinture de Kuiper et des Centaures. La spectroscopie de réflectance des corps du système solaire est un moyen très efficace pour déterminer la composition de leurs surfaces (minéraux, glaces, composants carbonés, et matériaux composés de macromolécules). Des modèles basés sur les théories de transfert radiatif simulent la diffusion de la lumière solaire sur la surface planétaire solide, ce qui permet alors de contraindre quantitativement la composition, l'abondance et l'état physique des matériaux présents sur la surface ainsi que sa microstructure. Les théories de diffusion d'Hapke et de Shkuratov qui sont communément utilisées pour modéliser les données spectrales des objets de Kuiper, des Centaures, et d'autres corps solides du système solaire sont discutées et comparées. Les deux théories sont alors utilisées pour reproduire les spectres du Centaure Pholus 5145. Le même mélange constitué de 5 composants (glaces, un composant carboné, un silicate, et un composant organique) permet de reproduire le spectre de cet objet avec les deux théories, cependant les abundances différent de manière importante. ***Pour citer cet article : D.P. Cruikshank et al., C. R. Physique 4 (2003).***

Keywords: Kuiper Belt; Centaur objects; Light scattering; Spectroscopy

Mots-clés : objets de Kuiper ; objets Centaures ; Diffusion de la lumière ; Spectroscopie

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1. Introduction

The objective of modeling the observed spectral reflectance of a planetary surface is to determine the composition (ices, minerals, metals, organic solids), the type of mixture (molecular, intimate, areal), the relative abundances of components, and approximate surface microstructure of the layers that reflect or scatter the incident sunlight in the visible and near-infrared spectral regions. Quantitative models also allow an evaluation of the surface temperature in some cases [1]. Depending upon the opacity, dimensions, and microstructure (e.g., crystalline or amorphous) of the particles composing the surface, the depth of the surface layer sampled by scattered incident sunlight can be a few micrometers or a few centimeters. Surfaces composed of small, highly opaque particles (e.g., the lunar maria) are sampled to micrometer depths, while surfaces covered with large, transparent crystals (e.g., Triton, with its solid N_2 surface [2]) are probed to depths up to several cm.

2. Radiative transfer in rough, particulate surfaces

Several photometric models describe in varying degrees of detail and precision the dependence of the bidirectional reflectance, R_t on the photometric geometry of a surface, where $R_t = I_t/\pi F$. R_t is also called the radiance factor, I_t is the intensity of light scattered from a surface element with a particular orientation (incident angle i, emission angle e, and phase angle α), and πF is the plane-parallel luminous flux.

The models of Hapke [3,4] and Shkuratov et al. [5] are especially useful in matching plausible, natural materials expected to be present in the outer Solar System to observational data on the surfaces of Kuiper Belt objects (KBOs) and Centaurs. These models, which are based on geometric optics, are applicable in the visible and near-infrared regions of the spectrum because the typical size range of the particles and other structures encountered or expected in planetary regoliths are significantly larger (tens of micrometers) than the wavelength of the light (see below). The available data for KBOs consists of photometric measurements at various wavelengths in the region 0.3–2.2 µm, and in a few cases, spectrophotometric data with spectral resolution $\lambda/\Delta\lambda \sim 100$ have been obtained to a maximum wavelength of 2.5 µm [6–9]. As observational techniques improve, with ground-based telescopes and telescopes in space, it will become possible to extend the data to longer wavelengths. For KBOs, all of the detectable radiation for $\lambda < 10$ µm (and for Centaurs $\lambda < 7$ µm) is diffusely reflected sunlight.

Applications of the Hapke model to quantitative analysis of (intimate) laboratory mineral mixtures give mass abundance estimates to better than 10% if the particle sizes of the components of the mixture are known [10–12]. When the Shkuratov theory is applied to laboratory reflectance spectra of mixtures, the abundance estimates are accurate to within 5–10%. At the same time, the calculated particle sizes fall within the range of actual sizes of the materials used in the mixtures [13].

