Supporting Information

Growth and Characterization of Centimeter-Scale Pentacene Crystals for Optoelectronic Devices

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1. Differential scanning calorimetry

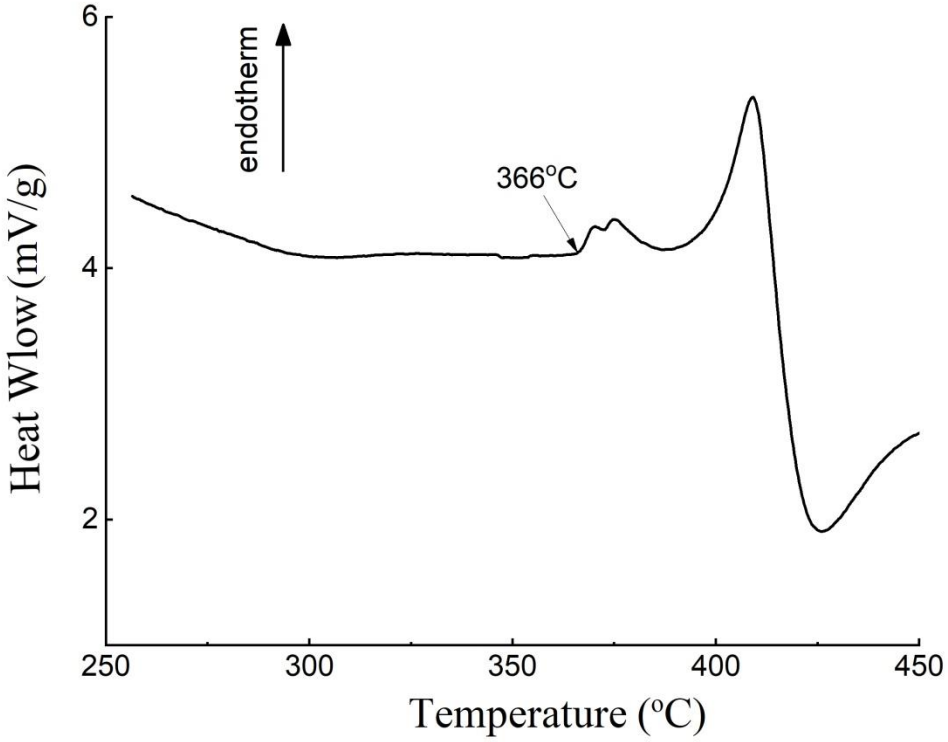


Figure S1. DSC curve of pentacene sample in sealed crucible.

2. Crystal growth

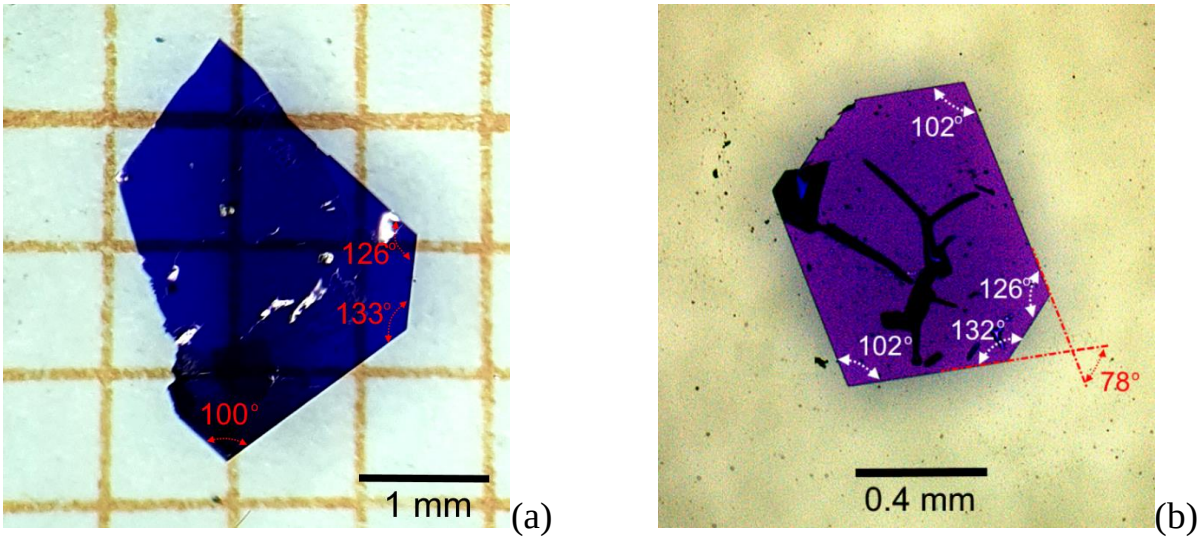


Figure S2. Pentacene crystals grown in a gradient thermal field.

