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Electronic structure of bathocuproine on metal studied by ultraviolet photoemission spectroscopy

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1. Introduction

The electrical properties at the interface between organic molecules and the metal electrode are important issue in the device performance. Recently, bathocuproine (BCP), whose bandgap energy is 3.5eV with the deep level of highest occupied molecular orbital (HOMO), is used as the interfacial layer between a fullerene (n-type semiconductor) layer and a metal electrode in organic solar cells [1, 2]. The chemical structure of the BCP is shown in Fig. 1. By inserting BCP layer with the thickness of several nanometers, the electrical conductivity of the organic solar cell and its power conversion efficiency were improved. The mechanisms, however, for the improvement in the electrical properties at the interface between BCP and metal electrode is not well understood yet. In this work, we studied the electronic structure at the interface between BCP and several kinds of metals by ultraviolet photoemission spectroscopy (UPS).

2. Experimental

The UPS measurements (hν=21.2eV) were carried out at the beam line 11C in KEK Photon Factory. Au, Ag, Al, In, Mg, and Ca were used as the electrode materials. The electrode metals were deposited on silicon substrates. BCP was deposited on the metal surface at room temperature with the deposition rate of 0.6nm/min. The base pressure in the UPS chamber was 1.2×10^{-10} Torr, and the pressure during deposition was 2.7×10^{-9} Torr. The thickness of the deposited layer was measured to be 4, 8, 16, 32, 50, 100Å by quartz vibrator.

3. Results and Discussion

Figs. 2(a) and (b) show the UPS spectra of BCP on Au (a) and Ca (b) based on the Fermi level position of the metal. The spectral shape corresponding to the bulk state of BCP was observed for the BCP thickness more than 50Å in both cases. The HOMO level of BCP was indicated by an arrow in the figure. There is no peak other than the Au and BCP related peaks in the UPS spectra of BCP/Au, however, a new peak was observed at around 1.5eV in the UPS spectra of BCP/Ca for the BCP thickness between 4Å and 50Å. The appearance of a new peak can be regarded as a generation of interface state.

Fig. 3(a) shows UPS spectra of BCP on Ca, Mg, Al, Ag, and Au in the region of the interface state. In addition to the case of BCP on Ca, interface states were observed for BCP on Mg, Al, and Ag as indicated by arrows in Fig. 3(a). The intensity of the interface state is normalized by that of the HOMO level. The intensity and the peak position are different each other probably due to the differences in the diffusion length of the metal atom and the strength of the interaction between BCP and metal [3].

Fig. 3(b) shows the work function of BCP on various metals. The values of the work function of BCP on Ca, Mg, In, Al, and Ag are almost the same and that on Au is different from others. Almost the same values of the work function of BCP may be due to the generation of the interface states.

BCP is well known as a strong chelating ligand forming coordinated compounds, therefore, it may be easy to form chemical bonding between BCP and metal atoms such as Ca, Mg, In, Al, and Ag. Such chemical bond may correspond to the interface state observed by UPS. The interface states are situated at around 1eV below the Fermi level of metal as shown in Fig. 3(a). This energy position corresponds to the position of 0.5eV above the lowest unoccupied molecular orbital (LUMO) of BCP. It may be possible to consider that electrons can through from LUMO of BCP to metal via interface state, that is, barrier height for electrons is lowered by the interface state. Such effect of the interface state results in the improvement of the device performance.

4. Summary

The electronic properties of BCP on metals were investigated by UPS. New interface states were observed in the case of BCP on Ag, Al, Mg, and Ca. The interface state may play an important role in improving electrical properties at the interface between BCP and electrode.

Acknowledgement

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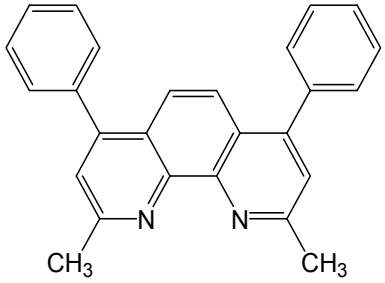

Fig.1 Chemical structure of Bathocuproine (BCP)

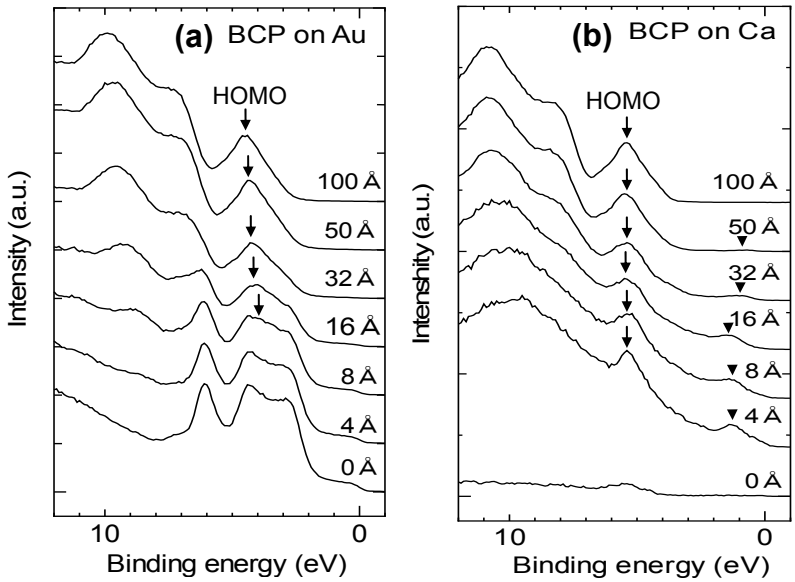

Fig.2 UPS spectra of BCP deposited on Au (a) and Ca (b) with various thickness of BCP

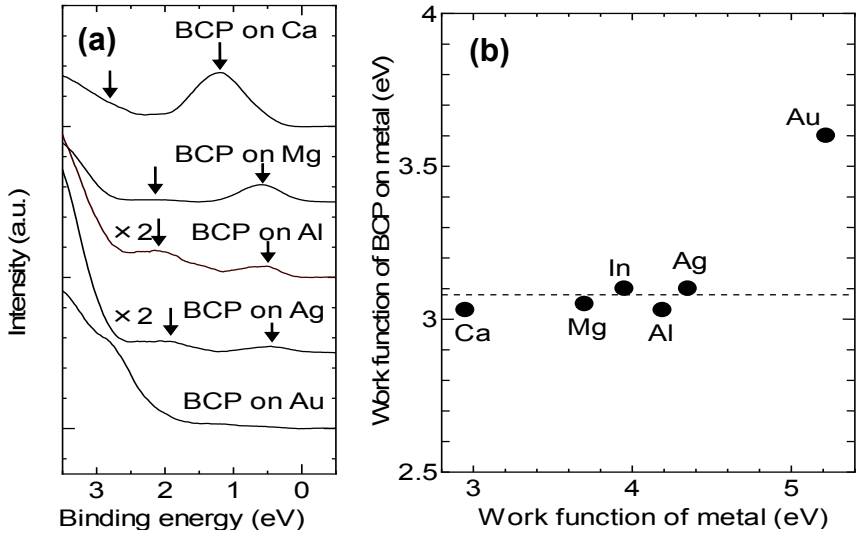

Fig.3 (a) UPS spectra of BCP on various metals, in the region of interface state. (b) Relation between work function of BCP on metal and work function of metal.