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.

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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