The effective equivalence of geometric irregularity and surface roughness in determining particle single-scattering properties

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Abstract: This study investigates the effects of geometric irregularity and surface roughness on the single-scattering properties of randomly oriented dielectric particles. Starting from a regular crystal with smooth faces, effects of roughening are compared with effects of perturbing the regular configuration of the smooth faces. Using the same slope distribution for small roughness facets and tilted faces provides a natural way to compare the effects on the single-scattering properties. It is found that the geometric irregularity and surface roughness have similar effects on the single-scattering properties of an ensemble of randomly oriented particles. In other words, particles with irregular geometries and those with surface roughness are optically equivalent if the slope distributions are the same. Furthermore, an ensemble of particles with irregular geometries can be used as an effective approximation for simulation of the scattering properties of roughened particles, and *vice versa*. This approach also provides new interpretation of the observed, relatively featureless and smooth, scattering phase functions of naturally occurring particles.

OCIS codes: (010.1290) Atmospheric optics; (290.0290) Scattering.

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1. Introduction

Atmospheric particles (e.g., water droplets, ice crystals, and aerosol particles) influence the Earth’s radiation budget and climate by scattering and absorbing both solar radiation and thermal emission. Because of the great variation of particle microphysical properties (e.g., size, shape and composition) and lack of quantitative observations of these properties, there are significant difficulties in the numerical representation of atmospheric particles and their scattering properties. This is especially true for non-spherical particles. Laboratory and in situ observations indicate that a large fraction of ice crystals and aerosol particles occurs with irregular geometry or some degree of surface roughness [1, 2], and that the particles show relatively featureless and smooth scattering phase functions [3–5]. For this reason smooth phase matrix elements are extensively used in radiative transfer and remote sensing applications, and show considerable success in representing the radiative effects of the atmospheric particles [6].

Various numerical models have been used to study the effects of surface roughness on the light scattering properties, which are based on idealized or realistic surface structures, as well as imaginary ones [7–12]. Whatever the models assume, the primary finding has been that one of the most significant influences of surface roughness on light scattering is to smooth out the peaks of the scattering phase function, for example, the substantial weakening or complete removal of the sharp peaks corresponding to the 22° and 46° halos produced by pristine hexagonal ice crystals within cirrus clouds. However, the scale of rough structures needed to remove the phase function peaks has typically been much larger than the scale observed on real ice crystals [5, 11]. This suggests that, in addition to surface roughness, there may be other mechanisms that cause the featureless scattering phase functions.

Due to complicated meteorological environment in which the particles are formed, as well as collision and coalescence processes, naturally occurring ice crystals often show irregular geometries, as has been widely reported in various in situ and laboratory measurements [13–15]. These irregular structures can be responsible for smoothing out the phase function peaks at certain scattering angles. Furthermore, because scattering peaks occurring at different scattering angles are related to particular particle geometries, averaging over an ensemble of particles with irregular geometry can lead to featureless ensemble-averaged phase function.

Thus, both surface roughness and irregular geometry observed for ice crystals and aerosol particles have similar influences on the scattering properties. It is therefore of theoretical interest and practical value to compare their effects on light scattering by atmospheric particles, and to find what relationships there may be between the two factors. The approach taken in this study is to start with a basic crystal shape that is a regular solid hexagon with smooth faces, and alter it in two ways. The first way is to roughen each face in a manner reminiscent of the tilted-facet method [7, 16] but producing a definite particle, as in the study by Liu et al. [11]. This results in a separation of scales between the face scale and the roughness scale. The second way is to alter the basic particle by tilting each entire face, with independently chosen tilts for each face. In this case the result is a particle with "irregular geometry," but there is no "small scale" roughness. More details are provided in the next section. One might consider the two approaches as extremes on a continuum in which the roughness scale increases from being much smaller than the facial scale to being the same as the facial scale, but this study will not pursue this point. In this study the basic shape is taken to be a regular hexagon with unit aspect ratio; the choice of a hexagon has a natural motivation in considering ice particles. Other aspect ratios and geometries could certainly be considered as basic, but the basic conclusions of this study should not be significantly affected.

The remainder of this paper is organized as follows. The models to generate roughened and irregular particles are described in Section 2. Section 3 presents results to show the optical equivalence of particle irregularity and surface roughness as far as their single-scattering properties are concerned. The conclusions of this study are given in Section 4.

