Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

Crystallisation kinetics in thin films of metastable phases: The polymorphism of dihexyl-terthiophene

Bernhard Wedl,[a] Roland Resel,*[a] Günther Leising,[a] Birgit Kunert,[a] Ingo Salzmann,[b] Martin Oehzelt,[c] Norbert Koch,[b,c] Antje Vollmer,[c] Steffen Duhm,[d] Oliver Werzer,[e] Gabin Gbabode,[f] Michele Sferrazza,[g] Yves Geerts,[f]

[a] *Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria*

[b] *Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor Straße 6, D-12489 Berlin, Germany*

[c] *Helmholtz Zentrum Berlin für Materialien und Energie - BESSY II, D-12489 Berlin, Germany*

[d] *Graduate School of Advanced Integration Science, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan*

[e] *Centre for Organic Electronics, The University of Newcastle, Callaghan, NSW 2308, Australia*

[f] *Chimie des Polymères, Faculte des Sciences, Université Libre de Bruxelles,Boulevard duTriomphe CP 206/0, 1050 Bruxelle, Belgium*

[g] *Département de Physique, Faculte des Sciences,Université Libre de Bruxelles, Boulevard du Triomphe, CP 223, B-1050 Bruxelles, Belgium*

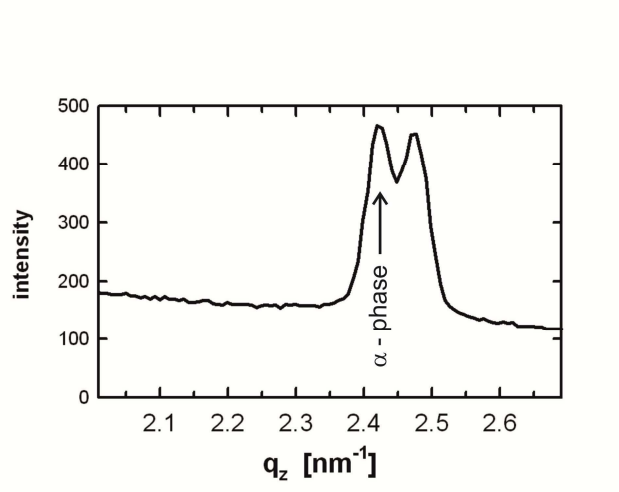

Figure S1: X-ray diffraction of a polycrystalline powder of the molecule dihexyl-terthiophene (DH3T) performed after heat treatment above the melting point.

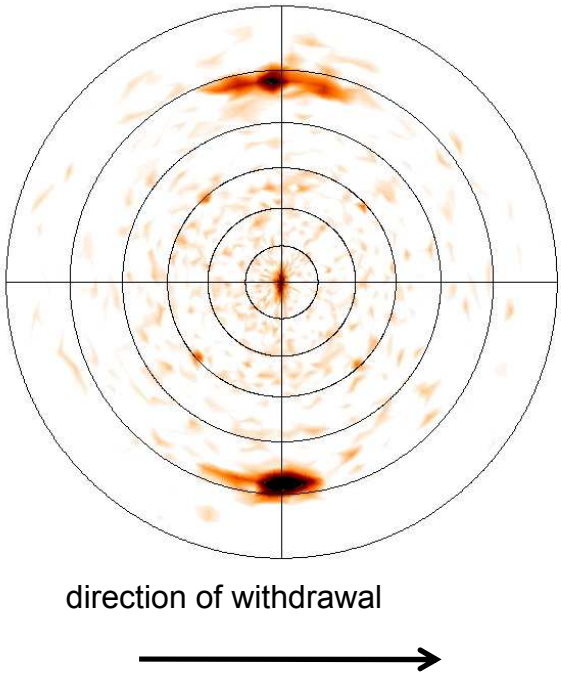

Figure S2: X-ray diffraction pole figure of a dip-coated film of the molecule DH3T (withdrawal velocity of 50 µm/sec) in respect to the direction of withdrawal. The measurement was performed at q = 26.0 nm^{-1} to monitor the spatial distribution of the -606 poles of DH3T crystallites. The strong features at χ / φ= 73° / 90° and 73° / 270° can be clearly assigned to the α-phase.