Hapke's model [3,4] is based on a two-stream approximation to the equations of radiative transfer, and enables the calculation of the reflectance of a particulate surface. In this paper and in other published work [6,14] we use Roush's [15] formulation of the Hapke model. The input parameters include the geometry of the illumination, the particle size distribution, porosity, and complex refractive indices of the constituent material(s). The model can accommodate mixtures of particles of different sizes and compositions that are thoroughly mixed at the micrometer scale (intimate mixtures). In intimate mixtures, an incident solar photon encounters grains of all composition before emerging from the surface.

The bidirectional reflectance of a surface at each wavelength λ is

$$r\left(i, e, \alpha, \overline{w}, h, S(0), \overline{\Theta}\right) = \frac{\overline{w}}{4\pi} \frac{\mu_o}{\mu_o + \mu} \left\{[1 + B(\alpha)]P(\alpha) + H(\mu)H(\mu_o) - 1\right\}, \tag{1}$$

where i is the angle of the incident light ($\mu_o = \cos i$), e is the angle of the emergent light ($\mu = \cos e$), α is the phase angle between i and e, $\overline{w}$ is the average single-scattering albedo of the surface, h characterizes the width of the non-linear increase in the reflectance phase curve with decreasing phase angle (the opposition surge) in terms of particle size distribution, surface porosity, and compaction rate with depth. $S(0)$ is the contribution of light scattered from near the front surface of individual particles at zero phase, $H(\mu_o)$ and $H(\mu)$ are the Chandrasekhar H-functions [16], and $\overline{\Theta}$ is the average topographic slope angle that characterizes surface roughness at subresolution scale. In order to determine many of these parameters independently (h, $\overline{\Theta}$, $B(\alpha)$, $P(\alpha)$) spectral observations over a wide range of phase angle and viewing geometry are required. While such a range of observations can be obtained in the laboratory or from orbiting spacecraft, typically only a very limited range of viewing geometries can be observed from Earth-based telescopes. Of the parameters in Eq. (1), the average single-scattering albedo $\overline{w}$ is the one most strongly influenced by composition and this is where the optical constants of the candidate materials are used. Grundy et al. [17] and Poulet et al. [18] show that the phase function depends strongly on the real part of the refractive index n. As n increases, the phase function becomes less forward-scattering; increasing n increases the reflection coefficient at particle surfaces, thus reducing the number of rays penetrating the particle and passing once through it. For models of Kuiper Belt objects and Centaurs one can assume $h = 0.05$ (a lunar-like surface), $S(0) = 1.0$, an isotropic phase function, and minimal internal scattering. The opposition surge, $B(\alpha)$ is calculated using the viewing geometry, h, and $S(0)$. Hapke [19] (Eq. (1))

uses $\overline{\Theta}$ to represent the average topographic slope angle of the surface roughness. For more specific details of this approach see Cruikshank et al. [20].

Another kind of surface configuration consists of materials of different composition and/or microphysical properties that are spatially isolated from one another. With this configuration an incident solar photon encounters only one surface component, but the emergent flux of scattered sunlight integrated over the whole illuminated surface includes light scattered from each kind of surface, weighted by the fraction of the surface covered with each kind. These areal, or geographically segregated surfaces are expected to be more typical for a real body in the Solar System, in contrast to a spatially homogenous, intimately mixed surface. Most real surfaces are surely much more complex than any of the current models can readily accommodate.

For areal mixtures, the reflectances of the individual components are calculated and then combined at each wavelength to give the total reflectance (R_T) of the spatially mixed surface:

$$R_T = (A * R_A) + (B * R_B) + \cdots (N * R_N), \tag{2}$$

where R_A, R_B, and R_N are the reflectances and A, B, and N represent the fractional areal extent or spatial coverage of each component, such that they sum to 1.0.

A third type of physical configuration consists of plane-parallel homogeneous layers, where one material overlies another; each layer can present different textures and compositions. The mean radiative properties of the layers are defined by the single-scattering albedo, the phase function, and the optical depth. Different methods have been used to solve the radiative transfer equations in a stratified medium: the adding method combined with the doubling method [21,22], a discrete-ordinate method [16,23], and the calculation of X and Y functions of Chandrasekhar [16,24]. In the Douté and Schmitt model [24] a better degree of realism is achieved for the single- and double-scattering contributions by using their real analytical expressions with a non-isotropic phase function.

