Modelling of doped organic solar cells

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Conjugated polymers or low-molecular compounds used in the active layer of organic solar cells contain numerous defects and impurities, which can act as dopants [1], for example, poly-(3-hexylthiophene) (P3HT) is easily doped by oxygen [2]. For inorganic solar cells, doping is essential for their performance. If for silicon solar cells adequate numerical models have been developed, it is not so for organic solar cells. Usually, the models for organic solar cells do not take into account doping, and only few papers analyse doping [1, 2]. We have developed numerical models for doped bulk and planar heterojunction organic solar cells and studied their performance [3].

Our numerical models are an extension of conventional models of organic solar cells with planar [4] and bulk heterojunctions [5], including field-dependent dissociation of bound electron-hole pairs at the heterojunction interface. For bulk heterojunction cells the metal-insulator-metal picture is used in which the active layer consisting of two materials (electron donor and acceptor) is considered as one semiconductor with properties of both materials. The model is based on the Poisson equation, current continuity equations, and equations for electron and hole current densities with drift and diffusion of charge carriers taken into account. The model accounts for ionized *n*- and *p*-type dopants, their energy levels are located in the band gap near the corresponding band edges. The *n*- and *p*-dopant concentrations N_n and N_p enter in the Poisson equation as follows

$$\frac{dE}{dx} = \frac{e}{\varepsilon\varepsilon_0} (p - n + N_n - N_p),$$

where *E* is the electric field strength, *e* is the electron charge, ε is the dielectric constant, ε_0 is the vacuum permittivity, *p* and *n* are concentrations of free holes and electrons, respectively.



Fig. 1. *J-V* characteristics at different *p*-type dopant concentrations N_{p} .

We studied the effect of doping using the material parameters of the most studied polymer-fullerene pair P3HT-PCBM. For an optimized P3HT-PCBM bulk heterojunction solar cell, the short current (J_{SC}), fill factor (*FF*), and efficiency drop with increasing dopant concentrations (Fig. 1). In the undoped cell, there is a constant electric field between the electrodes so that efficient bound electron-hole pair separation takes place

within the whole active layer. In the doped cell, the electric field is screened by free charges introduced by dopants in a part of the active layer, and at high doping the charge generation is efficient only within a thin region of the active layer, where a Schottky barrier is formed. However, for non-optimized bulk heterojunction cells, namely at low or unbalanced charge mobilities, or non-ohmic contacts, doping can enhance the cell efficiency. This is due to the fact that the electric field in the Schottky barrier region is much higher than in the undoped cell so that it can partly compensate the negative effect of non-optimized mobilities or contacts.

For bilayer cells in the case of majority carrier doping, i.e. when the electron transport layer (made of acceptor material) is *n*-doped and/or the hole transport layer (made of donor material) is *p*-doped, the J_{SC} , V_{OC} , and *FF* are increased with dopant concentrations (Fig. 2). Moreover, majority carrier doping compensates the negative effect of non-ohmic contacts, e.g. when the work functions of electrodes are equal and do not create a built-in potential. The improvement of bilayer cell performance with majority carrier doping is a result of the increased interfacial electric field between the layers. This field enhances the dissociation rate of bound electron-hole pairs, and hence the photocurrent increases. In the opposite case, i.e. minority carrier doping (acceptor is doped with *p*-type dopants, and/or donor is doped with *n*-type dopants), the J_{SC} and *FF* decrease with increasing dopant concentrations, the current-voltage curve becomes *S*-shaped.



Fig. 2. *J-V* characteristics of the bilayer solar cell at different dopant concentrations.

Thus, doping can strongly influence the performance of organic solar cells and should be taken into account in their optimization. The developed numerical device model could serve a useful tool for this purpose.

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