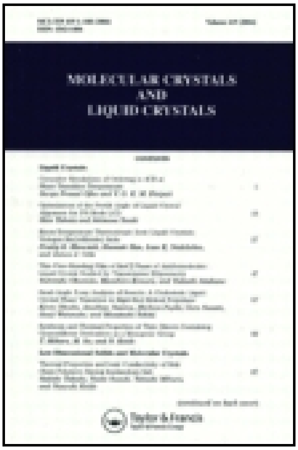

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

# Optical constants of conjugated polymer/fullerene based bulk-heterojunction organic solar cells

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Version of record first published: 18 Oct 2010

To cite this article: H. Hoppe, N. S. Sariciftci & D. Meissner (2002): Optical constants of conjugated polymer/fullerene based bulk-heterojunction organic solar cells, Molecular Crystals and Liquid Crystals, 385:1, 113-119

To link to this article: http://dx.doi.org/10.1080/713738799

*Mol. Cryst. Liq. Cryst.*, Vol. 385, pp. [233]/113–[239]/119

1058-725X/02 $12.00 + .00
DOI: 10.1080/10587250290113268

# OPTICAL CONSTANTS OF CONJUGATED POLYMER/ FULLERENE BASED BULK-HETEROJUNCTION ORGANIC SOLAR CELLS

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*The performance of organic solar cells consisting of multiple layers, which are a few hundred nanometers thick, is determined by strong optical interference effects. In order to model their optical and photoelectrical behavior, we determined the optical constants of all components of this system. This was done by fitting model dielectric functions to reflection and transmission spectra of all layers in the solar cell device. We put a special emphasis on understanding the optical behavior of the photoactive bulk heterojunction film, which consists of a composite of semiconducting polymers with fullerenes.*

*Keywords*: optical constants; dielectric function; plastic solar cell; refractive index; UV-vis spectroscopy; modelling

## 1. INTRODUCTION

Recently the polymer/fullerene bulk heterojunction "plastic solar cell" has triggered an increasing attention within the scientific community, and a lot of fundamental experiments to understand charge transfer and transport are performed on this or similar systems [1–2]. However, to best of our knowledge the optical constants of this plastic solar cell is not published in the literature, yet. They are important to understand the optical behavior of these thin film systems, which are strongly influenced by interference effects [3,9]. Only isolated data for the components of these cells can be found determined from spectroscopic ellipsometry on ITO (see e.g. [4–6]), on PEDOT [7], on (highly stretch oriented) poly(*p*-phenylene vinylene)

We gratefully acknowledge the help of Patrick Denk and Roman Rittberger (both QSEL, Linz) for some preparations in the lab. Our research was supported by the Bundesministerium für Bildung und Forschung in Germany (contract numbers 01SF0026). Part of this work was performed within the Christian Doppler Society's dedicated laboratory on Plastic Solar Cells funded by the Austrian Ministry of Economic Affairs and Quantum Solar Energy Linz GmbH.

(PPV) [8,9] and some derivatives [10] and on the MDMO-PPV:PCBM [(3,7-dimethyloctyloxy methyloxy poly(paraphenylene vinylene):(1-(3-methoxycarbonyl) propyl-1-phenyl [6,6]$C_{61}$)] blend as used in the bulk-heterojunction solar cell [11]. In this paper the optical constants of all layers are determined from a sequence of glass, ITO, PEDOT:PSS, MDMO-PPV:PCBM (1:4 by weight) and of aluminium, as used in standard architecture and as described previously [2]. In addition, modelling of the reflection of the actual solar cell allows us to directly determine the layer thicknesses in our devices.



## 2. EXPERIMENTAL

MDMO-PPV was provided by Covion (Germany), PEDOT:PSS (Baytron) was purchased from Bayer (Germany) and PCBM was purchased from J. C. Hummelen (Univ. of Groningen, The Netherlands). Films were prepared by spin coating from chlorobenzene solutions of the pristine materials as well as of the 1:4 weight ratio blend of MDMO-PPV and PCBM as used in our standard plastic solar cells [1–2]. PEDOT:PPS was spin cast from an aqueous solution 0,5% by weight. As a substrate, fused silica was used, which has been cleaned with iso-propane in an ultrasonic bath previous to spin coating. In order to determine the optical constants of the ITO-glass (MERCK, Germany), the ITO was etched away completely, to first allow for the determination of the optical properties of the substrate glass alone. Then the complete ITO-glass has been measured. Near normal incidence (7°) transmission and reflection spectra of the spin cast films on fused silica and of the substrates were recorded with a Cary 3G spectrophotometer (Varian, Inc., Palo Alto, USA) in the range between 300 and 900 nm. Organic layer thicknesses have been verified using a tapping mode AFM (NanoScope 3100, Digital Instruments, Santa Barbara, USA), by measuring the depths of scratches within the film. The fitting of model dielectric functions to the transmission and reflection spectra as well as the determination of the active layer thickness from reflection measurements of a complete solar cell was performed using the software SCOUT2 (M.Theiss, Aachen, Germany). The model dielectric functions consist of a constant dielectric background contributing to the real part of the dielectric function, and of so-called Kim-oscillators [5], which describe the optical absorption for the electronic transitions. A Kim-oscillator is an extension of the simple harmonic oscillator model for vibrational modes and it allows a continuous shift of the line shape between a Gaussian and a Lorentzian profile. Once the dielectric functions are obtained, the complex refractive index $\widetilde{\mathbf{n}} = \mathbf{n} + \mathbf{i} \star \mathbf{k}$ is calculated easily from the connections between the dielectric function and the optical constants, that are given by: $\varepsilon^{|} = \mathbf{n^2} - \mathbf{k^2}$ and $\varepsilon^{||} = \mathbf{2nk}$.

