Lower hole-injection barrier between pentacene and HDT-modified gold with lowered workfunction

Ki Pyo Hong,[1] Jong Won Lee[1], Sang Yoon Yang[1], Kwonwoo Shin[1], Hayoung Jeon[1], Se Hyun Kim[1], Chan Eon Park[1,*]

[1]Department of Chemical Engineering,
Pohang University of Science and Technology, Pohang, Korea

Introduction

Through photoemission spectroscopy (PES), we studied the injection barrier at interface between gold and pentacene with 1-hexadecanethiol (HDT), which is well-known material to form self-assembled monolayer (SAM) on gold and has 2.3 D dipole along molecular axis[1], leading to a low work function of metal so expected to have larger injection barrier between pentacene and metal at interface. From this study, it was revealed that pentacene on HDT-modified gold showed smaller hole injection barrier than that of none-treated even though the modified gold has 0.8 eV lower work function which is opposed to that a metal with lower work function gives higher hole injection barrier.

Experimental

The gold substrate was prepared by evaporation onto a SiO_2 wafer with an adhesion layer of a 30 nm titanium film deposited on the wafer before the deposition of 100nm gold. After deposition, the gold substrates were then immediately immersed into a 3×10^{-3} mol solution of HDT, purchased from Aldrich, in ethanol for 2 days. The substrates were thoroughly rinsed with ethanol and dried with a N_2 flow. Then substrates were loaded into a UHV chamber (base pressure of ~10^{-10} Torr) at the 4B1 beam line in the Pohang Accelerator Laboratory (PAL). The pentacene films were deposited at a rate of 0.1Å/s and each growth step, the sample were characterized in situ using UPS, 21.2 eV in normal emission and XPS, 650 eV. Also, 20 nm thick pentacene film on both gold and HDT-modified gold was characterized through XRD at the 10C1 beam line (wave length ~1.54 Å) in PAL.

Results and discussion

From the ultra-violet photoemission spectroscopy (UPS) (He I) electron distribution curves (EDC), work functions of bare gold and HDT modified gold were determined and the values are 4.86 eV for the bare gold and 4.06 eV for the modified gold. From the UPS EDC, the hole injection barrier at interface was 0.83 eV for pentacene on bare gold. In contrast, the hole injection barrier was 0.67 eV for pentacene on HDT-modified gold with no polarization-related shift observed. Figure 1 shows the molecular level positions from results of those UPS measurement.

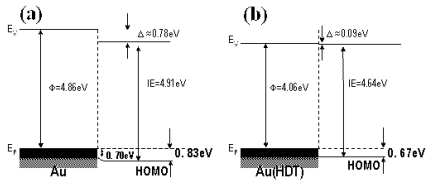

Figure 1. (a) Band diagram of the interface between pentacene and gold and (b) band diagram of the interface between pentacene and HDT-modified gold

This smaller injection barrier on HDT-modified gold with lower work function can be explained by two factors. The first factor is absence of large vacuum level shift observed generally when pentacene was deposited at early stages on gold.[2] The other is the difference in ionization energy due to different crystalinity. We obtained information on the crystalinity of pentacene through X-ray diffraction (XRD) experiment. From the XRD pattern, we calculated coherence length and we explained smaller ionization energy with this coherence according and polarization energy.[3] Alternatively, this lower ionization energy can be explained as electronic splitting of HOMO in terms of "delocalized" of band theory.[4]

Conclusions

We have performed UPS in-situ experiment to measure hole injection barrier between pentacene and HDT-modified gold. From this work, we found out that injection barrier between metal and pentacene is not determined only by work function of metal but also characteristics of metal surface and crystalinity of organic semiconductor which determines position of HOMO level.

References

[1] D. M. Alloway, M. Hogmann, D. L. Smith, N. E. Gruhn, A. L. Graham, R. Colorado, Jr., V. H. Wysocki, T. R. Lee, P. A. Lee, N. R. Armstrong, *J. Phys. Chem. B* **2003**, 107, 11690

[2] W. R. Salaneck, K. Seki, A. Kahn, J. J. Pireaux, *Conjugate Polymer and Molecular Interfaces,* Marcel Dekker, NY, USA, **2002**

[3] N. Sato, K. Seki, H. Inokuchi, *J. Chem. Soc., Faraday Trans.* **1981**, 77, 1621

[4] J. Cornil, J. Ph. Calbert, J. L. Bredas, *J. Am. Chem. Soc.* **2001**, 123, 1250