Thin PTCDA Films on Cu(111)

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Thin films of pi-conjugated organic molecules and polymers have found a wide application in optoelectronic devices such as organic light emitting diodes, displays, organic field effect transistors, etc. In this work, we report on a surface science study of 3,4,9,10-perylene tetra-carboxylic acid-dianhydride (PTCDA) thin films grown on Cu(111).

Fig. 1 shows the carbon *K*-edge NEXAFS spectra for a multilayer PTCDA on Cu(111) taken at different x-ray incident angles. Several prominent x-ray absorption peaks attributed to C1s to π* transitions can be observed. By consulting with earlier literature, these resonances can be identified as follows. The peaks at 284.3 and 285.7 eV are related to C1s to LUMO of perylene core. The peaks at 287.7 eV and 288.7 eV are associated with the transitions from carboxylic C1s to higher LUMO.

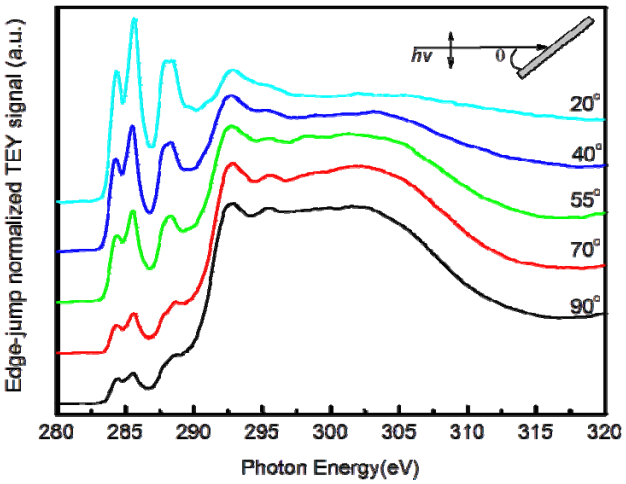

Figure 1. Carbon *K*-edge NEXAFS spectra of multilayer PTCDA on Cu(111) at different incident angle.

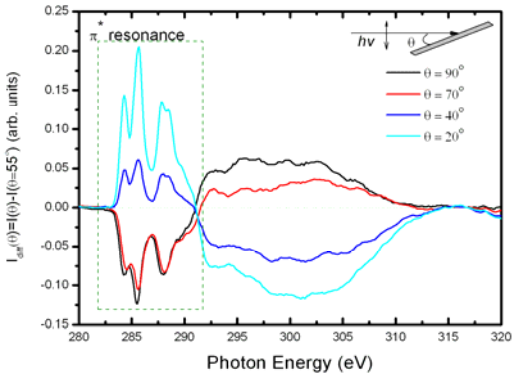

Figure 2. The angular dependence of intensity re-plotted in the form of difference spectra.

Fig. 2 shows a replot of the angular dependence of intensity in the form of difference spectra. The analysis of the angular dependence clearly shows both the perylene core and anhydride follow the same trend, validating the coplanar nature of the PTCDA due to the weak interaction of the multilayer with the copper substrate.

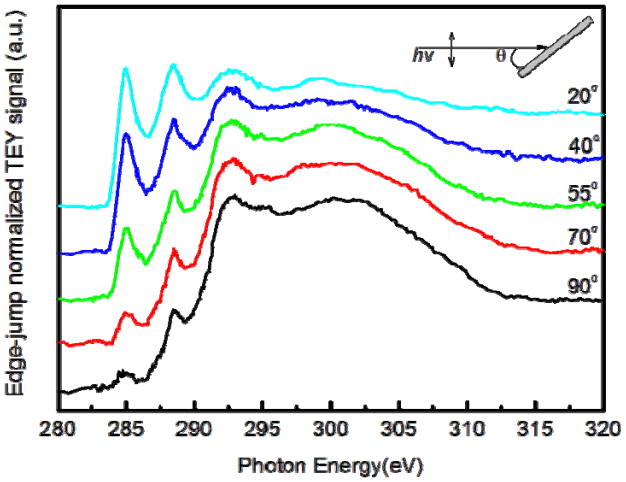

Figure 3. Carbon *K*-edge NEXAFS spectra for monolayer PTCDA on Cu(111).

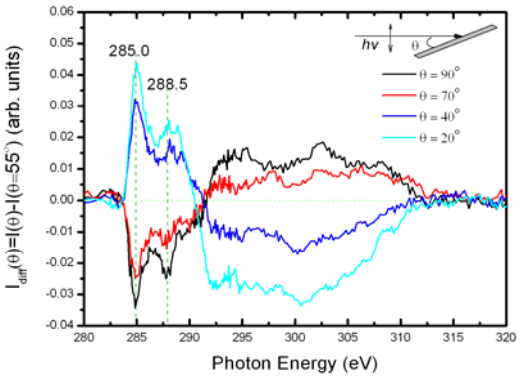

Figure 4. The difference spectra for the monolayer PTCDA on Cu(111) deduced from a replot of Fig. 3

Several conclusions can be drawn. First, in comparison with multilayer spectra, monolayer spectra exhibit a significant difference in the lowest 1s→π* transition due to the bonding to the surface. Second, in difference spectra, the angle dependence of 1s→π* transition from perylene at around 285 eV is different from that of carbonyl located at 288.5 eV, suggesting a different orientation between perylene and carbonyl. Third, the perylene core of the PTCDA monolayer sits flat on Cu(111) but the carboxyl group seems to bend out of plane because of charge transfer to the substrate. Further analysis based on O *K*-edge spectra reveals that a significant out-of-plane bending angle of about 20° for C=O group of PTCDA monolayer