DOI: 10.1478/C1V89S1P024

AAPP | Atti della Accademia Peloritana dei Pericolanti
Classe di Scienze Fisiche, Matematiche e Naturali
ISSN 1825-1242

Vol. 89, Suppl. No. 1, C1V89S1P024 (2011)

SCATTERING MATRIX MEASUREMENTS AND LIGHT-SCATTERING CALCULATIONS OF CALCITE PARTICLES

D. D. DABROWSKA,[a*] O. MUÑOZ,[a] F. MORENO,[a]
T. NOUSIAINEN,[b] E. S. ZUBKO,[bc] AND A. C. MARRA[d]

ABSTRACT. We present measurements of the complete scattering matrix as a function of the scattering angle of a sample of calcite particles collected near Lecce, Italy. The measurements are done at a wavelength of 647 nm in the scattering angle range $3^\circ - 177^\circ$. FESEM and SEM images show that the sample consists largely of flake-like particles. Ten different flake-like geometries are randomly generated and their scattering properties are simulated with DDA for sizes from 0.1 μm to 1 μm. Some preliminary comparisons of the simulations and the measurements are shown.

1. Introduction

Calcite is a main component of limestone (98 $\%$ [1]) and is commonly considered to be particularly important for its link with climate evolution and water resources on Mars. Moreover, dust from the North Sahara is rich in calcite [2] and the Saharan desert is one of the main sources of natural aerosols for the Earth's atmosphere [3]. In this work we study a calcite sample produced by grinding from bulk material collected near Lecce, Italy [4].

We measure the size distribution of the calcite sample using a Mastersizer 2000 from Malvern instruments. The Mastersizer measures the phase function of the sample at 633 nm in a certain scattering angle range paying special attention to the forward diffraction region and uses either Lorenz-Mie or Fraunhofer theory to retrieve the volume distribution that best fits the measurements [5]. From the measured size distributions we calculate the values of the effective radius r_{eff}, and effective variance v_{eff} as defined by [6]. The results are presented in Table 1.

Calcite is a uniaxial birefringent material, so it has one optical axis and, instead of one refractive index, it has a dielectric tensor specified by two principal dielectric functions, the ordinary and extraordinary refractive indices. These refractive indices change with wavelength, the ordinary refractive index varying roughly between 1.57 and 1.47, while the extraordinary refractive index varies between 1.88 and 1.62 in the 0.2–3.3 μm wavelength range [7].

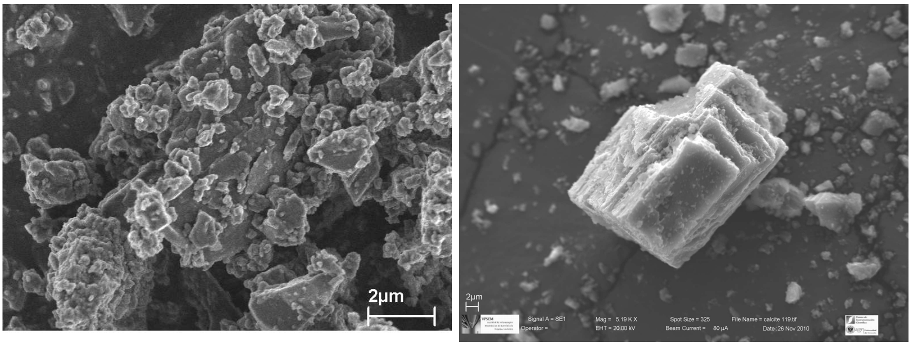

Figure 1. FESEM (left) and SEM (right) images of the calcite sample. The white bars correspond to 2 μm.

In Figure 1, we show an example of Field Emission Scanning Electron Microscope (FESEM) and Scanning Electron Microscope (SEM) images of our sample of calcite particles. As shown, a high percentage of the calcite particles present flake-like structures.

