DTU Energy
Department of Energy Conversion and Storage

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 an 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.

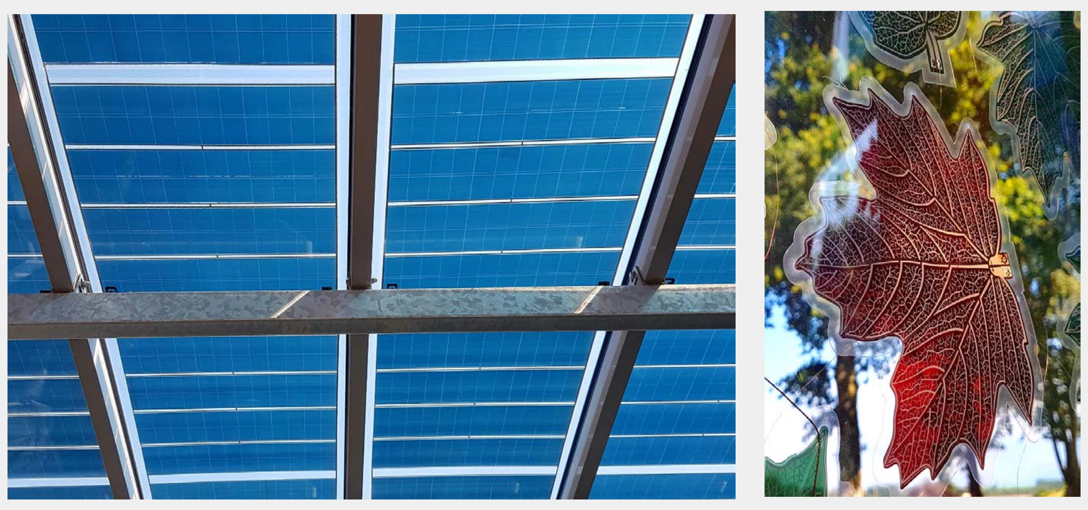

Figure 1: Organic solar cell installations in the city of Pau, France. Left a transparent sun roof and right a artistic solar leave, both fabricated by OPVius. Pictures taken by Anders S. Gertsen.

Challenge

The transition from laboratories to large scale fabrication methods fails to deliver high efficient solar panels. Reason being that the fundamental properties of a high functional organic solar cell is still unknown. We aim to investigate the morphology of the active layer as function of several parameters.

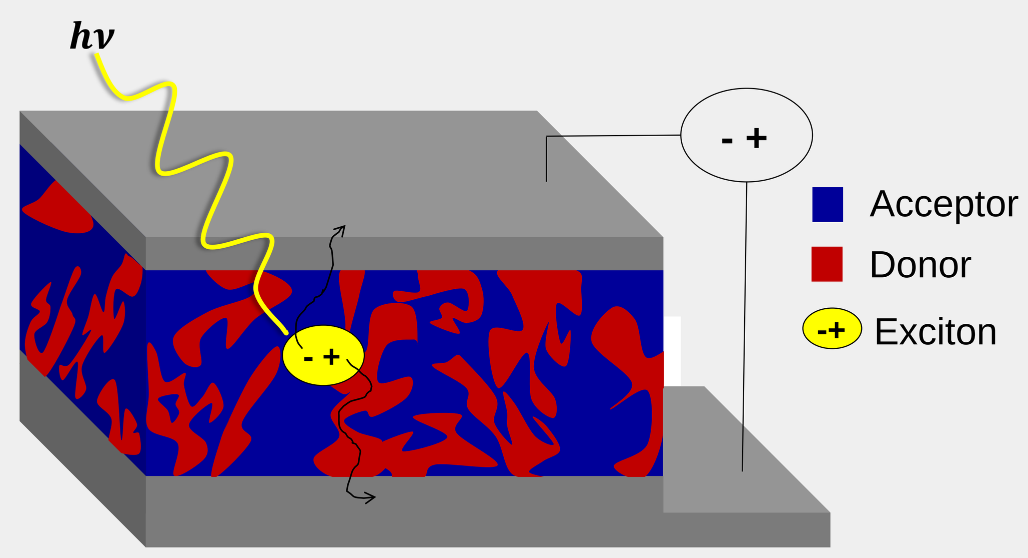

Figure 2: Working principle of an bulk heterojunction solar cell where an exciton is generated from where the electron and hole are transported to the respective anode and cathode.

