

NEXAFS Study of Orientational Ordering Effected by Rubbing in Pentacene/Octadecyltrichlorosilane Thin Films

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Last few years have seen an increasing activity in the research of organic semiconductor materials because of their potential applications in molecular electronics. It is now generally agreed that the transport efficiency of charge carriers is sensitively dependent on the molecular orientation order in the organic materials. To this end, a NEXAFS study of pentacene grown on top of organic thin film of *n*-alkyltrichlorosilane (OTS) self-assembled on oxidized Si(100) was carried out. Both the monolayer and multilayer of OTS were used and subsequently treated with and without mechanical rubbing before being served as organic-modified substrates. NEXAFS measurements in both polar- and azimuthal-angle scanning modes were attempted to address the issues of molecular alignment along surface normal and of anisotropic alignment possibly induced by rubbing.

Fig. 1 presents the polar-angle dependent carbon *K*-edge NEXAFS spectra for pentacene of 6-layer thick (A), and one monolayer thick (B) grown on unrubbed OTS. The polarization dependence analysis of the resonance intensity indicates that the aromatic plane of pentacene tilts away from substrate surface by 61° for the monolayer case, and 73° for the 6-layer case, respectively. It needs to be stressed that the OTS layer underneath the pentacene also contributes to the carbon NEXAFS signal and the component contribution needs to be titrated out first before a meaningful appraisal of pentacene contribution can be made. The orientation of pentacene determined is schematically shown in Fig. 2.

Figure 1. Polar angle dependent carbon *K*-edge NEXAFS spectra for 6-layer pentacene (A) and one monolayer pentacene (B) grown on unrubbed OTS.

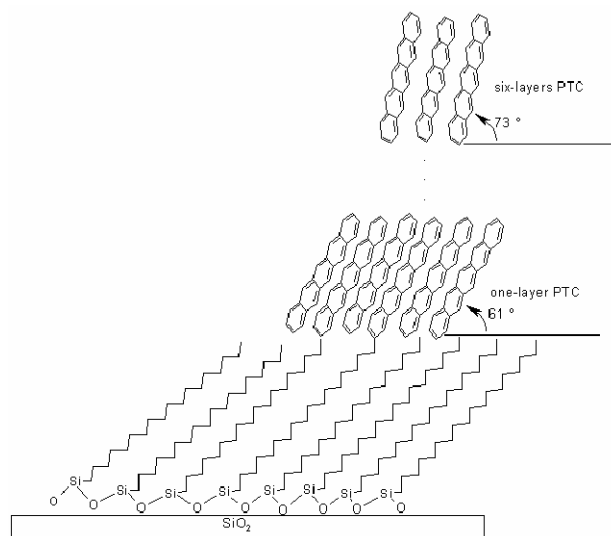


Figure 2. Schematic representation of the orientation of pentacene films on unrubbed OTS, determined from a careful fitting of data in Fig. 1.

Fig. 3 shows the azimuthal angle dependence of carbon *K*-edge NEXAFS spectra for 6-layer pentacene on rubbed OTS. Clearly, there is no observable trend for the intensity change with the azimuth, suggesting that the rubbing of OTS does not induce an anisotropic distribution of orientation of pentacene molecules.

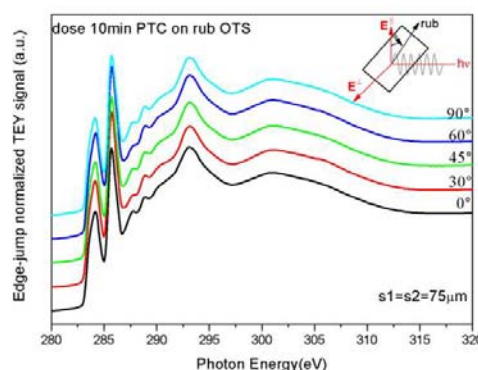
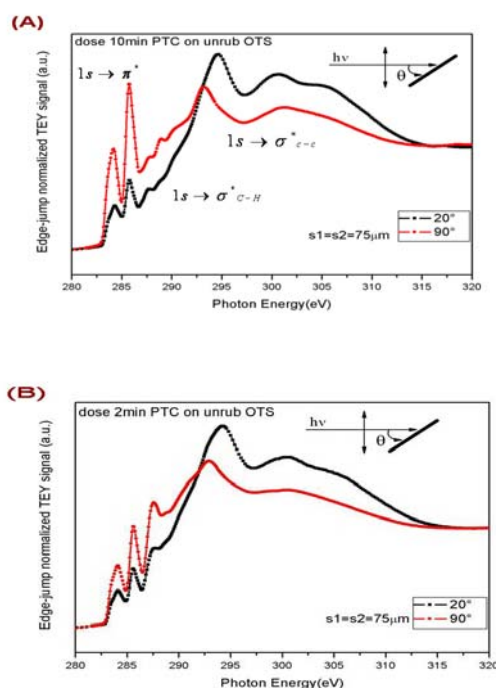


Figure 3. Azimuthal-angle dependent carbon *K*-edge NEXAFS spectra for PTC of 6-layer thick grown on rubbed OTS.