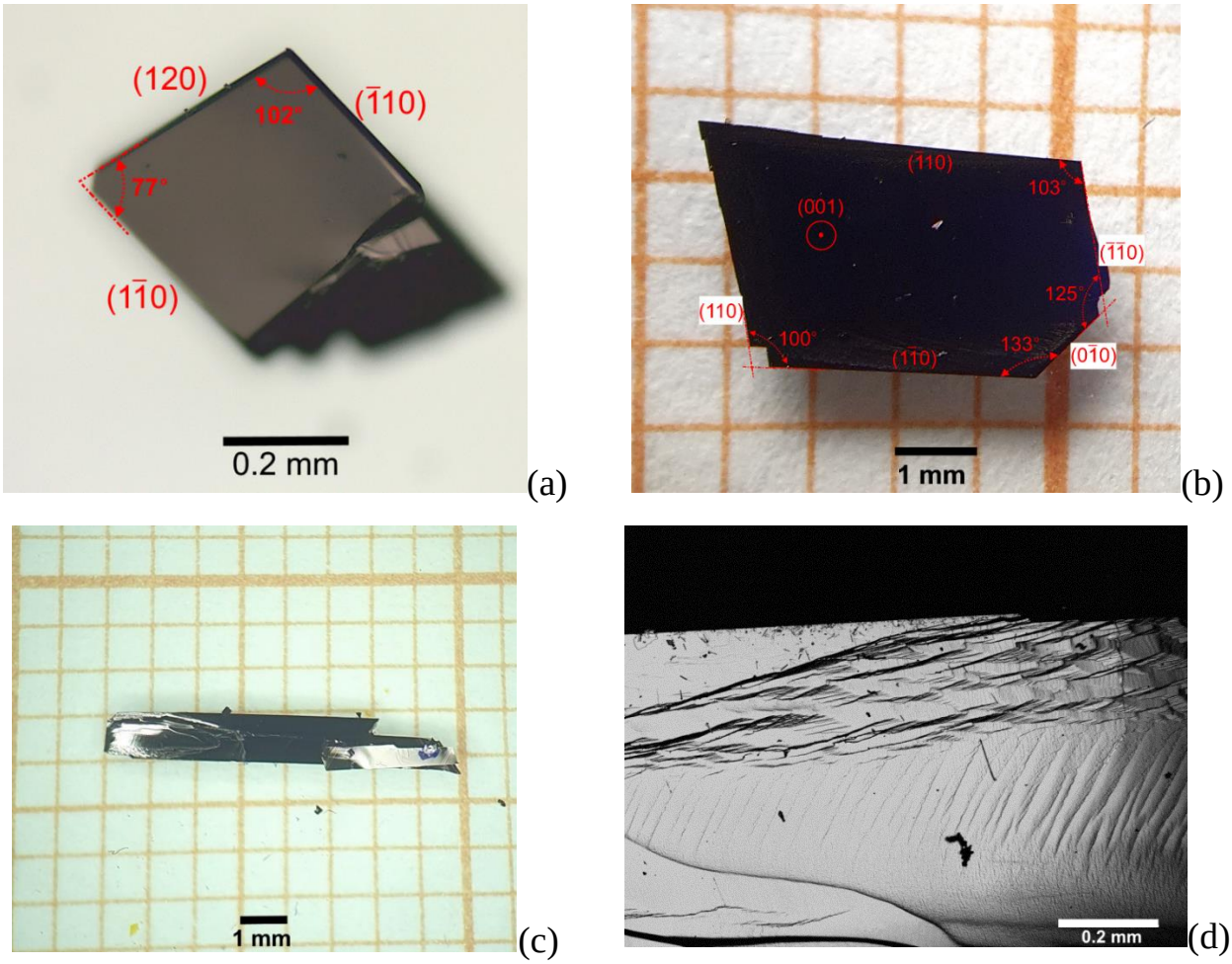


Figure S3. Crystals grown in a in a two-zone thermal field: (a), (b) flat Pc crystals with indication of angles between faces and indexes of faces; (c) elongated lamellar Pc crystals; (d) enlarged confocal image of surface of thick Pc crystal.

