Quantifying the impact of the surface roughness of ice crystals on the backscattering properties for lidar-based remote sensing applications

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Abstract

Impacts of small-scale surface irregularities, or surface roughness, of atmospheric ice crystals on lidar backscattering properties are quantified. Geometric ice crystal models with various degrees of surface roughness and state-of-the-science light-scattering computational capabilities are used to simulate single-scattering properties across the entire practical size parameter range. The simulated bulk lidar and depolarization ratios of polydisperse ice crystals at 532 nm are strongly sensitive to the degree of surface roughness. Comparisons of these quantities between the theoretical simulations and counterparts inferred from spaceborne lidar observations for cold cirrus clouds suggest a typical surface roughness range of 0.03–0.15, which is most consistent with direct measurements of scanning electron microscopic images. The degree of surface roughness needs to be accounted for to properly interpret lidar backscattering observations of ice clouds.

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Key Points:

- Sensitivities of the backscattering properties to the surface roughness of atmospheric ice crystals are theoretically investigated.
- The depolarization ratio is markedly sensitive to the degree of surface roughness of ice crystals.
- The lidar and depolarization ratios observed by CALIOP are well explained with the ice model with degree of surface roughness 0.03–0.15.

Abstract

Impacts of small-scale surface irregularities, or surface roughness, of atmospheric ice crystals on lidar backscattering properties are quantified. Geometric ice crystal models with various degrees of surface roughness and state-of-the-science light-scattering computational capabilities are used to simulate single-scattering properties across the entire practical size parameter range. The simulated bulk lidar and depolarization ratios of polydisperse ice crystals at 532 nm are strongly sensitive to the degree of surface roughness. Comparisons of these quantities between the theoretical simulations and counterparts inferred from spaceborne lidar observations for cold cirrus clouds suggest a typical surface roughness range of 0.03–0.15, which is most consistent with direct measurements of scanning electron microscopic images. The degree of surface roughness needs to be accounted for to properly interpret lidar backscattering observations of ice clouds.

Plain Language Summary

Lidar (Light Detection and Ranging) instruments on satellites use reflected, or backscattered, laser beams to investigate ice clouds in the atmosphere. However, it has long been a challenge to interpret lidar signals, called backscattering properties, to accurately infer ice cloud characteristics. This study uses theoretical simulations to investigate how small-scale surface irregularities of ice crystals affect the lidar signals reflected from ice clouds. These simulations demonstrate the significant impacts of the small-scale surface irregularities of ice crystals on backscattering. Comparisons between the theoretical simulations and satellite lidar observations confirm the necessity to assume a moderate degree of small-scale surface irregularities to explain lidar observations of typical ice clouds.

1 Introduction

Atmospheric ice crystals often exhibit small-scale surface irregularities or roughness (Cross, 1968; Magee et al., 2014), which are caused mainly by depositional growth and sublimation under super- and sub-saturated conditions. Roughening of ice crystal surfaces has been observed via laboratory experiments (Pfalzgraff et al., 2010; Schnaiter et al., 2016; Butterfield et al., 2017) and in-situ measurements in cirrus clouds (Ulanowski et al., 2014; Magee et al., 2021). Compared to pristine ice crystals with smooth surfaces, those with roughened surfaces tend to have featureless phase function near backscattering angles, which corresponds to smaller asymmetry factor values. It has been demonstrated that surface roughness is a critical factor affecting passive remote sensing of ice cloud properties (Yang et al., 2008; van Diedenhoven et al., 2013; Hioki et al., 2016) and estimation of ice cloud radiative effects (Yi et al., 2013; Järvinen et al., 2018).

