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Mass spectrometry to investigate crystallinity of OLED molecules: a novel application of ToF-SIMS measurements.

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Crystalline modifications in OLEDs induce loss of efficiency, but also modifications in the mass spectra. The objective is to propose a methodology to characterise them using ToF-SIMS and principal component analysis to treat the data. This allowed crystalline and amorphous phases to be distinguished and potentially give insight as to the crystallisation mechanism.

OLED displays have known many developments and improvements, increasing their efficiency. Nevertheless, several challenges in OLED development remain hot topics, in particular the stability of their emitting layers¹. Damage in the emitting layer can be caused by degradation of the emitting molecule, diffusion of dopants or molecules from other layers, oxidation or crystalline modification for example. To prevent such degradation, the first step is to understand the mechanisms through adequate characterisation. Among the many characterisation techniques that can be used, ToF-SIMS is especially well suited to address these questions. Indeed, this mass spectrometry technique is extremely surface sensitive with good mass resolution, with the capability to perform depth profiling with excellent depth resolution (few nm). In the same time, imaging is also possible with good lateral resolution (below 70 nm). These capabilities means that chemical modifications can be investigated, such as molecular degradation and oxidation, but also questions of diffusion between layers. Crystallinity-related modifications have been little studied by ToF-SIMS, though they are known to induce changes in the mass spectra². The goal is to propose a way to characterise crystalline modifications using ToF-SIMS. To this end, an emitting molecule, NPB, was deposited on a Si substrate and left to crystallise in room conditions. Crystallites were imaged in ToF-SIMS (see Figure 1). The acquired mass spectra were analysed using principal component analysis (PCA) and Shannon entropy. These two analysis enable the amorphous and crystalline phases to be distinguished and even gives hints as to the crystallisation mechanism.

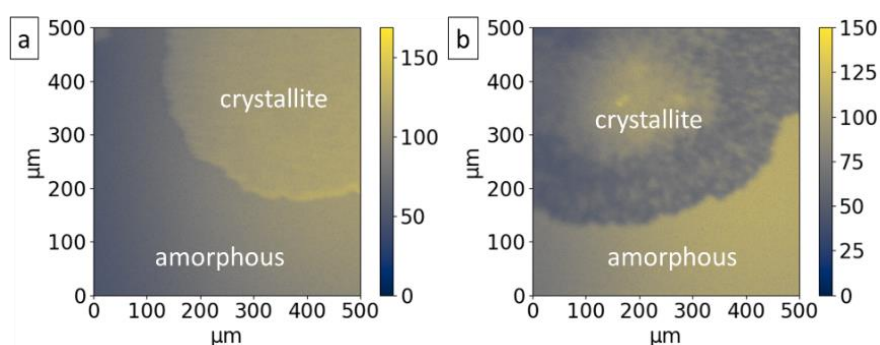


Figure 1: Map of the total intensity for two images acquired (a) in the positive and (b) in the negative mode.

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