Supporting Information
for
"Statistical measures of spottiness in diffraction rings", Bridget Ingham

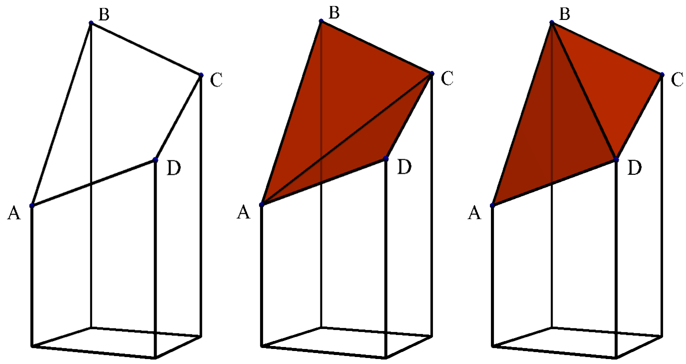
Calculation of surface area

For each binned grid element ABCD, the areas of the triangles ABC, ACD, ABD and BCD are calculated using Heron's formula:

$$Area = \sqrt{p(p-a)(p-b)(p-c)}$$

where $p = \frac{a+b+c}{2}$

and a, b and c are the lengths of the sides of the triangle. The two sums (ABC+ACD and ABD+BCD) are then averaged.



Additional parameters used to calculate the diffraction patterns in Figures 3 and 5

X-ray wavelength = 0.824 Å
Sample size = 1.5 mm
Sample-detector distance = 136.0 mm
Instrument broadening = 0.1 deg
d-spacing of the reflection being calculated = 2.027 Å (Fe 110)
Multiplicity of the reflection being calculated = 12
Accuracy parameter (used to limit the range over which each Gaussian peak is calculated, for time efficiency) = 0.001
Output file size in pixels = 81 × 521
2θ (radial) range = 22.9 - 24.1 deg
γ (azimuthal) range = 25 - 155 deg

Both computer programs (for extracting statistical parameters and for calculating diffraction rings from an input size distribution) are written in Java (1.6) and can be obtained by contacting the author.