## 3. RESULTS AND DISCUSSION

The optical constants of all layers of which the solar cells is built up, have been determined. In Figure 1 the transmission and reflection spectra and

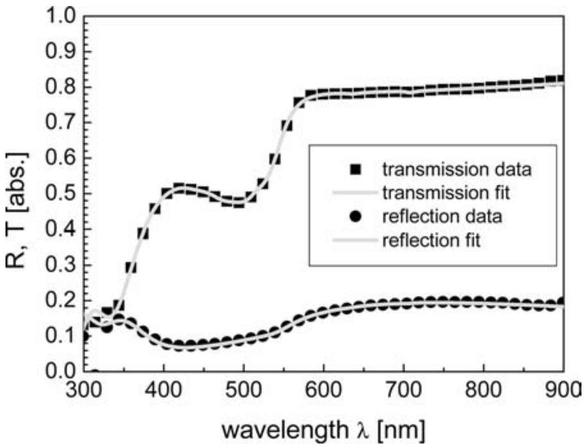


**FIGURE 1** Measured and fitted transmission and reflection spectra of a thin film of the MDMO-PPV:PCBM mixture (1:4 weight ratio), spin coated from chlorobenzene solution onto fused silica substrates.

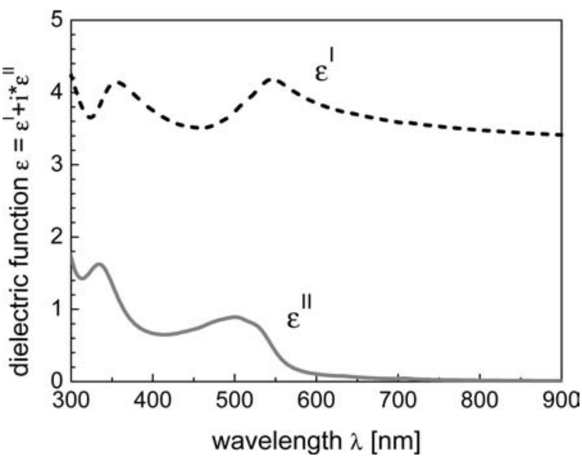


**FIGURE 2** Real ($\varepsilon^{|}$) and the imaginary part ($\varepsilon^{||}$) of the model dielectric function of the MDMO-PPV:PCBM 1:4 blend in a 110 nm thick film spin cast from a chlorobenzene solution 1,4% by weight.

the respective fits from the model dielectric function are shown for the MDMO-PPV:PCBM (1:4 weight ratio) mixture, obtained for a film spin cast from chlorobenzene solution with an approximate thickness of 110 nm. The resulting dielectric function for this material is presented in Figure 2, showing the real ($\varepsilon^{|}$, dotted line) and the imaginary ($\varepsilon^{||}$, full line) part.

In the same way, the refractive index n and extinction coefficient k of the other materials were obtained. Figure 3 shows n and k of the glass substrate, of the ITO and the PEDOT:PSS, while in Figure 4 the n and k values



