

Determination of the crystal structure of substrate-induced pentacene polymorphs in fiber structured thin-films

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The intrinsic charge transport properties in organic crystals as calculated by numerical methods depend strongly on the molecular packing and arrangement in the crystal. Pentacene, showing one of the highest charge carrier mobilities among organic semiconductors, is known to crystallize in at least four polymorphs, which can be distinguished by their layer periodicity $d_{(001)}$. Only two polymorphs grow as single-crystals and their crystal structure has been solved. The substrate-induced 15.4 Å polymorph is the most relevant for organic thin-film transistor (OTFT) applications, however its crystal structure has remained incomplete as it only grows as a fiber structured thin-film. Here we extend the crystal truncation rod x-ray scattering technique to fiber structured thin-films. We determine the complete crystal structure of this polymorph grown on various substrates and find that the molecular arrangement within the unit cell is substrate dependent.

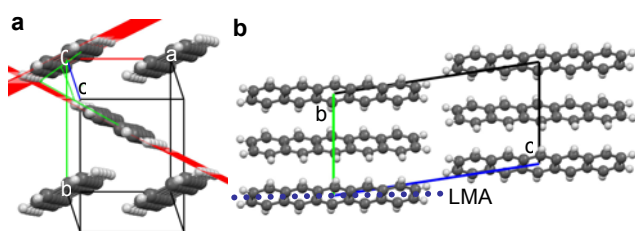


Figure 1: 3D view of 15.4 Å pentacene thin-film polymorph on SiO_2 . (a) top view, the herringbone angle between the two red molecule planes is illustrated in green. (b) side view, the long molecular axis (LMA) is illustrated as a dotted line.

References

- [1] S. Schiefer, M.Huth, A. Dobrinevski, B. Nickel
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