2. Roughness and geometric irregularity

The tilted-facet (TF) algorithm based on the geometric-optics method is one of the most efficient and widely used models for simulating the effects of surface roughness on light scattering. Ray by ray, it accounts for each reflection-refraction event by calculating the result of encountering an imaginary facet randomly tilted about the local normal with a slope chosen from an assumed probability distribution [7, 10, 16]. The particle surface itself is unchanged, and different rays encountering the same point on the surface are treated using different slopes. There is no single "roughened particle" that all rays meet. The normal distribution has been the most widely used, but the more general Weibull distribution has also been used [17]. Liu et al. [11] developed a generalized random wave superposition model to study light scattering by roughened particles over the entire size range, and in this method explicit rough structures are generated. They showed that when the structures are used in a numerical model, with the discretization implicitly creating small local facets, the slopes of facet elements actually follow the normal distribution:

$$P(s_x, s_y) = \frac{1}{\pi\sigma^2}\exp\left[-\frac{s_x^{\,2} + s_y^2}{\sigma^2}\right], \tag{1}$$

where, in terms of a facet-based coordinate system with spherical angle coordinates θ and φ (See Fig. 1), the slopes s_x and s_y along the x- and y-directions are given by:

$$s_x = |\tan\theta|\cos\varphi, \qquad s_y = |\tan\theta|\sin\varphi$$

and σ^2 is the variance. The central parameter characterizing surface roughness is σ^2. This model of surface roughness used by Liu et al. [11] is the same one that is used in the current study. Figure 2(b) shows an example of the roughened hexagonal column with σ^2 = 0.4. The

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parameter σ^2 is also central in characterizing geometric irregularity, as explained next, giving a quantitative way of comparing the two forms of particle geometry.

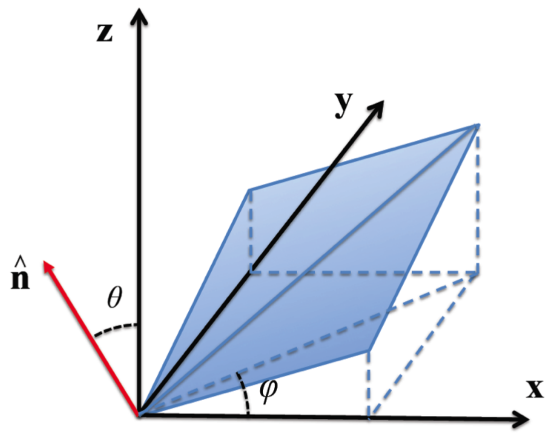

Fig. 1. Geometry of tilted surface element of a rough particle or titled face of an irregular smooth particle.

In previous studies of the effects of irregularity, a number of highly complicated irregular geometries, e.g. Poisson-Voronoi tessellation, agglomerate debris particles, Gaussian random field particles and fractal particles, have been used to model the light scattering properties of mineral dust or ice crystals [18–21]. We use a relatively simpler model, allowing only perturbations of facial orientations, leaving the faces themselves smooth. Adopting the idea used in the TF algorithm, we generate irregular particles by randomly tilting surfaces of regular ones, but in distinction from the TF algorithm, the tilts are features of the particle generated, and are fixed throughout the scattering simulation.

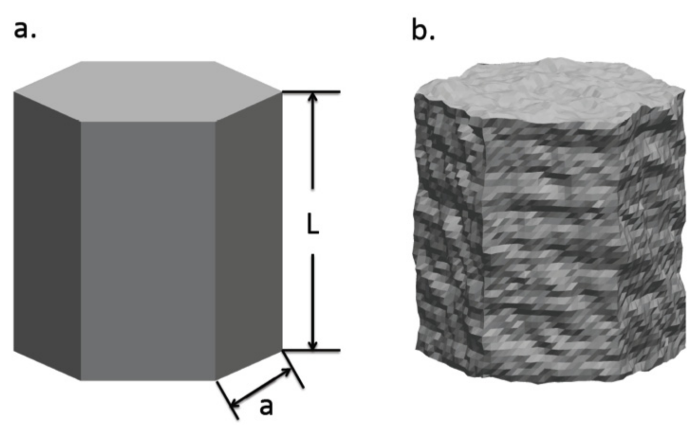

Fig. 2. Geometry of a smooth and roughened column with an aspect ratio of 1. The rough surface has $\sigma^2 = 0.4$.