The Hapke model in particular has been subjected to many tests and verifications in the laboratory, in comparisons with astronomical data, and at the theoretical level. For example, Hillier [25] compared the Hapke bidirectional reflectance of a medium consisting of a macroscopically smooth layer of spherical particles containing isotropic internal scatterers with a Monte Carlo method, and showed that the Hapke calculation underestimates the scattering at high phase angles. This suggests that the fundamental scattering volume should be governed by more forward-scattering particles. The discrepancy is most significant for low-albedo surfaces (which are often best fit by Hapke theory), suggesting that the single-scattered component is somewhat underestimated. In Hapke theory, this discrepancy can be addressed by increasing the asymmetry parameter g, which describes the effective anisotropic scattering behavior of a particle or collection of particles, and which governs the single-scattering phase function. However, because g enters only once in the Hapke model, an increase in this parameter will decrease the whole spectrum in the same proportions, thus requiring the use of smaller grains to compensate. Thus, for a given set of refractive indices, the only parameter that can be varied is the particle size.

The Shkuratov theory is based on the slab model for the local scattering properties and on the principle of invariant imbedding for the derivation of the reflectance of the particulate surface. Specifically, the average single-scattering albedo of a single particle is a linear combination of the forward- $(r_{f,i})$ and back-scattered $(r_{b,i})$ components of each grain type weighted by it's areal fraction (f_i)

$$\overline{w} = \frac{\sum_{i=1}^{n} f_i (r_{b,i} + r_{f,i})}{\sum_{i=1}^{n} f_i}. \tag{3}$$

The treatment of particle scattering asymmetry is different, however. The Shkuratov model incorporates the phase function symmetry not as a free parameter, but as a dependent variable that is calculated directly from the refractive indices as a function of grain size and composition in a self-consistent way. It can be characterized by the ratio $(r_f - r_b)/(r_f + r_b)$, which can be interpreted as a representation of the asymmetry parameter g. Poulet et al. [18] evaluated the role of g in the Shkuratov model by calculating the reflectance of a surface with g as a free parameter while keeping the calculated grain size constant. Fig. 1 [18] shows the result, with normalized spectra of surfaces made of pure water ice particles (upper panel) and for particles of a complex organic solid called Titan tholin (lower panel) for different values of g. This parameter affects the dark and bright parts of a spectrum in a non-uniform way; decreasing g makes the continuum of the water ice less blue in the near-IR, while the UV/near-IR slope of the Titan tholin spectrum is less red. Thus, making the particles more backscattering will allow light to leave the regolith with fewer internal scatterings between grains, and therefore with less absorption. This effect is strongest for dark particles for which the single-scattering component is proportionately more important than for bright particles. At the same time, the color of a surface of bright particles with even a weakly coloring component can be greatly magnified by forward-scattering, which leads to more internal scatterings of photons before the escape. This in turn leads to differences in the depths of absorption bands (such as H_2O ice) that are normally attributed to variations in grain size.

Both Shkuratov and Hapke theories relate the single-scattering albedo $\overline{w}$ to particle properties by means of a slab model, and in this respect there is little difference between the two theories. The principal difference between the Hapke and Shkuratov theories lies in the role of the *phase function* of individual regolith particles, where the scattering of sunlight occurs. In Hapke,

