ESRF	**Experiment title:** In-operando organic solar cells: simultaneous structure and spectroscopy characterization during polychromatic light soaking	**Experiment number**: MA-5560
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Report:

During this experiment, we have studied the structural evolution of the organic photovoltaic system PM6:Y6 during polychromatic light-soaking. We have successfully designed a new chamber for this purpose. The chamber allows to mount four samples at the same time on a custom-designed printed circuit board (Figure 1a) and perform GIWAXS experiments while illumination of the samples using four different light-sources (Figure 1b).

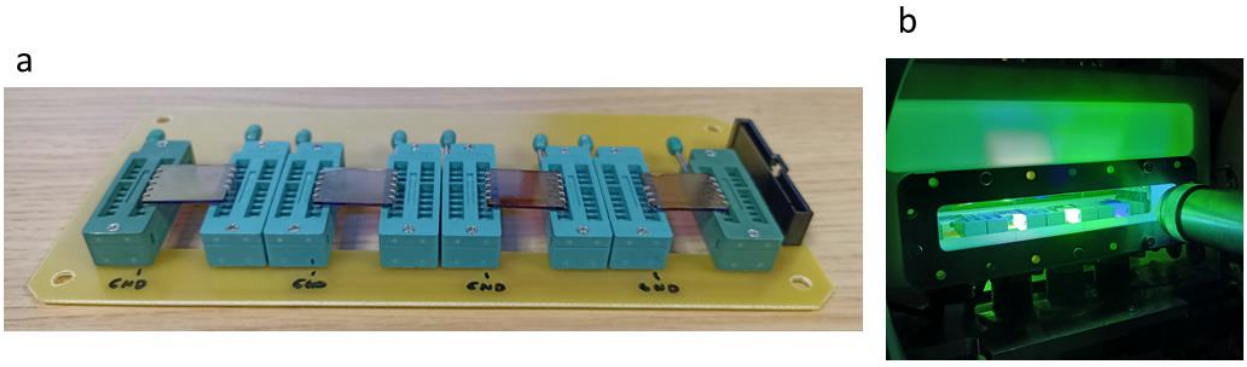

Figure 1. (a) Sample holder with four mounted samples. The samples are clamped by electrical legs, which are inserted into the green sockets. The sockets are solded into the circuit printed board. (b) Rear view of the chamber, with the mounted samples, each one illuminated by a different source of light.

We decided to focus on the same photovoltaic system (PM6:Y6) to get a full characterisation of the light-soaking impact using four different experimental parameters: excess of polymer, excess of acceptor, with and without using solvent-additive. According to previous experiments, these four scenarios represent four different morphological/structural behaviors. For example, in a polymer-rich cell without solvent additive, the diffusion and crystallization of the acceptor is forbidden. On the other hand, the crystallization if favourable in Y6-rich cells using solvent additive.

Therefore, we applied routines of 5-10 hours of light-soaking to four equivalent samples deposited using the same parameters. Three of these samples were illuminated by green, infrared and ultraviolet LEDs, and a fourth

one was kept in dark conditions. The idea was to perform a rigoruous analysis on the evolution of the diffraction pattern (Figure 2), before any electrical performance.