Surface roughness effects on the shortwave scattering properties of ice crystals have been theoretically investigated based mainly on the principles of geometric optics (Macke et al., 1996; Yang & Liou, 1998), because rigorous light-scattering computational methods lead to an enormous computational burden for typical ice crystal sizes in the ultra-violet to near-infrared spectral regime. However, geometric optics methods compute inaccurate single-scattering properties of ice crystals near the backscattering angle due to inherent limitations, particularly a lack of consideration of coherent backscattering enhancement (CBE). The more sophisticated Physical Geometric Optics Method (PGOM), implemented by either the surface-integral or volume-integral approach, fully considers phase interference of outgoing waves (Yang & Liou, 1996, 1997), and produces consistent numerical results (Yang et al., 2019). PGOM has been numerically implemented for relatively simple ice particles (e.g., columns and plates) and aggregates of convex particles (e.g., 8-column aggregates; see Yang et al., 2019 and references cited therein).

The challenge in light-scattering computations for nonspherical particles, particularly in the case of large size parameters, has long hampered the accuracy of inferred ice cloud properties from lidar observations. Specifically, the physical interpretation of the backscattering properties of ice crystals, such as the lidar and depolarization ratios, is largely empirical (Zhou & Yang, 2015; Ding et al., 2016), leading to substantial uncertainties in inferred ice cloud quantities. As surface roughening in ice crystals is prevalent globally in ice clouds (van Diedenhoven et al., 2020), this study aims to quantify the impact of surface roughness based on a combination of state-of-the-science rigorous and approximate light-scattering computational algorithms applied to geometrically roughened ice crystal models.

2 Methods

2.1 Geometrically roughened ice crystal models

In this study, the degree of surface roughness is defined in terms of the variance (σ^2) of the two-dimensional Gaussian distribution $P\left(Z_x, Z_y\right)$ of local planar surface slopes (Liu et al., 2013; Saito & Yang, 2022a), which originates from a rough ocean surface model (Cox & Munk, 1954) and is described as

$$P\left(Z_x, Z_y\right) = \frac{1}{\pi\sigma^2} e^{-\left[\left(Z_x^2 + Z_y^2\right)/\sigma^2\right]}, \tag{1}$$

where $Z_x = \partial Z/\partial x$ and $Z_y = \partial Z/\partial y$ are the slopes of local planar facets along two axes orthogonal to the normal direction Z in reference to an un-tilted regular crystal facet described below. The original facets of a regular hexagonal column are discretized into many small triangular facets with a maximum facet length of approximately 1/40 of those original facets. These small facets are tilted according to the probability density of the surface slope defined by a 2D Gaussian distribution with the specified σ^2. Technical details on geometrically roughened ice crystal models are discussed in Liu et al. (2013). In this study, the macroscopic crystal shape is a regular hexagonal column with an aspect ratio of unity. Note that Okamoto et al. (2020) have investigated the backscattering properties of many other particle shapes without surface roughness.

Figure 1 illustrates geometrically roughened hexagonal column models with various degrees of surface roughness ranging from $\sigma^2 = 0$ (smooth) to 0.5 (severely roughened). A crystal surface with a higher degree of surface roughness has more complex texture. Neshyba et al. (2013) developed a stereographic method to estimate the surface roughness using scanning electron microscopic (SEM) images of an ice crystal, and found that surface roughness is well represented by a Weibull distribution with a shape parameter 0.7–0.95 (Butterfield et al., 2017). The Weibull distribution with a shape parameter of unity is equivalent to the 2D Gaussian distribution.

