2D and 3D light absorption modeling of interdigitated full organic solar cells

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Introduction

A promising architecture for organic solar cells (OSC) is the interdigitated heterojunction approach, which joins the advantages of bulk heterojunction and planar bilayer devices. This approach provides a proper exciton dissociation interface without sacrificing direct paths for carriers' collection [1]. Several studies have demonstrated an increase in the efficiency of these cells [2]. Nevertheless, the interdigitated dissociation interface can be also a potential source of light trapping that can enhance OSC efficiency.

By means of numerical modelling, we investigate light absorption in interdigitated heterojunction full organic solar cells. Simulations are carried out by using the finite-element method [3], which allows evaluating the magnitudes on the devices as a function of the position. To determine the best configuration, we compare different cells which are obtained by varying the Donor-Acceptor interface geometry. The donor and the acceptor materials are poly(3-hexylthiophene) (P3HT) and 1-(3-methoxycarbonyl)-propyl-1-phenyl-(6,6)C_{61} (PCBM) respectively. This study is intended to improve our devices which are achieved via nanoporous anodic alumina templates (NAAT) [4,5] (Fig.1a and Fig.1b).

In this study we compare the absorbed light, from a standard AM1.5 light source model, in the P3HT layer by using two models: a 2D and a 3D one. The 2D one (Fig. 1c) is a simplification of a real 3D device where the nanostructured interface is composed of alternating blocks of each organic material. The advantages of this model over the 3D one are an easier geometry definition, shorter computing times and smaller simulation files. On the other hand, since it is a 2D definition, nanopillars are actually grooves. A more realistic 3D model is presented in Fig. 1d, where a more complex geometry represents the nanopillars. In both cases we model a structure of indium tin oxide (ITO), Poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS), P3HT, PCBM and a back contact of aluminium (Al). The parameters under study are α (nanopillar diameter), β (structure period (2D) or interpillar distance (3D), where β = 2α) and *T* (nanopillar height including the supporting base).

Results and discussion

Fig. 2 shows the total absorbed light power (Q_{TOTAL}) in the P3HT layer as a function of the nanopillars height (*T*) for several nanopillar diameters (α). Fig. 2a) corresponds to the 2D model. We can see that all the curves have a similar trend with two local maxima for *T* around 80 nm and 230 nm. A local minimum for *T* close to 130 nm is also present in all cases. The maximum absorption is achieved for α = 12.5 nm while the lower absorption is clearly for α = 125 nm.

Fig. 2b) shows Q_{TOTAL} for the 3D model. In this case we can see that not all the curves have the same trend. For α = 12.5 nm and 50 nm the maximum absorbed light take place for *T* = 70 nm and 260 nm while there is a local minimum for *T* = 150 nm. However, for the biggest diameters the local maxima are achieved for a pillar height of 50 nm and 190 nm, and the minimum Q_{TOTAL} take place for *T* = 110 nm. The amount of absorbed light for each height is also different, being higher for the 3D model.

So, if we compare the results of the two models, the 2D and the 3D ones, we can find some similarities. However, the fact that in one model we have grooves while in the other there are nanopillars introduces differences in the results. Hence, a 2D model of a real 3D interdigitated OSC can be a first approximation but it is not accurate enough to replace a 3D model.

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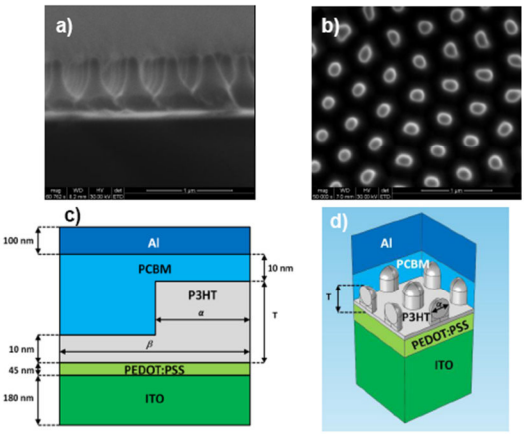

Figure 1: Environmental scanning electron microscopy (ESEM) images of P3HT nanopillars with the structure glass/ITO/PEDOT:PSS/P3HT-pillars made with NAAT, a) cross section and b) top view. Schematic unit cell (periodic conditions) of the structure ITO/PEDOT:PSS/P3HT/PCBM/Al for c) the 2D and d) the 3D models.

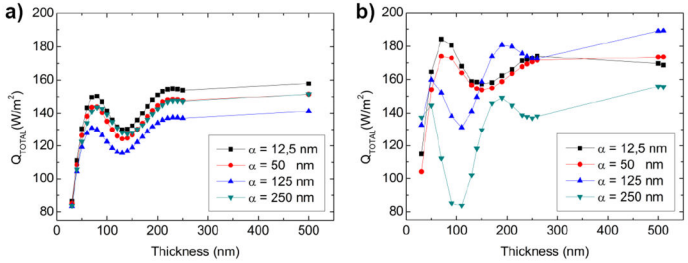

Figure 2: Total absorbed light power (Q_{TOTAL}) in the P3HT layer of a) the 2D and b) the 3D models as a function of the nanopillars height (*T*) for several nanopillar diameters (α).

References

[1] H. Hoppe, N. S. Sariciftci, J. Mater. Res., 19 (2004) 1924–1945.

[2] J. S. Kim, Y. Park, D. Y. Lee, J. H. Lee, J. H. Park, J. K. Kim, K. Cho, Adv. Funct. Mater., 20 (2010) 540–545.

[3] COMSOL (COMSOL Inc.), MA, USA. Available: http://www.comsol.com

[4] R. Palacios, P. Formentín, T. Trifonov, M. Estrada, R. Alcubilla, J. Pallarés, L. F. Marsal, Phys. Status Solidi Rapid Res. Lett., 2 (2008) 206–208.

[5] A. Santos, P. Formentín, J. Pallarés, J. Ferré-Borrull, L. F. Marsal, Sol. Energy Mater. Sol. Cells, 94 (2010) 1247–1253.