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Optical constants of particulate minerals from reflectance measurements: The case of calcite

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Abstract

In this work we describe a new method for the derivation of the optical constants of a particulate sample by means of the Hapke theory, starting from directional-hemispherical reflectance measurements. This approach has been applied to calcite fine grains, whose spectra have been obtained in our laboratory in the spectral range 0.3−2.3 μm.

Keywords: Optical constants; Minerals; Calcite

1. Introduction

The search for signs of the stable presence of liquid water in the early Martian environment is an extremely important issue, which can give precious information about the geological and climatological evolution of Mars and could have very important implications on the development of some form of life on the planet.

Today the extremely harsh conditions of temperature and atmospheric pressure on the surface of Mars do not allow the stable presence of liquid water which usually freezes and then quite rapidly sublimates, except that in the polar regions where ice is relatively stable. However, strong evidences, mainly supported by remote sensing images, suggest the possibility that, in the past, Mars may have experienced episodes of warmer and wetter climate with a thicker atmosphere able to provide a strong greenhouse effect and to stabilize liquid water on the surface. This hypothesis seems to be supported by the presence of sinuous and dendritic channels, apparently carved through slow erosion by water running across the surface, along with paleolacustrine basins which could have hosted relatively large bodies of liquid water for a significant period of time [1–3].

In this scenario evaporites, such as carbonates, sulphates and other salts, could therefore play a crucial role in determining the history of the Martian atmosphere, geology, and hydrology. Actually, the presence of evaporite deposits on the Martian surface, particularly in sites such as depressions and craters, could strongly

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indicate that bodies of liquid water were once present on the early Martian surface for a sufficiently long period of time; in turn, due to the present strong instability of liquid water on the surface, this could imply an ancient climate much warmer and wetter than the current one.

In order to better understand the climatic evolution of the planet it would be therefore important to collect new remote sensing data and to continue the spectral search for evaporite minerals.

For radiative transfer computations, needed to model spectra of Martian dust, optical constants of minerals, probably present in the dust, are helpful.[1] They serve as the basis for the calculation of the necessary absorption and scattering efficiencies for different size and shape distributions of the dust particles.

Not all the optical constants of the interesting minerals are available since the needed calculations are quite time consuming; moreover, much care has to be taken using optical constants present in literature, because they may refer to bulk material instead than to the particulate state and this could be of great relevance in reproducing the spectral behaviour of Martian dust. In fact, the thermal inertia estimated for the Martian surface [4,5] indicates an average diameter of 400 μm for the surface grains. On the other hand, detailed measurements of an aerosol size distribution are difficult in the Martian atmosphere, since the average size of the suspended particles depends on the temporal and spatial variations of the climatic conditions (global storms, dust devils, etc.). Therefore, some size distributions with a small number of parameters are ordinarily used. Many authors over the past 20 years have used a variety of observations to constrain the mean effective radius r_{eff} and variance of the size distribution of the dust. The values, derived for r_{eff} in the literature, range from 0.2 to 2.75 μm, depending on the wavelength interval of observation going from ultraviolet [6] to thermal infrared [7]. Recently an analysis of data acquired by the Mars Global Surveyor seems to indicate a typical dust particle size $r_{eff} = 1.5 \pm 0.1\,\mu m$, with significant variations between the northern and the southern latitudes [8].

In this context the knowledge of the complex refractive index (“complex optical constants”) of a typical carbonate rock, such as limestone, may help in elucidating the problem of the presence of these minerals on Mars. Limestone, in fact, is a carbonate-bearing material mainly composed of calcium carbonate ($CaCO_3$), generally in the form of very small calcite grains.

In general, in the attempts of reproducing the spectra of fine Martian dust, the synthetic absorption and emission spectra have been calculated by means of the optical properties of particulate materials computed starting from the optical constants of bulk samples. This approach has been questioned by many authors (see, for example, [9]), since it is well known that particular caution has to be exercised in extrapolating laboratory results concerning bulk samples to conditions where small particles occur. The question has genuine physical roots. In fact, the incoming radiation can induce lattice vibrations in the particulate material, the so-called “surface modes”, specific to the shape and size of the grains. This problem can be overcome if the optical constants of minerals directly derived for particulate samples are known.

In a first attempt, infrared transmission spectra measured for limestone particles with an average radius of 0.06 μm were used to retrieve optical constants of submicron grains [10]. The dispersion theory was applied in this case, under the assumption of the spherical shape of the grains and hence according to Mie theory. The data were also used for a tentative identification of carbonates on Mars. However, a Scanning Electron Microscopy (SEM) analysis of these limestone grains has shown that the particle shapes are different from spheres. As a matter of fact the real grains, whether on Mars or in laboratory samples, in general are not spherical and for this reason Mie theory can be used in principle only as a first approximation for the derivation of the optical constants. In this respect optical constants of the same submicron sample of calcite have been calculated for two types of continuous distributions of ellipsoids [11]. It was shown that in the spectral region around the bands at 32 and 44 μm, whose assignment to surface modes raises no doubt, the optical constants derived for various shape distributions are markedly different from each other.

In this work we describe a new method for the derivation of the optical constants of a particulate sample by means of Hapke theory [12], starting from directional-hemispherical reflectance measurements.

[1]The terms *dielectric constant*, *refractive index*, and *optical constants* are used interchangeably throughout this paper. Of course, the quantities in question are not constant in any useful sense. The dielectric function ($\varepsilon = \varepsilon' + i\varepsilon''$) and the complex index of refraction ($m = n + ik$) are linked by the relation $\varepsilon = m^2$.