ESRF	**Experiment title:** Time-space resolved structural study of the active layer of organic photovoltaic devices	**Experiment number**: MA-1096
Beamline:	**Date of experiment**: from: 24/11/2010 to: 30/11/2010	**Date of report**: 20/02/2013
Shifts: 18	**Local contact(s)**: WRIGHT Jonathan	*Received at ESRF:*

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Report:

In the present experiment, performed on the beamline ID11, spatially-resolved diffraction studies of thin films constituting the active layers of organic photovoltaic (OPV) devices were conducted. Due to the constraints imposed by the geometry of the OPV cell (the thickness of each layer lied in the range from 50 nm to 200 nm), the use of a tightly focused X-ray beam was required to perform spatially-resolved diffraction experiments. In order to probe each layer comprising the device cross section the beam direction was set parallel to cell surface (x-y plane). By progressively shifting the device in the vertical (z) direction, the X-ray beam probed all the layers of the sandwiched specimen, from the top to the bottom electrode.

An X-ray energy of 35 keV was selected using the Laue-Laue monochromator of the beamline. A vertical line focus was obtained using planar silicon lenses. The X-ray beam was defined by slits in front of the lenses and a 1 mm pinhole was mounted between lenses and sample to remove diffraction from the slit blades. Behind the sample, a compound detector system allowed the translation among different detectors. A high-resolution Sensicam X-ray camera (1.3 μm pixel size) was used for alignment purposes. A fibre optic coupled CCD area detector was used for the diffraction measurements. Once the optimal alignment was reached, the corresponding sample position was set for diffraction by locating the height of the ITO layer in the substrate using the Indium fluorescence signal. The X-ray beam size and profile were critical parameters in order to be able to attain a spatial resolution close to 100 nm needed for our experiment. The X-ray probe characteristics were obtained using the signal from the ITO thin film. The spatial profile of the incident beam was measured by recording the indium fluorescence as a function of the position of the ITO film (thickness about 140 nm) with respect to the beam. Accounting also for the ITO film thickness contribution and fitting with a pseudo-voigt peak convoluted with a 140 nm wide rectangular function a beam FWHM of 112(5) nm is found (Figure1). This was a relevant result, being the smaller beam size obtained up to now on ID11.

As a result of the proposed approach we were able to probe the stuctural properties of the OPV cells photo-active film at the nanoscale. In particular, by scanning the nanometre sized focal spot of the used synchrotron X-ray beam across the OPV device cross-sectional area, the structural properties of the different organic layers and interfaces were precisely detected. In addition to this, the respective modifications induced on the structural properties of the organic layers as a consequence of thermal annealing were studied, in order to be correlated with the photovoltaic performance of the respective OPV cells.

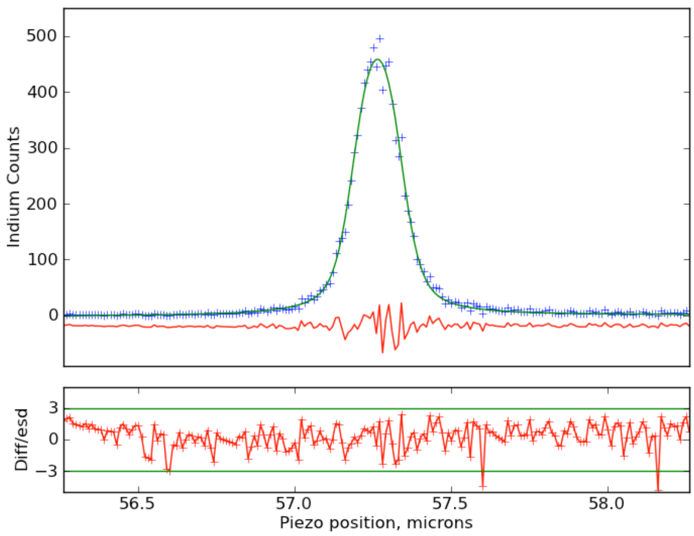

Figure 1. Spatial profile of the incident beam: best fit results obtained in the case of the convolution of the pseudo-voigt with a rectangular function.

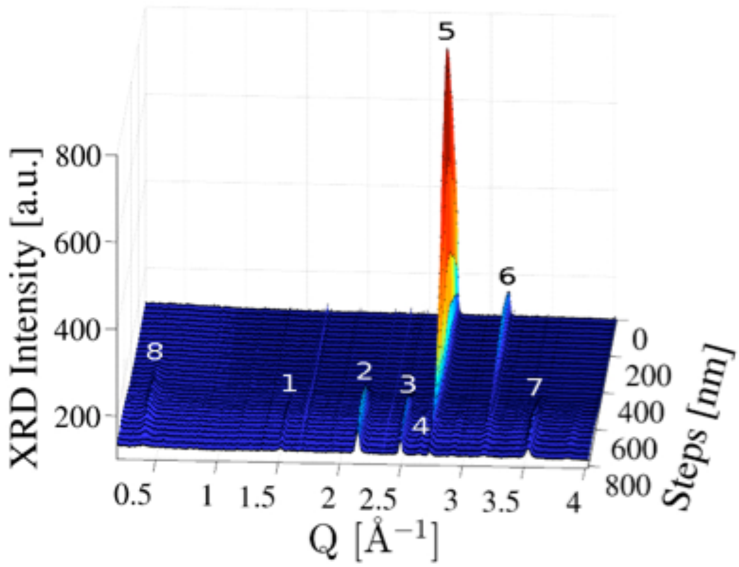

Figure 2. Sequence of X-ray Diffraction patterns acquired during the cross-sectional scan of the devices.

Reference:

B. Paci*, D. Bailo, V. Rossi Albertini, J. Wright, C. Ferrero, G. D. Spyropoulos, E. Stratakis, E. Kymakis, submitted to Advanced Materials.