Journal of Quantitative Spectroscopy & Radiative Transfer 115 (2013) 93–95

Contents lists available at SciVerse ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Notes

Q-space analysis of scattering by dusts

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ARTICLE INFO

Article history:
Received 4 July 2012
Received in revised form
30 August 2012
Accepted 2 September 2012
Available online 8 September 2012

Keywords:
Light scattering
Q-space analysis
Phase function
Mineral dust

ABSTRACT

This note applies Q-space analysis, wherein the scattered intensity is plotted versus the scattering wave vector $q=(4\pi/\lambda)\sin(\theta/2)$ on a double log plot, to phase function data for scattering from irregularly shaped dusts. This analysis yields a power law description of the dust scattering as it has for aggregates and spheres. This implies that Q-space analysis can yield a simple and comprehensive description of scattering in terms of power laws with quantifiable exponents for a wide variety of shapes. It also calls for an explanation of the power law for irregular dust particles and the numerical exponent.

1. Introduction

The description of light scattering by particles evolves from the simple limit of those much smaller than the wavelength of light, the Rayleigh limit, to spherical particles of arbitrary size and refractive index describable by the classical Mie equations, to the much more complex yet common irregular geometries such as aggregates and a multitude of non-spherical shapes. These can include soot, mineral dusts, volcanic ash, snow and ice crystals, and biological micro-organisms distributed in size from submicron to millimeters. The foremost agenda in the light scattering literature for the past few decades has been how to describe and calculate scattering from irregularly shaped particles, including aggregates. Significant computational advances have been made, and very useful experimental programs have allowed for comparison with computation. However, a simple description encompassing all shapes has yet to be obtained. In this brief note we suggest that a simple description encompassing all shapes might lie with what we have called a Q-space analysis [1,2]. We support this suggestion by showing that the phase function scattered from four well known dust samples can be simply described by quantifiable power laws in Q-space, similar to the simple descriptions that also occur for aggregates and spheres.

2. Q-space analysis

Q-space analysis involves plotting the scattered intensity, not as a function of the scattering angle θ, but instead as a function of the scattering wave vector

$$q=2k\sin(\theta/2) \tag{1}$$

on double-log plots [1,2]. Here $k=2\pi/\lambda$ where λ is the wavelength. Note that the units of q are inverse length.

When this is done, aggregates show power laws in the scattered intensity at large q with negative slopes equal to the aggregate fractal dimension [3]. As q decreases the power law transforms through a curving Guinier regime to a flat Rayleigh regime as q approaches zero. The Guinier regime, which is dominated by simple diffraction, occurs near $qR_g \approx 1$ and thus contains cluster size information in R_g, the radius of gyration of the aggregate.

When the Q-space analysis is applied to the scattered intensity from spheres of arbitrary size and refractive index, the Mie solution [4], power laws again appear in the envelops of the plots (ignoring the "ripples" and the

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http://dx.doi.org/10.1016/j.jqsrt.2012.09.001

enhanced backscattering) and a simple description results [1,2]. One finds similar plots for spheres of wide ranging size and refractive index if the so-called phase shift parameters are equal. The phase shift parameter is

$$\rho = 2kR(m-1) \tag{2}$$

where m is the refractive index and R is the sphere radius. As for aggregates, at small q the scattered intensity in the forward lobe Rayleigh regime is constant as q approaches 0 and a Guinier regime occurs near $qR \approx 1$. For $qR > 1$ the scattered intensity falls off with a power law as $(qR)^{-2}$ until this functionality crosses over at $qR \approx \rho$. For $qR > \rho$ the scattered intensity falls off as $(qR)^{-4}$. If $\rho < 1$, there is no -2 power law and the Guinier regime crosses over directly to the -4 power law with increasing q.

These situations indicate that Q-space analysis leads to a simple and comprehensive description of the scattered intensity in terms of quantifiable power laws that encompasses both arbitrary spheres and aggregates. Now we show that Q-space analysis is equally effective in giving a simple description of certain common types of dusts.

3. Application of Q-space analysis to dusts

Scattering by dusts has seen extensive experimental study. In four notable instances [5–9] experimental data have been averaged to create tables of the "synthetic" phase function, essentially the scattered intensity as a function of the scattering angle. The tabulation of Volten et al. [5] was the average of 14 phase functions measured at two different wavelengths, 441.6 nm and 632.8 nm. The data of Munoz et al. [6] were obtained for a sample of Saharan sand particles collected from the Libyan Desert with a narrow distribution of sizes around 100 μm in radius. Munoz et al. [7,8] studied ash particles from a number of volcanoes. Laan et al. give data for Martian analogue palagonite particles [9]. All mentioned phase functions are found in the website for the Amsterdam–Granada light scattering database advertised in [10]. For the 14 phase function average of [5] we used a wavelength of 441.6 nm while we used 632.8 nm for the other data sets to calculate q according to Eq. (1). We then plotted the scattered intensity listed in Table 3 of [5] and Table 1 of [6] and the tables at the website in [10] for the other two versus q to yield a Q-space analysis of these data. These results are shown in Figs. 1 and 2.

