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# Light scattering by particles with small-scale surface roughness: Comparison of four classes of model geometries

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## ABSTRACT

We compare four different model geometries for particles with small-scale surface roughness. The geometries are based on regular and stochastic surface perturbations, as well as on 2D- and 3D-roughness models. We further compare T-matrix and discrete dipole computations. Particle size parameters of 5 and 50 are considered, as well as refractive indices of $1.6+0.0005i$ and $3+0.1i$. The effect of small-scale surface roughness on the intensity and polarisation of the scattered light strongly depends on the size parameter and refractive index. In general, 2D surface roughness models predict stronger effects than 3D models. Stochastic surface roughness models tend to predict the strongest depolarising effects, while regular surface roughness models can have a stronger effect on the angular distribution of the scattered intensity. Computations with the discrete dipole approximation only cover a limited range of size parameters. T-matrix computations allow us to significantly extend that range, but at the price of restricting the model particles to symmetric surface perturbations with small amplitudes.

## 1. Introduction

Small-scale surface roughness is a morphological feature that is found in many different types of particles in nature, such as mineral aerosol particles in planetary atmospheres, cosmic dust particles, regolith particles on the surface of terrestrial planets and asteroids, and ice-cloud particles rimed with supercooled water droplets. The impact of small-scale surface roughness on the scattered intensity and polarisation can, in some cases, even dominate over the effect of the particles' overall non-spherical shape. This is particularly the case for particles with high absorption cross-sections [1,2] and for particles composed of optically hard material [2].

Computing the optical properties of such particles is among the most challenging problems in electromagnetic scattering research. The roughness features are often smaller than the wavelength of light, so that the light scattering problem cannot be solved by use of the geometric optics approximation. On the other hand, the size parameter $x=2\pi r/\lambda$ of the particles is often large compared to unity. (Here, $r$ denotes the volume-equivalent radius of the particle, and $\lambda$ is the wavelength of light.) For particles with large $x$, numerically exact solutions of Maxwell's equations are often plagued by ill-conditioning problems or high CPU-time requirements. Owing to these numerical limitations, very little is known about the significance of small-scale surface roughness for the optical properties of particles of different size parameters, morphologies, and chemical compositions. Studies for

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particles with large size parameters are particularly rare. A ray optics approximation (ROA) modified with partial Lambertian reflection/refraction has been used by [3,4], and another ROA model incorporated a radiative transfer approach [5], to study the impact of small-scale surface roughness for dust particles much larger than the wavelength. The former model was rather phenomenological and the latter assumed roughness elements to be independent scatterers, so neither model can be expected to provide fully accurate and reliable predictions for the impact of roughness.

Most theoretical studies have been limited to high-order, spherical 2D-Chebyshev particles [1,6,2]. More advanced model geometries involve spheroidal 2D-Chebyshev particles [1], spherical 3D-Chebyshev particles [7], Gaussian random particles [8,9], and spheres covered by smaller spherical particles [10]. Investigations of 2D-Chebyshev particles revealed that the phase function initially changes and eventually converges as the order of the perturbing Chebyshev polynomial is increased. This indicates that the optical properties of particles are sensitive to the presence and the amplitude of a surface perturbation with a sub-wavelength scale, but they do not seem to depend on the detailed structure of that perturbation. This raises the question if it makes much of a difference how one chooses the representation of small-scale surface roughness in a model. For instance, does it matter if we employ particles with a 2D- or a 3D-surface roughness? Does it make a difference if our model particles have a regular or a stochastic roughness structure?

Due to numerical constraints, almost all studies of particles with small-scale surface roughness have either been limited to size parameters of $x \lesssim 15$ or have been based on non-physical parameterisations or independent multiple scattering treatments that leave out part of the physics involved. Recent work reported in [7] was based on numerically exact T-matrix calculations for 3D-Chebyshev particles with size parameters up to $x=70$. This substantial increase in the range of size parameters has been achieved by a numerical approach that makes combined use of group theoretical methods [11,12] and a perturbation formulation [13] of the null-field method. The perturbation approach reduces numerical ill-conditioning problems, but it is limited to surface perturbations with small amplitudes. The group theoretical approach reduces CPU-time by 4–6 orders of magnitude, depending on particle size and on the order of the perturbing polynomial. However, it is limited to particles with symmetric surface perturbations and base geometries. Despite these limitations, the method offers the potential for investigating the effects of small-scale surface roughness for a significantly extended range of size parameters by use of numerical methods based on rigorous electromagnetic scattering theory.

The studies in [1,6,2,7,10] were based on T-matrix computations with the null-field method, while [8,9] made use of the discrete dipole approximation (DDA). Exploiting geometric symmetries and formulating a perturbation approach for small-scale surface roughness is relatively straightforward in the null-field method and in other T-matrix methods. Also, optical properties of randomly oriented particles can be computed analytically with higher accuracy and efficiency [14,15]. However, the null-field method is, in general, limited to star-shaped particles that do not deviate too strongly from spherical shape, and it is mostly applied to homogeneous particles. The DDA, on the other hand, is a highly flexible method that has no such limitations. However, the DDA is a computationally demanding method that does not lend itself easily to exploiting geometric symmetries, and it requires time-consuming numerical orientation-averaging. Thus, either method offers specific advantages for computing light scattering by particles with small-scale surface roughness.

This short review of recent work on particles with small-scale surface roughness leaves several questions unanswered, of which we will address the following ones in the present study:

- What are the differences and similarities of particles with a 2D- and 3D-surface roughness, and of particles with regular and stochastic surface perturbations? In which optical properties do the differences (if any) manifest themselves, and how does the comparison of different surface-roughness models depend on the size parameter and the refractive index of the particles?
- What are the strengths and limitations of the null-field method and the discrete dipole approximation in applications to particles with small-scale surface roughness? What are the main sources of error in either method, and what is the range of size parameters that can be covered for particles with irregular, small-scale surface roughness?

To keep this work computationally manageable, we will limit our study to mineral particles. The details on the selection of our case studies, model geometries, and numerical methods are given in Section 2. Computational results are presented in Section 3 and discussed in Section 4. Concluding remarks are given in Section 5.

## 2. Methods

The aim of this study is two fold. First, we want to investigate the suitability of both the T-matrix approach and the discrete dipole approximation (DDA) for particles with small-scale surface roughness. Second, we want to compare the optical properties computed with different model geometries for small-scale surface roughness with varying degree of sophistication and computational complexity.

### 2.1. Computational methods

We compute the T-matrix by the use of Waterman's null-field method [16], also known as the extended boundary condition method. The advantages of this method are that the computation of orientation-averaged optical properties can be performed analytically [14,15], and that particle symmetries can be systematically exploited [12,17]. A disadvantage is that the method can become numerically ill-conditioned for particles that deviate strongly from