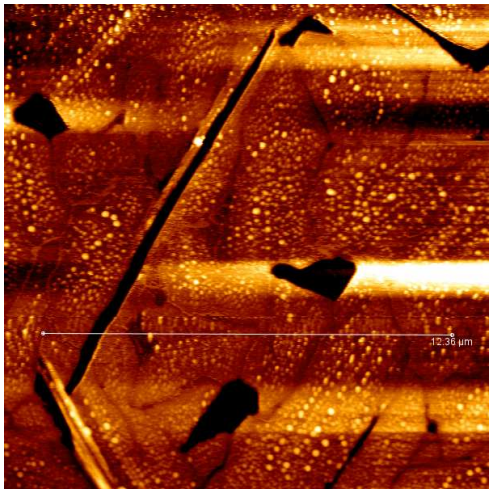

Figure S3: Atomic force microscopy micrograph of a vapour deposited film of DH3T with a layer thickness of 44nm. The image covers an area of 15µm x 15 µm.

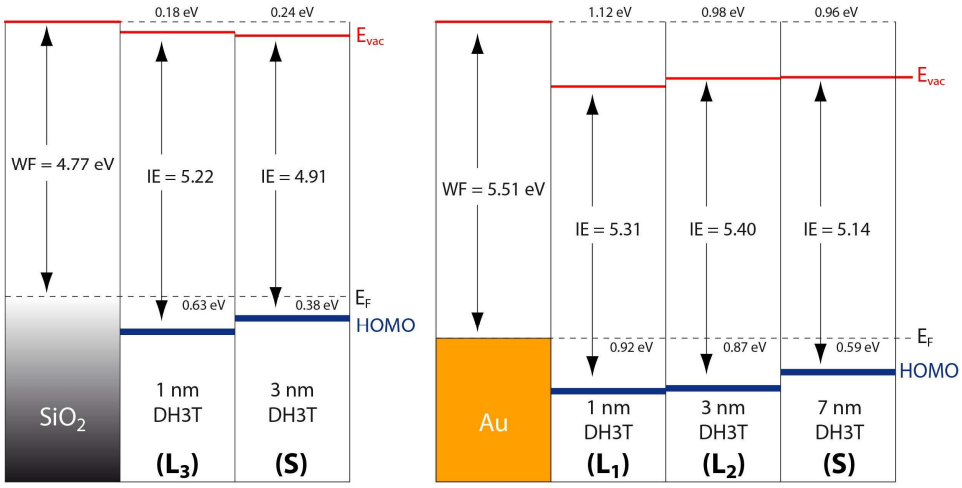

Figure S4: Schematic energy level diagrams for DH3T films of different thickness on SiOx (left) and polycrystalline Au (right) deduced from the UPS spectra depicted in Figure 8a. Both shifts of the vacuum level (E_{vac}) and changes in the ionization energy (IE) occur upon subsequent growth, which is explained by orientational transitions of DH3T (see main text). HOMO denotes the highest occupied molecular orbital, E_F the Fermi level, and L_1, L_2, L_3, and S the different molecular orientations discussed in the main text.

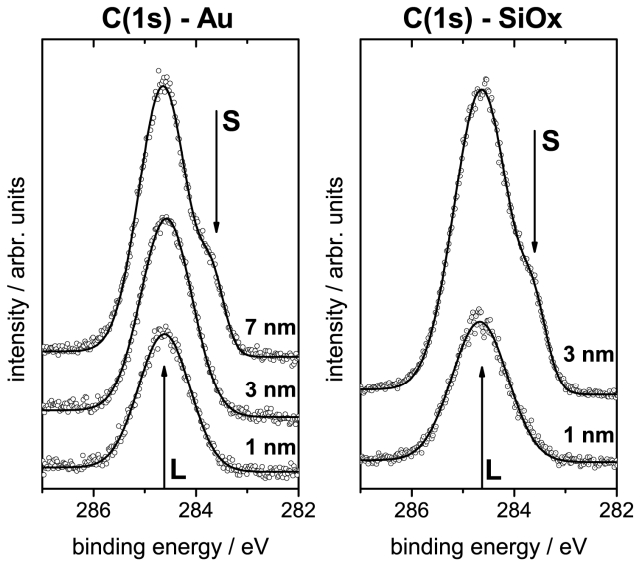

Figure S5: XPS-C(1s) results for DH3T thin films of different thickness prepared by physical vapour deposition on flame-annealed polycrystalline gold (left) and SiO_x (right) substrates demonstrating an orientational transition from lying (L) to standing (S) DH3T upon subsequent growth.