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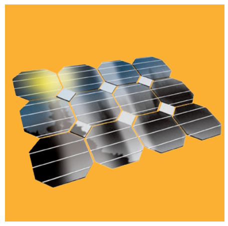
Spectroscopic Ellipsometry

P3HT:PCBM Bulk Heterojunction Solar Cells Characterization by Spectroscopic Ellipsometry



Application Note

Photovoltaic SE25

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Abstract

The performance of organic solar cells based on the blends of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) is strongly influenced by blend composition and thermal annealing conditions. For high-efficiency solar cells, a nanoscale interpenetrating network with crystalline order of both constituents is the desirable architecture for the photoactive layer. To that end, recent studies have focused on how to tailor and control the morphology of the P3HT:PCBM blend, the material combination that has led to the highest power conversion efficiency values reported thus far (4-5%).

In this note, we demonstrate the use of ellipsometry as a powerful and sensitive metrology means of monitoring blend morphology, phase separation as well as crystallinity.

Spectroscopic Ellipsometry is an optical technique for the characterization of thin films, mainly used to determine film thickness and optical constants of single or multilayer stacks.

Experimental

A HORIBA Scientific UVISEL Spectroscopic Phase Modulated Ellipsometer has been used to characterize three organic photovoltaic samples including: P3HT/c-Si, PCBM/c-Si and P3HT:PCBM/c-Si. Ellipsometric measurements were performed at an angle of incidence of 70°, across the spectral range 190-2100 nm.

UVISEL Spectroscopic Ellipsometer

Ellipsometric Modelling and Results

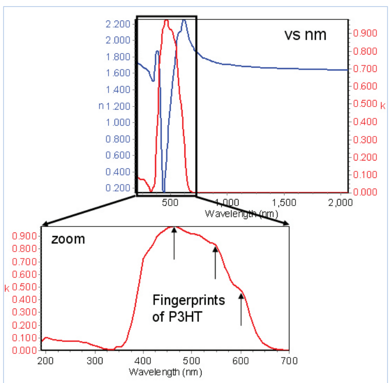
The goal for the characterization of the first two samples were to find the film thickness and optical constants of P3HT and PCBM materials.

1st sample

934.6 Å P3HT
Si

The model found is a single layer of P3HT deposited on c-Si. The thickness found is 934.6Å and optical constants of P3HT were modeled using the new amorphous dispersion formula. The modeling was performed in two-steps: a normal dispersion fit over 0.6-2.3eV to extract film thickness, and then a point by point fit above 2.3eV to extract film index over full range.

P3HT Optical constants

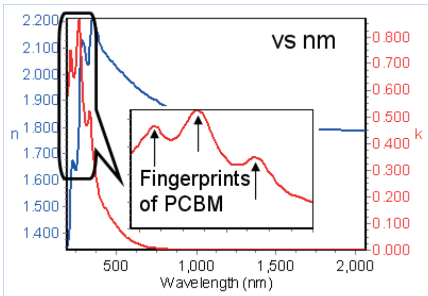


2nd sample

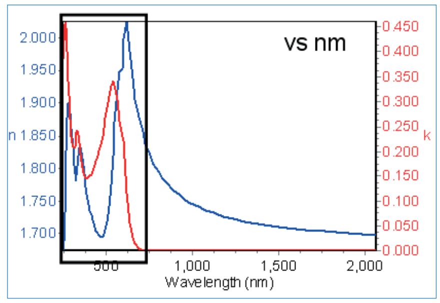
505.9 Å PCBM
Si

The 2nd sample is represented by a single layer model of PCBM deposited on c-Si. The thickness found of the PCBM film is 505.9Å and the PCBM optical constants were modeled by a new amorphous dispersion formula.

PCBM Optical constants



"Effective" Optical constants of P3HT:PCBM Blend



3rd sample

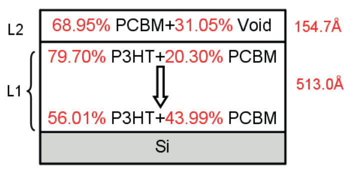
Two different analysis protocols were used to model the blend P3HT:PCBM structure.

The 1st protocol analysis is based on the use of the **effective medium theory**, allowing to **mix pure P3HT and PCBM in a layer to represent the blend P3HT:PCBM structure**. In the 2nd protocol, the blend is considered as **one single, homogenous** material, represented optically through one single dispersion function (new amorphous).

Analysis protocol I: Effective Medium Theory

The model used to represent the blend P3HT:PCBM film on c-Si is shown below. The best fit is based on a bi-layered model. The layer 2 (L2) represents surface layer consisting of PCBM and void (i.e., air). The layer 1 (L1) is a linear gradient, with P3HT concentration increasing whereas PCBM decreasing towards surface layer.

The individual P3HT and PCBM optical constants are fixed to previously determined in samples 1 and 2, whereas percentages are varied to render blend index changes.



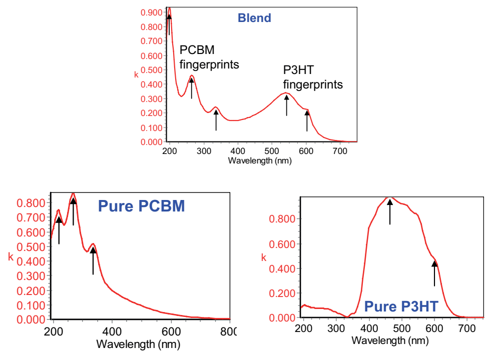
In conclusion, the protocol I renders investigation of final morphology (grading, phase separation, etc.) of P3HT:PCBM blend.

Analysis protocol II

Results for thickness and optical constants obtained are shown below.

639.6 Å P3HT:PCBM
Si

It is important noticing that Fingerprints of constituents are visible on effective optical spectra of P3HT:PCBM blend.



The protocol II provides insights into blend film composition and crystallinity through monitoring of fingerprints of each component (peak amplitude, broadening, etc.)

Conclusion

A HORIBA Scientific spectroscopic ellipsometer allows characterization of **blend morphology, phase separation as well as crystallinity of organic PV solar cells**, which are important properties to increase solar cell efficiency.

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