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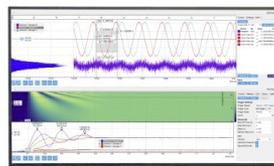
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## An optical spacer is no panacea for light collection in organic solar cells

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The role of an optical spacer layer has been examined by optical simulations of organic solar cells with various bandgaps. The simulations have been performed with the transfer matrix method and the finite element method. The results show that no beneficial effect can be expected by adding an optical spacer to a solar cell with an already optimized active layer thickness. © 2009 American Institute of Physics. [DOI: 10.1063/1.3073710]

The enhanced collection of solar energy in thin organic films is a desirable goal for organic photovoltaic conversion based on bulk-heterojunction materials. In these devices, a thin active layer is sandwiched between electrodes and light entering through a transparent electrode is absorbed in the active layer, forming charge carriers that are collected. The collection is enhanced by high electric fields and short distances for transport, which requires thin films of the active material. This reduces the optical absorbance of the films and less photocurrent can be generated. Approaches to increase the optical absorption in thin films have been developed using scattering elements, light traps<sup>1</sup> and plasmon couplers.<sup>2</sup> Another approach is based on the concept of optical spacers. The thin film stack in an organic photovoltaic device controls the power dissipation profile of the incoming electromagnetic radiation. The optical power dissipation profile can be calculated with the help of a transfer matrix method, as demonstrated in studies of bilayer photovoltaic devices.<sup>3,4</sup> The optical modeling has since been extended to bulk heterojunction devices,<sup>5–10</sup> including tandem solar cells.<sup>11,12</sup> Bilayer donor-acceptor heterojunctions only allows charge generation close to the interface due to a limited diffusion length of the exciton. The external quantum efficiency of charge generation is proportional to the optical dissipation close to this interface, which can be controlled by device geometry. By varying the thicknesses of the layers, a local optical maximum or minimum may coincide with the location of the donor-acceptor interface.<sup>13</sup> The location of the extrema is however highly dependent on the wavelength of light. It was suggested that the optical spacer effect can be beneficial when considering the full wavelength range of optical absorption in the active material in solar cells.<sup>14–16</sup>

Here we show by simulations that only in the case that the thickness is chosen away from local maxima of optical power dissipation can the dissipation be enhanced by an optical spacer. If the thickness and geometry are chosen to give optimal power dissipation, no such advantage is found. This is in agreement with recent reports.<sup>17,18</sup> We demonstrate this by optical simulations of devices built from three different bulk heterojunction materials, the standard P3HT:PCBM, APFO-3:PCBM, and the low bandgap APFO-Green5:PCBM. The first two materials share a higher bandgap, with absorption starting at 650 nm, but with quite different absorption

characteristics and therefore also dielectric functions. The third material is a low bandgap material, and the onset of absorption occurs at 850 nm. We represented the optical spacer by a thin layer of TiO<sub>2</sub>. The thickness of the optical spacer and the active bulk heterojunction material has been varied. The cathode is Ag and the anode is poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) (40 nm) located on indium tin oxide (ITO) (140 nm), supported by a thick glass substrate.

Our optical simulations are performed with the transfer matrix method, for P3HT:PCBM, and by a finite element method, solving Maxwell's equations numerically for APFO-3:PCBM and APFO-Green5:PCBM. The two methods of calculations here used give identical results when applied to the same problem, and we used the numerical simulations in order to enable analysis of more complex problems, such as non-normal incidence of light and anisotropic layers.<sup>19</sup> Dielectric functions for P3HT:PCBM, APFO-3:PCBM, and APFO-Green5:PCBM have been established in previous studies.<sup>8,19</sup> Optical absorption spectra of the three materials are shown in Fig. 1 together with the chemical structure of the polymers. Using the optical material properties as input data, we calculate the optical power dissipation in the active layer in devices with varying thickness of optical spacer and active layer as a function of wavelength. We then calculate the upper limit to photocurrent generation ( $J_{scmax}$ ), by multiplying the spectral response with the AM1.5 G solar spectrum (Fig. 2). We thereby implicitly assume an internal quantum efficiency of 100%, and the photocurrents are therefore larger than those obtained in real devices. This assumption does not alter the conclusions concerning the optical effect of the spacer layer. We note that for thick layers of P3HT:PCBM, photocurrent densities of 110 A/m<sup>2</sup> are predicted. A lower  $J_{scmax}$  of 100 A/m<sup>2</sup> is predicted for APFO-3:PCBM and a higher  $J_{scmax}$  of 160 A/m<sup>2</sup> is predicted for APFO-Green-5:PCBM because of a lower and a higher, respectively, degree of spectral overlap with the solar irradiation.