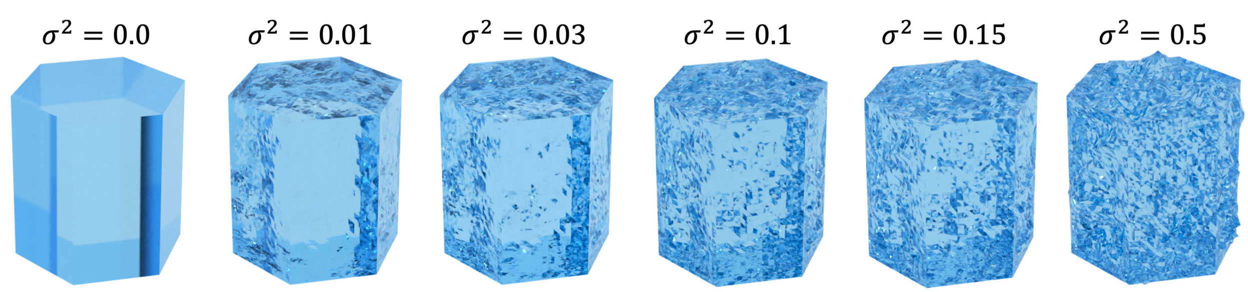

Figure 1. Illustration of geometric hexagonal column ice crystal models with degree of surface roughness 0, 0.01, 0.03, 0.1, 0.15, and 0.5.

2.2 Computational methods

To simulate the single-scattering properties of roughened ice crystals, we use the numerically accurate Invariant-Imbedding T-matrix Method (IITM; Johnson, 1988; Bi & Yang, 2014; and references cited therein), for the largest possible size parameter cases. As the computational burden increases exponentially with the size parameter, previous studies limited simulations of geometrically roughened ice crystals to size parameter kD up to ~150, where the modified wavenumber is $k = 2\pi/\lambda$, D is the particle maximum dimension, and λ is the wavelength. Leveraging the computational capabilities provided by the Texas A&M University High-Performance Research Computing (TAMU HPRC) facilities, we perform scattering property simulations with IITM for roughened ice crystals with kD up to approximately 316.

For larger size parameters, we use the Improved Geometric Optics Method (IGOM; Yang & Liou, 1996) which is a simplified form of PGOM. However, IGOM considers the ray spreading effect but the ray-tracing procedure neglects the phase interference among scattered waves associated fundamentally with different outgoing rays. This simplification results in inaccuracy in backscattering directions. Saito and Yang (2022b) derived a semi-physical CBE correction formula from Maxwell's equations to substantially reduce the systematic biases in the backscattering properties computed with IGOM. With a combination of IITM for small-to-moderate size parameters ($kD \leq 316$) and IGOM with a CBE correction (hereinafter referred to as IGOM+CBE) for large size parameters, the single-scattering property simulations for roughened ice crystals across the entire practical size parameter range are performed. For smooth particles, IITM with an efficient scheme utilizing axial symmetry is performed for $kD \leq 464$, and PGOM is performed for larger size parameters.

3 Results and Discussion

3.1 Phase matrix of roughened ice crystals

Figure 2 shows the six nonzero phase matrix elements of compact hexagonal ice crystals with various degrees of surface roughness at wavelength 532 nm, which are computed with IITM. Size parameter $kD = 316$ in these simulations corresponds to an ice crystal maximum diameter of 26.8 μm. Halo peaks appear at scattering angles of approximately 22° and 46° in the phase functions of smooth to moderately roughened ice crystals ($\sigma^2 < 0.1$) but are suppressed for more roughened ice crystals (Bi & Yang, 2014). The angular variations of the phase matrix at larger scattering angles seem sensitive to smaller degrees of surface roughness. For example, the phase matrices at scattering angles around halo peaks are similar between smooth and slightly roughened ($\sigma^2 = 0.01$) cases, while they are different at backward scattering angles (e.g., > 120°). Moreover, in Fig. 2a, the phase functions near the backscattering angle show distinct differences between smooth and all roughened ice crystals.