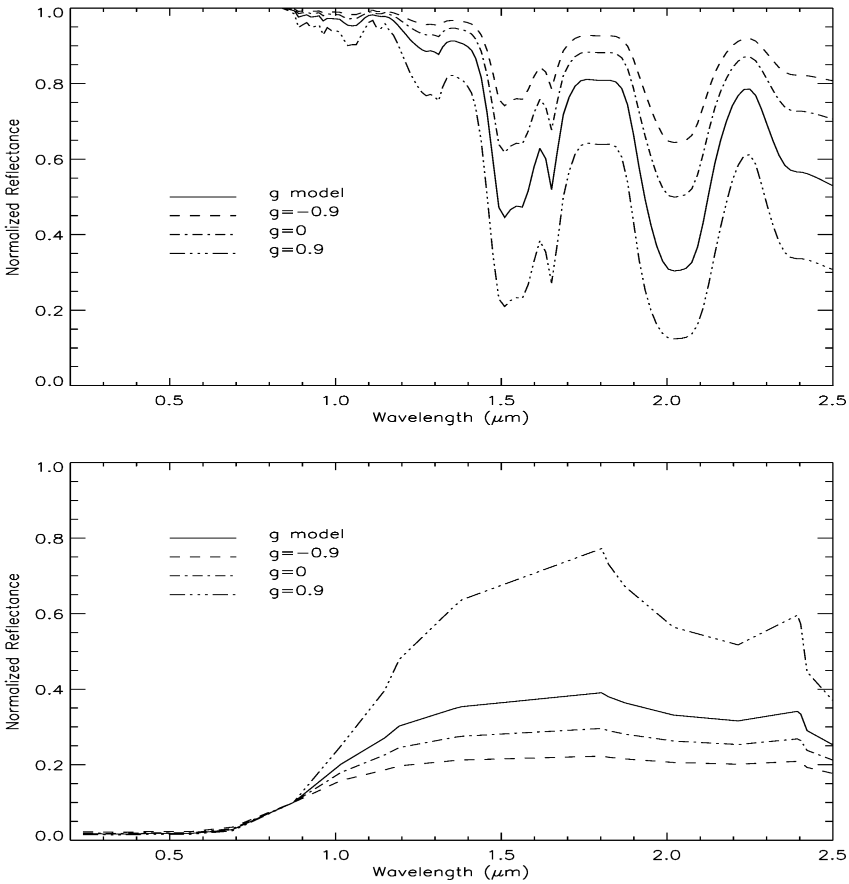

Fig. 1. This figure from Poulet et al. [18] shows the dependence of the normalized reflectance of pure H_2O ice on g (upper panel). The label 'g model' defines the spectrum calculated by using the Shkuratov model. The grain size is 10 μm. The lower panel shows the same range of g values, but for Titan tholin. Reprinted from [18] with permission from Elsevier.

the particle phase function is derived from best fits to reflectance data (over a wide range in phase angles), but comes into play only in the singly scattered light. The particle phase function thus derived is valid for surfaces of low albedo, where single-scattering dominates, and less valid for surfaces of high albedo in which multiple-scattering occurs; in Hapke's theory, the multiple-scattering term treats particles as isotropic scatterers. Most Solar System bodies studied with the Hapke theory show that the asymmetry parameter g is negative (although Verbiscer et al., [26], found a positive g for terrestrial snowbanks, consistent with lab results and theoretical models). Most lab studies, however, suggest that regolith grains should be forward-scattering, particularly in the $s = 0$ limit normally assumed (no internal scattering). Grundy et al. [17] used a Monte Carlo ray-tracing model to confirm that the phase function of irregular particles of size $\gg \lambda$ have strong forward-scattering lobes.

In Hapke models of planetary surfaces, a backscattering phase function is generally used to represent the single-scattering component, while for higher orders of scattering an isotropic phase function is assumed. The Hapke model requires proportionally less red material than the Shkuratov model to achieve a fit for the red objects that are typical among asteroids and other objects in the outer Solar System. With the Hapke model and a given set of refractive indices, a fit to a red planetary object usually requires a decrease in particle size, in extreme cases leading to the conflict with the geometric optics condition noted above. Shkuratov models of red, low-albedo objects generally avoid this problem, although even with the different formulation of the particle scattering properties, Poulet et al. [18] could not reproduce the very strong red color of the exceptional object 5145 Pholus using intimate mixtures of particles greater than a few micrometers in size. Instead, they modeled mixtures of different materials conceptualized as small inclusions of a strongly colored material (such as a tholin) in a larger particle of more transparent material (e.g., H_2O ice) (see discussion of effective medium below).

