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Optimization of matrix spraying on OLEDs to increase the ionization in ToF-SIMS for tandem MS applications.

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Introduction

ToF-SIMS is an excellent tool for surface chemical characterization, and has been recently adapted to perform tandem MS measurements. Therefore the ionization of heavier fragments becomes crucial, especially when analyzing biological or polymer samples. The use of matrices is one way to increase the ionization, hence the intensity, of the fragments of interest. The applicability of matrices commonly used for MALDI has already been demonstrated as efficient for biological samples, but their use for OLED materials has never been reported. The goal is to optimize the use of matrices for OLED materials in ToF-SIMS measurements, which will help to better understand the ageing of these devices with a view to increasing device lifetime.

Methods

Alq₃ surfaces and six other typical OLED materials – $Ir(mppy)_3$, HATCN, F_4 TCNQ, NPB, STTB and TCTA – were sprayed with four different matrices: α -Cyano-4-hydroxycinnamic acid (CHCA), 2,3- dihydrobenzoic acid (DHB), N-(1-Naphthyl)ethylenediamine dihydrochloride (NEDC), and the solvent used for spraying a mixture of water and acetonitrile 50% v/v. Three different passes of spraying were made: 6 passes, 2 passes, 1 passes and no passes. The surfaces were analyzed in ToF-SIMS using a PHI nanoTOF 2, by acquiring spectra, profiles and large area images.

Preliminary data (results)

Firstly, the characteristic fragments of the different matrices studied were identified to make sure they do not interfere with the main fragments of the molecules of interest. Then the intensity of the ions of those molecule were thoroughly investigated. It appears that there is an optimum of matrix concentration around two passes of spraying for all the matrices as well as the solvent sprayed samples. The behavior of the intensity of the molecules differs between positive and negative modes. For the molecules that are more easily identified in the positive mode $(Alq_3, Ir(mppy)_3, NPB, STTB and TCTA)$, the intensities of their fragments are at the highest when only the solvent is sprayed. For these molecules, no clear pattern of intensities was found in the negative mode. F_4 TCNQ and HATCN are more easily identified in the solvent appears as the best solution to obtain higher intensities for the characteristic ions. Looking at the images and the profiles

acquired, the surfaces undergo significant changes in topography and crystallinity when sprayed with matrices (see Figure 1). These changes are less visible on the samples sprayed with only the solvent. Therefore, the solvent gives the best results both in terms of ionization enhancement and in terms of minimal sample modification.

Please explain why your abstract is innovative for mass spectrometry?

The use of MALDI matrices, or just the solvent, can be interesting in some cases to enhance ionization during TOF-SIMS analysis of OLED materials.



(a) Alq_2^+ ion, images of the different matrices sprayed.