Interfacial electronic structures at Fe/pentacene/Fe interfaces

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[Introduction]

The discovery of giant magnetoresistance (GMR) in 1988 is considered to be the beginning of new, spin-based electronics.[1,2] The application of organic in the spin valve arose great interest among researchers due to their long spin diffusion length. Since the first reported organic spintronic device in 1999,[3] devices fabricated from a variety of organic materials have been extensively investigated.

We investigate the interfacial electronic structures of the hetero-junction Fe/pentacene/Fe on Cu(100) substrate, using photoemission spectroscopy (XPS, UPS and NXEAFS). No chemical reaction was observed at both pentacene on Fe and vice versa interfaces. The hole injection barrier was about 0.95 eV between deposited pentacene and bottom Fe thin film. C K-edge NEXAFS revealed that the long axis of pentacene molecule was perpendicular to the surface plane.

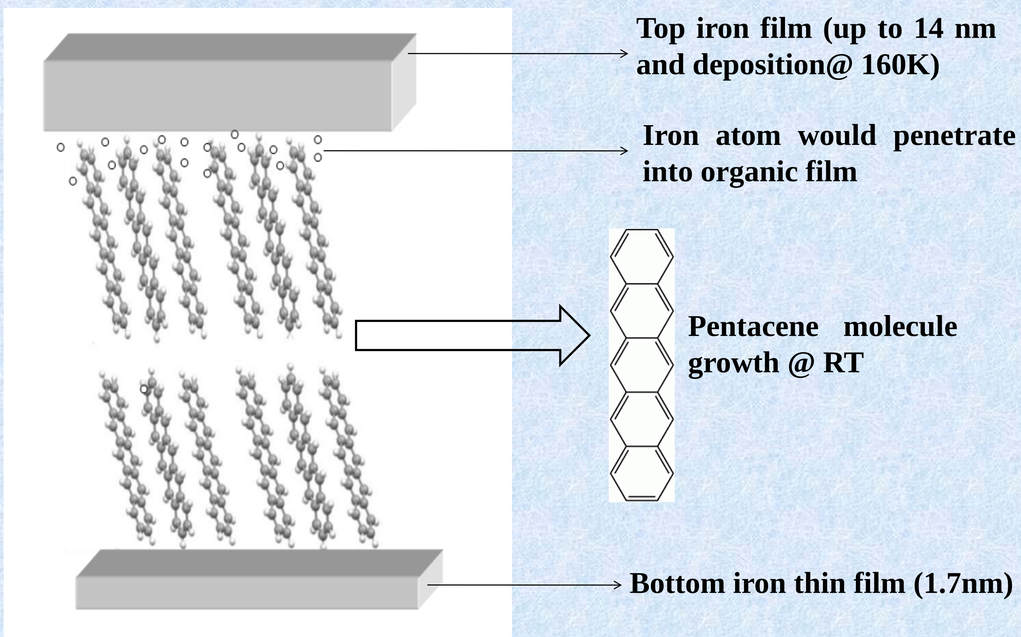
[Experiment]

Experiments were carried out in a UHV chamber with a base pressure of 1×10^{-10} mbar at the ***SINS*** beamline[4] of ***Singapore Synchrotron Light Source(SSLS)***.

The Cu(100) single crystal was sputtered and annealed for several circles and checked with XPS contaminations was negligible at the surface. The thickness of the Fe film was calibrated by the intensity decrease of the Cu 3p peaks. Pentacene was degassed at 150˚C during 12 hours before the experiment. The growth rate of pentacene at 190˚C was 10nm/10mins calculated from the attenuation of the Fe 3p peak. Firstly, 1.7nm Fe was deposited on Cu(100) substrate followed by the pentacene deposition, during which process both film growth and photoemission measurement were conducted at room temperature. While in the last step the manipulator was cooled down to 160 K using liquid nitrogen during the deposition of iron on pentacene thin film.

