3B, 13A/2009S2-007, 2011G026

Interfacial electronic properties of fullerene/bathocuproine/Ag heterostructures studied by ultraviolet photoemission spectroscopy

Shenghao Wang[1], Takeaki Sakurai[*1,2], Ryusuke Kuroda[1] and Katsuhiro Akimoto[1]

1. Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan
2. PRESTO, Japan Sceience and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan

1 Introduction

Organic solar cells (OSCs) have great potential in the photovoltaic market due to the advantages of low cost, easy fabrication, and compatibility with large-scale and flexible substrates. It is a key issue for organic electronic devices to understand the electronic properties of interfaces, because they strongly affect the charge transfer and collection. Bathocuproine (BCP), as a buffer layer inserted between fullerene (C_{60}) layer and the cathode layer, can improve the power efficiency of OSCs. However, the role of BCP buffer layer still remains unclear. Gaining insight into the interfacial properties of C_{60}/BCP/metal heterostructures is necessary for understanding the role of BCP and further improving the performance of OSCs. It has been demonstrated that the performance of OSC was dependent on the thickness of BCP. In present work, we studied the influence of BCP thickness on the energy level alignment of C_{60}/BCP/Ag heterostructures using synchrotron-based in situ ultraviolet photoemission spectroscopy (UPS)[1]. We found that relatively thin BCP layer has favourable energy level alignment for the OSCs.

2 Experiment

The UPS experiments were carried out at beamline 3B of the Photon Factory. *Ex* situ cleaned Si(100) wafers were used as substrates. The C_{60}/BCP/Ag heterostructures were formed by depositing BCP on Ag and subsequently depositing C_{60} with increasing thickness from 0.4 to 5 nm onto BCP/Ag stack layers in the UHV chamber. BCP layers with thicknesses of 0.8 and 5 nm were formed in two samples; these represent thin and thick layers, respectively. Prior to deposition, BCP (Wako Corp., sublimated grade) and C_{60} (Sigma-Aldrich, 99.5 %) were purified three times by vacuum gradient sublimation. The deposition rates for both materials were 0.01 nm/s and the thicknesses were monitored by a quartz-crystal microbalance. UPS spectra were measured in an analysis chamber (< 9.0×10^{-10} Torr) using the photon energy of 30 eV.

3 Results and Discussion

Fig. 1 shows UPS spectra of C_{60} layers with various thicknesses deposited on BCP/Ag stack layers with 0.8 and 5 nm for BCP layer thickness. The abscissa is the electron binding energy (*BE*) relative to the Fermi level (E_F) of Ag. From Fig. 1(a), small peaks at about 1.8 eV can be clearly observed near the E_F, indicating the generation of gap states. Apart from the gap states, there is hardly any other change and shift for the spectrum after depositing 0.4 nm C_{60}. The peak of the highest occupied molecular orbital (HOMO) for C_{60} exhibits no shift as the thickness is increased up to 5 nm, indicating the pinning of E_F.

To the contrary, no small peak can be observed near the E_F and obvious peak shifts for the BCP features can be seen upon the deposition of C_{60}, implying that the molecular orbitals of BCP change. After depositing 0.8 nm C_{60}, the HOMO peak of BCP abruptly shifts to lower *BE* by 0.6 eV. When the C_{60} layer thickness is increased from 1.6 to 5 nm, the HOMO peak of C_{60} shifts to lower *BE* by 0.2 eV. The change of the HOMO peak indicates that band bending occurs for both BCP and C_{60} at the interface of C_{60}/BCP heterojunction. This band bending will enlarge the offset of the lowest unoccupied molecular orbital (LUMO) levels of C_{60} and BCP at the interface, and therefore generate a Schottky barrier for electrons transport, which is undesirable for the device performance.

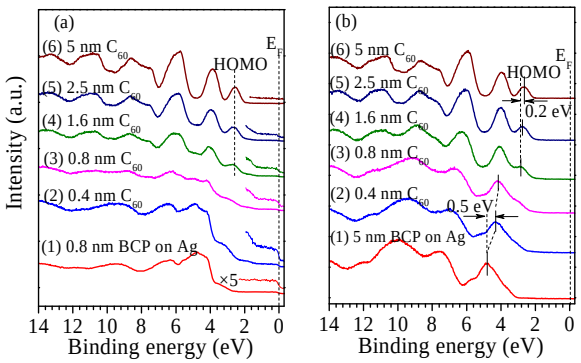

Fig. 1 UPS spectra of C_{60} layers with various thicknesses deposited on (a) BCP (0.8 nm)/Ag stack layers and (b) BCP (5 nm)/Ag stack layers

References

[1] S. Wang, T. Sakurai, R. Kuroda, and K. Akimoto. Appl. Phys. Lett. **100**, 243301 (2012).

* sakurai@bk.tsukuba.ac.jp