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INVESTIGATING CRYSTALLIZATION WITH MASS SPECTROMETRY: A NEW WAY TO CHARACTERIZE OLED MOLECULES

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Summary: Light emitting devices have known constant developments over the years, especially organic light emitting devices (OLEDs). Even though those developments enabled commercial availability, there are still remaining challenges. One of them is the stability of the emitting layer^[1]. The stability of these layers can be reduced by degradation of the emitting molecule over time, diffusion of metallic dopants or organic molecules from other layers, oxidation or crystalline modifications for instance. To prevent such degradation, the capacity to characterize them is paramount. Among the existing characterization techniques, Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is well suited to tackle these issues. Indeed, this mass spectrometry technique is extremely surface sensitive, while able to perform imaging with good lateral resolution, up to 50 nm, and perform depth profiling with excellent depth resolution, up to a few nanometers. Taking advantage of these possibilities, one can investigate thoroughly chemical modifications, such as oxidation, molecular degradation or even diffusion. Crystallization is known to induce modifications in the mass spectra^[2], hence the images and the profiles, but this very phenomena has never been studied on OLED molecules. The goal is to study the crystallization and its mechanism of a known OLED molecule, NPB. This molecule was deposited on a silicon substrate, and let to crystallize at room conditions. Mass spectra were acquired in imaging mode in ToF-SIMS. These data were analyzed using principal component analysis (PCA) and then multivariate curve resolution (MCR). To support the mass spectral data, X-ray Photoelectron Spectroscopy (XPS) and Atomic Force Microscopy (AFM) experiments have also been performed. This allowed to clearly identify the amorphous and the crystalline areas, while obtaining hints on the reaction mechanism.

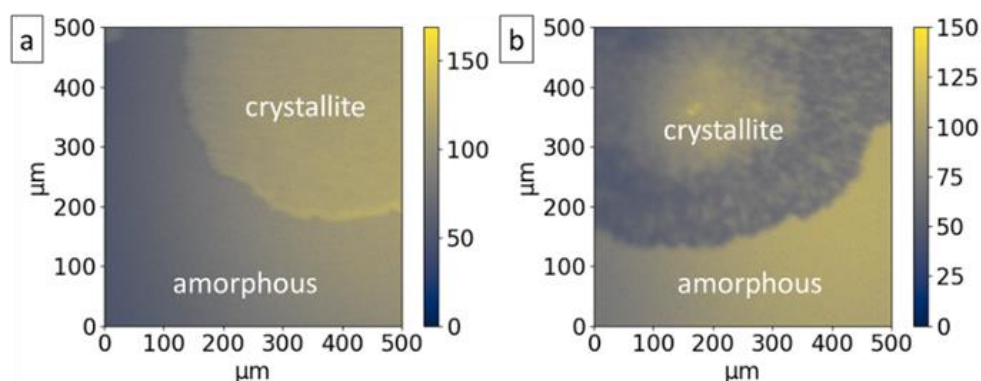


Fig. 1 Map of the total secondary ion intensity for two images acquired (a) in the positive and (b) in the negative mode in ToF-SIMS.

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