[Result and Discussion]

A. Schematic of our tri-layer structure on Cu(100)



B. Fe/pentacene interface (pentacene on Fe thin film)

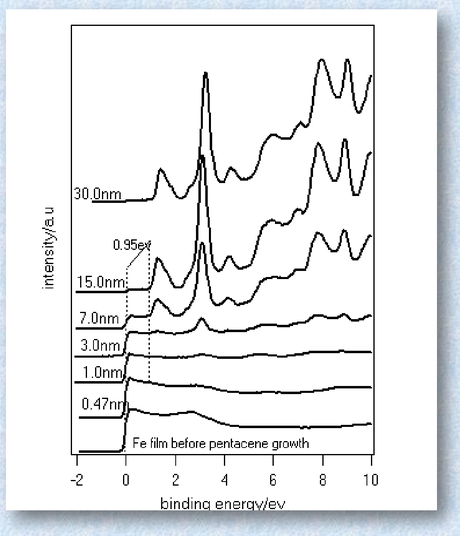


Fig. 1 valence band of pentacene molecules

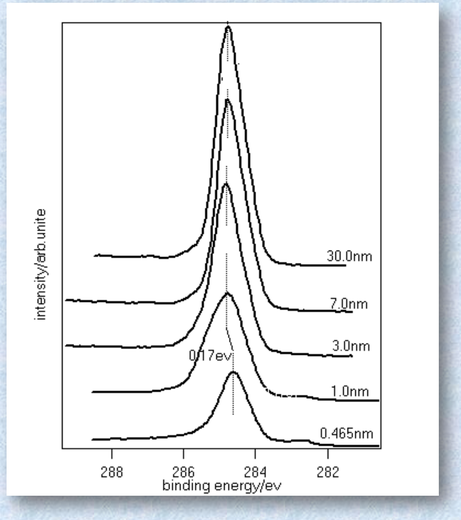


Fig. 2 C 1s spectra of pentacene deposited on Fe thin film

In Fig. 1, the hole injection barrier (from Fermi level to the onstet of HOMO) of pentacene on iron film is estimated to be 0.95 eV. A subtle shift of the C 1s peak toward higher binding energy with the increment of pentacene thickness in Fig. 2 could be explained by the decreasing of the polarization energy of the molecules due to weakening of screening effect from the metal substrate.

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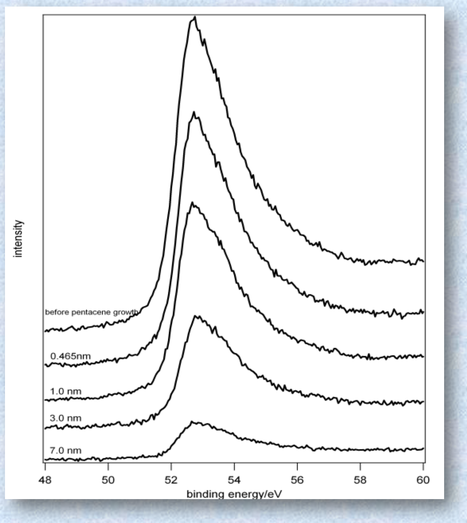


Fig. 3 Fe 3p spectra during pentacene growth

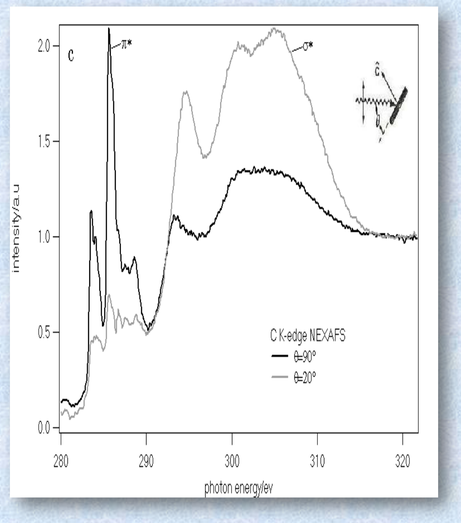
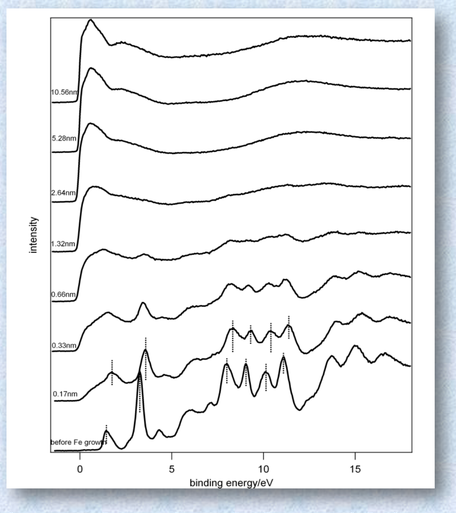