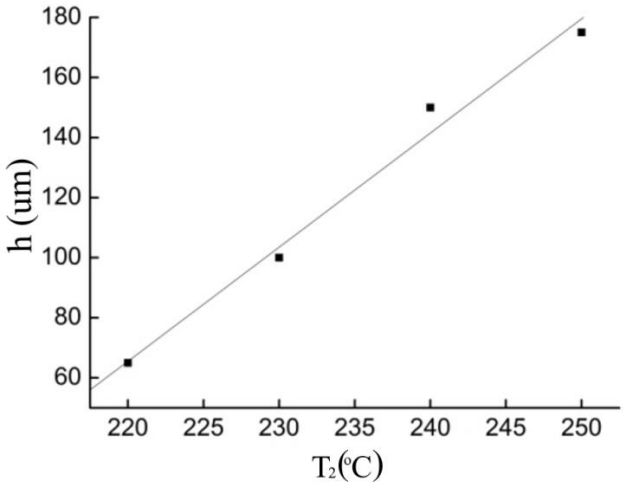


Figure S4. The dependence of the average thickness of the largest pentacene crystals in the growth zone on the temperature of the cold zone.

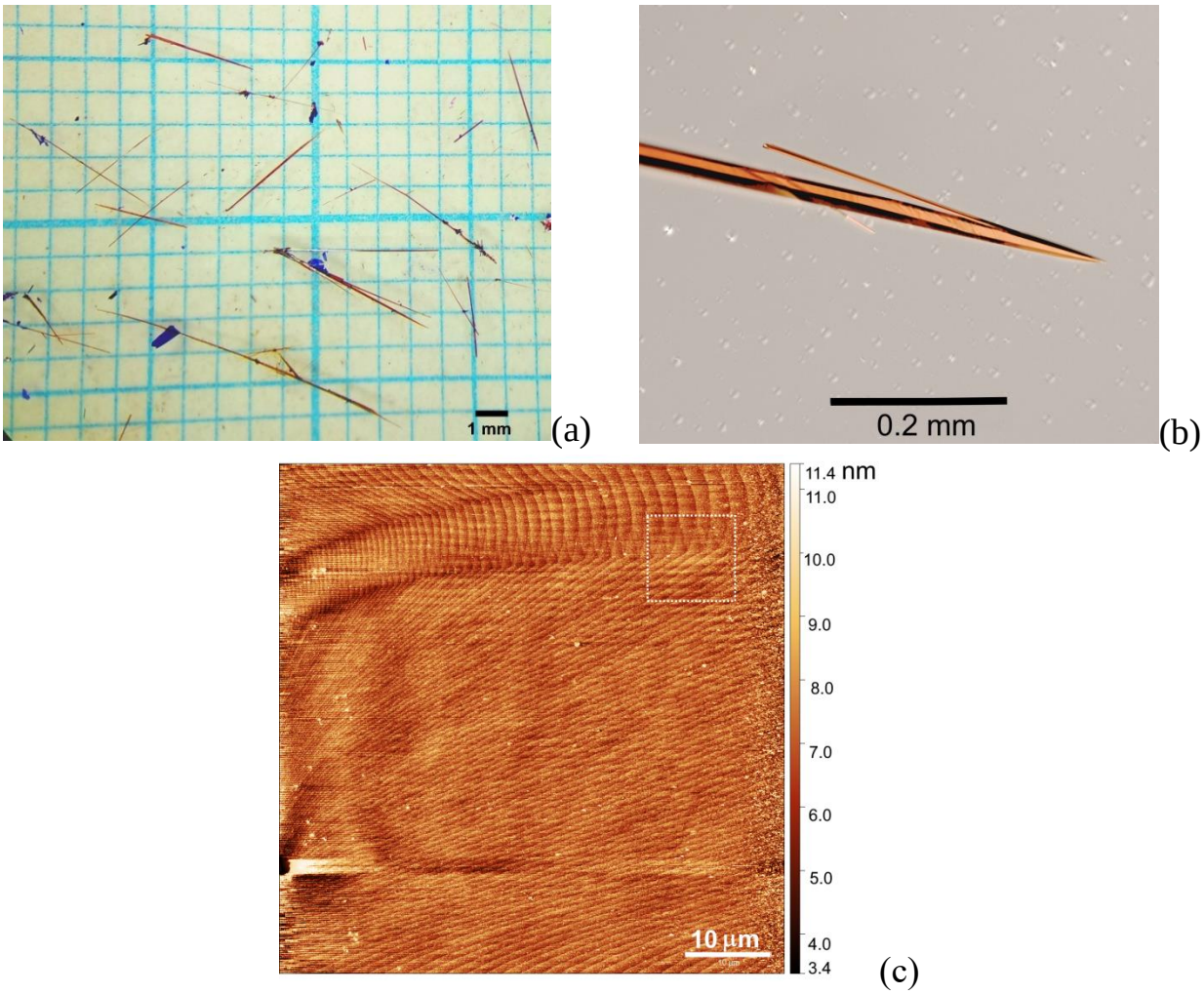


Figure S5. Images of golden needle crystals: (a) a collection of needle-shaped crystals with lamellar dark blue crystals on some of them; (b) enlarged optical image of crystal tip; (c) topographic AFM image of the surface of a developed crystal face (the scanning area covers almost the entire crystal in width).

