



Letter

Determination of the optical constants of bulk heterojunction active layers from standard solar cell measurements



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ABSTRACT

The determination of the optical constants $n(\lambda)$ and $k(\lambda)$ for organic bulk heterojunction (BHJ) active layers from standard solar cell measurements is presented. We show for a small molecule based as well as for polymer solar cells that the complex refractive index can be derived from the external quantum efficiency (EQE) in combination with current–voltage curves obtained from a series of devices with different active layer thicknesses. The results are compared to those obtained via established techniques and the impact of differences in $n(\lambda)$ and $k(\lambda)$ on the solar cells is shown by simulation of the current density using a transfer matrix model.

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1. Introduction

The power conversion efficiency of organic solar cells (OSC) has been steadily improved over the last decade. Efficiencies around 9% have been reported for small molecule (SM) [1] as well as for polymer [2] based single-junction OSCs. To be competitive with established photovoltaic systems a power conversion efficiency of 15% on the lab scale is desired. However, these numbers require tandem solar cells (TSC) with complementary absorbing subcells to harvest more solar energy. Employing tandem structures, efficiencies of 10.6% [3] and 12% [4] have been accomplished for polymeric- and SM-OSC, respectively.

In order to get a deeper insight into the processes that influence the device performance as well as to optimize organic solar cells, optical simulations are inevitable. Due to the use of thin films and a reflecting top electrode the light distribution within the stacked device is strongly influenced by interference effects. Especially in tandem solar cells the distribution of the electric field of the incoming

light plays an important role. The subcell producing the lower current limits the overall current of the tandem device. Therefore, both active layers need to be placed in the TSC stack where most of the light can be absorbed [5].

The optics of a solar cell can be simulated by a transfer matrix (TM) model which requires as input parameters the optical constants of all materials involved in the device stack along with their respective thicknesses [6]. The parameters of the most commonly used materials in organic solar cells, e.g. electrode materials, can be found in literature. Therefore, the determination of the extinction coefficient $k(\lambda)$ and refractive index $n(\lambda)$ of new active layer materials is the first step to an optical simulation of the device.

Several techniques for the determination of optical constants are available, where varying angle spectroscopic ellipsometry (VASE) represents the most commonly used method. In order to obtain the dielectric function with VASE or any other related method, thin films with thicknesses of some 100 nm of the material under investigation must be prepared on specific substrates, usually quartz glass or Si(100) wafer. Alternatively, the optical constants can be derived from transmittance spectra as well, e.g. by

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employing the layer of interest on a partially reflective substrate to promote interference effects for an unambiguous determination of the complex refractive index [7]. However, the substrate itself can influence the process of film formation and thus the optical parameters of the grown layer. It is therefore desirable to determine the optical parameters of layers that are incorporated within an actual device stack.

In this communication, we demonstrate that the complex refractive index of active layers of bulk heterojunction (BHJ) OSCs can be calculated from the external quantum efficiency (EQE) spectra and JV -curves using a custom made program based on a reverse transfer matrix (RTM) model. The resulting optical constants are compared to those obtained via established techniques (VASE) and the impact of deviations in $n(\lambda)$ and $k(\lambda)$ (RTM vs. VASE) on organic solar cells is shown by simulation of the current density using a transfer matrix model.

2. Theoretical approach

2.1. Fitting absorption spectra using a reverse transfer matrix model

The program is based on the TM model introduced by Pettersson et al. [6] This model allows to calculate the internal electric field distribution and absorption within an arbitrary stack of thin layers with known optical constants. Here, the model is used in a Matlab [8] code in reversed mode: If the optical properties of all layers in a device stack are given except for one layer, but its layer absorption can be deduced, our code is able to determine $n(\lambda)$ and $k(\lambda)$ of the unknown layer. In this work the required absorption spectra are calculated for the active layer (AL) within an organic solar cell stack from standard solar cell measurements (details will be discussed in the following Section 2.2). Ideally, several devices with varying active layer thicknesses should be prepared to minimize the parameter space. The active layer absorption spectra $Abs_{exp}^i(\lambda)$ for devices with active layer thicknesses d_i (with “ i ” being the device counter) will then serve as the fitting target in the algorithm. A flowchart of the program sequence is presented in Scheme 1. In the first step of the program, we choose a constant initial value for $n_{init} = 1.75$ and calculate an initial spectrum for $k_{init}(\lambda)$ from $Abs_{exp}^i(\lambda)$. These data

are then passed to the RTM algorithm together with the layer thicknesses d_i and all known optical parameters of the device stack. The algorithm then varies $n_{AL}(\lambda)$ and $k_{AL}(\lambda)$ and d_i to fit the layer absorption $Abs_{exp}^i(\lambda)$ and thus gaining the refractive index, extinction coefficient and thickness of the optically unknown layer in the stack. For detailed information about the individual steps of the program the reader is referred to the Supporting Information section of this paper.

2.2. Calculating absorption from EQE- and JV-measurements

Since the absorption of the active layer within the solar stack is needed for the RTM program, several assumptions/simplifications have to be made:

- (i) Every photogenerated exciton reaches the donor/acceptor (D/A) interface and is dissociated into free charge carriers. The resulting charge carriers can be extracted at high internal voltages (negative voltage bias) yielding an internal quantum efficiency (IQE) of 100% for the saturated photocurrent $J_{photo,sat}$.

This assumption allows to estimate IQE at short-circuit conditions (IQE_{SC}) by normalizing the photocurrent J_{SC} to the saturated photocurrent $J_{photo,sat}$ at negative bias:

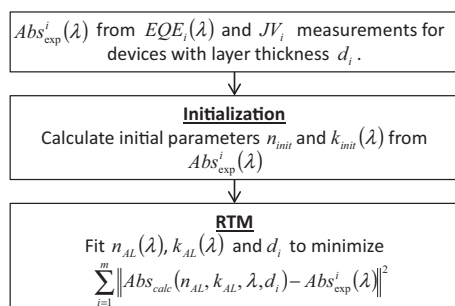
$$IQE_{SC} = \frac{J_{SC}}{J_{photo,sat}} \quad (1)$$

In the literature this value is often referred to as dissociation/collection probability $P(E,T)$ [9,10]. This assumption is arguable due to the short exciton diffusion length in organic semiconductors. Therefore, this approach is only reasonable for bulk BHJ active layers with rather fine intermixing of the donor and acceptor material.

- (ii) The internal quantum efficiency (IQE) is assumed to be constant over the full wavelength range where the active layer absorbs.

$$IQE(\lambda, V) = IQE(V). \quad (2)$$

There is an ongoing discussion in the literature whether or not this assumption is realistic. The general opinion is that a charge transfer state between the donor and the acceptor component is the last step before the dissociation into free charge carriers [11,12]. However, it still remains uncertain whether or not excess energy from excitation is beneficial for charge separation. Multiple groups reported on “hot exciton dissociation” in BHJ solar cell blends, which would result in larger IQE values at higher photon energies [13–15]. In contrast, several groups found wavelength independent IQEs for various materials in BHJs [12,16,17]. Recently, Armin et al. showed that after careful consideration of the parasitic absorption, i.e. absorption of non-photoactive layers, the IQE of PCDTBT:PC₇₁BM (poly [N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)]:phenyl-C71-butyric acid methyl ester) based BHJ solar cells is indeed wavelength independent [18]. Additionally, their results imply that the saturated photocurrent reflects the highest current



Scheme 1. Program sequence of the RTM method.

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