Fig. 4 C K-edge NEXAFS of pentacene @ nominal thickness 15 nm

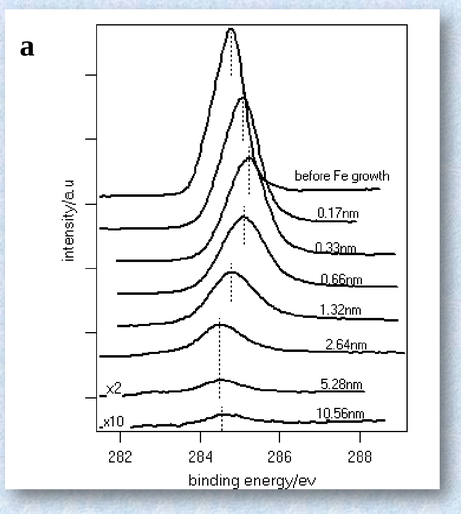
The shape of Fe 3p shows little difference in Fig. 3 indicating there is no chemical reaction between pentacene and iron. As calculated from angle-resolved C K-edge NEXAFS taken at a nominal thickness of 15nm, the angle between the long axis of pentacene molecule and surface plane is about 83±5˚.

C. Pentacene/Fe interface (Fe on pentacene thin film)



In Fig.5, HOMO levels of pentacene shift toward higher binding energy at low coverage of iron atoms, which is could be explained by the downward band bending at the interface caused by iron atoms doping. And Fe 3p shows little change except intensity increment (not shown here).

Fig. 5 Valence band along with iron growth on pentacene film



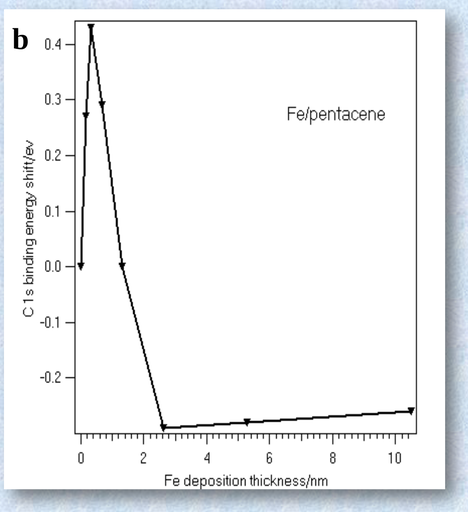


Fig. 6(a), (b) C 1s evolution and binding energy shift as a function of Fe thickness

During Fe deposition on pentacene thin film, the C1s binding energy shifts according to an interesting kinked behavior along with Fe thickness increment, as demonstrated in Fig. 4a and 4b. The initial shift of C 1s toward higher binding energy until a maximum 0.43 eV is as a result of surface doping of pentacene film by the penetrating iron atoms. With further deposition of Fe, C 1s shifts back to lower binding energy because polarization energy contribution arising from metallic film begins to dominate.

[Conclusion]

In this work, we investigated the interfacial band structure of Fe/pentacene/Fe hetero junction and our results could contribute to a more comprehensive understanding of the electronic (XPS, UPS) and morphological environment (NEXAFS)at the interface between ferrometals and organics.

However, there is no data of work function available so that to obtain a complete band alignment diagram of this tri-layer structure becomes impossible. In this case, it is urgent to work on this aspect in order to complement this experiment in the future.

1. *M. Baibich, et al. Physical Review Letter 61, 2472 (1988)*
2. *J. Barnas, A. Fuss, et al. Physical Review B 42, 8110 (1990)*
3. *K. Tsukagoshi, B. W. Alphenaar, et al. Nature 401,572 (1999)*
4. *X. J. Yu, O. Wilhelmi, H. O. Moser, et. al, J. Electron Spectrosc. Relat. Phenom. 144–147, 1031 (2005)*