Monte Carlo simulations of multiple light scattering by large non-spherical particles

M. Mikrenska* and P. Koulev

Institute of Mechanics, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria.

We apply Monte Carlo ray tracing in order to simulate multiple light scattering by ensembles of randomly oriented non-spherical particles with large size parameter. The numerical results obtained show a common tendency for different particle shapes: the degree of polarization decreases when the mean free path decreases.

INTRODUCTION

The single-scattering approximation is the commonly used approach to particle characterization and identification [1-3]. The study of the individual polarization properties at light scattering shows strong dependence of the polarization properties on the shape, size, and refractive index of the scatterers [4-7]. However, multiple scattering is an inherent effect [8] for many natural objects (e.g., atmospheric aerosols and clouds). This effect persists in laboratory measurements as well. Therefore, one should account for multiple-scattering events. Multiple scattering in participating media is generally a complex phenomenon. Theoretical aspects of the general problem of multiple light scattering are presented in [9,10]. Numerical calculations of multiple scattering by spherical particles were reported in [11,12]. The present work is aimed at studying how the multiple scattering affects the polarization properties of an ensemble of particles with non-spherical shape.

In this paper, we extend our previously developed three-dimensional computational model for single light scattering [4-6] to examine the effect of multiple scattering by an ensemble of particles with cubic and rounded cubic shape and sizes larger than the wavelength on the intensity and polarization phase functions.

COMPUTATIONAL MODEL

We consider light scattering of an ensemble of particles randomly and sparsely distributed throughout a finite scattering volume V. The light source is a non–polarized laser. The scattering particles are supposed to be dielectric, homogeneous, transparent or weakly absorbing. They are also assumed to be cubes or rounded cubes with sizes much larger than the wavelength which allows the laws of geometric optics to be applied. The rounded cube is defined as a section of cube and sphere. The roundness parameter is characterized by the degree of roundness defined as:

* Corresponding author: Maya Mikrenska (mikr@imbm.bas.bg)

$$k = \frac{a}{d}, \qquad (1)$$

where a is the cube side and d is the diameter of the sphere.

The algorithm for multiple scattering is based on the tracing of paths for a large number of rays in correspondence with geometric-optics laws. Ray tracing is done in three-dimensional geometry. For each ray-particle interaction, we apply a Monte-Carlo algorithm for single scattering by cube [4] or rounded cube [5,6]. At each optical interface, Snel's law determines the possible propagation direction and the changes of light intensities parallel and orthogonal to the scattering plane are calculated by means of Fresnel's formulas. The coefficients in Fresnel's formulas are used as probabilities for the choice of the outcome of the ray – optical interface interaction: reflection or transmission (refraction).

The free path *fp* of the ray at multiple scattering is determined by means of the mean free path *mfp* as follows:

$$fp = -\log(1-rand)*mfp, \qquad (2)$$

where *rand* is a random number, uniformly distributed in [0,1].

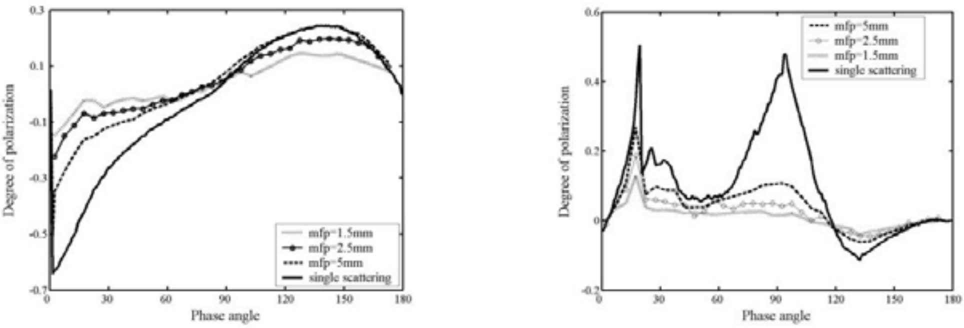
When the traced ray leaves the scattering volume V, it is referred to the corresponding phase angle. The contribution of each traced ray is accumulated in angular bins and the final result for the degree of polarization is obtained.

