Modelling and Loss Analysis of Meso-Structured Perovskite Solar Cells

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Abstract

Recently, the pursuit of organic-inorganic perovskite solar cells has been significantly advanced because of the promising high-efficiency potential of the perovskite materials. Based on the structure of dye sensitized solar cells, Miyasaka et al. in 2009 firstly incorporated a perovskite material into a solar cell, thereby achieving 3.8% conversion efficiency. Afterwards, many groups contributed to the development of perovskite solar cells and as a result, its efficiency increased quickly to 22.1% in this year. In addition to the advancement in experimental studies, the modelling and numerical simulation of perovskite solar cells are crucial, as it can aid in elucidating the device physics, unveiling its intrinsic material properties and predicting the device performance.
In view of the lack of an in-depth mathematical device model for meso-structured perovskite solar cells and the ongoing discussion of the dominant type of recombination mechanism in those solar cells, we firstly derive a generic mathematical device model for meso-structured perovskite solar cells. Secondly, we calibrate and validate the resulting model with the help of COMSOL Multiphysics. Inside COMSOL, we use the Transport of Diluted Species interface to compute the concentration of electrons and holes inside the solar cell, coupled with Poisson's Equation interface to model the electric potential within the cell. At various interfaces, the continuity of electric potential and the electric field are enforced, while the corresponding jumps of electron/hole flux and of the electron/hole concentration are also defined. There are a total of 36 physical parameters required for our mathematical model in which 29 of them can be measured or taken from literature and the remaining 7 more parameters are unknown. Calibration of these unknown parameters was performed by solving a non-linear curve-fitting problem in the least-squares sense in LiveLink for MATLAB.
After calibration and validation with experimentally measured current-voltage curves, we are able to elucidate within the mathematical framework the dominant type of recombination mechanism and the location where this dominant type of mechanism takes place. Last but not least, a subsequent loss analysis for meso-structured perovskite solar cells is derived based on the COMSOL simulation results. It indicates that, in our fabricated solar cell, the interfacial recombination between the perovskite/mesoporous titanium dioxide within the mesoporous absorber layer constitutes the main loss channel. This interfacial recombination accounts for up to 46% of all recombination losses at maximum power, thereby exceeding the recombination inside the perovskite capping layer with 31% loss.

Figures used in the abstract

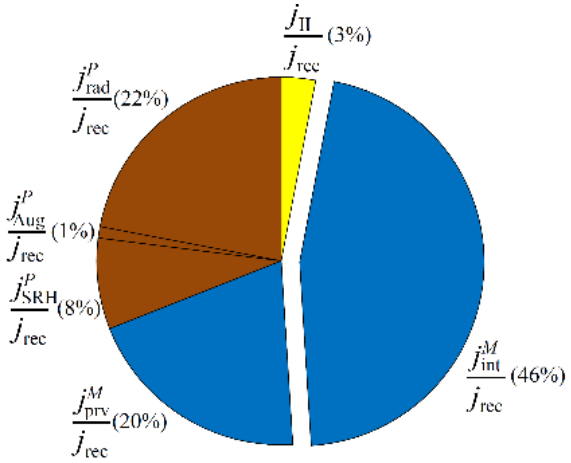

Figure 1: Percentage contribution of various recombination loss channels under open-circuit condition.