3. Elemental analysis

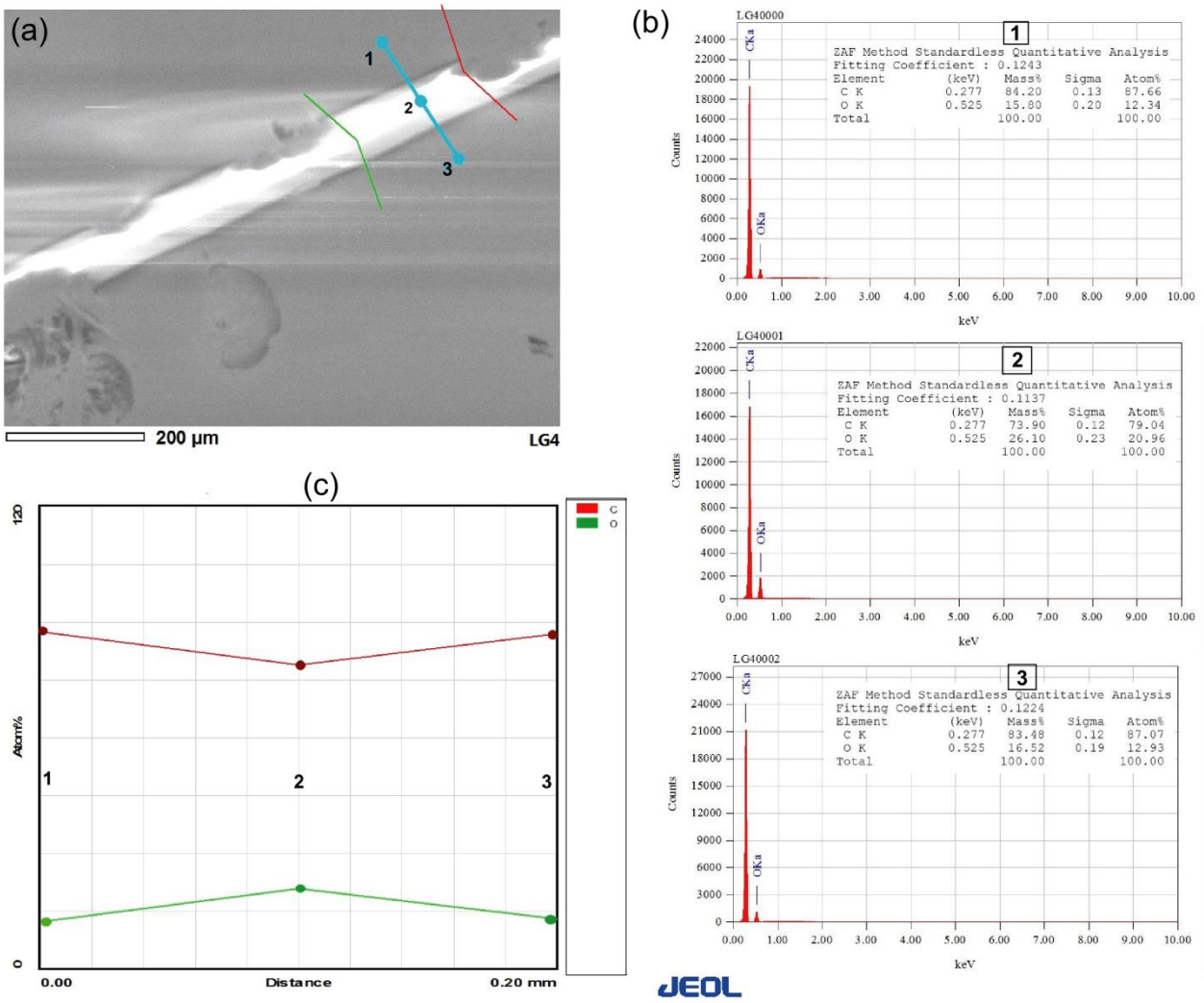
