Initial investigation into using Fourier spectra as a means of classifying ice crystal shapes

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Abstract

Fast Fourier Transforms of azimuthal light scattering patterns are investigated as a method for classifying cirrus cloud ice crystals. Small Ice Detector Mk. 2 data is compared to modelled reference data of various aspect ratio, size and basal indentation.

1 Introduction

Characterization of the shape of cloud ice crystals is important with respect to their effect on radiative forcing in the atmosphere. Due to the small size of the crystals, direct imaging suffers from resolution constraints [1]. Because of this, few instruments are capable of recording useful information regarding the smaller particles. Small Ice Detector Mk. 2 (SID-2) relies on light scattering from individual particles, and so can observe particles in the 1µm-50µm size range. The detector consists of 24 azimuthally arranged elements collecting information between 9° and 19.8°, with a further 3 elements spanning the 5.5°-9° range (though the latter are not considered in this investigation.)

A computational model has been developed at the University of Hertfordshire to include diffraction on facets in a ray tracing model [2][3]. This model allows generation of scattering patterns from crystals with known morphology and orientation, which can then be compared with measurements. A reference database of patterns from various crystal sizes, basal indentations and aspect ratios has been developed for this purpose. A laboratory rig has also been assembled to measure the scattering pattern from ice analogue crystals (crystals with similar optical properties to ice but stable at room temperature [4]) in known orientations, for scattering angles from 5° to 120°. Modelled patterns are then compared to imaged patterns from the analogues for verification purposes.

2 Reference database

The Ray Tracing with Diffraction on Facets (RTDF) model was used to create a database of patterns for crystals with known shape. Each crystal is a hexagonal prism, with variable size, aspect ratio and degree of basal indentation. Basal indentation refers to an indentation of the hexagonal basal facets. This indentation takes the form of a hexagonal pyramid extending from each of the basal facets towards the centre of the crystal. The complete set is comprised of modelled data from crystals of 9 sizes (4.5µm, 7µm, 11µm, 16µm, 23µm, 27µm, 32µm, 35µm, & 40µm), each with a range of 5 aspect ratios (length:diameter 8:1, 3:1, 1:1, 1:3, 1:8), and 8 degrees of basal indentation (0%, 5%, 10%, 17%, 25%, 33%, 41% & 49% of the total length) over 80 evenly spaced orientations - a total of 28800 individual patterns. For the computation, a cluster of 40 processors was used, for duration of 32 hours, so expansion of the reference data is feasible. The model has been compared to imaged scattering patterns from ice analogue crystals suspended in a custom built laboratory rig. Before inclusion in the database, each computed 2D scattering pattern is reduced to its equivalent SID-2 response, the modulus of the fast Fourier transform (FFT) calculated and normalised to the zero order coefficient – figure 1 [6].

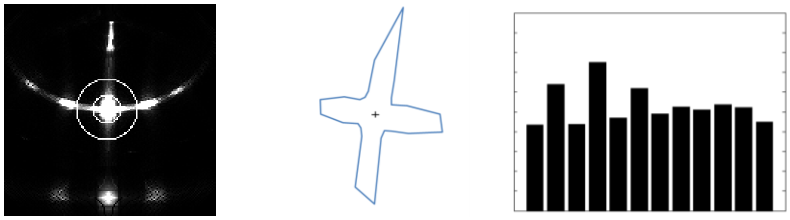

Figure 1, from left to right – 2D scattering pattern from modelled column (rings represent area recorded by the SID-2 detector), polar plot of square root intensity of SID-2 pattern, normalised FFT spectrum of polar plot

3 Test of FFT fitting as a method of crystal classification

FFT fitting is performed by finding the smallest RMS difference between the FFT spectrum of a subject particle and reference FFT spectra.

To test the fitting as a viable method of crystal classification, a further set of crystals was modelled, of the same aspect ratio and basal indentation, but a different range of sizes. This was then fitted to the database, and the error for each fitting inspected. The error is defined as the sum of the distances separating the fit from the expected bin (in three dimensions of Aspect Ratio, Basal Indentation and Size) multiplied by the number of particles in that bin – Eq (1).

$$Error = \sum_{1}^{\#Bins} \frac{\sqrt{\Delta AR^2 + \Delta BI^2 + \Delta Sz^2} \times Size\ of\ Bin}{Number\ of\ Patterns} \tag{1}$$

Initial investigations showed that three reference sizes (4.5μm, 11μm and 23μm) provided a poor fitting for a set of modelled test crystals. To increase the accuracy, an additional two sizes (7μm and 11μm) were added to the reference data, which improved the fitting considerably – Figure 2. This indicates that the FFT patterns are heavily dependent on size as well as aspect ratio and basal indentation, even when normalised.

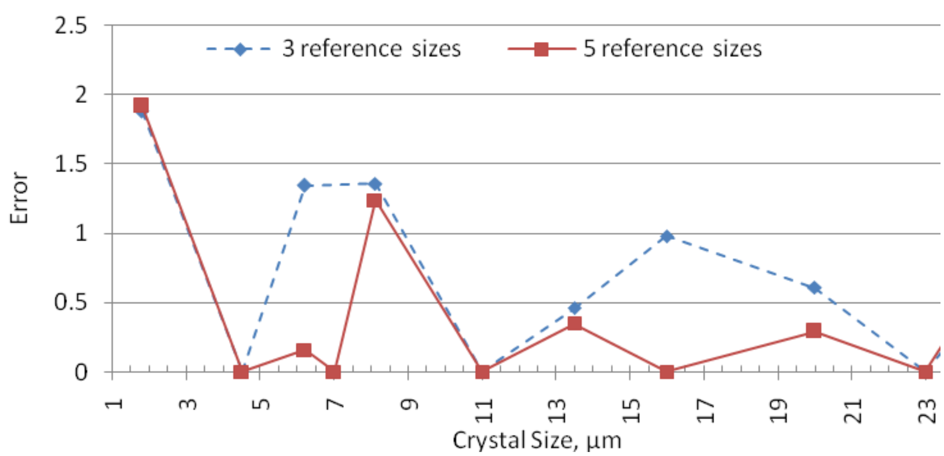

Figure 2. Comparison of fitting error between modelled test crystals over a range of sizes and the reference database before (3 reference sizes) and after (5 reference sizes) the addition of two crystal sizes to the reference database.

