Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 331 (2018) 281–308
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Solution map analysis of a multiscale Drift–Diffusion model for organic solar cells

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Received 27 July 2017; received in revised form 17 November 2017; accepted 19 November 2017
Available online 2 December 2017

Abstract

In this article we address the theoretical study of a multiscale drift–diffusion (DD) model for the description of photoconversion mechanisms in organic solar cells. The multiscale nature of the formulation is based on the co-presence of light absorption, conversion and diffusion phenomena that occur in the three-dimensional material bulk, of charge photoconversion phenomena that occur at the two-dimensional material interface separating acceptor and donor material phases, and of charge separation and subsequent charge transport in each three-dimensional material phase to device terminals that are driven by drift and diffusion electrical forces. The model accounts for the nonlinear interaction among four species: excitons, polarons, electrons and holes, and allows to quantitatively predict the electrical current collected at the device contacts of the cell. Existence and uniqueness of weak solutions of the DD system, as well as nonnegativity of all species concentrations, are proved in the stationary regime via a solution map that is a variant of the Gummel iteration commonly used in the treatment of the DD model for inorganic semiconductors. The results are established upon assuming suitable restrictions on the data and some regularity property on the mixed boundary value problem for the Poisson equation. The theoretical conclusions are numerically validated on the simulation of three-dimensional problems characterized by realistic values of the physical parameters.

Keywords: Organic semiconductors; Solar cells; Nonlinear systems of partial differential equations; Multi-domain formulation; Drift–Diffusion model; Functional iteration

1. Introduction

Within the widespread set of applications of nanotechnology, the branch of renewable energies certainly occupies a prominent position because of the urgent need of addressing and solving the problems related with the production and use of energy and its impact on air pollution and climate. We refer to [1] for the analysis of the state-of-the-art in the complex connection between industrial and domestic usage of energy and global climate change. Renewable energies comprise a set of different physical and technological approaches to production, storage and delivery of sources of

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https://doi.org/10.1016/j.cma.2017.11.026
0045-7825/

supply to everyday's life human activities that are alternative to the usual fossil fuel, and include, without being limited to: solar, hydrogen, wind, biomass, geothermal and tidal energies. A comprehensive survey on the fundamental role of nanotechnology in understanding and developing novel advancing fronts in renewable energies can be found in [2].

In this article we focus our interest on the specific area of solar energy, and, more in detail, on organic solar cells (OSCs). OSCs have received increasing attention in the current nanotechnology industry because of distinguishing features such as good efficiency at a very cheap cost and mechanical flexibility due to roll-to-roll fabrication process, which make them promising alternatives to traditional silicon-based devices [3]. The macroscopic behaviour of an OSC depends strongly on the photoconversion mechanisms that occur at much finer spatial and temporal scales. According to the physical description of [4–6], such mechanisms basically consist in: (1) generation and diffusion of excited neutral states in the material bulk; (2) dipole separation at material interfaces into positive and negative charge carriers; and (3) transport of charge carriers in the different material phases for subsequent collection of electric current at the output device terminals (positive charges at the anode and negative charges at the cathode).

In the following pages we proceed along the line of the series of works [7–10] and we carry out the mathematical analysis of the model proposed in [8] and studied in two-dimensional geometrical configurations, under the assumption that the computational domain is a three-dimensional polyhedron divided into two disjoint regions separated by a two-dimensional manifold that represents the material interface at which the principal photoconversion phenomena take place. The structure considered in the present work is described in Section 2 and can be regarded as a faithful representation of a realistic OSC. The mathematical model, described in Section 3, and then subsequently in Sections 4 and 5, is an extension of the classic Drift–Diffusion (DD) system of partial differential equations (PDEs) used for the investigation of charge transport in semiconductor devices for micro and nano-electronics [11–14]. It consists of a multidomain differential problem in conservation format for four distinct species: excitons, polarons, electrons and holes. Excitons and polarons are neutral particles; polarons may dissociate into electrons (negatively charged) and holes (positively charged) at the interface and the resulting free charges are free to move in their respective material phases under the action of a internal potential drop (related to the work function gap between the two phases) and of an external electric field due to an applied voltage drop. Electrons and holes are electrostatically coupled through Gauss' law in differential form (Poisson equation) and kinetically coupled through recombination/generation reactions occurring at the interface.

The resulting problem is a highly nonlinearly coupled system of advection–diffusion–reaction PDEs for which, in Section 6, we provide in the stationary regime a complete analysis of the existence and uniqueness of weak solutions, as well as nonnegativity of all species concentrations, via a solution map that is a variant of the Gummel iteration commonly used in the treatment of the DD model for inorganic semiconductors [13]. The results are established upon assuming suitable restrictions on the data and some regularity property on the mixed boundary value problem for the Poisson equation. The theoretical conclusions are numerically validated in Section 7 on the simulation of three-dimensional problems characterized by realistic values of the physical parameters whereas in Section 8 some concluding remarks and indications for future extensions of model and analysis are illustrated.

2. Geometry and notations

Let $\Omega \subset \mathbb{R}^3$ denote the organic solar cell volume (called from now on the *device*). We assume that Ω is a bounded, connected, Lipschitzian open set.

Inside Ω we admit the presence of an open, regular surface Γ (called from now on the *interface*) that divides Ω into the two regions (connected open sets) Ω_n and Ω_p in such a way that $\Omega = \Omega_n \cup \Gamma \cup \Omega_p$. The unit normal vector oriented from Ω_p into Ω_n is denoted by ν_Γ. A graphical plot of the three-dimensional (3D) domain comprising the interface is depicted in Fig. 1(a). The boundary of Ω is the union of two disjoint subsets, so that $\partial\Omega = \Gamma_D \cup \Gamma_N$. The unit outward normal vector on $\partial\Omega$ is denoted by ν. Specifically, Γ_D represents the contacts of the device, i.e. *anode* $\Gamma_A = \Gamma_D \cap \partial\Omega_p$ and *cathode* $\Gamma_C = \Gamma_D \cap \partial\Omega_n$. We assume that anode and cathode have nonzero areas and that Γ_D and Γ are strictly separated. Furthermore, Γ_N is the (relatively open) part of its boundary where the device is insulated from the surrounding environment. We put $\Gamma_n = \Gamma_N \cap \partial\Omega_n$ and $\Gamma_p = \Gamma_N \cap \partial\Omega_p$. A graphical plot of a two-dimensional (2D) cross-section of the device domain comprising the interface and the boundary is depicted in Fig. 1(b).

The notation of function spaces in the present paper is as follows. We define $\mathcal{W}^q$ ($q \geq 2$) as the closure of the set

$$\left\{ w|_\Omega : w \in C^\infty\left(\mathbb{R}^3\right),\ \operatorname{supp}(w) \cap \Gamma_D = \varnothing \right\}$$