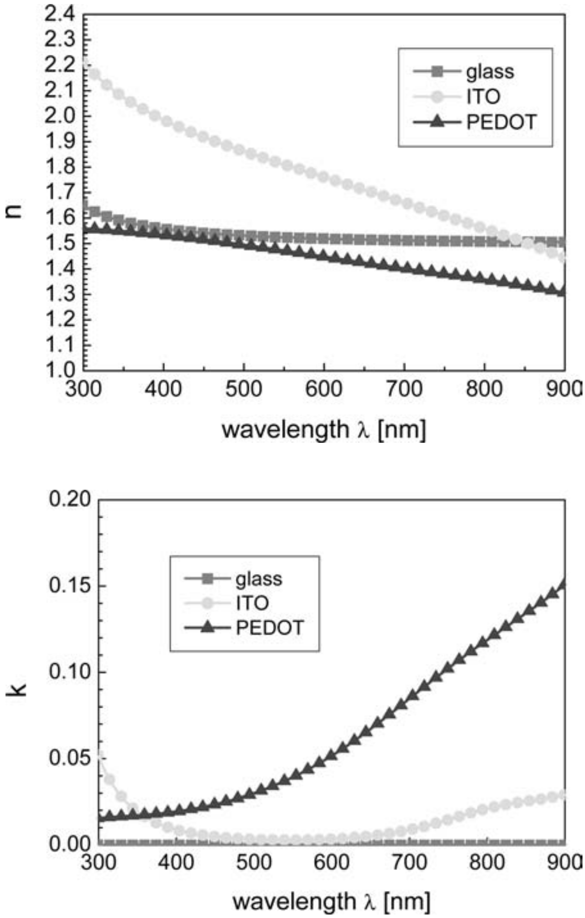


**FIGURE 3** Optical constants of the ITO-substrate glass (triangles), the ITO (circles) and the PEDOT:PSS (squares) layer, determined by fitting model dielectric functions to the respective transmission and reflection data.

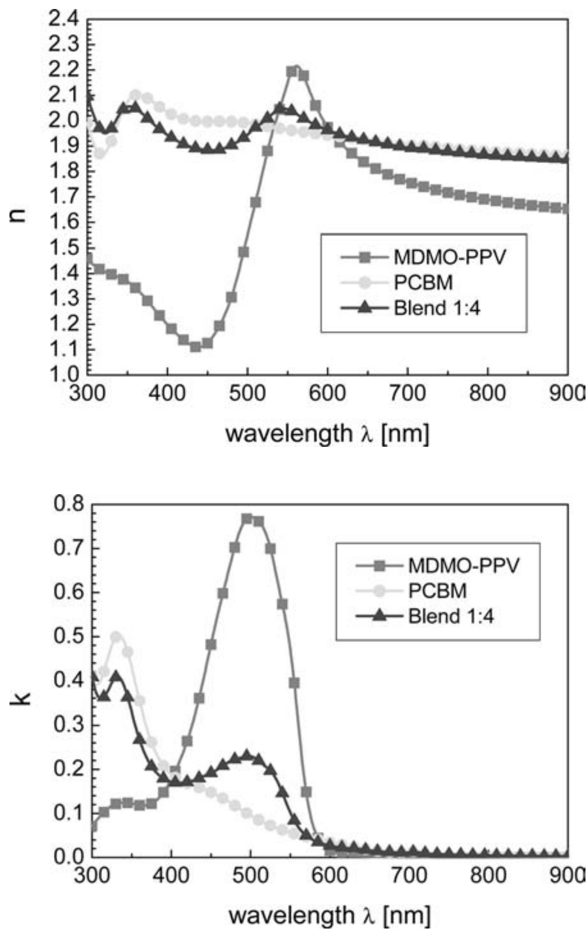


**FIGURE 4** Optical constants of pristine MDMO-PPV (squares), PCBM (circles) and the MDMO-PPV:PCBM 1:4 blend, determined by fitting model dielectric functions to the respective transmission and reflection data of single layer films on fused silica.

of the bare MDMO-PPV and PCBM, as well as of their 1:4 mixture are shown.

For a full set of known optical constants or dielectric functions, the optical determination of a certain layer thickness within a multilayer system is feasible. This was done by fitting reflection spectra of complete solar cells. As an example the experimental reflection spectrum of a solar cell, and the corresponding fit, are presented in Figure 5 where the only free fit

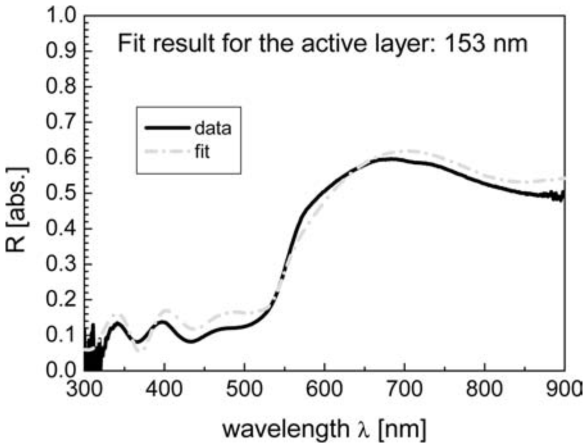


**FIGURE 5** Measured (full line) and fitted (dash-dots) reflection spectra of a complete solar cell structure illuminated from the glass side. The only fit parameters were the layer thicknesses of ITO, PEDOT:PSS and of the MDMO-PPV:PCBM layer.

parameters were the layer thicknesses of the ITO, of the PEDOT:PSS and of the active layer. By knowing of e.g. the ITO-layer thickness (which is practically constant), the number of parameters can be reduced even further. The deviations are assumed to be due to some roughness effects of the layers and to some thickness variations, as the actual measurement takes place on a spot of about 5 mm × 5 mm.

## 4. CONCLUSIONS

Optical constants of all layers in an organic solar cell have been determined and are presented. As such, the knowledge of the quantitative optical properties in these films has a useful application for the determination the film thickness of each layer within a complex multilayer device. Furthermore, this opens up the possibility of optimization of the layer thicknesses for optimal absorption and interference effects on the efficiency of the solar cells.

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