Figs. 1 and 2 show that essentially perfect power laws for more than two orders of magnitude describe the dust scattered intensity until a small enhanced backscattering regime is encountered at large q. Unfortunately, the data for each set were limited to angles of 3°–5° and larger so that no data were obtained in the Guinier and Rayleigh regimes ($qR_g \leq 1$). Regardless, the figures show that the Q-space analysis uncovers power laws in the scattering phase function for dusts. Recall that conventional plotting (I or F_{11} versus θ) of the scattering phase function for dust scattering, and for that matter scattering from spheres and aggregates, yields non-descript curves. Thus these figures extend the range of the Q-space analysis to irregular dust particles for providing a simple and comprehensive description of scattering for many different particle shapes.

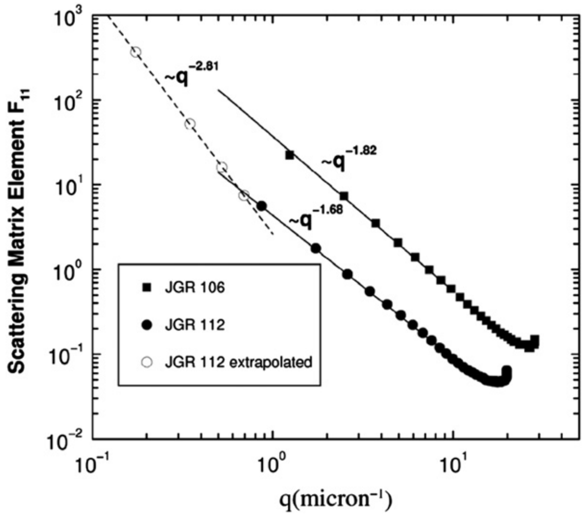

Fig. 1. "Synthetic" scattered intensity (scattering matrix element F_{11}, arbitrary units) versus the scattering wave vector q for an average of 14 dusts (JGR 106 [5]) and Saharan dust (JGR 112 [6]). Solid points are averaged data, open points are extrapolations made by the authors of [6].

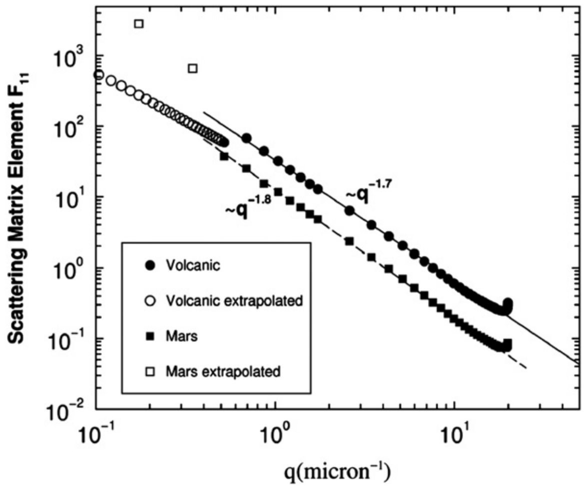

Fig. 2. "Synthetic" scattered intensity (scattering matrix element F_{11}, arbitrary units) versus the scattering wave vector q for volcanic [7,8] and Martian [9] dusts. Solid points are averaged data, open points are extrapolations made by the authors in [10].

The open symbols are extrapolations to small angles less than 3°–5° found in the Amsterdam–Granada light scattering database [10]. From the point of view of the Q-space analysis, the extrapolations have a much different power law and appear miss-guided. Whether they are or not can only be resolved by experiment.

We limited our analysis to four well known average phase functions. However, the dusts have different origins with different sizes and refractive indices yet they show the same behavior when plotted in the Q-space. This and the near equality of the power law exponents suggest these values might be universal for dusts or at least dusts of a certain morphology. Future comparisons with other data sets and new data sets is certainly warranted.

The dust power law exponents are 1.75 ± 0.05. This range is equal to the power laws observed for diffusion limited fractal aggregates [3] with fractal dimensions in the range 1.7–1.8. However, the real space morphologies are much different. Aggregates are composed of smaller primary particles stuck together to form an open, ramified aggregate structure. The dusts on the other hand are compact, single particles with rather random surfaces and non-spherical symmetries. Future work should attempt to explain the dust power laws in terms of the dust structure.

4. Conclusion

This note applied the Q-space analysis to data for the scattering phase function of four well known average phase functions of irregularly shaped dusts. The analysis yielded a quantifiable power law description of the dust scattering as it had for aggregates and spheres. Thus Q-space analysis can yield a simple, comprehensive and quantitative description of the scattered intensity for a wide variety of shapes.

Acknowledgments

I thank Gorden Videen for suggesting that I submit this work and reading the manuscript before submission. I thank William Heinson for graphing the data.

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