For the P3HT:PCBM (1:1) active layer without an optical spacer, local maxima of photocurrent are expected at 70 and 220 nm thicknesses. Addition of an optical spacer only reduces the photocurrent at these points, as seen in the color labeled graph [Fig. 2(a)]. For the more dilute APFO-3:PCBM (1:4), the local maxima of photocurrent is found at 75 and 220 nm, and for APFO-Green5:PCBM (1:4) the maximum is found at 115 nm. By adding an optical

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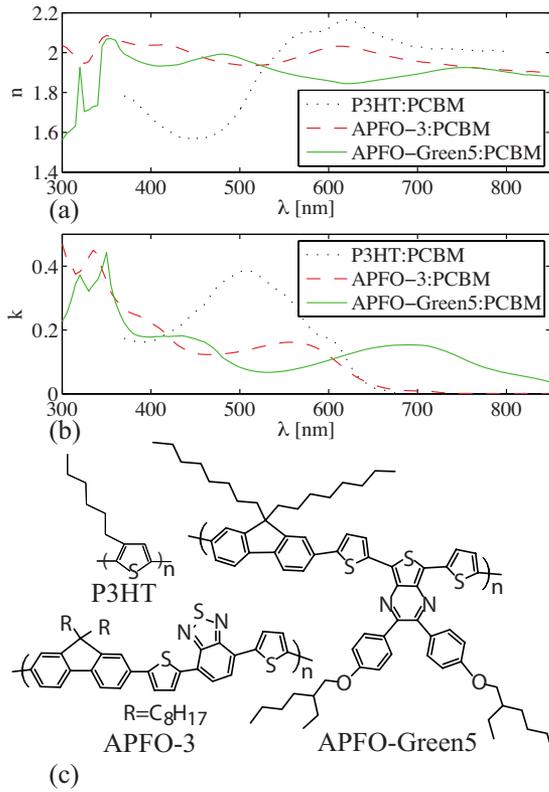


FIG. 1. (Color online) (a) Refractive index and (b) extinction coefficient spectra of the three polymer blends. (c) Molecular structure of the polymers.

spacer, the photocurrent can also only be reduced in these cases. Off the local maxima, the results are somewhat different. The main reason for not using the optical maximum is, of course, poor collection of charge carriers, which will be the case in thicker devices with lower electric fields and longer distances for charge collection, and hence also a higher probability for trapping and recombination. At low thickness, below the first local maximum, a small increase in optical absorption and photocurrent is expected, as the maxima are shifted toward smaller thicknesses. For the same reason there is a small enhancement in the photocurrent just below the second maximum. In the case of APFO-3:PCBM, this occurs at active layer thicknesses between 120 and 200 nm and the current is enlarged from 74 to 78 A/m<sup>2</sup> at 150 nm, with a 10 nm thick spacer. As the absorption is shifted toward smaller thicknesses a larger absorption may be found at the point where a cell without a spacer layer shows a minimum, if a sufficiently thick spacer is used, e.g. this is seen when a spacer layer of 50 nm is used in the APFO-3:PCBM cell. Here the maximum photocurrent increases from 65 to 78 A/m<sup>2</sup> at 150 nm active layer thickness. For APFO-Green5:PCBM the enhancement is seen for thicknesses ranging from 190 to 290 nm with a current shift from 125 to 133 A/m<sup>2</sup> at a 200 nm active layer thickness with a 50 nm spacer.

