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# C K-NEXAFS of *n*-Alkane on Graphite (0001)

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## Introduction

Self-assembly of alkyl chains on an inert solid surface is one of fundamental phenomena in surface science and nano technology. A monolayer of long *n*-alkane on a graphite surface with a density 10 % larger than that of an *n*-alkane crystal was reported for more than 30 years ago[1]. More recently, the structure of a monolayer was investigated by neutron diffraction and scanning tunneling microscopy, and it was revealed that *n*-alkane molecules are stacked in a lamella with the all-trans conformation and the long axis lying parallel to the graphite (0001) surface[2,3]. However, the intermolecular spacing in a lamella as well as the orientation of the short axis is still controversial until now.

The values 0.426 nm and 0.464 nm, both of which are smaller than 0.48 nm of the bulk, have been reported for the intermolecular spacing of an *n*-alkane lamella. The former is typical for the monolayer formed from the solution or liquid, while the latter is for that obtained by the vapor deposition. The smaller value corresponds to the perpendicular orientation of the short axis and larger one parallel. More direct determination of the orientation of the molecule requires complementary spectroscopic techniques including near edge X-ray absorption fine structure (NEXAFS). Carbon K-edge NEXAFS has been hardly used partly because of the difficulty of distinguishing the carbon atoms of an *n*-alkane monolayer from those of a graphite substrate.

In this study, we have measured the C K-NEXAFS spectra of a vapor deposited monolayer of *n*-$C_{36}H_{74}$ on graphite (0001). The signal from the monolayer was separated by using the depth profile of photoelectrons emitted in proportion to the absorption.

## Experimental

A piece of highly oriented pyrolytic graphite cleaved in the air was degassed in the ultrahigh vacuum chamber at 1000 K. *n*-$C_{36}H_{74}$ was evaporated from the glass cell on the clean surface at room temperature. C K-NEXAFS was measured with a partial electron yield method at BL-7A. Electrons were collected by a micro channel plate and a fluorescence back screen was imaged by a CCD camera to observe the distribution of electrons as a function of the escape depth.

## Results and Discussion

A black line in Fig. 1(a) shows the C K-NEXAFS spectra of *n*-$C_{36}H_{74}$ physisorbed on graphite (0001). Three peaks are assigned to the resonances of the excitation of the 1s electron to the $\pi^*_{CC}$, $\sigma^*_{CH}$/Rydberg, and $\sigma^*_{CC}$ orbitals. Figure 1(b) exhibits the depth profiles of the photoelectrons for two particular excitation energies. Since the $\sigma^*_{CH}$/R resonance at 288 eV is observed only for the *n*-$C_{36}H_{74}$ overlayer, a red line is inclined to a grater channel number which corresponds to a more shallow escape depth. In contrast, photoelectrons excited with the energy of 305 eV mainly come from the substrate. Each profile for each excitation energy was fitted by these two profiles by using the least square fitting method and the extracted curves are shown as a blue line (substrate) and a red line (*n*-$C_{36}H_{74}$) in Fig. 1(a). Detailed analysis with gscf3 calculations will be reported later.

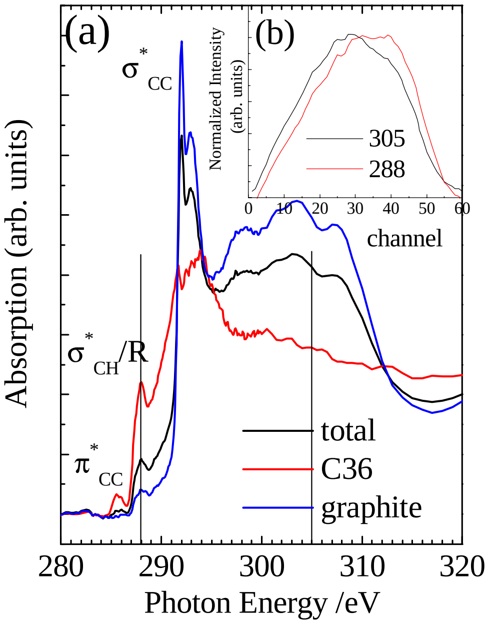

Figure 1. (a) C K-NEXAFS spectra of as measured (black line), extracted curve for the substrate (blue line), and for *n*-$C_{36}H_{74}$ (red line). (b) Depth profile of photoelectrons excited at the energy 288 eV, which represents the signal from the *n*-$C_{36}H_{74}$ overlayer, and 305 eV, which mainly contains the signal from the substrate.

## References

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