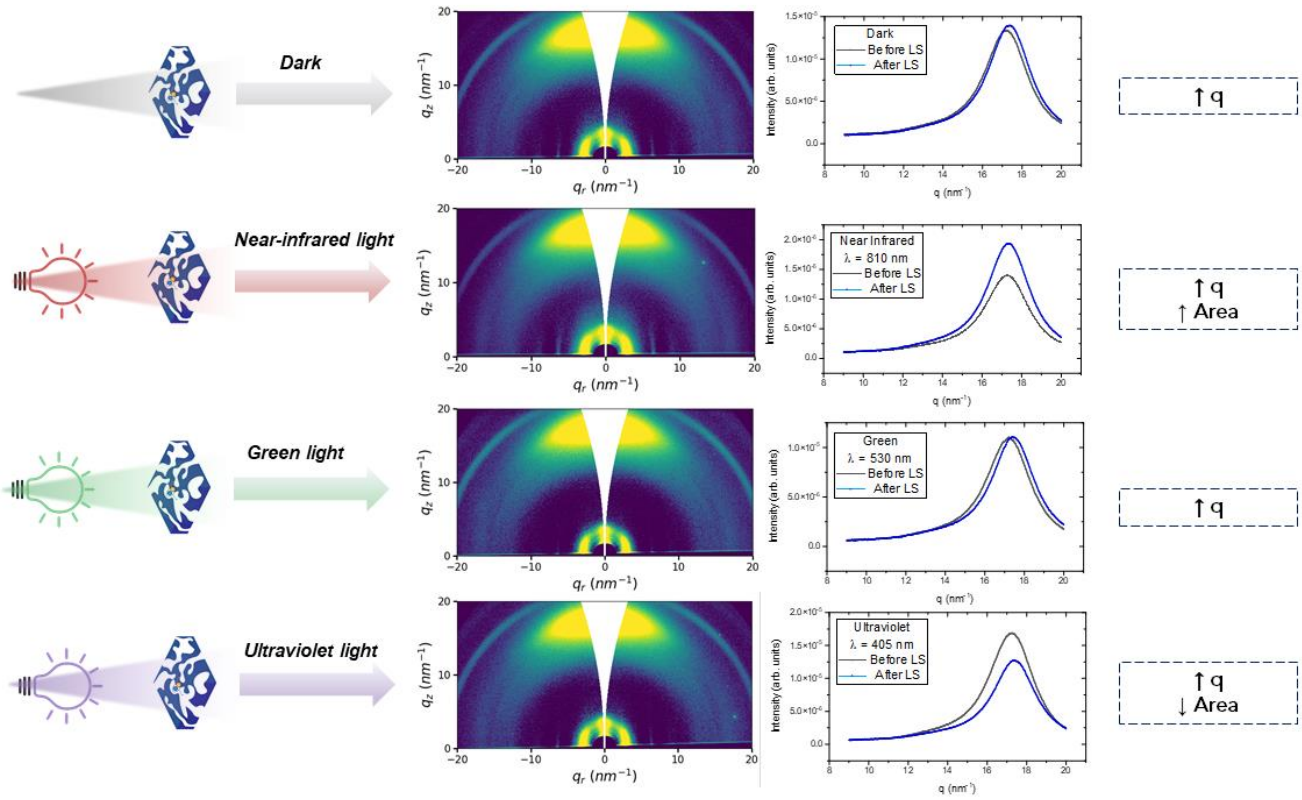

Figure 2. 2D GIWAXS patterns and intensity profiles from PM6:Y6, 2:1, 0%CN thin films after light-soaking using three different wavelengths.

While we are still analyzing the collected data, and trying to find the most efficient and accurate way of fitting the Bragg peaks, we can show already some interesting results regarding the structural evolution of the photovoltaic system as a function of the applied light wavelength (Figure 2).

We are showing in Figure 2 a focused analsysis of the vertical diffraction peak at q≈17nm^{-1}. From previous experiments, we know that the intensity profile can be deconvoluted on a gaussian peak, associated to the amorphous component of every organic material, and a Pseudo-Voigt peak, associated to the vertical stacking between conjugated planes. In our experiment, we are proving that this latter peak is evolving in a different way after using different excitation wavelengths. While on every case, the peak is shifting to higher q's, the area of the peak is increased after infrared excitation, is decreased after ultraviolet excitation and stays similar after green or no light excitation at all. This frequencial deconvolution allows to prove how the near infrared light is able to increase the fraction of diffractive material, presumably through local temperature increase, while the ultraviolet light is inducing an opposite effect. While we have to test these behavior for every measured photovoltaic system, these preliminar analysis are quite interested to understand the instability mechanism on organic solar cells.

Unfortunately, we could not test the performance on these systems. Although we had solar cells to test, fabricated at the Institute of Materials Science of Barcelona, we had issues with the connector cable from the circuit board to the external electronic control system. For that reason, although we spent one day on it, we could not measure reliable electric data. We expect to complete this part of the experiment in future proposals.