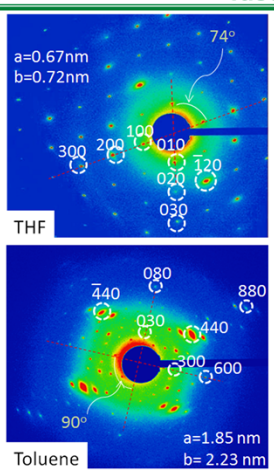
CNMS Staff Science Highlight

Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor



Selected area electron diffraction patterns of TES ADT thin films slowly crystallized from THF and toluene solutions in [001] zone.

Work performed at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory.

Scientific Achievement

We report a solvent-type-dependent polymorphism of a long fused-ring organic semiconductor and its crucial effects on charge transport.

Significance and Impact

A newly discovered polymorph of 5,11-bis(triethylsilyl-ethynyl) anthradithiophene (TES ADT) obtained using toluene solvent-assisted crystallization exhibits up to 10-fold higher hole mobility in organic thin film transistor devices than devices fabricated with other solvents. These results underscore the importance of crystalline polymorphism of organic semiconductors as a critical factor in determining the structure and properties of the resultant organic electronic devices.

Research Details

- A method for obtaining the new polymorph of TES ADT and its structure was discovered.
- Identified mechanism for charge transport enhancement based on intrinsic packing of the resultant TES ADT polymorphs.
- Density functional theory UV-Vis absorption and simulation.

J. Chen, M. Shao, K. Xiao, A. J. Rondinone, Y-L. Loo, P. R. C. Kent, B. G. Sumpter, D. Li, J. K. Keum, P. J. Diemer, J. E. Anthony, O. D. Jurchescu, J. Huang, *Nanoscale*, DOI: 10.1039/c3nr04341j

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Highlight Narrative: Polymorphism is widely encountered in organic solids due to the relatively weak intermolecular interactions (van der Waals type). In this work, we demonstrate that the specific intermolecular interactions between the solvent and aggregated clusters in the initial stage of crystallization can cause a remarkable polymorphism during the solution crystallization of TES ADT. This control over polymorphism is important because crystalline packings/polymorphs of TES ADT when processed at room temperature critically affect device performance, changing the maximum hole mobility by up to 10 times under the same testing conditions.

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