A STUDY OF LIGHT SCATTERING BY WAVELENGTH-SIZED PARTICLES COVERED BY MUCH SMALLER GRAINS USING THE SUPERPOSITION T-MATRIX METHOD

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ABSTRACT. By using the results of a direct, numerically exact solution of the Maxwell equations we analyze the behavior of the light scattering characteristics for polydisperse spherical particles covered with a large number of smaller grains. We show that the effect of the presence of microscopic dust on the surfaces of wavelength-sized particles depends on the particle absorption and the relative size of irregularities. In our computations, a new parallel superposition T-matrix code developed for use on parallel computer clusters is applied.

1. Introduction

It is well known that many natural and artificial particles exhibit both overall nonsphericity of shape and small-scale surface irregularities. The latter can manifest themselves in the form of microscopic grains dusting the surfaces of the larger host particles [1, 2]. The effects of overall nonsphericity of wavelength-sized particles on the optical cross sections and the elements of the Stokes scattering matrix have been studied extensively and have been demonstrated to be quite significant (e.g., [3] and references therein). At the same time, the effects of microscopic surface irregularities are much less investigated. By using the geometric optics technique there have been attempts to analyze the effects of surface imperfections on light-scattering characteristics of particles with sizes substantially greater than the incident wavelength [4, 5]. In our work [6], the numerically exact superposition T-matrix method was used to compute the scattering cross sections and the Stokes scattering matrix for polydisperse weakly absorbing spherical particles covered with a large number of much smaller weakly absorbing grains. We have shown the optical effect of the presence of microscopic dust on the surfaces of wavelength-sized, weakly absorbing particles to be much less significant than that of a major overall asphericity of the particle shape. In this work, we study the effect of particle absorption and size parameter scale of irregularities on light scattering properties of such particles. Furthermore, on the basis of numerous computations, our objective is to test a new parallel Fortran-90 code developed for use on parallel computer clusters, described in [7] and publicly available on-line [8].
2. Methodology and Computational Results

In order to analyze the possible optical effects of the presence of microscopic grains covering the surface of the wavelength-sized particles, similarly to [6] we adopt a scattering model in the form of a sphere with the size parameter $X_1$ dusted by $N_g = 49$ much smaller grains with the size parameter $X_2$. Employing a random-number generator, we generate such scattering target composed of $N$ particles ($N = 1 + N_g$) where the small non-overlapping grains are placed on the surface of the larger host particle. The angular distribution and polarization state of the light scattered by a particle group in random orientation in the far-field zone is fully described by the so-called normalized Stokes scattering matrix

$$F(\theta) = \begin{pmatrix} a_1(\theta) & b_1(\theta) & 0 & 0 \\ b_1(\theta) & a_2(\theta) & 0 & 0 \\ 0 & 0 & a_3(\theta) & b_2(\theta) \\ 0 & 0 & -b_2(\theta) & a_4(\theta) \end{pmatrix},$$

where $\theta$ is the scattering angle, and the Stokes parameters are defined with respect to the scattering plane. The zeros denote scattering matrix elements negligibly small (in the absolute sense) relative to the other elements at the same scattering angle. The $(1,1)$ element $a_1(\theta)$ is the phase function normalized according to

$$\frac{1}{2} \int_0^\pi \sin \theta a_1(\theta) d\theta = 1$$

To compute the light scattering characteristics expressed in terms of the elements of the scattering matrix, we use the efficient superposition $T$-matrix method developed for multi-sphere groups [7, 8, 9]. To eliminate oscillations typical for monodisperse particles, the scattering characteristics are averaged over a standard power-law distribution [3] with an effective size parameter $X_{1,eff} = 10$, effective variance $\nu_{eff} = 0.05$, and host size parameters in the range $X_1 \in [6.61; 14.39]$. The numerical integration over sizes is based on a Gaussian integration formula with 100 quadrature points. Recall that in [6] the refractive index of the host particle and small grains was adopted to be $m = m_R + im_I = 1.55 + i0.0003$, and the ratio of their size parameters $X_{1,eff}/X_{2,eff}$ was constant and equal to 10. In this work, we consider such two cases:

i) in order to analyze the effect of particle absorption, we perform computations of the scattering characteristics for $m_R = 1.55, m_I = 0.3$ and $X_{1,eff}/X_{2,eff} = 10$;

ii) to investigate the influence of the size of microscopic irregularities on the surface of the host particle, the refractive index is adopted to be the same as in [6] ($m = 1.55 + i0.0003$) but the ratio of the size parameters $X_{1,eff}/X_{2,eff} = 5$.

Some of the results of our computations are given in Table 1. For comparison, we also present the data for uncontaminated polydisperse host (i.e. when the number of grains $N_g = 0$) computed from the Lorenz Mie theory as well as the numerical data obtained early in [6]. The values of the extinction, $C_{ext}$, and scattering, $C_{sca}$, cross sections correspond to a wavelength of 0.628 $\mu$m. It is seen that the increasing size parameter scale of irregularities influences the values of $C_{ext}, C_{sca}$, single scattering albedo $\omega$, and asymmetry parameter $g$. At the same time the presence of strong absorption does not result in appreciable effect of irregularities on the values of $C_{ext}, C_{sca}, g$ and $\omega$. 

In Table 1 we depict the results of computations of all non-zero elements of the Stokes scattering matrix both for "uncontaminated" and contaminated hosts with \( m_I = 0.0003, 0.3 \), and \( X_{1,\text{eff}}/X_{2,\text{eff}} = 5 \) and 10. Let us discuss these data briefly. It is seen that the optical effects of surface contamination become stronger with increasing the value of particle absorption and the size parameter scale of irregularities, and the effect of the size of irregularities is larger as compared with absorption which is least pronounced for the phase function \( a_1(\theta) \). It is interesting to note that increasing the relative size of irregularities results in virtually neutral behavior of linear polarization \(-b_1(\theta)/a_1(\theta)\) in the range \( \theta < 150 \). The most noticeable indicator of nonsphericity is the deviation of \( a_2(\theta)/a_1(\theta) \) from...
100%, which increases with increasing the size of grains and decreases with increasing absorption; this is also characteristic, e.g., of randomly oriented spheroids.

We must note that all our computations have been performed using a new Fortran-90 superposition $T$-matrix parallel code developed for use on parallel computer clusters. A detailed description of this code is given in [7, 8]. We have used a computer cluster consisted of eight nodes with the total number of cores in the cluster = 64 (2.5GHz) and the total amount of RAM = 64 GB. Here because of the space shortage, we can only note that if a parallel cluster is characterized by $N_1$ number of nodes and $N_2$ number of cores in each node, then the computing time decreases proportionally to $N = N_1N_2$, and the available storage increases proportionally to $N$. In conclusion, we can state that our numerous computations show both high accuracy and high efficiency of applying this code.

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References
