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Direct simulation Monte Carlo ray tracing model of light scattering by a class of real particles and comparison with PROGRA^2 experimental results

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Abstract

The Direct Simulation Monte Carlo (DSMC) model is presented for three-dimensional single scattering of natural light by suspended, randomly oriented, optically homogeneous and isotropic, rounded and stochastically rough cubic particles. The modelled particles have large size parameter that allows geometric optics approximation to be used. The proposed computational model is simple and flexible. It is tested by comparison with known geometric optics solution for a perfect cube and Lorenz–Mie solution for a sphere, as extreme cases of the class of rounded cubes. Scattering and polarization properties of particles with various geometrical and optical characteristics are examined. The experimental study of real NaCl crystals with new Progra^2 instrument in microgravity conditions is conducted. The experimental and computed polarization and brightness phase curves are compared.

Keywords: Direct simulation Monte Carlo; Ray tracing model; Rounded cubes; Polarization phase function; Brightness phase function; Rough particles

1. Introduction

Knowledge of the individual light scattering properties of particles with various shapes and refractive indices is of great importance for optical particle characterization and identification. It is useful for many applications in astronomy, meteorology, photographic science, powder material technologies, etc.

The dependence of the degree of linear polarization defined by

$$P_l = \frac{I_\perp - I_\parallel}{I_\perp + I_\parallel} \tag{1}$$

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on the angle between the sample illumination and the scattering light acquisition directions is called the polarization phase function. In (1) $I_{\parallel}$ and $I_{\perp}$ are the intensity components, polarized parallel and perpendicular to the scattering plane, respectively.

The scattered light intensity is defined by

$$B = I_{\perp} + I_{\parallel}. \tag{2}$$

The angular dependence of B is called the brightness phase function. Both polarization and brightness phase functions hold essential information about the nature and physical properties of the scattering particles.

Solving of the light scattering problem is a non-trivial task, especially in the case of non-spherical particles. Both experimental measurements and numerical calculations of polarization and brightness phase functions are invaluable tools for the study and identification of particles with complex shapes.

Different techniques of measurements are available in order to obtain such polarization and brightness phase functions. In particular, measurements can be conducted at ground with particles levitated by an air flow [1] or an air draught [2]. But, it is difficult and almost impossible to levitate in random manner weighty particles with mean diameter greater than few tens of microns. Then, for the larger particles, we conduct measurements in microgravity, in order to produce clouds of randomly oriented particles [3]. These measurements are necessary in order to validate numerical models [4].

Light scattering theories and main numerical methods are reviewed and compared in [5–8]. The Direct Simulation Monte Carlo (DSMC) method [9] is originally developed for rarefied gas flow in engineering and space science and widely used later for modelling of condensed gas flows and neutron scattering in a reactor.

The geometric optics ray tracing technique has been used to study the scattering properties of variously shaped micro-crystals with large size parameters [10–13].

The combination of DSMC with ray tracing [14] has now become a flexible and powerful tool for the simulation of light scattering by particles much larger than the wavelength. The main advantages of this approach are its relative simplicity, flexibility and great capabilities to effectively simulate scattering and polarization by particles with complex shapes and optical properties. Moreover, this class of models is of a growing interest due to increasing computer power. It has been applied for the study of spherical particles [15], particles whose shapes are approximated by a number of polygonal facets [16,17], particles with inclusions [18], etc.

In this paper, we present a DSMC model for three-dimensional single scattering of natural light by suspended randomly oriented, optically homogeneous and isotropic, rounded and stochastically rough cubic particles and the results of the experimental study (Section 2) of crystals of NaCl (Fig. 1).

As can be seen in Fig. 1a, only a small fraction of the NaCl particles have shapes close to a perfect cube. Some particles are rounded to different degrees. Another fraction of the particles possess near spherical shapes. The individual particle size and roughness degree are also variable. The cubic particles are the smallest and smoothest.

Description of the model and the computational procedure for single light scattering by a class of stochastically rough and randomly oriented rounded cubes is given in Section 3. Both absorbing and

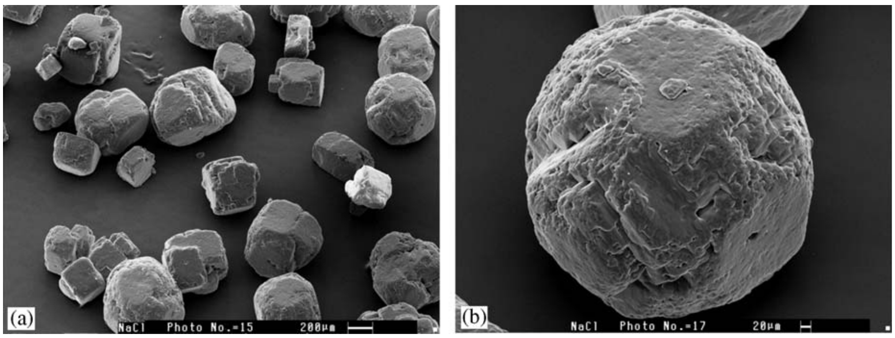

Fig. 1. Scanning electron micrograph (SEM) images of NaCl crystals. (a) Ensemble of crystals; (b) magnified image of single, close to spherical crystal.