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Atomic and electronic structures of TTC/Cu(001) interface

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Introduction

Alkanes are expected for insulator materials in the application of light, flexible devices. Though reduction of a work function, softization of the C-H vibration etc. have been reported, there remains uncertain points for the organic/metal interfaces. Among the alkanes, we concentrated on teteratetracontane (TTC; a long normal chain alkane (n=44)), which is a typical organic insulator expected for the various applications and has been studied as a model system of an organic insulator/metal interface. In the present study, we aimed at obtaining detailed knowledge for atomic and electronic structures of the interface of TTC and substrate metal using S K-edge NEXAFS and XPS. A 1 ML thick TTC film can be epitaxially grown on Cu(001), thus, TTC/Cu(001) interface is an ideal system to study the electronic structure of the organic insulator/metal interface.

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). C K-edge NEXAFS spectra were obtained by the partial electron yield method using a micro-channel plate. C 1s XPS were taken at the normal emission using a hemispherical electron energy analyzer (GAMMADATA SCIENTA, SES-2002).

Results and Discussion

RHEED measurements showed that a single-crystalline TTC film grew heteroepitaxially on Cu(001) with its molecular long axis parallel to the [110] azimuth of Cu(001). The observed streaks in RHEED patterns indicated that the 1 ML film was atomically flat, that is, a well-defined insulator/metal interface was prepared.

Figure shows the polarization dependence of NEXAFS spectra for 1 ML thick TTC/Cu(001) together with that for multi layer TTC. In the TTC film spectrum, sharp C1s-to-σ * (C-H) and broad C1s-to-σ * (C-C) peaks are observed at 288 eV, and 293 eV. Intensity of the σ*(C-H) peak is larger for grazing x-ray incidence (30°), while the σ*(C-C) peak is larger at the normal x-ray incidence. The σ*(C-C) peak is assigned to the transition whose transition moment is parallel to the molecular long axis.

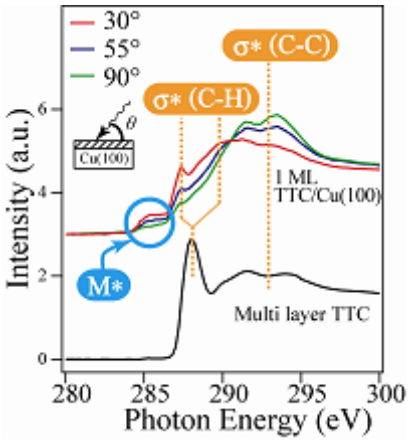

Figure: The polarization dependence of C-K edge NEXAFS spectra for 1 ML thick TTC/Cu(001) together with that for multi layer TTC. All the spectra are normalized by their edge-jump.

According to this peak assignment, the average inclination angle of the TTC molecules from the surface is determined to be 20(±10)°.

We then discuss the electronic structure of these interfaces. For the 1 ML TTC film, σ*(C-H) peak splits into two peaks; 288.0 eV peak splits into 287.2 eV and 289.8 eV peaks. This peak splitting might come from interaction of the molecule with the substrate. The σ*(C-H) orbital is the lowest unoccupied molecular orbital (LUMO). The LUMO and highest occupied molecular orbital (HOMO) would significantly interact with the metal substrates, compared with other orbitals. For the 1 ML film grown on metal substrates, LUMO of TTC interacts with the metal substrates, and thus, bonding and anti-bonding orbitals are formed. The splitting peaks could be assigned to these bonding and anti-bonding orbitals. XPS measurement showed a charge transfer from metal substrate to TTC film, indicating the strong interaction between them.

In addition to these peaks, another well pronounced pre-peak (M*) can be observed just below the bulk edge onset for the 1 ML thick TTC film. This peak should correspond to the metal induced gap states (MIGS). The details are described in another report comparing with octane/metal interfaces.

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