7A/2003G259

Metal induced gap states at organic insulator/metal interface

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Introduction

At the alkali halide/metal interfaces, we have revealed the existence of metal induced gap states (MIGS) [1]. Alkali halide is a typical ionic crystal, while a solid organic material is a typical molecular crystal. It is, thus, attractive to know whether MIGS are also formed at the organic insulator/metal interface, and to compare the character of MIGS at the organic/metal interface with that at the alkali halide/metal interface. In the present study, we have studied the electronic structure of a typical organic insulators *n*-alkane; octane (C_8H_{18}) and tetratetracontane (TTC; $C_{44}H_{90}$).

Experiment

The experiments were performed with an UHV chamber at the soft x-ray beam line BL-7A of the Photon Factory. TTC was evaporated on Cu(001) with the substrate temperature of 300 K using a Knudsen cell. Real-time observation of crystallinity and orientation of the films was done by reflection high energy electron diffraction (RHEED). The octane 1 ML and multi layer films were prepared by exposing Ni, Cu(111) substrates to gaseous octane at 180 K and 120 K, respectively. C K-edge NEXAFS spectra were obtained by the partial electron yield method using a micro-channel plate.

Results and Discussion

Figure shows the pre-edge feature of 1 ML thick octane/Cu, Ni(111) and TTC/Cu(001). Well pronounced pre-peaks appeared just below the bulk edge onset for all films. Since NEXAFS qualitatively provides information on the density of states of unoccupied states, the appearance of the pre-peak below the edge indicates that new states are formed below the vacuum level and above the Fermi level. The intensity of the pre-peak was obtained by subtracting the bulk component from the spectra, and it is shown in the figure. The intensity ratio of the pre-peak is 0.30 : 0.27 : 0.45 for octane/Cu(111) : octane/Ni(111) : TTC/Cu(001).

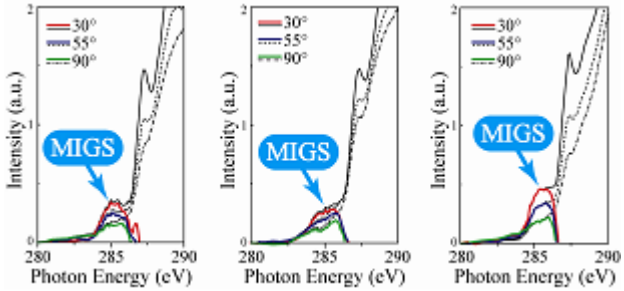

Figure: Pre-edge feature of 1 ML thick octane/Cu(111), octane/Ni(111), and TTC/Cu(001).

We then discuss the origin of the pre-peak observed by NEXAFS. If a chemical bond is formed between an organic molecule and Ni, Cu metal substrates, metal 3d band would interact with the orbital of the organic molecule. Ni 3d band locates at Fermi level, while Cu 3d band locates at about 3 eV below Fermi level. Since the pre-peak observed by NEXAFS originates from unoccupied orbital, intensity of the pre-peak would increase with a decrease in energy difference between LUMO of *n*-alkane and 3d band, that is, Fermi level and 3d band. Therefore, intensity of the pre-peak for octane/Ni(111) would be larger than that for octane/Cu(111), if the pre-peak originates from chemical bonding states. However, there is little difference in the intensity of the pre-peak between octane/Ni(111) and octane/Cu(111), suggesting that the pre-peak does not originate from chemical bonds. Furthermore, the adsorption energies of *n*-alkane molecules on metal surfaces are rather small and the molecule-surface interaction is considered to be quite weak and categorized to be not chemisorption but typical physisorption. In addition, the appearance and shape of the pre-peak for organic insulator/metal are similar to those for alkali halide/metal system, where MIGS are formed at the interface. The above results and discussion indicate that the pre-peak observed by NEXAFS originates from the states formed by the proximity to a metal. The states can be qualitatively understood as MIGS. MIGS are thought to accompany metal wave functions whose (exponential) tails penetrate into the insulating side of the interface. We can reveal that MIGS are formed at the organic insulator/metal interface.

Finally, we discuss the character of MIGS at the organic insulator/metal interface. First, the pre-peak appears irrespective of the number of carbon, suggesting general formation of MIGS at the organic insulator/metal interface. Second, the formation of MIGS does not depend on whether the metal band is d band or sp band. Third, from the results of polarization dependence of NEXAFS, the MIGS extends along the interface normal direction.

References

[1] M. Kiguchi *et al.*, Phys. Rev. Lett. 90 (2003) 196803.

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