Using mechanical deformation to elucidate structure-property relationships in polymer semiconductors

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Organic semiconductors are touted to for their potential to significantly advance flexible electronic applications including displays and solar power, among others. It is well established that the morphology of organic semiconductor films strongly influences their electrical properties. Elucidating precise morphological features that dictate device performance has been difficult given the disorder inherent in these materials. The ductility of the films, which in part makes them very attractive for flexible device applications, also provides a unique opportunity to elucidate a number of structure-property relationships in these materials.

In this study, we use large strains of over 50% to isolate morphological features within the films and study how these features dictate electrical properties. The focus of the research is on semicrystalline polymer poly(3-hexylthiophene) (P3HT), and P3HT-fullerene (PCBM) blend films. We use large strains applied to the films to strongly orient the crystalline P3HT within the films. The strain alignment process is illustrated in **Figure 1**.



Figure 1. Illustration of the P3HT strain process. The organic semiconductor film is first cast on an initial substrate. A PDMS stamp is then used to remove and strain the film. The strained organic semiconductor film is then printed onto a second receiving substrate for analysis.

To develop of clear morphological picture of these films, a number of characterization tools are employed including UV-visible spectroscopy, spectroscopic ellipsometry, and X-ray diffraction. The strained films are applied as the semiconductor layer in organic thin film transistors (OTFTs) and photoactive layer in organic photovoltaic (OPV) devices. The morphological analysis along with detailed device characterization provides several insights into morphological features of organic semiconductors driving device performance.

In the strained P3HT films that are applied to OTFT applications, we find that the field effect mobility is efficient with the conjugated ring plane perpendicular (edge-on) and parallel (face-on) to the gate dielectric. This result suggests that charge mobility is significantly higher along the polymer backbone direction over other crystallographic directions. Strained P3HT:PCBM films are applied in organic solar cells. Films strained by over 50% have a large dichroic ratio, and power conversion anisotropy. Differences in absorption and power conversion efficiency depending on the incident light polarization allow for a number of insights into the energy conversion process.