Enhanced Phase Purity in Sexithiophene Thin Films through Laser Illumination

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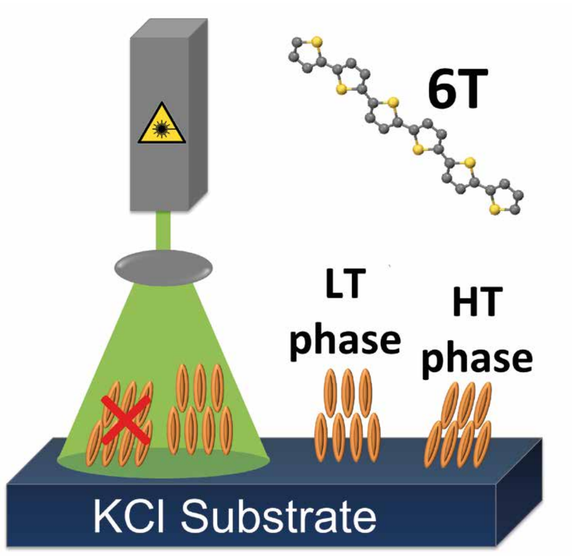
Growth Control through Light



Controlling the growth and crystallinity of organic molecules helps to increase the efficiency of organic thin film devices such as OLEDs or OFETs and has been addressed as on of the current challenges in thin film growth. Besides substrate temperature and molecular deposition rate there is an ongoing quest for additional ways to influence the molecular growth process [2]. With our study [1] we introduce light as new control parameter and show that the phase purity of α-sexithiophene (6T) can be increased through irradiation.

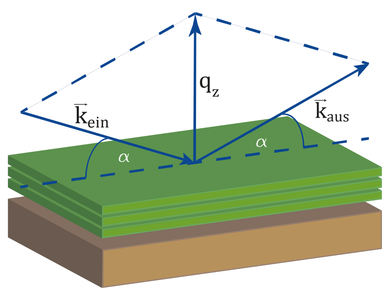
Methods

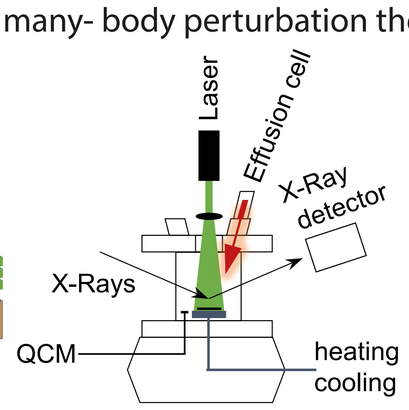
Growth
- Organic Molecular Beam Deposition (OMBD), base pressure of 10^{-8} mbar
- 6T on cleaved potassium chloride (KCl) substrate

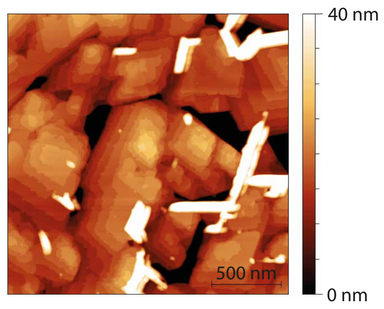
Growth Monitoring
- Real time, *in situ* x-rays experiments at MS beamline, Swiss Light Source

Growth Control
- 523nm Laser Light Source (1W/cm²)

Simulation
- Optical properties simulated with **`exciting`** code in the framework of density-functional and many- body perturbation theory (MBPT) [3]



