

Optical Characterization of Organic Electronic Thin Films

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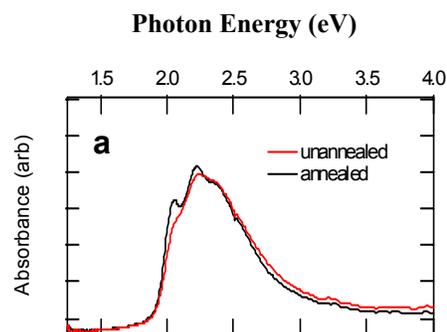
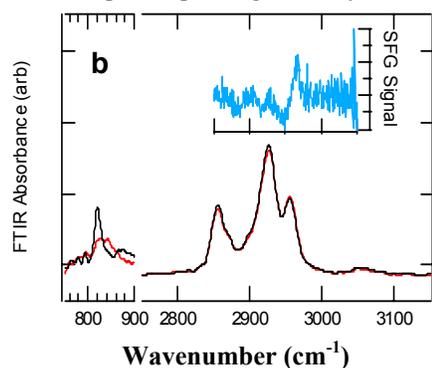
CSTL Program: *Measurement Science for Future Standards and Technology*

CSTL researchers demonstrate that vibrational spectroscopies can provide new insight into the structure of OE films and potentially may provide the basis for evaluation and monitoring of OE films by manufacturers.

x-ray diffraction techniques, the ‘gold standard’ for structural determination, are difficult with very thin films. Additionally, as many target applications require flexibility in the OE film, true crystalline order (which gives rise to diffraction) may be undesirable. In this exploratory research project, optical techniques originally developed for the characterization of molecules adsorbed at surfaces are explored as tools for the structural characterization of thin films.

Poly3hexylthiophene (P3HT) has emerged as a prototypical OE material. Transistors made from this material can achieve performance levels close to those of amorphous silicon. Data from traditional structural characterization tools, however, have not shown strong correlations with the electrical performance of P3HT films. Surprisingly, low relative molecular mass, highly crystalline films have poorer performance than high relative molecular mass films that appear highly amorphous.

Shown in the figure to the right (a) are absorption spectra for a high relative molecular mass P3HT film before and after annealing. The fine structure that appears near 2.0 eV after annealing has been attributed to an electronic excitation that spans multiple chains and is indicative of good interchain order. Shown in the main panel of the figure (b) are infrared spectra probing the alkyl side groups (features at 2800 cm^{-1} to 3000 cm^{-1}) and the thiophene ring (823 cm^{-1}).



Infrared spectroscopy allows selective study of different parts of the polymer chain, but averages the information over the entire film. The alkyl side chains show little change upon annealing, indicating that, contrary to the behavior in bulk crystals, the alkyl groups do not drive the ordering of the thin films. Detailed analysis establishes that the alkyl groups are highly disordered. There is significant change in the thiophene ring feature, indicating that the chains adopt a more card-edge stacking structure upon annealing. The inset to Figure 1 (b) shows nonlinear vibrational spectra of the alkyl groups (SFG = sum-frequency generation). Unlike infrared spectroscopy, the nonlinear spectroscopy is only sensitive to the surface of the thin film. The presence of

the feature near 2960 cm^{-1} indicates that, while the alkyl groups are disordered in the interior of the film, they are highly ordered at the surface. The combination of the three spectroscopies (visible, infrared, and nonlinear) provides a detailed picture of the evolution of the structure that can be related to the electronic properties of the film.

Future work will be performed within the context of the FY05 NIST Competence Program on *Metrology to Enable the Realization of Organic Electronics Devices*.

The next challenges include correlating the spectroscopic results with direct measurements of the electrical performance of the films to establish the structural characteristics of high performance films. The optical techniques for orientation determination will be validated against direct techniques based on x-ray absorption. Models for the quantitative separation of the buried and free interfaces of ultrathin films via nonlinear optics will be developed and extended to higher order processes such as coherent anti-stokes Raman scattering.