As mentioned in the introduction, this study considers a hexagonal column with a unit aspect ratio (i.e. $L/2a = 1$ in Fig. 2(a)) as the prime regular geometry. The corresponding roughened particle with $\sigma^2 = 0.4$ is shown in Fig. 2(b). Each surface of the hexagonal column is randomly tilted following a given slope distribution, and, to have the same normal distribution as Eq. (1), θ and φ, the polar and azimuth angles to determine a tilted surface, can be chosen according to

$$\cos\theta = \frac{1}{\sqrt{1-\sigma^2 \ln \varepsilon_1}}, \tag{2}$$

$$\varphi = 2\pi\varepsilon_2, \tag{3}$$

where ε_1 and ε_2 are random numbers distributed uniformly between zero and one [16]. With the center position of a surface fixed and the tilted angles given by Eqs. (2) and (3), a new surface can be determined. The vertexes and edges of the new irregular particle can be obtained by calculating the intersecting points and lines of corresponding surfaces. We eliminate resultant particles that are significantly different from a hexagonal column, by using only those that are convex and have two hexagonal and six tetragonal surfaces. After the construction, the volume and surface area of the particle are generally changed, so the irregular particle is scaled to have the same effective diameter as that of the regular one. The effective diameter of the particle is defined to be $1.5 \times V/A$, where V is the particle volume and A is the particle's projected area, i.e. the average of areas of projection over all projection angles.

The size parameter of a hexagonal column is defined as $2\pi L/\lambda$, where L is the length of a column and λ is the incident wavelength: the size parameter of an irregular particle constructed from a hexagonal column is taken to be the same as that of the original column. Figure 3 illustrates some examples of randomly generated irregular hexagonal columns with different values of σ^2 (0.01, 0.1 and 0.4 from top to bottom). The figure illustrates the variability in actual shape that comes from sampling the corresponding slope distribution. Even with such a simple method of construction, the irregular particles show quite different geometries, and, as the value of σ^2 increases, the hexagonal columns become highly irregular.

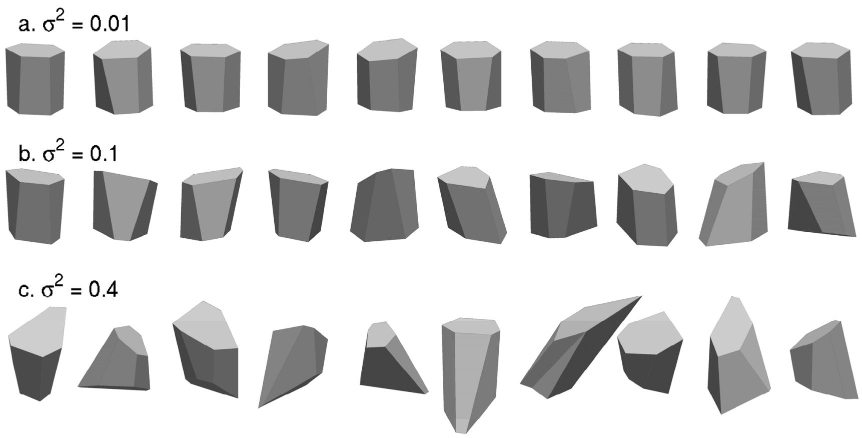

Fig. 3. Examples of randomly generated irregular hexagonal columns.

With geometries of irregular and roughened particles explicitly given, it is straightforward to calculate their light scattering properties. In this study both the pseudo-spectral time domain method (PSTD) [22–24] and the improved geometric-optics method (IGOM) [25, 26] are used. Due to the approximations involved in the ray-tracing technique, the IGOM is only appropriate for large particles, whereas the PSTD, directly solving Maxwell's equations in the time domain, is in principle applicable to light scattering by arbitrarily shaped and sized particles, with a feasibility limit imposed by current computer technology that size parameters be not much larger than 200 [23, 24].

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A refractive index of m = 1.31 (i.e. ice at visible wavelengths) is used for all simulations. All scattering properties calculated are those for randomly oriented particles, and we will mainly discuss two important elements of the scattering phase matrix: phase function P_{11} and the degree of linear polarization $-P_{12}/P_{11}$. The integral scattering properties will not be discussed, because the extinction efficiency for particles we considered are all close to 2, and no absorption is considered in this study.