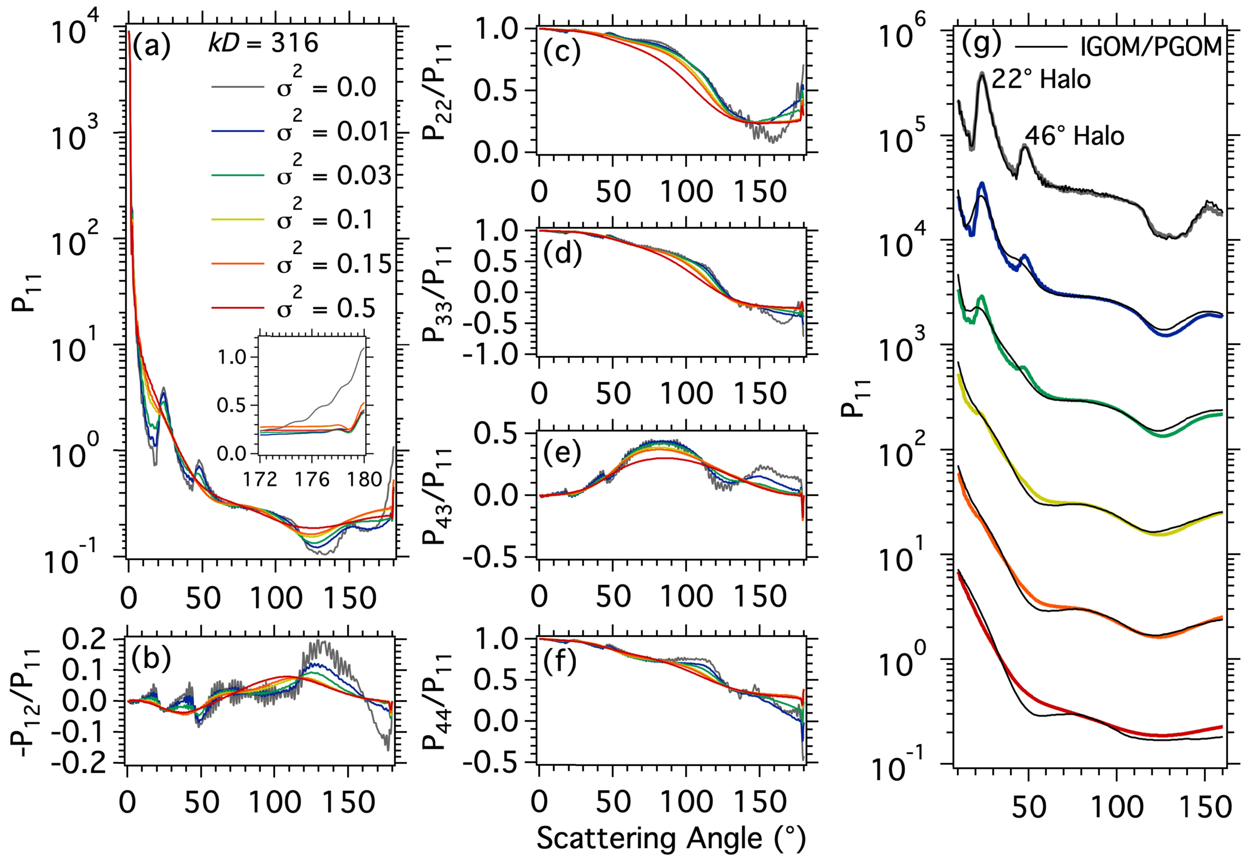

Figure 2. (a-f) Six independent phase matrix elements (labeled on y-axis) of ice crystals with various degrees of surface roughness denoted with different colors. (g) Phase function (P_{11}) curves computed with Invariant Imbedding T-matrix Method (bold lines with colors same as in panel (a)) and geometric optics methods (black lines) for the same six degrees of roughness, which are offset one order of magnitude apart.

