I. INTRODUCTION

More comprehensions of the halide perovskites accompany the robust improvement of their solar cells, whose record of the single junction [1] and 2-terminal tandem [2] are 22.7% and 25.2%, respectively. Halide perovskite materials (ABX$_3$) share a similar cell structure with the classic mineral oxide perovskite (ABO$_3$). The cation A site is typically composed of organic methylammonium (MA), formamidinium (FA), or inorganic Cs or Rb cations. Generally, lead (Pb) sits inside halide perovskites under different operation conditions, which is quite different from the traditional silicon or III-V materials. The ion migration is assumed to contribute to one of the major instabilities of perovskite solar cells (PSCs), the abnormal hysteresis effect [9], which means the current-voltage (J-V) characteristics depends on the scan rate, the scan direction or the precondition. With such effect, the effective photon-to-electron conversion efficiency could be questioned.

In the study, the drift-diffusion approximations and the continuity equations of electrons and holes are extended in the simulator atlas to consider ions moving inside the perovskite layer. One of the most widely studied compounds, MAPbI$_3$ perovskite is chosen to investigate the ion migration within the TiO$_x$/MAPbI$_3$/Spiro-OMeTAD architecture. The simulated ion migration and the corresponding hysteresis effect are presented and discussed.

II. MODELING AND DISCUSSION

The architecture is experimentally studied as mentioned in the previous report [10]. The anatase TiO$_x$ (165 nm-thick) is the electron transport layer, and the Spiro-OMeTAD (50 nm-thick) is the hole transport layer, sandwiching the absorber MAPbI$_3$ (total 335 nm-thick). The 135 nm-thick MAPbI$_3$ is related to the part inside the porosity of mesoporous TiO$_x$ layer. The electrodes are Ohmic. The photo-induced carrier generation processes are introduced by the complex refractive index of the materials, in addition to the bimolecular recombination, and the trap-assisted recombination in the bulk and at the TiO$_x$/MAPbI$_3$ interface.

The schematic architecture of PSC is drawn (Fig. 1), along with the simulated band alignment and the electric field (E$_{bd}$). Two E$_{bd}$ spikes in a logarithm scale are related to two hetero-junctions, while the E$_{bd}$ is uniform in the middle. In the dark and short circuit (Fig. 2 a-c), carriers are depleted under built-in potential, and the negative ions accumulate near the TiO$_x$ layer, where the ionized dopants are positive. Under illumination of one sun and 1.5 V bias (Fig. 2 d-f), the perovskite layer is filled with photo-generated carriers, and the negative ions shift towards to the positively biased anode.

After preconditioned under one sun and 1.5 V bias for 20 seconds, the J-V characterization is performed from 0 to 1.5 V then back to 0 V. The hysteresis effect is observed in the experiments and simulations (Fig. 3). The variation of the open circuit voltage is well reproduced, while the difference of the short-circuit current might come from the thickness of the perovskite layer.
the MAPbI\textsubscript{3} layer or the device surface area. The simulated J-V characteristic above 1 V shows a similar trend to the experiments, indicating a saturation of the ion migration. According to the simulation in the study, the interface recombination at TiO\textsubscript{x}/MAPbI\textsubscript{3} is mandatory to reproduce the hysteresis effect, besides the ion migration. This might interpret the observation of ion migration in the inverted PSCs, however, who are almost free of the hysteresis effect. The interface condition between perovskite and PCBM is assumed to be better than that at TiO\textsubscript{x}/MAPbI\textsubscript{3} interface.

Fig. 1. a) Schematic architecture of PSCs, b) the simulated band alignment and c) the electric field profile. The band alignment and the electric field share the same x-axis. Spiro is short for Spiro-OMeTAD.

Fig. 2. Potential, carrier and ion density a-c) in the dark and short circuit, d-f) under light and 1.5 V bias. C\textsubscript{n} indicates major part of the negative ions.

Fig. 3. Experimental and simulated hysteresis J-V characteristics. FW is the forward scan and BW is the backward scan. Before any scan, the devices are preconditioned under one sun and 1.5 V bias for 20 seconds. The y-axis in b) uses a logarithm scale.

REFERENCES