3. Results

The scattering properties of irregular particles with different realizations can be quite different. Figure 4 shows some examples of P_{11} and $-P_{12}/P_{11}$ for irregular hexagonal columns with a size parameter of 100. Three values of σ^2, i.e. 0.1, 0.2 and 0.4, are used to generate irregular geometries, and results of 20 realizations are illustrated for each case by colored thin curves. Figure 4 clearly shows the variations of P_{11} and $-P_{12}/P_{11}$ for different particle realizations, which mostly occurs at scattering angles around 20° and backward directions. With an increase in σ^2, the variations of P_{11} are not significantly enhanced whereas P_{12}/P_{11} becomes more divergent. The black thick curves in the figure are averaged values of the 20 realizations, and can be understood as the mean scattering properties of an ensemble of randomly oriented irregular particles. All averaged values show smooth and featureless phase functions, which are similar to observed ones for dust particles and ice crystals [2, 4]. This indicates that an ensemble of particles with irregular geometries is a potential choice to model the light scattering properties by atmospheric particles.

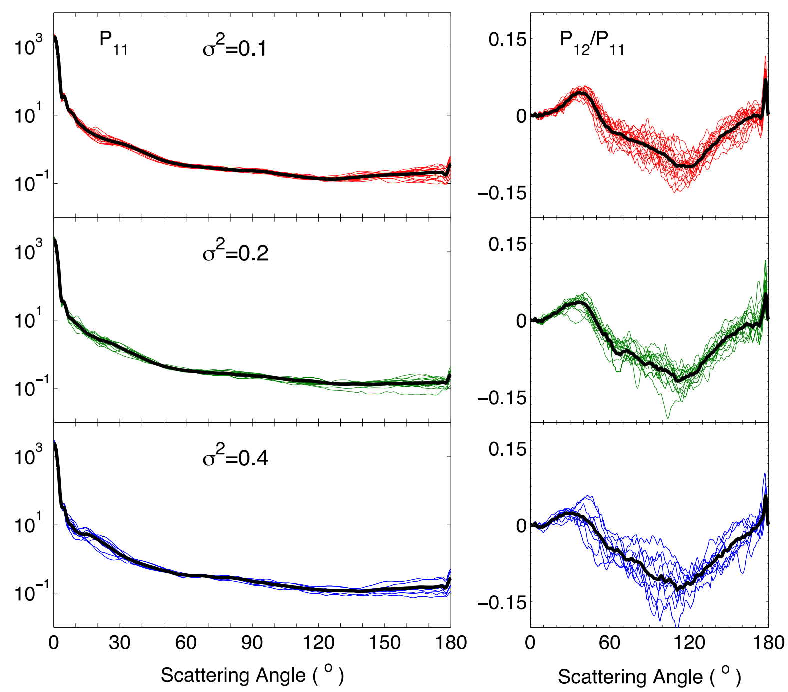

Fig. 4. P_{11} and P_{12}/P_{11} of irregular hexagonal columns with different degree of irregularity. The size parameter of the corresponding regular column is 100, and the PSTD is used for the simulation.

P_{11} and $-P_{12}/P_{11}$ of an ensemble of irregular particles (the averaged values from Fig. 4) and roughened ones are compared in Fig. 5, where results of the corresponding regular smooth particle are also shown. The size parameter of the hexagonal columns is kept the same at 100, and all simulations are performed using the PSTD. The effect of roughness realization is relatively minor, and only results of a single roughened particle are simulated. The weak peaks at 22° and 46° that are clearly shown by the regular smooth particles are smoothed out by both irregular geometry and surface roughness. With σ^2 being 0.1, the phase functions of the irregular and roughened particles agree closely, whereas $-P_{12}/P_{11}$ shows some differences. As particles become more irregular (σ^2 = 0.4), the scattering in the backward directions becomes weaker, and slight differences from that of roughened particles emerge. This indicates that the irregular geometry and surface roughness defined in this study have similar effects on the single-scattering properties of particles, in other words, the irregular geometry and surface roughness are optically equivalent.

