Band diagram of an Alq3/Nb:STO interface studied by in situ photoemission spectroscopy

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Introduction
Organic semiconductors (OSC) have attracted enormous attention in the past few decades because of their potential applications to organic-based devices, such as organic light-emitting diodes. In these devices, formation of interfacial dipole layers between OSCs and metal electrodes dominates device performance, and a great number of studies have been devoted for understanding the origin of the interfacial dipole [1]. Conductive perovskite oxides are expected as candidates for electrode materials in organic devices, since they possess the advantage of high transparency and high chemical stability. However, there are few studies on the band alignment at OSC/oxide interface.

In this study, we report on the band alignment at the interface between tris(8-hydroxyquinolinato)-aluminum(III) (Alq3) and conductive Nb-doped SrTiO3 (Nb:STO) determined by in situ photoemission spectroscopy (PES) measurements.

Experimental
The Nb:STO substrate was annealed at 1050 °C and an oxygen pressure of 1 × 10⁻⁷ Torr to ensure an atomically flat TiO₂-terminated surface, and was subsequently annealed at 450 °C and 760 Torr to restore the surface oxygen stoichiometry. Alq3 thin films with various thicknesses were deposited on the Nb:STO substrate by vacuum vapor deposition with the deposition rate of 0.1 Å/s using Knudsen cell heated at 250 °C. Subsequently, PES measurements were carried out in situ using MgKα (hv = 1253.6 eV) and He I (hv = 21.2 eV) with an energy resolution of 1.3 eV and 0.1 eV, respectively. The valence band spectra of Alq3/Nb:STO sample was measured ex situ by synchrotron-radiation photoemission system installed at BL2C at photon energy of 600 eV with an energy resolution of 0.25 eV. The film thicknesses were calibrated by ex situ grazing incidence X-ray reflectivity measurements.

Results and discussion
The valence band spectrum show systematic changes with increasing the Alq3 film thickness, and finally become bulk Alq3 spectra at 14-nm thickness. The several distinct peaks originated from Alq3 molecular orbital (MO) were clearly observed and these energy positions were in good agreement with the MO calculation [2]. In the 14-nm thick film, highest occupied molecular orbital (HOMO) onset was located at located at 2.2 eV below Fermi level. The difference of work function between Alq3 and Nb:STO was estimated to be 0.6 eV from secondary electron emission spectra. Furthermore, corresponding peak shift was observed in core level spectra with increasing the Alq3 thickness. From these experimental results, we determined the band diagram of the Alq3/Nb:STO interface as shown in Fig. 1, and found the formation of interface dipole with 0.6 eV.

Fig. 1. Band diagram of an Alq3/Nb:STO interface. The value of the band gap for Alq3 were referred to that in Ref. 2.

References

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