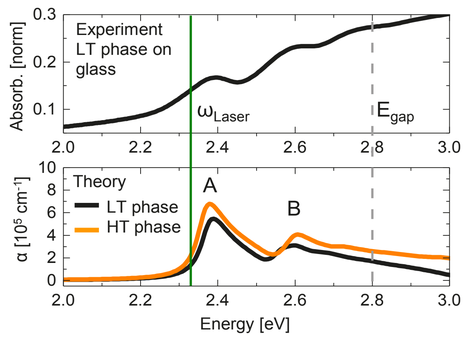




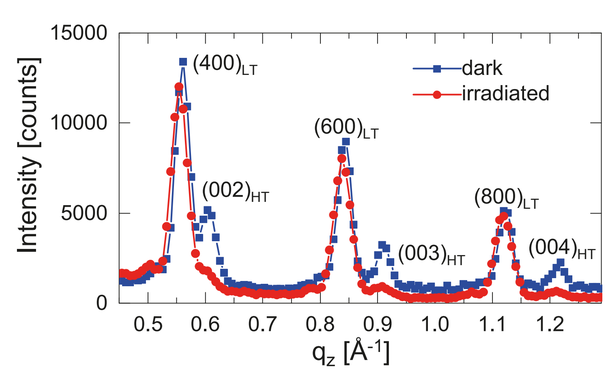
AFM image of 6T film on KCL

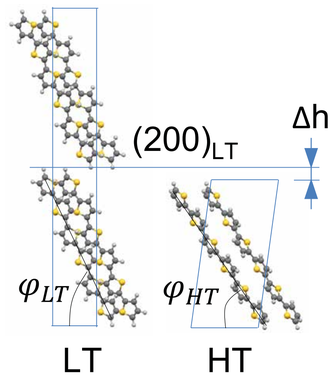
Optical Absorption of 6T Polymorphs

- Separate simulation of the absorption spectra of the 6T HT and LT polymorphs, since there is no experimental access to the isolated HT phase absorption spectrum
- Differing molecular tilt angle of the two phases leads to 20 % higher optical absorption of the HT phase

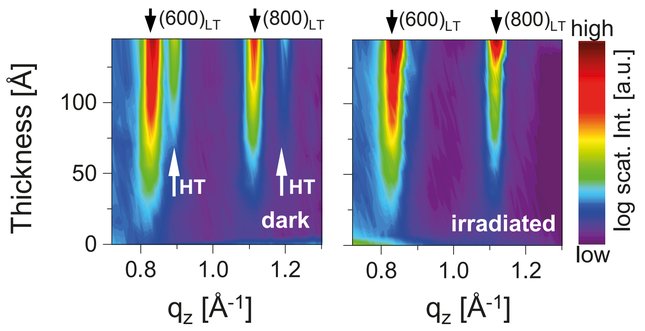


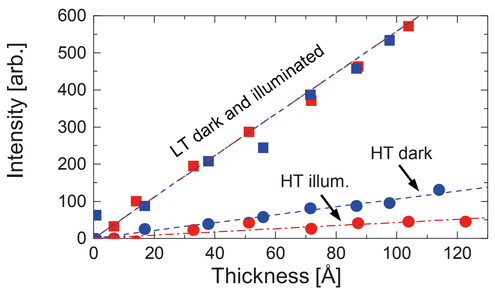
Phase-Purification by Illumination





- HT & LT polymorph of 6T coexist on KCl
- Irradiation with light reduces occurence of 6T HT phase
- Real-time *in situ* x-ray diffraction experiments highlight the suppression of the 6T HT crystal phase through light during the whole growth process

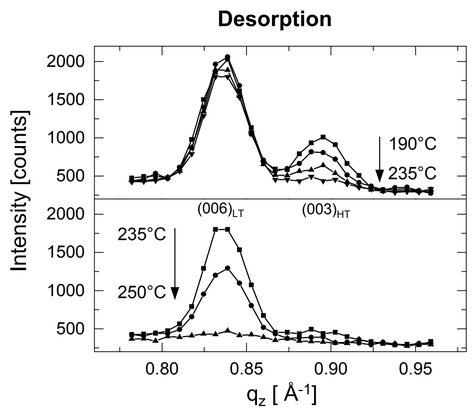




Thermal Stability of 6T Polymorphs

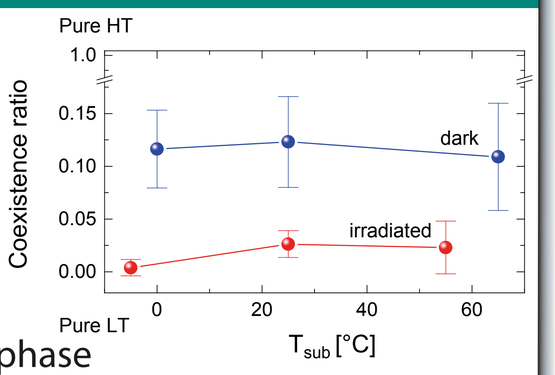
Differing desorption temperatures for LT and HT phases of 6T on KCL

- HT phase desorbs between 190°C and 235 °C
- LT phase desorbs between 235°C and 250 °C



Conclusion

- Phase purification by illumination is a robust effect over wide temperature range



Mechanisms of HT phase supression
- Phase Selective Optical Absorption => stronger heating of HT phase
- Lower thermal stability of 6T HT polymorph => suppressed nucleation

Perspectives
- Patterning through local growth control
- Increasing phase purity in other molecular materials

References

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