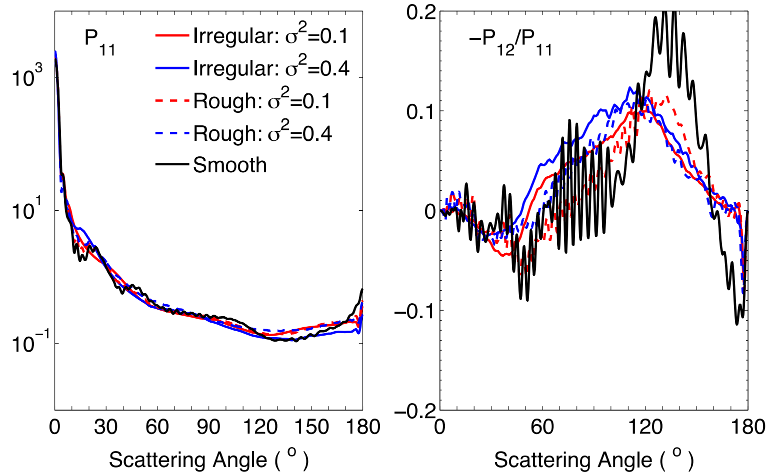

Fig. 5. Comparison of the P_{11} and P_{12}/P_{11} of irregular, roughened and smooth hexagonal columns with a size parameter of 100 simulated by the PSTD.

Figure 6 is the same as Fig. 5 but for hexagonal columns with a size parameter of 1000, and the IGOM is used for the simulations. As particle sizes become much larger, halos of the smooth particle become much stronger. P_{11} and $-P_{12}/P_{11}$ for irregular and roughened particles agree closely for both σ^2 values, and this further supports our claim of the optical equivalence of surface roughness and irregular geometry. The closer agreement is mainly because IGOM considers the scattering as reflections and refractions of "rays" on particle surfaces, and, with the same slope distribution for particle surfaces (i.e. surfaces from the ensemble of irregular particles or small facets on roughened ones), the scattering energy will be distributed in similar ways.

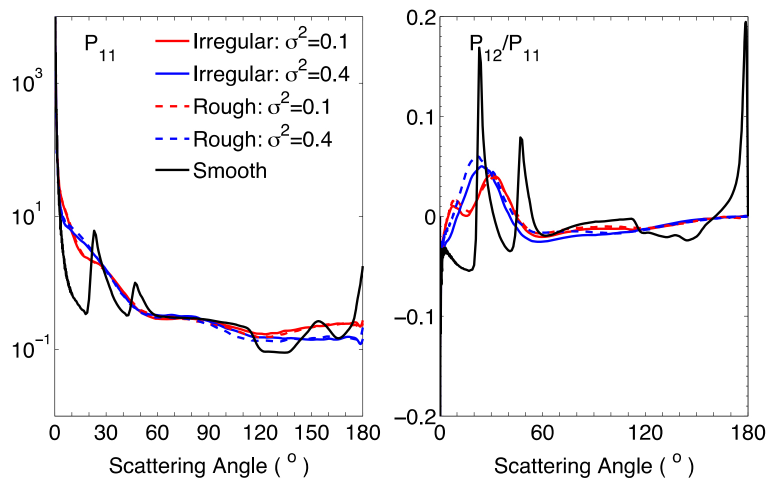

Fig. 6. Comparison of the P_{11} and P_{12}/P_{11} of irregular, roughened and smooth hexagonal columns with a size parameter of 1000 simulated by the IGOM.

4. Conclusions

We compare the single-scattering properties (mainly the angular-dependent scattering phase matrix elements P_{11} and P_{12}) of particles with roughened surface and irregular geometries. To perform a clean comparison, we choose a common slope distribution for small facets or surfaces for the roughened and irregular particles respectively, and generate particles that are geometrically comparable, in that they are specified by the same value of σ^2. Numerical results from both the PSTD and IGOM show that the roughening of the surface and irregularization of facial geometry have similar influences on the scattering phase matrices of a hexagonal column. In this sense, the two perturbation forms are optically equivalent. The implication is that an ensemble of particles with irregular geometries can be used as an alternative method to model light scattering by roughened particles, and *vice versa*. Furthermore, we call special attention to the fact that these conclusions are based on the particular forms of geometric perturbation and surface roughening used in this study, and further investigation will be need to determine the robustness of the conclusions.

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