Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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

Boyu Peng[1], Zongrong Wang[1] and Paddy Kwok Leung Chan[1, *]

1 Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong.

Correspondence and requests for materials should be addressed to Prof. P. K. L. Chan (email: pklc@hku.hk)

Supplementary Information

COMSOL simulation

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

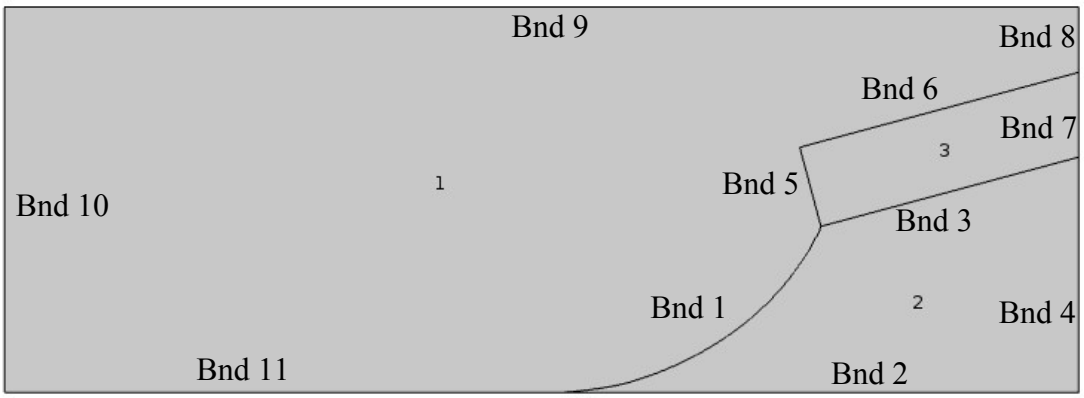

Figure 1. Model construction with COMSOL simulation. Domains 1, 2, and 3 are air, silicon and tetralin, respectively.

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:

$$\rho\left(\frac{\partial v}{\partial t} + v \cdot \nabla v)\right) = \nabla \cdot \sigma + F \quad (1)$$

$$\nabla \cdot v = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (2)$$

where $\boldsymbol{v} = (u, v)$ is the velocity, ρ is the density of tetralin, $\boldsymbol{\sigma}$ is the stress tensor, and $\boldsymbol{F}$ 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:

$$\rho C_p v \cdot \nabla T = k\nabla^2 T \tag{3}$$

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:

$$JL = -k\nabla T \cdot n \tag{4}$$

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:

$$D\nabla^2 c = 0 \tag{5}$$

where c denotes tetralin vapor concentration in air, and D is the diffusivity of solvent molecule (tetralin) in air (2.65×10^{-5} m^2/s). Initial concentrations of Domain 1, and Bnd 8, 9, and 10 are determined from the saturated vapor pressure of tetralin at 25^{o}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:

$$j = D\left(\frac{\partial c}{\partial x}n_x + \frac{\partial c}{\partial y}n_y\right) \tag{6}$$

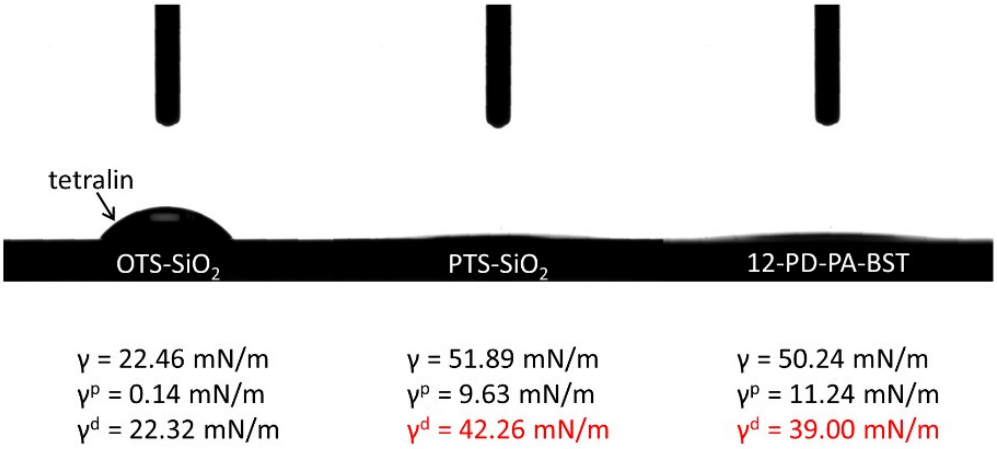

Figure 2. Tetralin contact angle on OTS treated SiO_2 and PTS treated SiO_2. Surface energy is acquired by measuring contact angles of polar liquid (deionized water) and non-polar liquid (diiodomethane) and determined by using Owens, Wendt, Rabel and Kaelble (OWRK) method. Dispersion terms in the surface energy of PTS/SiO_2 and 12-PD-PA/BST (red in color) improve wetting property of tetralin solvent.

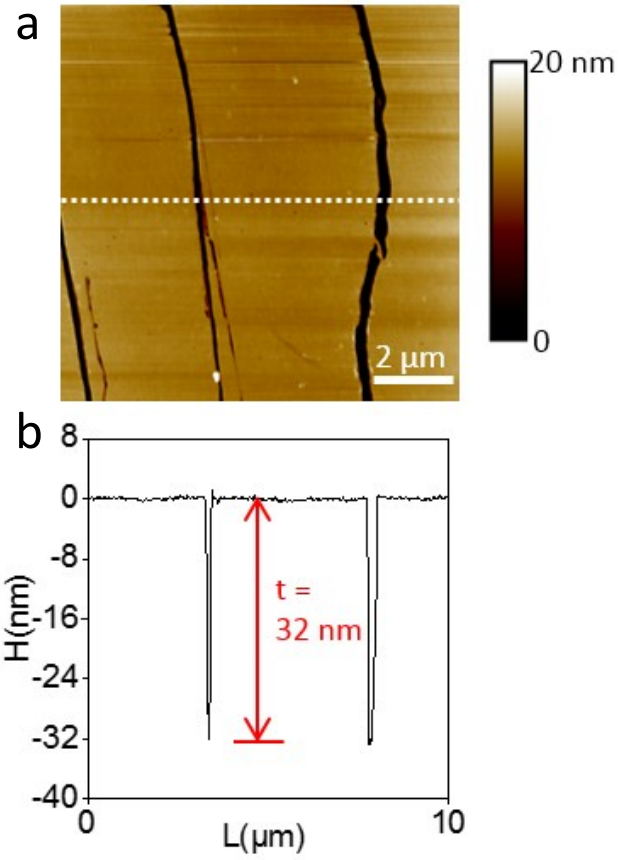

Figure 3. Morphology of optimized crystal. AFM image (a) and thickness profile (b) of continuous C_{10}-DNTT crystal. Despite nanoscale cracks, RMS roughness of crystal is < 0.2 nm.