Returning to the geometric optics issue, we note that both the Shkuratov and Hapke theories require for full validity that the scattering particles have dimensions substantially larger (at least a factor of ~ 10) than the wavelength of the light. As the particle size approaches the wavelength of light, the theories are thus not directly applicable to measurements and must be used with care. In particular, the abundance of the fine-grained material may be underestimated because of a decrease in the spectral contrast as particle size decreases. Mustard and Hays [27] modeled the near-infrared spectra of samples having very fine particles using a combination of Mie theory to determine the single-scattering albedo, and a Hapke model to calculate the reflectance spectra. The results are qualitatively good, but extracting reliable quantitative information on the physical and compositional properties in this optical regime remains an issue. A limitation of the Mie–Hapke model is that the Mie solution explicitly assumes particles that are separated by several particle radii, which is clearly not the case in planetary regoliths. Particles with dimensions of the order of the wavelength of the light and smaller are predicted to scatter as Rayleigh particles, rather than as independent, forward-scattering Mie particles. However, laboratory studies of particulate surfaces in progress [28,29] have called this prediction into question. Photometry of ultra-small particles of both low and high albedo over a range of phase angles is showing that as the particle size decreases there is no indication of a transition from a Mie to a Rayleigh scattering regime. These new results are prompting a reevaluation of the theory of scattering of light by planetary regoliths.

3. Effective medium theory

Shkuratov et al. [5] address the significant differences in the assumptions on the physical mixing in multicomponent surfaces, and the important effects the mixing has on the resulting synthetic spectra when compared with observations. For example, inhomogeneous particles that commonly occur in nature can take many forms, such as inclusions of one material in a host matrix of another material. There are several approaches to approximating the average dielectric constant of the combined media by using weighted averages of the dielectric constants of the various constitutents. The most widely used are the models of Maxwell Garnett [30] and Bruggeman [31], although there are several others as described in Bohren and Huffman [32] and Hapke [4]. Under the conditions imposed by the many underlying assumptions in effective medium theory, e.g., particle sizes are $\gg$ wavelength, inclusions are homogenously distributed and randomly oriented, etc., the general Maxwell Garnett expression for multicomponent spherical inclusions in a matrix is

$$\bar{\varepsilon} = \varepsilon_m \left[1 + \frac{3 \sum_{i=1}^{n} f_i \frac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}}{1 - \sum_{i=1}^{n} f_i \frac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}} \right], \tag{4}$$

where ε_m is the dielectric function of the matrix, ε_i is the dielectric function of a given inclusion, and f_i is the volume fraction of the component. The Bruggeman expression [31] is

$$\sum_{j=1}^{n} c_j \frac{\varepsilon_j - \bar{\varepsilon}}{\varepsilon_j + 2\bar{\varepsilon}}, \tag{5}$$

where c_j and ε_j are the concentration and dielectric function of the jth component, respectively, and $\bar{\varepsilon}$ is the average dielectric function. Hapke [4] notes that neither of these effective medium theories address the way in which the scattered intensity is modified by further scattering as it propagates through the medium.

4. Model calculations of the spectrum of 5145 Pholus

The choice of scattering theory, as well as the choice of the mixing modes and other parameters of the scattering particles, has a significant effect on the calculated abundances of the components. To illustrate some differences in the abundances of a complex surface derived in the Shkuratov and Hapke models, we show in Fig. 2 the spectral reflectance of 5145 Pholus together with two models. Pholus is a ~ 140 km diameter body whose orbit crosses the orbits of Saturn and Uranus, and has a period of 92.7 years. It is thought to be a former member of the Kuiper Belt population, and is designated a Centaur object. For a solid body of overall low reflectivity (albedo), its spectrum is particularly rich in terms of overall shape and the presence of diagnostic absorption bands.