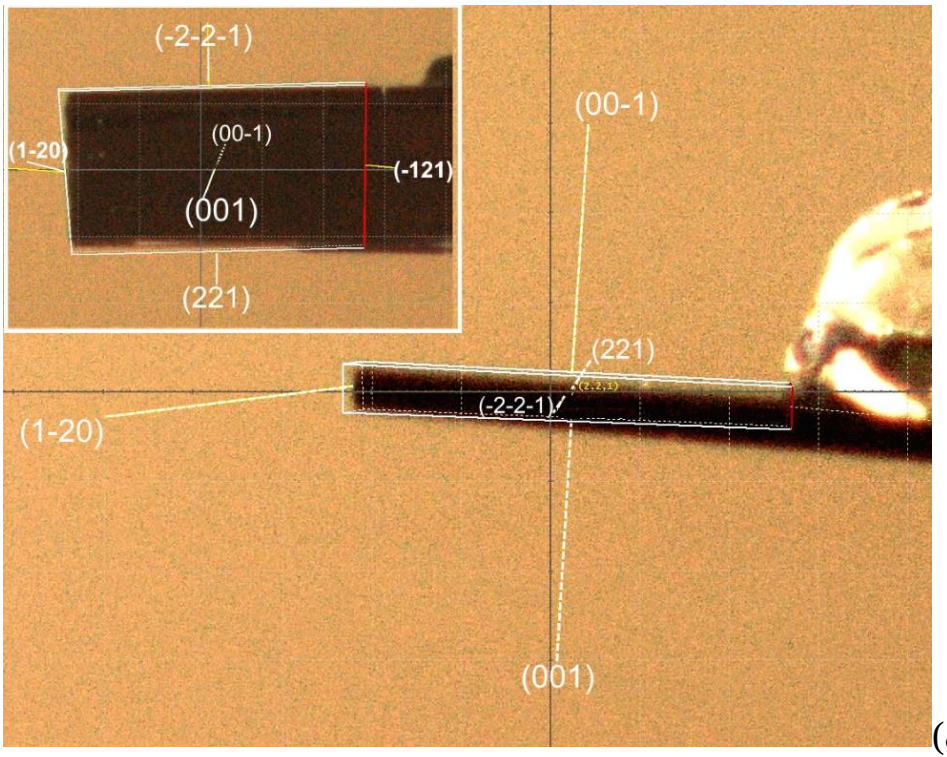
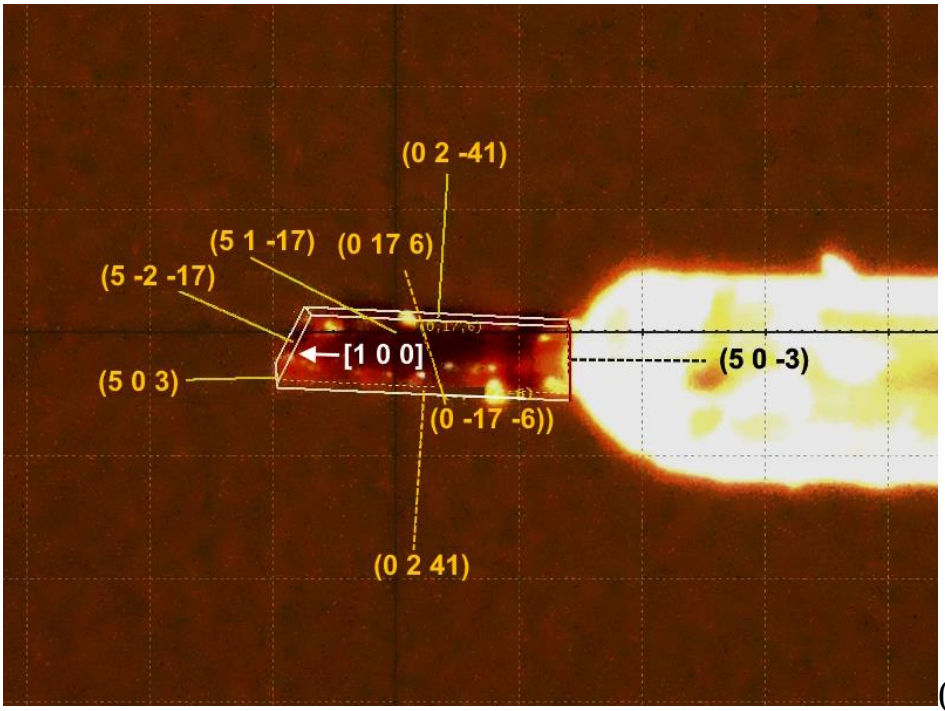