Because of the size dependence the error in fitting will increase as crystal sizes extend beyond the range of reference sizes. Expanding the database below 2.3μm is currently not feasible since the RTDF model becomes inaccurate for two dimensional scattering below this point.

4 Laboratory scattering measurements

Scanning electron microscopy has been employed to obtain precise dimensions of analogue crystals to enable comparison between modelled and experimental data. Once measured, crystals were placed in the scattering rig, and their scattering patterns imaged. The crystals were rotated in order to get a range of patterns from known orientations. Crystals were then modelled for use with the RTDF program, and scattering patterns were produced. Comparison of the imaged and modelled patterns shows a good fit.

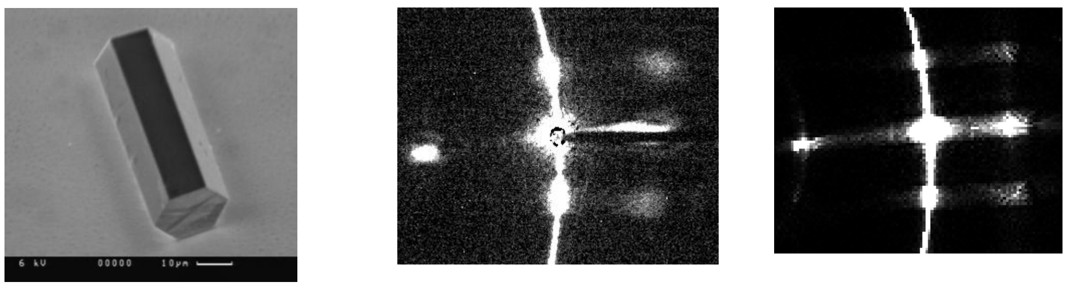

Figure 3 (left) Scanning Electron Microscope image of 2:1 aspect ratio ice analogue column, (middle) experimental 2D scattering pattern from ice analogue column with long axis at 40° to incident beam. Note that the dark line from the centre of the image to the right is a rod supporting the crystal on a glass plate, (right) RTDF modelled 2D scattering pattern of equivalent crystal.

5 Application of fitting data to SID-2 experimental data from a cloud chamber

During the HALO-01 campaign at the AIDA cloud chamber [5], small ice crystals were produced and recorded by numerous instruments, including SID-2. During experiment 18 flat plates were observed by the PHIPS imaging probe [7], which is in agreement with the FFT fitting of SID-2 data from that experiment - Figure 4. In addition, IR spectroscopy indicates a presence of 1:1 ratio compacts around 11μm as seen in the SID-2 data. FFT fitting is limited to a maximum RMS of 0.046, which includes approximately 50% of the data from the experiment.

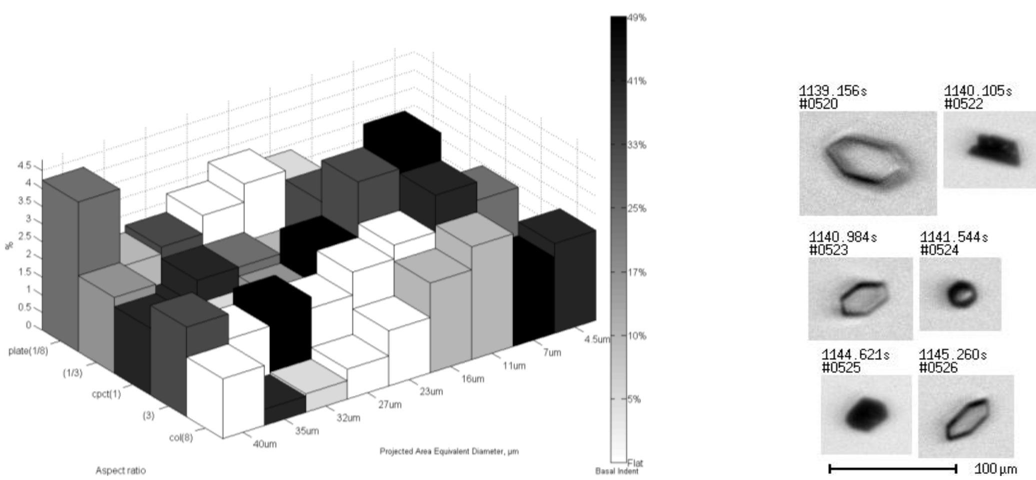

Figure 4 (left) – Best fits of FFT spectra of data recorded by SID-2 at HALO-01 campaign at the AIDA cloud chamber (right) – PHIPS data from the same time period shows large plates

6 Conclusions

A set of reference scattering patterns was computed using the RTDF model. These were verified by comparing them to experimental scattering patterns from ice analogues. Retrieval of crystal shape from azimuthal scattering patterns from SID-2 cloud probe data was investigated by least squares fitting of the patterns to the reference set. FFT was used to remove the dependence of scattering patterns on rotation about the axis of the SID-2 detector. The fitting method is shown to be able to recover crystal aspect ratio and depth of basal indentation while being dependent on size.

Acknowledgements

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