Instability Analysis of Perovskite Solar Cells via Drift-diffusion Numerical Simulation of Impedance Spectroscopy at Short-circuit

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Abstract

Perovskite solar cells (PSCs) remain at the forefront of emerging photovoltaic technologies[1] due to their high power conversion efficiency and versatile applications. However, challenges persist not only in achieving stability but also in understanding the ionic-electronic transport mechanisms governing their performance. In this study,[2] we present the results of numerical drift-diffusion simulations in relation to the study case of NiO_x-based PSCs with various interface passivation treatments.[3] Our simulations approach qualitatively and quantitatively several experimental measurements of impedance spectroscopy (IS) under short-circuit conditions at different illumination intensities, along with bias-stress accelerated operational stability tests under constant illumination. Drift-diffusion simulations suggest that interface modification with the hole transport material may reduce conductivity, ion mobility within the perovskite layer, and electron mobility within the NiO_x layer. Notably, capacitance and resistance exhibit peak values and minimum values, respectively, within specific ranges of mobile ion concentration. Our findings provide a systematic approach for characterizing instability mechanisms in PSCs using IS under short-circuit conditions.

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