The reflectance spectrum of Pholus compiled from observations by several investigators and calibrated in terms of geometric albedo (determined from observations of the thermal emission of the object) has been modeled with the Hapke code and a combination of five different components [6]. The data and the Hapke model are shown in Fig. 2. The model consists of two principal components. The first component, covering 38.5 ($\pm$5)% of the surface, is an intimate mixture of olivine, Titan tholin, H_2O ice, and CH_3OH ice. The second component is carbon black, covering 61.5 ($\pm$5)% of the surface, spatially isolated from the first component. Titan tholin, a complex organic solid material synthesized by energy deposition in a mixture of gaseous N_2 and CH_4 (abundance ratio 9:1) [33] absorbs strongly in the ultraviolet and violet spectral regions, giving the model the steeply rising section (0.45–1.2 µm), that is, its red color. H_2O ice produces the absorption bands at 1.55 and 2.0 µm; frozen CH_3OH produces the double band at 2.27 and 2.33 µm, magnesium-rich olivine (Fo_{82}) absorbs between 0.8 and 1.4 µm, and the carbon

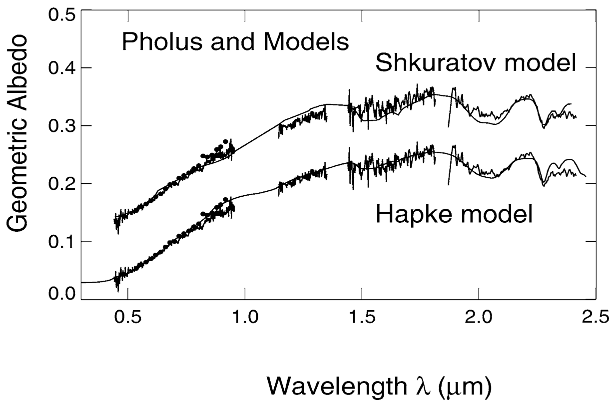

Fig. 2. Hapke and Shkuratov models of the Centaur 5145 Pholus. The data and the Shkuratov model are offset upward by 0.1 in geometric albedo. The uncertainties in the Pholus data, different wavelength segments of which are taken from various sources (and have varying levels of signal precision) can be estimated from the point-to-point scatter.

Table 1
Abundances of the components in spectral models of 5145 Pholus. Reprinted from [18] with permission from Elsevier.

	H_2O ice	Titan tholin	CH_3OH ice	Olivine	Carbon
Hapke model					
Abundance (%)	6	6	6	20.5	61.5 ± 5
Grain size (μm)	10	1	10	20	–
Shkuratov model					
Abundance (%)	42$^{(*)}$	26	12	5	15
Grain size (μm)	10	50	50	100	$\geqslant 10$

$^{(*)}$ H_2O ice with 16% small inclusions of Titan tholin.

contributes to lowering the geometric albedo. The Titan tholin particles used in this Hapke model are only 1 μm in size, in violation of the geometric optics principles of the model.

The same spectral data have also been modeled using the Shkuratov code [18], with Titan tholin incorporated as inclusions in the H_2O ice as well as in independent grains. This technique avoids the problem of grains that are too small, yet it produces the required amount of absorption at the short wavelengths to match the observational data. The Shkuratov model, which is an intimate mixture of the same materials used in the Hapke model, is shown as the top trace in Fig. 2.

The grain sizes and abundances derived for Pholus from the Hapke and Shkuratov models are given in Table 1 [18]. The Shkuratov model achieves the spectral fit and low overall albedo with much less carbon by using significantly larger grains for most components, but uses substantially more Titan tholin to achieve the strong absorption toward the violet. This comparison effectively illustrates the variation in the abundances of the components that results from the choice of modeling technique, as well as the choices of grain sizes.

5. Summary

Quantitative models of the spectrum of scattered sunlight from the surfaces of Kuiper Belt objects, Centaurs, and other airless bodies in the Solar System permit an evaluation of the compositions, mixing of the components, and other parameters of interest concerning these bodies. The calculations require the complex optical refractive indices of the surface constituents (ices, minerals, organic solids) over a wide range in wavelength. As the wavelength interval of the data and models increases, so does the information that can be derived. Several mathematical techniques have been developed for modeling planetary surfaces with varying degrees of complexity and completeness; the codes of Hapke and Shkuratov have been verified by laboratory observations and have proved to be especially useful.

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