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Chemical bonding at NTCDA/metal interfaces

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Introduction

Planar π-stacking organic molecules have been shown to be excellent model compounds for studying the growth and optoelectronic properties of organic semiconducting thin films on metal substrates. Recently, perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) has been investigated as a model compound in organic diodes. In this study, we investigated the properties of 1,4,5,8-naphthalene-tetracaboxylic-dianhydride (NTCDA) films on Au and In metals which are useful materials for electrode. NTCDA molecule consists of both the naphthalene part and the anhydride group, and it is correlated with PTCDA simply by replacing the perylene part with naphthalene one (Fig. 1).

Experimental

All measurements were performed at room temperature in ultrahigh vacuum at a base pressure of 3×10^{-10} torr. NTCDA films were prepared by vacuum deposition.

Results and Discussion

Fig. 2 shows the C 1s XPS spectra for NTCDA on Au and In. The C 1s spectrum of NTCDA film at the deposition of 200Å on Au consists of two distinct peaks labelled (1) and (2), as has been reported previously [1]. These peaks can be assigned to the two different carbon atoms of NTCDA, that is, carbon in C-O bonding and in C-C bonding, respectively, as shown in Fig.1, referring to the electronegativity of oxygen and carbon atoms. These two peaks are observed even at the 10Å deposition on Au, and both the ratio of their intensities and the splitting energy are almost the same between the 10Å and the 200 Å deposition. These results indicate that the MOs of the NTCDA are not much modified by adsorption on Au surface. Therefore, it is considered that the interface between NTCDA film and Au is structurally abrupt and not reacted.

In Fig. 2, the C 1s XPS spectrum for the NTCDA deposition of 50Å on In is also shown. Though the full width at half maximum of the peak (2) is almost the same as that on Au, the peak (1) becomes very broad and shoulder-like structure. This suggests that the carboxylic anhydride of NTCDA molecule contributes to the reaction between NTCDA and In atom. The contribution of the carboxylic anhydride to the bonding is also confirmed by the O 1s spectra, which suggests that the oxygen atoms at the C=O contributes to the bonding between NTCDA molecule and In atom.

Summary

From the XPS results, it can be concluded that the reactivity of NTCDA with metal strongly depends on the ionization energy of metal atom, and that the oxygen atoms in the C=O bonding contributes to the bonding with In atom.

References

[1] D. Gador et al., J. Electron Spectrosc. Relat. Phenom. 96 (1998) 11.

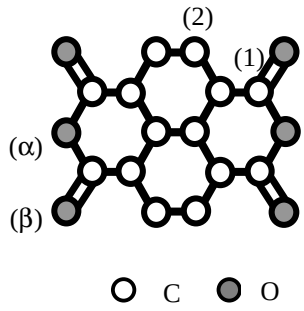

Fig. 1

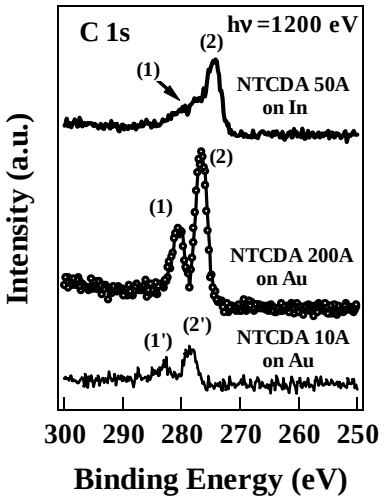

Fig. 2

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