Figure S6. Elemental analysis of a golden needle crystal: (a) SEM image of crystal; (b) EDS elemental spectroscopy at the position shown in (a); (c) distribution of carbon and oxygen atoms inside (2) and outside the crystal (1,3). The crystal was placed on the surface of the carbon tape.

4. X-Ray Diffraction and crystal structure



(a)



(b)

Figure S7. Images of a single crystals of pentacene (a) and PD (b) with face indices determined in the X-ray diffraction experiment.

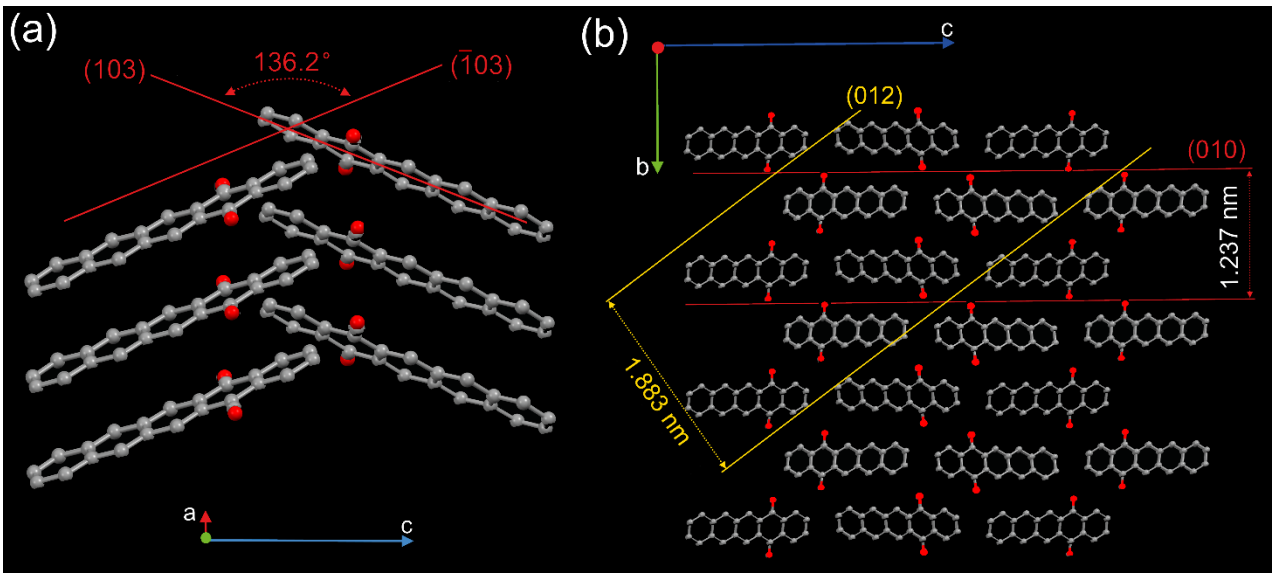


Figure S8. PD crystal structure model at 85 K: projections of the structure on the planes (010) (a) and (100) (b).

5. Electrical properties

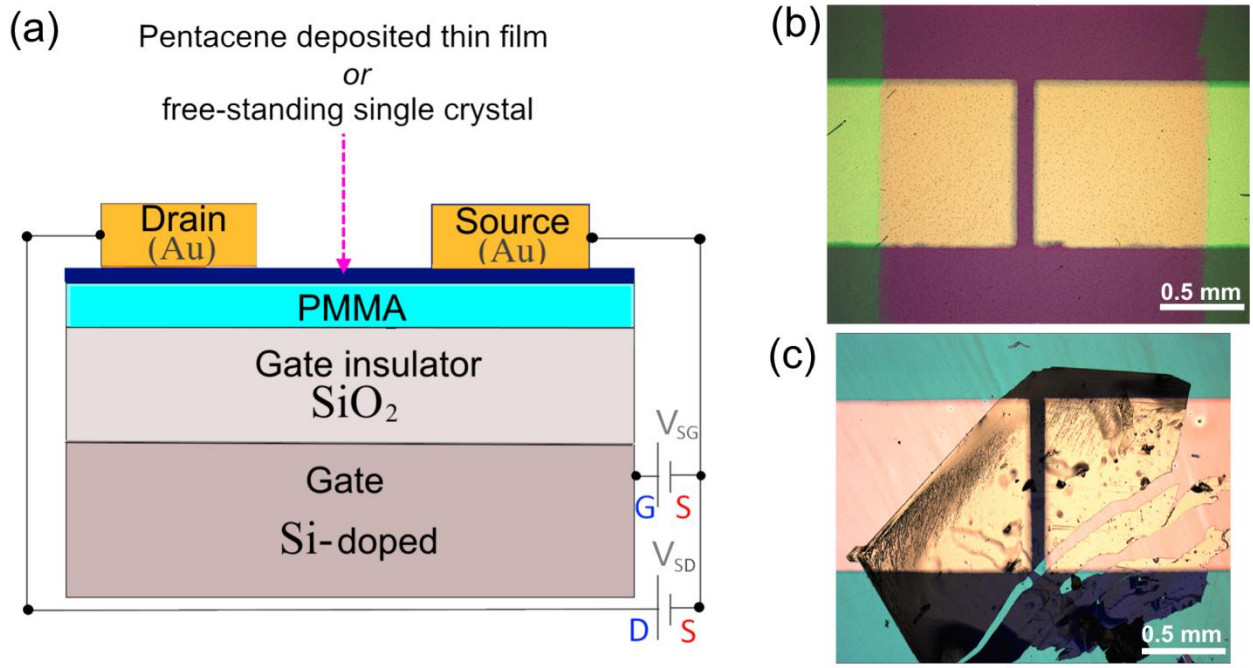


Figure S9. Diagram of the field-effect transistor device (a); photo-images of pentacene field-effect transistors based on thermally deposited polycrystalline layer (b) and single crystal (c).