In Fig. 2g, comparisons of the phase functions of smooth and roughened ice crystals are consistent between IITM and PGOM/IGOM across scattering angles for $\sigma^2 = 0.1$–0.5 and at backward scattering angles 90–160° for less roughened cases. Interestingly, the halo peaks computed with IITM show similar angular widths but weaker magnitudes of their peaks as roughness increases. In comparison, the counterparts computed with IGOM tend to be broadened and more rapidly suppressed when the degree of surface roughness increases, particularly for the 46° halo peak (van Diedenhoven, 2014).

van de Hulst (1957) states that a pencil of light with its basal width of the order $l\lambda$ can retain its ray characteristics over a distance of the order $l^2\lambda$ according to the Fresnel–Huygens principle, where l and λ are the geometric width of the ray and wavelength of light. Ding et al. (2020) further validate this statement using the vector Kirchhoff integral equation. A major difference in particle geometry between smooth and roughened ice crystals is the sizes of the individual planar facets of a particle. With L defined as the maximum length of a facet of an ice crystal, we obtain $L^2\lambda \gg kD$ for a smooth ice crystal with $L = 23.19$ μm but $L^2\lambda < kD$ for roughened ice crystals with $L = 0.58$ μm in the present case. From the geometric optics perspective, distinct halo peaks quantified with IITM imply that the refraction of electromagnetic waves is determined mainly by the macroscopic shape rather than the small facets of the ice crystal rough surface, when the surface roughness is not significant and has a scale comparable to λ. For better understanding of these halo peaks for a roughened ice crystal from the physical perspective, the Debye series expansion of the T-matrix (Bi et al., 2018; Bi & Gouesbet, 2022) may be a useful approach.

3.2 Lidar backscattering properties

The lidar ratio S and depolarization ratio δ are two fundamental backscattering properties for lidar-based remote sensing applications. For a single ice crystal, these ratios are defined as

$$S = \frac{4\pi}{\omega P_{11}(\pi)}, \quad (2)$$

$$\delta = \frac{P_{11}(\pi) - P_{22}(\pi)}{P_{11}(\pi) + P_{22}(\pi)}. \qquad (3)$$

Figures 3a–b plot the lidar and depolarization ratios associated with roughened ice crystals computed with IITM and IGOM+CBE and the counterparts associated with smooth ice crystals computed with IITM and PGOM. In Fig. 3a, the lidar ratios of roughened ice crystals substantially deviate from those of smooth ice crystals with size parameters $kD > 100$. In the range of kD up to 316 simulated with IITM (corresponding to D up to 26.8 μm at wavelength 532 nm), a decreasing lidar ratio with larger size parameters for smooth ice crystals originates presumably from the significant contribution of the second-order corner reflection (Borovoi et al., 2013). In Fig. 3b, the depolarization ratios exhibit pronounced sensitivities to the degree of surface roughness for size parameters $kD > 20$. The depolarization ratio levels off between 0.2 for smooth and 0.55 for severely roughened ice crystals with $kD \geq 100$.