It should be pointed out that the Monte-Carlo computational procedure described is capable of accounting for arbitrary shape, size, and refractive index distribution of the scatterers. The present approach is quite similar to the one developed in [13]. Both algorithms keep track of the phase jumps so that the elliptic polarization is taken into account. However, the averaging over all orientations is different: the cluster in [13] is previously generated, while in the present Monte-Carlo algorithm each ray hits particle with arbitrary orientation. Besides, we do not use facets to approximate rounded parts of the scatterers which might reduce the required computer time and/or memory.

NUMERICAL RESULTS AND DISCUSSION

The computational model is applied to examine multiple light scattering by different ensembles of randomly oriented particles. At first, computer simulations of multiple light scattering by different ensembles of randomly distributed perfect cubes and rounded cubes (roundness parameter $k = 1.11$) are performed and the effect of the mean free path (i.e., volume fraction of particles) on the intensity and polarization phase function is examined. In all computer simulations the refractive index of the particles is taken to be $n = 1.54$ which corresponds to crystals of NaCl at the wavelength of 0.63 μm. The refractive index of the surrounding media is $n = 1$. The scattering particles occupy a spherical region V with diameter $D = 1$ cm. The number of the traced rays in all numerical experiments is 10^7.

Figure 1a shows calculated values of the polarization phase function for different mean free paths of the rays traced. For comparison, the polarization phase function which corresponds to single scattering by randomly oriented cube is also presented in Fig. 1a. The performed computer simulations show that the specific features of the polarization phase function at single light scattering by cube retain at multiple scattering by ensembles of cubes. The strong negative peak of polarization at backscattering and positive maximum in forward direction typical for single light scattering by cubes retain at multiple scattering by cubes. When the mean free path decreases (i.e. the volume fraction of the scatterers increases), the absolute values of the degree of polarization significantly decrease. The results obtained are quite similar to those reported for clusters of cubes [13].



(a) **(b)**

Figure 1. Polarization phase functions for different mean free paths. The scattering particles are cubes **(a)** or rounded cubes with roundness parameter $k = 1.11$ **(b)**. The scatterers with refractive index $n = 1.54$ are randomly distributed within a sphere with diameter of 1 cm.

Similar to the observed tendency for ensembles of perfect cubes, multiple scattering by rounded cubes (Fig. 1b) does not affect the qualitative behavior of the polarization curves, especially, when the mean free paths are relatively large. A decrease in the mean free path also leads to a significant decrease in the absolute values of the degree of polarization. It should be noted that the observed tendency is confirmed by the numerical experiments performed for different degree of roundness.

The second series of numerical experiments is aimed at studying the effect of multiple scattering by randomly distributed cubes on the intensity and polarization phase function. The calculated values of the polarization phase functions of randomly oriented cubic particles for different finite volumes are presented in Fig. 2. The side of the cubes is 20 μm. The volume fraction (packing density) of the particles is $p = 0.1$. For comparison, polarization phase function for semi-infinite medium [13] is also presented.

In conclusion, the results of computer simulations indicate a common tendency for different shapes of the scatterers: For relatively large mean free paths, the main features of the polarization curve retain at multiple scattering but the degree of polarization decreases considerably and tends to zero with a decrease of the mean free path. The computational model is capable of contributing to a more realistic treatment of the observed or laboratory-measured polarization data. Moreover, it allows consideration of mixture of different shapes and optical properties of the scattering particles.

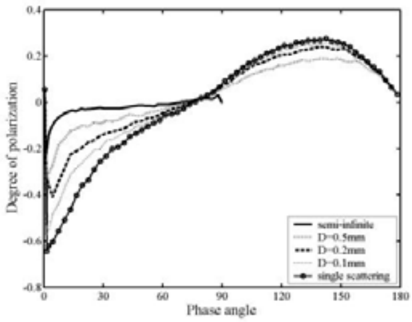


Figure 2. Polarization phase functions for different finite volumes (spheres with diameter *D*) and semi-infinite medium. The scattering particles are cubes with refractive index *n* = 1.5.

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