A compact model for organic field-effect transistors with improved output asymptotic behaviors

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The performance of organic field-effect transistors (OFETs) has known impressive progress over the last two decades. At the present time, a key topic in OFET research is device-to-system integration, which aims at realizing circuit-level systems such as displays, large-area sensors, RFID tags by using high-performance OFETs. A compact model captures the overall electrical behavior of a device into a fully analytical form and provides methods for analyzing unit devices and building higher-level circuits in SPICE-type simulators. There is a lack of widely accepted OFET models up to now and therefore, accurate and physically based compact modeling of OFETs is of great interest for organic circuit development. In this work, we report on an advanced compact model for OFETs with improved output asymptotic behaviors. Based on the unified model and parameter extraction method, we use a modified output asymptotic function that enables a precise fit of the finite saturation conductance and the low-voltage output conductance. The model covers all regimes of OFETs by a single analytical function. A systematic parameter extraction method is detailed with an example of curve fitting for pentacene-based flexible OFETs. The results show that the model-calculated curves are in excellent agreement with the experimental data, which confirms the validity of the model over a wide operation range.

Electronic states at the grain boundaries in the polycrystalline naphthalene

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Organic crystalline semiconductors based on small molecules are promising materials for electronic and optical devices such as organic light emitting diodes (OLEDs), organic thin film transistors (OTFTs) and organic sollar cells (OPVs). One of the limiting factors for charge carrier transport in polycrystalline organic semiconductors based on small molecules are grain boundaries. We investigated the electronic structure of grain boundaries in polycrystailline organic semiconductor naphthalene. Energy of the system was modelled using TraPEE potential for the interaction between atoms. Atomic structure was obtained by a Monte Carlo method. Electronic structure was obtained using the Charge patching method (CPM) [1], which is based on Density Functional Theory (DFT).
Results for small systems (1000 molecules) indicate that grain boundaries produce trap energy states within the band gap of the material. These states are localized on molecule pairs (called trapping pairs) at the grain boundaries with the distance between molecules significantly smaller than the distance between two adjacent molecules in a naphthalene crystal. Strong correlation between trapping pair mutual distance and trap state energy relative to the top of the valence band energy was found. As a consequence, on the basis of the densities of trapping pairs, densities of trap states for bigger systems (100 000 molecules) were calculated.

[1] N. Vukmirovic, L. Wang, J. Chem. Phys. **128**, 121102 (2008)