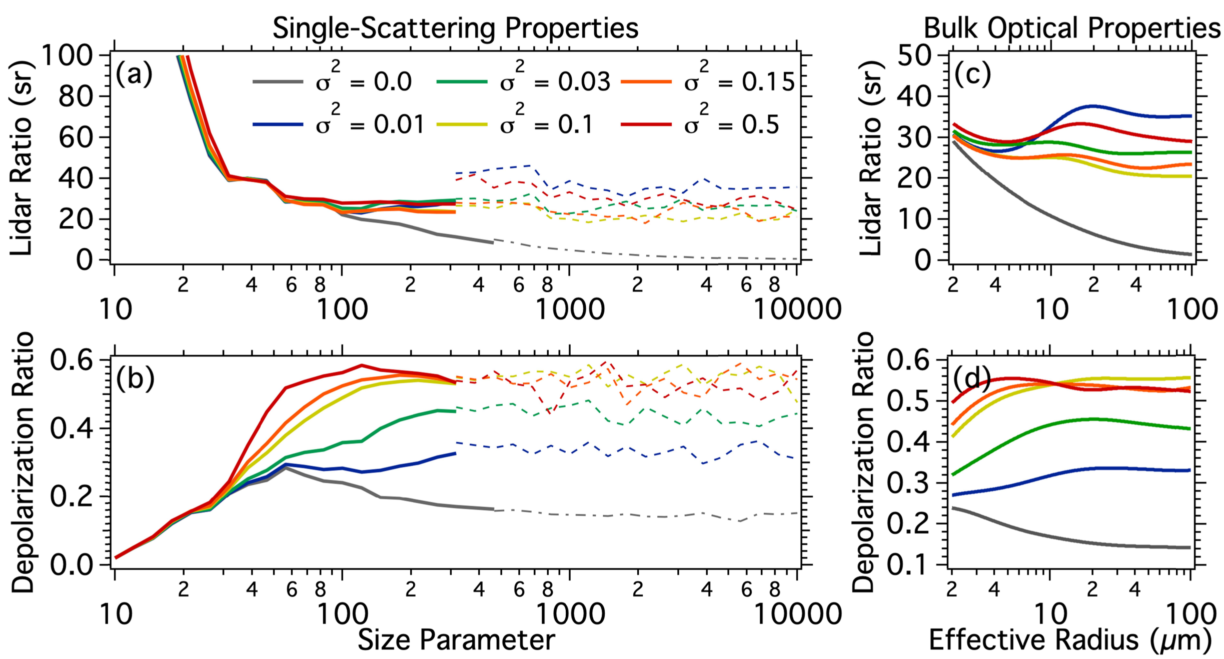

Figure 3. The single-scattering (a) lidar and (b) depolarization ratios (y-axis scales), for various degrees of surface roughness (colors stated in (a)) computed with (bold solid lines) rigorous and

(dashed lines) geometric optics methods, for size parameters 10 to 10000 (x-axis scales). (c-d) Bulk optical properties corresponding to (a-b), for effective radius 2 to 100 μm (x-axis scales).

The backscattering properties of roughened ice crystals computed with IGOM+CBE are consistent with IITM at the size parameter upper limit, except with lidar ratios (Fig. 3a) for $\sigma^2 = 0.01$ and 0.5 that may be associated with simplified assumptions in the CBE correction. Because of weak ice absorptivity at wavelength 532 nm, the backscattering properties tend to approach their respective asymptotic values for larger size parameters, as indicated by IGOM+CBE simulations. In Fig. 3b, moderate fluctuations in the IGOM+CBE backscattering properties originate from Monte Carlo noise associated with the ray-tracing process (Saito & Yang, 2022b).

Bulk optical properties of polydisperse ice crystals are obtained from a weighted average over the single-scattering properties of smooth and roughened ice crystals. The particle size distribution (PSD) is assumed to be a gamma distribution with an effective variance of 0.26 (Saito & Yang, 2022a) obtained from in-situ observations of ice cloud PSDs (Heymsfield et al., 2013). The bulk lidar and depolarization ratios of the polydisperse ice crystals are computed based on Eqs. (1–2) with replacing the single-scattering properties with the bulk ice crystal counterparts. Figures 3c–d show the bulk backscattering properties of smooth and roughened hexagonal column ice crystals for effective radii 2–100 μm. The backscattering properties of roughened ice crystals show a weak dependence on effective radius > 20 μm. In contrast, those of a smooth ice crystal consistently show a negative correlation with effective radius.

3.3 Comparison with spaceborne lidar observations

We compare the theoretical backscattering properties of smooth and roughened ice crystals with the counterparts estimated from the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) observations (Winker et al., 2009). We use the version 4.20 CALIOP level-2 cloud layer 5km product and select single-layer transparent cirrus clouds with a middle cloud temperature $T \leq -60$ °C, where ice particles are typically small (Platt et al., 1987, 2002) as less water vapor is available for ice crystal growth in a colder atmosphere. The lidar ratio is derived from the constrained retrievals utilizing the two-way transmissivity of ice clouds (Young & Vaughan, 2009). The particulate depolarization ratio is derived from the measured volume depolarization ratio with the Rayleigh scattering contribution subtracted (Hu et al., 2009).

