Modeling of transient photocurrent in organic semiconductors incorporating the annihilation of excitons on charge carriers

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Bulk heterojunction organic solar cells are considered as promising photovoltaic structures due to their properties, such as low-cost production, flexibility and relatively high solar energy harvesting. However, the organic photocells operate with different mechanisms than conventional solar cells based on inorganic materials [1]. The excitons play a key role in molecular devices, for example, the photogeneration of charge carriers takes place mostly from a dissociation of charge bounded pairs (excitons) at the boundaries between donor and acceptor phases. In addition, excitonic effects, which occur in the bulk of photovoltaic devices, can also influence on other photoelectric properties.

Here, we investigate the role of annihilation process of excitons on charge carriers in organic semiconductors. Recently, it has been shown that such an effect can visibly influence on the Langevin bimolecular recombination in the considered structures [2]. In this work, we have developed the numerical drift-diffusion model of transient photocurrent that traditionally incorporates the photogeneration and recombination processes of electrons, holes and excitons [3, 4], and additionally, the interaction process between excitons and charge carriers which leads to the annihilation of interacting excitons. The Poisson equation has been applied for solving the electric potential and electric field distributions between electrodes. The development of electrons, holes and excitons in time and space has been found from the continuous equations.

In the following study, we will demonstrate the results of photovoltaic parameters (short-circuit current, open-circuit voltage, fill-factor and efficiency of solar cell) as a function of annihilation rate constant and exciton mobility. The time evolution and the steady-state space distribution of charge carriers will be also presented to explain the role of exciton annihilation process.

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