2. Laboratory measurements

In Figure 2, we present the measured scattering matrix elements as functions of scattering angle of our sample of randomly oriented calcite particles. The measurements have been performed at the IAA Cosmic Dust Laboratory located in Granada. Detailed information on the experimental procedure is given in [5]. The measurements are performed in the scattering angle range 3-177° at a wavelength of 647 nm. The scattering matrices fulfill the Cloude coherency matrix test [8] within the experimental errors at all measured scattering angles. The measured phase function $F_{11}(\theta)$ is normalized to unity at 30°. In general, the calcite sample presents the typical behavior of irregular mineral dust, i.e., the $F_{11}(\theta)$ presents a strong forward peak with almost no structure at side and back scattering angles showing a slight increase when approaching the backward direction. The degree of linear polarization for unpolarized incident light, $-F_{12}(\theta)/F_{11}(\theta)$, presents the typical bell shape with a maximum around 90° and with the negative branch near backscattering direction. Moreover, the $F_{44}(\theta)/F_{11}(\theta)$ is larger than the $F_{33}(\theta)/F_{11}(\theta)$ at side and backscattering angles. The experimental data will be available in digital form in the Amsterdam-Granada light scattering database at www.iaa.es/scattering.

Method	r_{eff} [μm]	v_{eff}
Fraunhofer	1.7	7.6
Mie	3.3	4.4

Table 1. Calculated effective radii r_{eff} and effective variances v_{eff} for the calcite sample.

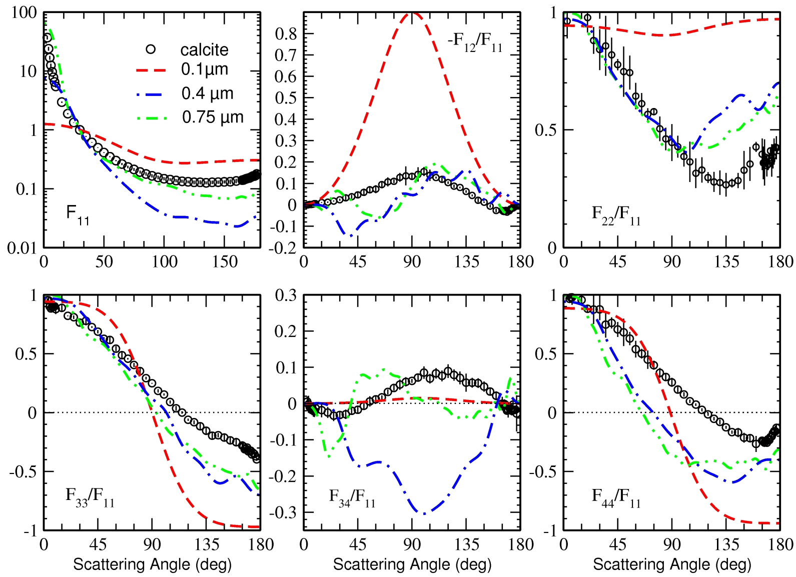

Figure 2. Measured (circles with error bars) and simulated (dashed lines) scattering matrices for the calcite sample. Measurements have been performed at 647 nm. The red, blue and green lines correspond to simulations for flakes with radii of 0.1, 0.4 and 0.75 μm, respectively, averaged over all the simulated geometries.

3. Simulations

We model the single-scattering properties of 10 different flake-like shapes shown in Figure 3 for 12 sizes from 0.1 to 1 μm. We consider only orientation-average results. A large number of orientations is needed to achieve well converged, orientation-averaged results for our model particles. The number of orientations used ranges from 512 for the smallest particles (0.1 μm) to 1485 for the largest (1.0 μm). In Figure 2 we illustrate the trends on the calculated scattering matrix elements when increasing the size of the particles. In our shaped-averaged calculations we use DDSCAT 7.1 that is an implementation of the discrete dipole approximation. DDASCAT 7.1 is flexible regarding the target geometry and allows calculations for birefringent particles. Large size parameters are, however, challenging due to high memory and computational requirements. In particular, good accuracy requires that sufficient amount of volume elements are used per wavelength to describe the target shape. We therefore consider sizes only up to 1 μm at this point. For a detailed description and limitations of the code we refer to [9].