Figure 4 shows the climatological distributions of the lidar and depolarization ratios of cold cirrus clouds observed by CALIOP in 2009. CALIOP points in an off-nadir direction to avoid substantial influence from horizontally aligned ice crystals (Saito & Yang, 2019) in the present analysis. The observed lidar and depolarization ratios are densely populated in a range S of 10–45 sr and δ of 0.3–0.6. The backscattering properties of smooth ice crystals are far from this range, but those of roughened ice crystals ($\sigma^2 =$ 0.01–0.5, and especially 0.03–0.15) tend to be within the range. Interestingly, this roughness range is also consistent with a range of estimated surface roughness from 0.01–0.3 using stereographic SEM measurements of ice crystals in a laboratory (Neshyba et al., 2013, Butterfield et al., 2017).

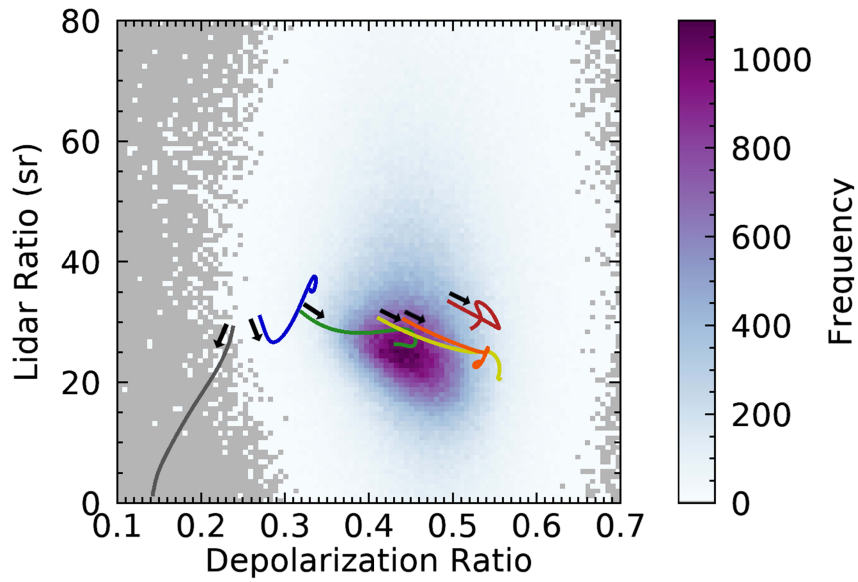

Figure 4. Two-dimensional histogram of the lidar and depolarization ratios of cold cirrus clouds obtained from CALIOP observations in 2009. Color lines are the theoretical counterparts along effective radii from 2–100 μm (arrows show the 2-μm starting points) with various degrees of surface roughness (same colors as in Figs. 2 and 3).

Previous studies show that smooth ice crystals with various aspect ratios exhibit limited variations of δ from 0.1–0.2 (Borovoi et al. 2013), with the exception of a smooth droxtal that shows lidar and depolarization ratios ranging from 30–40 sr and approximately 0.4, respectively (Okamoto et al., 2020). However, smooth droxtals are considered to be rare in ice clouds, as they produce specific halo peaks (Zhang et al., 2004) that are rarely observed (Sassen et al., 2003). This suggests that droxtals in ice clouds have some degree of surface roughness. Thus, we conclude that surface roughness has pronounced impacts on the backscattering properties of ice crystals and must be considered to infer the microphysical properties of ice clouds from lidar backscattering signals.