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

$$I(\vec{q}) = \langle |F|^2 \rangle S(q_{\parallel}),$$

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

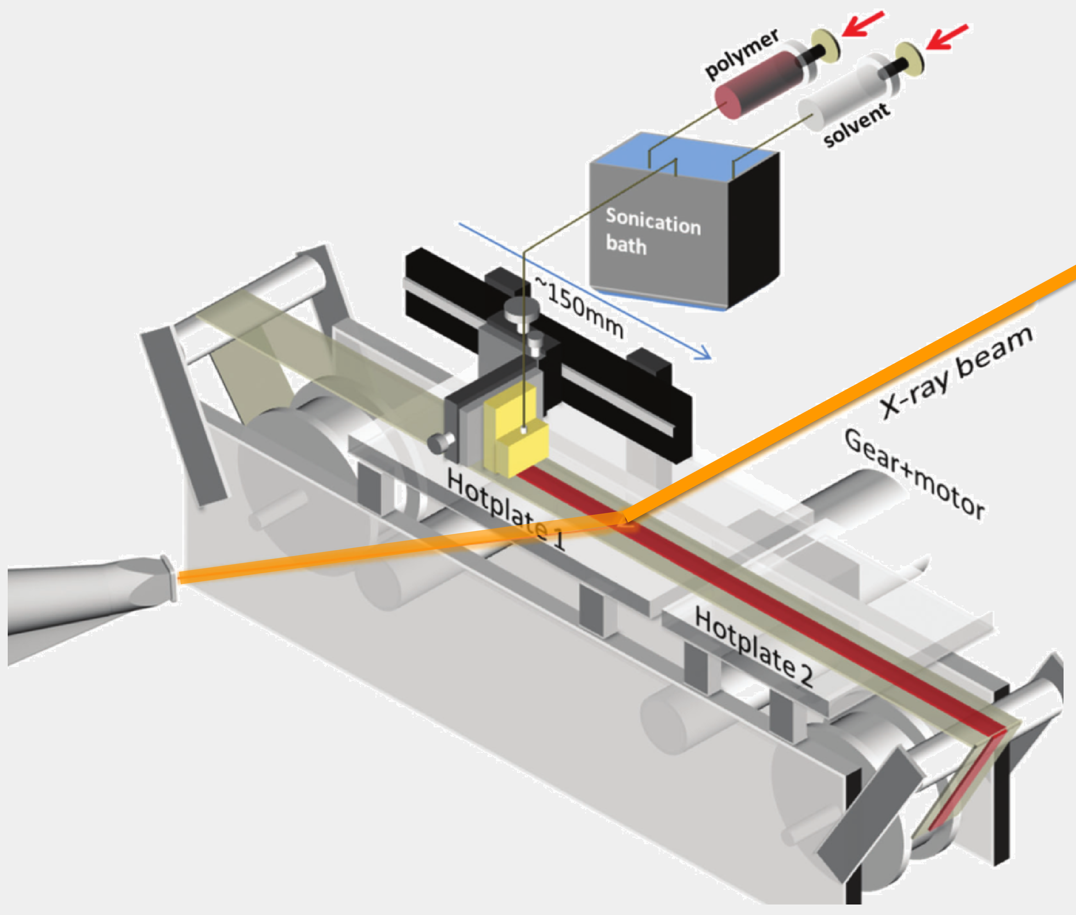

Figure 3: Illustration of *in situ* Roll to toll GISAXS experiment. Illustration published by: *Lea H. Rossander, et al 2017, DOI: 10.1039/c7ee01900a.*

To probe the large parameter space which determines the morphology we are using an *in situ* roll to roll (R2R) doctor blading technique, coupled to a gracing incidence small angle scattering experiment (GISAXS). From this method the solvents concentration ratio, film thickness, drying times and temperature can be adjusted while printing.

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.

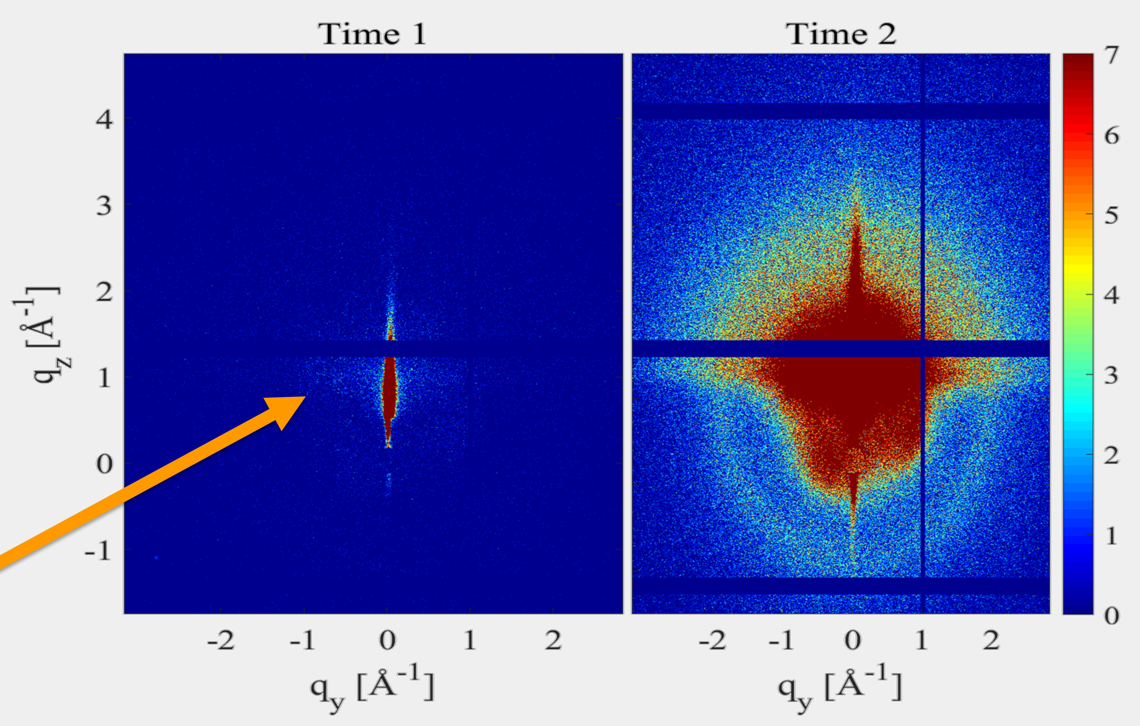

Figure 4: Two examples of 2D data from in-house data. This represents how data is gathered in gracing incidence small angle x-ray scattering experiment. In this example one parameter is change and it will be interring to model the exact morphology.

Analysis – Future work

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

$$F(\vec{q}) = \int_V \exp(i\vec{q} \cdot \vec{r}) d^3 r$$

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.

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