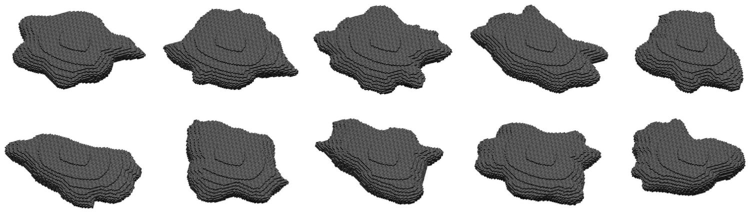

Figure 3. The randomly generated model shapes used in simulations.

At this point, we assume that calcite is isotropic. The complex refractive index is fixed to $m = 1.655 + 0.0i$. The real part corresponds to that of the ordinary ray [7]. The imaginary part of the refractive index is set to zero, on the basis that pure calcite is very weakly absorbing at visible wavelengths. In the next step we plan to consider the fully birefringent case.

4. Conclusions and future work

Because the DDA computations cover only part of the size distribution of the samples, the scattering matrices of the model particles and the measured values are not expected to coincide. However the simulated scattering matrix for larger particles tends to be more similar to the measurements.

We plan to average the calculations over the measured size distribution of our calcite sample (up to 1 μm). Moreover, the same procedure will be applied for the birefringent case. We also plan to expand our simulations to more geometries to take into account the non-flake particles of our calcite sample making it more realistic.

A more detailed treatment with more examples will be provided in a forthcoming paper.

References

[1] V.Orofino, A.Blanco, S.Fonti, R.Proce and A. Rotund. The infrared optical constants of limestone particles and implications for the search of carbonates on Mars, Planet.Space Sci. Vol. 46, No. 11/12, pp. 1659-1669,(1998)

[2] T.Nousiainen, E.Zubko, J.V.Niemi, K.Kupiainen, M.Lehtinen, K.Muinonen and G.Videen, Single-scattering modeling of thin, birefringent mineral-dust flakes using the discrete-dipole approximation, J.Geophys.Res.,VOL.114,D07207, (2009)

[3] T.Nousiainen, Optical modeling of mineral dust particles, J.Quant.Spectrosc.Radiant.Transfer., 110, 1261-1279, (2009)

[4] A.C. Marra, R. Politi, A. Blanco, R. Brunetto, S. Fonti, G.A. Marzo, V. Orofino, Optical constants of particulate minerals form reflectance measurements: The case of calcite, J.Quant.Spectrosc.Radiant.Transfer. 100,250-255 (2006)

[5] O.Muñoz, F.Moreno, D.Guirado, J.L.Ramos, H.Volten, J.W.Hovenier, The IAA cosmic dust laboratory: Experimental scattering matrices of clay particles, Icarus 211,894-900, (2011)

[6] J.E.Hansen and L.D.Travis, Light scattering in planetary atmospheres. Space Sci.Rev. 16,527-610, (1974)

[7] G.Ghosh, Dispersion-equation coefficients for the refractive index and birefringence of calcite and quartz crystals, Optics Communications 163 (1999) 95-102, (1999)

[8] J.W.Hovenier, C.V.M. van der Mee and H.Domke, Transfer of polarized light in planetary atmospheres: Basic concepts and practical methods. Kluwer Springer, Dordrecht,(2004)

[9] B.T. Draine and P.J. Flatau, User Guide for the Discrete Dipole Approximation Code DDSCAT 7.1, (2010)

[a] Instituto de Astrofísica de Andalucía, CSIC
Glorieta de la Astronomía s/n
18080 Granada, Spain

[b] Department of Physics
P.O. Box 48
FI-00014 University of Helsinki
Finland

[c] Institute of Astronomy
Kharkov National University, 35 Sumskaya St.
Kharkov, 61022
Ukraine

[d] Institute of Atmospheric Sciences and Climate (ISAC) of the Italian National Research Council (CNR)
UOS Lecce,
Str. Prov. Lecce-Monteroni km 1.2, 73100, Lecce,
Italy

* To whom correspondence should be addressed | Email: dominika@iaa.es

Paper presented at the ELS XIII Conference (Taormina, Italy, 2011), held under the APP patronage; published online 15 September 2011.

© 2011 by the Author(s); licensee *Accademia Peloritana dei Pericolanti*, Messina, Italy. This article is an open access article, licensed under a Creative Commons Attribution 3.0 Unported License.