Reichardt et al. (2002) reported two distinct correlations among the lidar ratio, depolarization ratio, and temperature of cirrus clouds from ground-based lidar observations. A strong positive correlation between the lidar and depolarization ratios occurring at warmer temperatures (above -40°C) is well explained by the presence of horizontally oriented planar ice crystals (e.g., Saito et al., 2017). However, a reported slight negative correlation between the lidar and depolarization ratios occurring at colder temperatures (below -50°C) has been an open question. Figure 5 shows correlations among backscattering properties, temperature, and surface roughness obtained from CALIOP observations of single-layer transparent cirrus clouds with $T \leq -40$ °C and theoretical backscattering simulations. The roughness variations can mimic the temperature dependence of the CALIOP-based backscattering properties of ice clouds. Although a definitive conclusion cannot be obtained from this analysis, a potential temperature dependence of the surface roughness of ice crystals could be a candidate to explain the slight anti-correlation of the lidar and depolarization ratios of cold cirrus clouds.

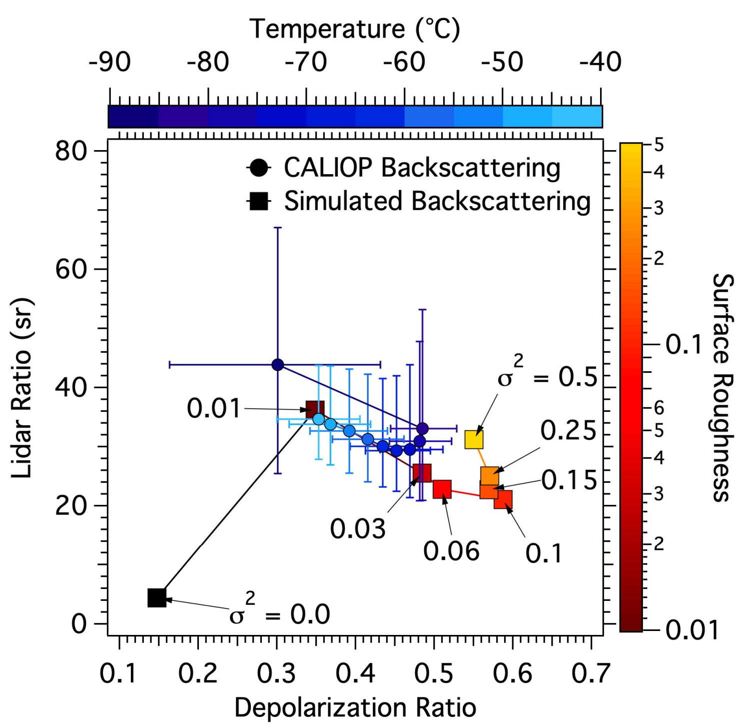

Figure 5. (circles) Median and quartile ranges of the lidar and depolarization ratios of ice clouds with various middle cloud temperatures (indicated by blue colors) obtained from CALIOP observations. (squares) Theoretical counterparts with various degrees of surface roughness (indicated by red colors) and an effective radius of 30 μm are coplotted.

4 Conclusions

This study performs single-scattering property simulations of smooth and roughened hexagonal column ice crystals over a wide size parameter range to investigate the impact of surface roughness on backscattering properties. State-of-the-science light-scattering computational methods and realistic ice crystal models reveal distinct differences in the lidar ratio between smooth and roughened ice crystals. The depolarization ratio is especially sensitive to the degree of surface roughness. Comparisons between theoretical backscattering properties with various degrees of surface roughness and those estimated from CALIOP observations imply that surface roughness is essential to robust explanation of observed lidar backscattering signals associated with cold cirrus clouds, and imply possible temperature dependence of dominant degrees of surface roughness of ice crystals.

The present study indicates a robust path forward for a better interpretation of lidar-derived backscattering signals by using the microphysical properties of ice crystals. Further research using sophisticated polarimetric lidar observations and these ice crystal backscattering property models should provide knowledge of a wider range of morphological characteristics of ice clouds.

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Open Research

The single and bulk scattering property data used in this study will be publicly available (https://doi.org/10.5281/zenodo.??????) after the acceptance of this manuscript (the data is temporarily available from Supplemental Information). CALIOP data are available through the NASA Langley Research Center Atmospheric Science Data Center (https://asdc.larc.nasa.gov/).

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