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Decomposition of ultrathin LiF cathode underlayer in organic-based devices evidenced by ToF-SIMS depth profiling

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Highlights:

- Chemical composition of the multilayer organic-based devices incorporating an ultrathin LiF cathode underlayer was analyzed using the time-of-flight secondary ion mass spectrometry (ToF-SIMS) with depth profiling.
- LiF layer is partly decomposed due to diffusion of lithium in the bulk of the device.
- Lithium diffuses down to the substrate surface, with accumulation at the interfaces.

Abstract

In this work we investigate the chemical composition of an archetypal thin-film organic device with the Ag/LiF cathode using the time-of-flight secondary ion mass spectrometry (ToF-SIMS) with depth profiling. The LiF cathode underlayer is partly decomposed because a significant amount of lithium is released into the bulk of the multilayer device. The released lithium diffuses all the way to the substrate, accumulating, as revealed by ToF-SIMS depth profiles, at the interfaces rather than uniformly doping the underlying layers. Particularly, the bottom anode becomes chemically modified.

Keywords: organic devices, ToF-SIMS, lithium fluoride, doping, diffusion

1. Introduction

Thermally evaporated lithium fluoride is widely used in organic electronic devices [1-10]. It may serve as an electron transporting layer or work-function modifier in small molecule based light-emitting diodes (OLED) [1-4], photovoltaic cells [4-8] or transistors [9,10]. However, the true role of ultrathin LiF layers in these devices needs to be better understood [4]. At least two questions arise: *i*) whether LiF with a thickness of only 1 nm can protect underlying organics from penetration of the top evaporated metal and *ii*) whether lithium or fluorine can react with (or dope) neighboring layers [1-3,5,7,11,12-19].

In this work, we applied the time-of-flight secondary ion mass spectrometry (ToF-SIMS) with depth profiling to study the chemical composition of a multilayer device containing an Ag/LiF/boron subphthalocyanine chloride (SubPcBCl) interface. The molecular structure of SubPcBCl is shown in Fig. 1 (inset). The choice of SubPcBCl was stimulated by *i*) an interest in mixed LiF:SubPcBCl systems described recently as a way to form effective contacts in OLEDs [3] and *ii*) observation of high open circuit voltages in photovoltaic cells based on SubPcBCl as a photoabsorber [7,8]. Ag/LiF bilayer electrodes are known in organic electronics [2,9,10,12-16], but much less than Al/LiF bilayer or composite electrodes [1-8,12-19]. To make the archetypal

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