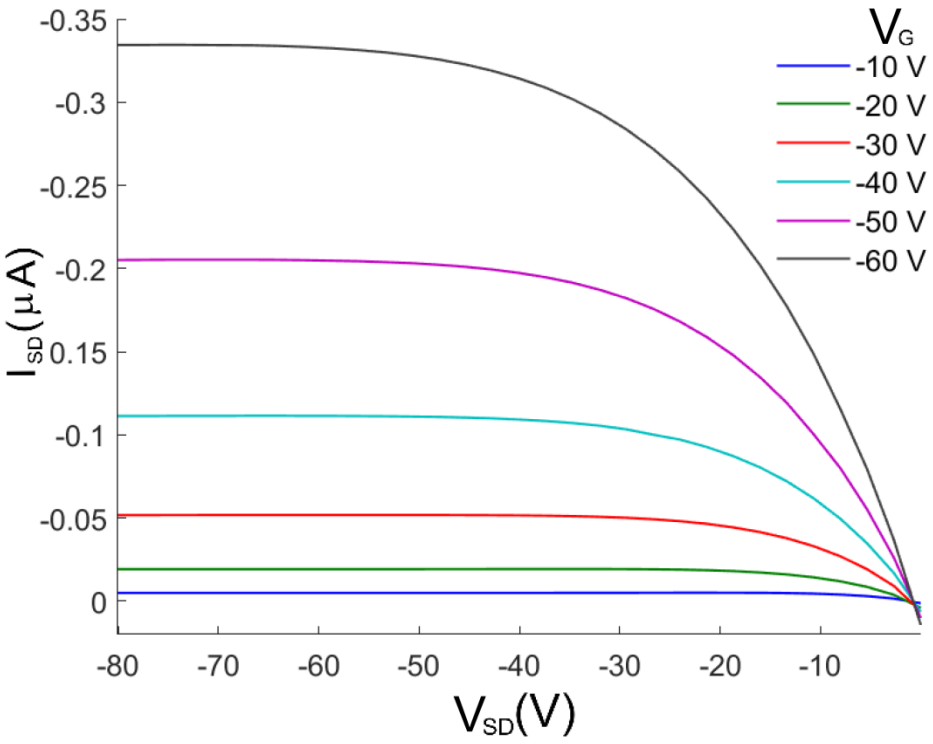
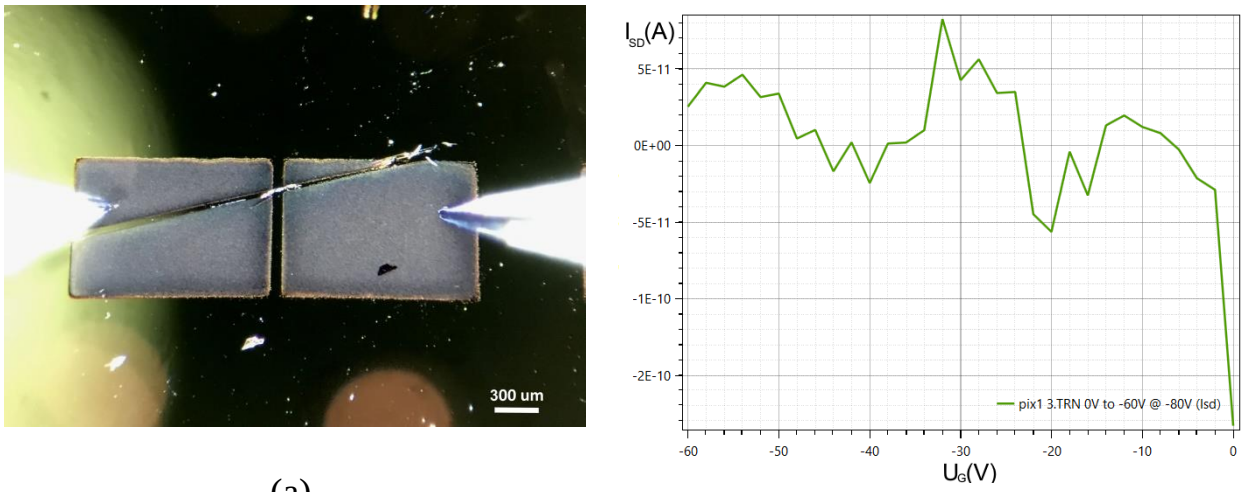


Figure S10. Output I-V characteristics for a thin polycrystalline layer based on the initial (unpurified) pentacene.



(a) (b)

Figure S11. Photo-image of a field-effect transistor based on a PD single crystal (a) and its I-V transfer characteristic (V_{SD}= -80 V).