Univ. of Minnesota:
Transverse Shear Microscopy. Visualizing grains in organic semiconducting layers

B. Stadlober

Microstructure imaging by Transverse Shear Microscopy

Although lots of studies exist that enlighten the growth mechanism, the crystalline structure and the morphology of organic polycrystalline thin films there is still a gap in information concerning direct imaging of the microstructure of ultra-thin coalesced organic semiconductor layers. Especially in thin film transistors the first few monolayers of the organic semiconductor are the ones which control the charge carrier dynamics and therefore a mapping of the respective orientation of grains and a visualization of the shape of grains in these layers would help to unravel the influence of grain morphology and grain boundaries on the charge carrier transport.

In this context the group of **D. Frisbie** from the **University of Minnesota** demonstrated that a novel scanning probe microscopy method, Transverse Shear Microscopy (TSM), produces striking, high contrast images of grain size, shape and orientation in 1-2 nm thick closed pentacene monolayers. In TSM the scanning direction of the force microscope probe tip is parallel to the cantilever axis, and the lateral deflection or twist of the cantilever is recorded. It is shown that the transverse shear and the mechanism of TSM contrast rely on mechanical properties of the material, specifically the in-plane elastic anisotropy. The sign and the magnitude of the TSM signal depend on the precise relationship between the scan direction and the crystallographic orientation and therefore TSM can be used to index directions on the (001) plane of pentacene crystals and grains.

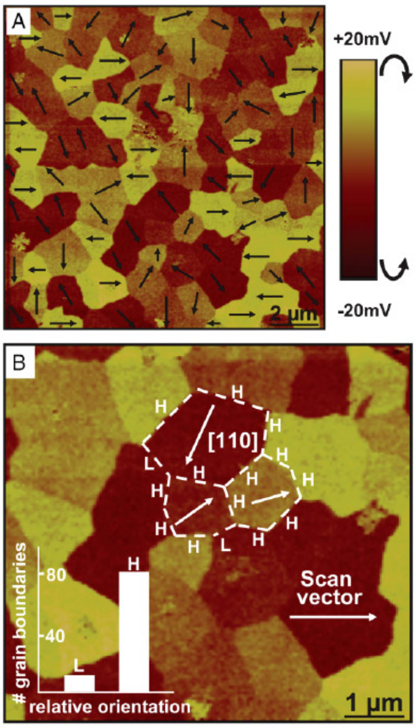

Figure 1: Grain Orientation Map and GB analysis. A) A TSM-generated Grain Orientation Map, where the arrows indicate the [110] direction ineach grain. The bright contrast corresponds to clockwise cantilever twisting, while the dark contrast corresponds to counter-clockwise cantilever twisting. B) TSM image showing high (H) and low (L) angle GBs. The histogram indicates that ~90% of the GBs present in the polycrystalline first monolayer of pentacene on SiO_2 are high angle. *Reprinted with permission from Advanced Materials 20, 4033 (2008). Copyright 2008 Wiley-VCH.*

Based on this, the authors produced a Grain Orientation Map of polycrystalline pentacene films (see Figure 1) where the contrast is related to the orientation of the crystallites. This allows determining the relative population of high and low angle grain boundaries (low angle means that the relative orientation between adjacent grains is less than 15°, whereas it is more for high angle grain boundaries). It is found that 90 % of the grain boundaries are high angle as is indicated by the inset of Figure 1 and 80 % have six faces as is expected from theoretical considerations based on calculated surface energies. It was concluded that under the growth conditions employed (deposition rate 0.01 Å/s) the pentacene grains in the first monolayer have adopted largely equilibrium grain shapes with faceting dictated by surface energies.

In this work for the first time the morphology and respective orientation of grains in the first closed monolayer of an epitaxial grown organic semiconductor was visualized and analysed quantitatively. Since it is this layer which is the most important for the control of the charge carrier transport in organic thin film transistors, detailed information about the shapes and size of the grains will help to understand the transport characteristics of pentacene TFTs with SiO_2 gate dielectrics.

Moreover, information about the angles between adjacent grain boundaries which govern the transport from grain to grain is useful to understand their influence on the hole mobility and on electron and hole trapping. Additionally, the authors claim to be the first to give an estimate of the diffusion energy of pentacene on SiO_2 (400 meV)

The authors succeeded to close a gap in understanding the microstructure of the first monolayer of polycrystalline organic thin films. Actually they applied TSM, a rather exotic scanning probe technique, to nicely visualize the shape and orientation of grains in pentacene monolayers thus providing valuable information upon the nature of grain boundaries in the accumulation region of organic thin film transistors. In addition, TSM was shown to be successfully applicable to other organic semiconductors for quantifying grain morphology, grain boundary density and grain boundary orientation. In fact the authors showed that any elastically anisotropic surface can generate a contrast in the TSM signal. These findings establish TSM as a new method for the quantitative characterization of microstructure in crystalline soft materials.

"Grain Orientation Mapping of Polycrystalline Organic Semiconductor Films by Transverse Shear Microscopy" ; V. Kalihari, E. B. Tadnor, G. Haugstad, C.D. Frisbie : ***Advanced Materials*** **20**, 4033 (2008).