Reconstructing images from in situ small angle x-ray scattering experiments

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Motivation
Organic solar cells are cheap, non-toxic, flexible, colourful, and show the potential to be mass produced, thus this technology have the potential to be major contributor in the renewable energy transformation. A few number of pioneering companies are producing organic solar cells, but in order to serve as a tool for the terawatt challenge, fundamental research is needed to reach a competitive levelised cost of energy. This project is dedicated to investigate the determining factors for an ideal morphology of the active layer and how to preserve these when going from laboratory scale to large scale production.

Introduction
Pioneering companies based on organic solar cells technology are slowly getting established. Despite their huge potential, these companies can not survive with out third part money. The key limiting factor is the levelised cost of energy.

Experiment
To investigate the morphology of the active layer while printing, gracing incidence small angle x-ray scattering is used. The probing x-ray beam will scatter in all directions and is recorded by a 2D detector. The intensity is given by

\[ I(\vec{q}) = \langle |F|^2 \rangle S(q), \]

where \( F \) contains information of shape and \( S \) about the structure of the morphology.

Data
2D images detectors captures the scattered x-rays. The scattering pattern contains, in theory, all information about the morphology of the illuminated volume. An example of 2D detector is shown below from two different times.

Analysis – Future work
The formfactor, \( F(\vec{q}) \), is the Fourier transform of the shape function for a given object. Every object geometry has a unique form factor.

\[ F(\vec{q}) = \int V \exp(i\vec{q} \cdot \vec{r}) d^3r \]

We would like to apply the methods from convex optimisation in order to reconstruct the shapes / the morphology of the active layer in organic solar cells as function of several parameters. If you have any suggestions or recommendations for how to proceed with applying convex optimisation methods for the reconstruction, please do not hesitate approaching me.