Simulation-assisted solution-processing method for large-area, high-performance C_{10}-DNTT organic semiconductor crystal


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Supplementary Information

**COMSOL simulation**

Three modules in COMSOL Multiphysics 4.4a are applied for the simulation.

![Model construction with COMSOL simulation](image1)

**Figure 1. Model construction with COMSOL simulation.** Domains 1, 2, and 3 are air, silicon and tetralin, respectively.

**Laminar flow**

Liquid profiles at different substrate temperatures and shearing speeds are captured by using a camera with high magnification lens. The images were turned into black and white, and then converted into DXF files, which can be inputted into COMSOL for model construction, as shown in Fig. 1. The solvent (Domain 2) is modeled as an incompressible Newtonian liquid by using Navier-Stokes equations:

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \nabla \cdot \mathbf{\sigma} + \mathbf{F} \tag{1}
\]

\[
\nabla \cdot \mathbf{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2}
\]

where \( \mathbf{v} = (u, v) \) is the velocity, \( \rho \) is the density of tetralin, \( \mathbf{\sigma} \) is the stress tensor, and \( \mathbf{F} \) is the gravitational force. Bnd 2 is set as the sliding wall with a specific speed to represent...
the shearing process. No slip conditions are applied to Bnd 3 and 4, but a slip condition is applied to Bnd 1.

**Heat transfer in fluids**

Heat transfer in liquid is solved (Domain 2). Convection and radiation at liquid-air interfaces are neglected. Heat transfer equation is solved as follows:

\[ \rho C_p v \cdot \nabla T = k \nabla^2 T \]  \hspace{1cm} (3)

\( C_p \) is the heat capacity of tetralin, \( T \) is the temperature, and \( k \) is the thermal conductivity. Bnd 2 and 3 are the temperature of the substrate and shearing blade respectively. Bnd 4 is thermal insulation. Evaporation induced heat loss is described as:

\[ J_L = -k \nabla T \cdot n \]  \hspace{1cm} (4)

\( J \) is the evaporative flux and solved in the following section, \( L \) is the latent heat of tetralin.

**Transport of diluted species**

Major governing equation of solvent transport in air (Domain 1) is:

\[ D \nabla^2 c = 0 \]  \hspace{1cm} (5)

where \( c \) denotes tetralin vapor concentration in air, and \( D \) is the diffusivity of solvent molecule (tetralin) in air \( (2.65 \times 10^{-5} \text{ m}^2/\text{s}) \). Initial concentrations of Domain 1, and Bnd 8, 9, and 10 are determined from the saturated vapor pressure of tetralin at 25°C. The concentration on Bnd 1 is determined from the vapor pressure and temperature relationship of tetralin, so that mass transport is coupled with heat transfer.

Evaporation flux is defined by:

\[ j = D \left( \frac{\partial c}{\partial x} n_x + \frac{\partial c}{\partial y} n_y \right) \]  \hspace{1cm} (6)
Surface energy is acquired by measuring contact angles of polar liquid (deionized water) and non-polar liquid (diiodomethane) and determined by using Owens, Wendt, Rabel and Kaelble (OWRK) method. Dispersion terms in the surface energy of PTS/SiO$_2$ and 12-PD-PA/BST (red in color) improve wetting property of tetralin solvent.
Figure 3. Morphology of optimized crystal. AFM image (a) and thickness profile (b) of continuous C$_{10}$-DNTT crystal. Despite nanoscale cracks, RMS roughness of crystal is < 0.2 nm.