Finally, we consider whether any hypothetical material could perform better as an optical spacer layer than TiO<sub>2</sub>. Our hypothetical material would have  $k$  of zero, meaning no light is dissipated in this layer and the thickness and  $n$  could be varied. With no absorbance in the optical spacer variation of either  $n$  or the optical spacer thickness serve only to shift the phase change in light within the spacer, and so they are degenerate effects. We therefore fix  $n$  and consider only the

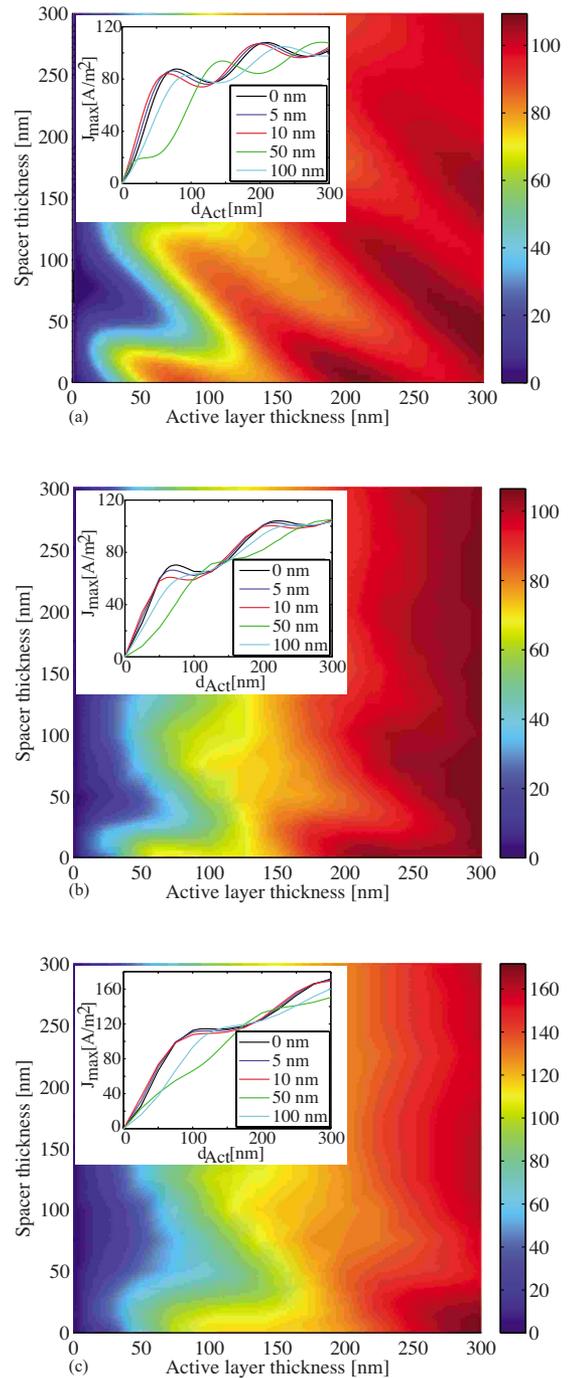


FIG. 2. (Color online) Maximum short circuit current density in bulk heterojunctions located on top of an optical spacer of TiO<sub>2</sub> for (a) P3HT:PCBM, (b) APFO-3:PCBM, and (c) APFO-Green5:PCBM mixtures. Insets show slices of the data at optical spacer thicknesses of 0, 5, 10, 50, and 100 nm.

effect of changing both layer thicknesses for our hypothetical material. The simulation results show that the calculated losses due to absorption in the TiO<sub>2</sub> in the thickness ranges that we considered are <3%, compared to an optical spacer with  $k=0$ .<sup>20</sup> This shows conclusively that no material can perform significantly better as an optical spacer than TiO<sub>2</sub>.

In conclusion, all three active layer materials showed the same behavior. In agreement with recent reports on some more materials, we suggest that the enhancement in photon collection using optical spacers is not a rewarding strategy for enhancing efficiency. Fine tuning of optical absorbance

can be possible for the case of layer thicknesses, which do not give optimal optical absorption. This small enhancement cannot motivate the fabrication complexity of incorporating an optical spacer. For materials where electrical transport and collection is too weak, a suboptimally thin active layer located on an optical spacer can be expected to give enhanced photocurrent.

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