Modeling the perovskite solar cell and the ion migration with physical approach based on FEM from Silvaco

Jihye Baik[1], Haeyeon Jun[1,2], Hindia Nahdi[1,3], Bernard Geffroy[1,4], Denis Tondlier[1] and Yvan Bonnassieux[1]

[1]LPICM-CNRS (UMR7647), Ecole Polytechnique, IP Paris, 91128 Palaiseau, France
[2]Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, BP 48 91192 Gif-sur-Yvette Cedex, France
[3]SEGULA Technologies, 19 Rue d'Arras, 92000 Nanterre, France
[4]Université Paris-Saclay, CEA, CNRS, NIMBE, LICSEN, 91191 Gif-sur-Yvette, France

The hybrid perovskites have emerged as the promising alternative materials of silicon-based solar cells in PV industry due to high absorption coefficient [1] and long carrier lifetimes and diffusion lengths [2]. Even though the power conversion efficiency of perovskite solar cells (PSCs) has increased rapidly to 25.2 % in 2020 [3], PSCs have still drawbacks such as J-V hysteresis of which origins are not fully understood yet but might be ion migration [4], [5]. Therefore, studying factors causing J-V hysteresis is required to develop strategies for resolving the issue.

In this work, modeling of ion migration in the PSCs with physical approach based on finite element method is studied. As the time-transient state is necessary to investigate the hysteresis, the simulation is performed in time-transient state by using Atlas, Silvaco. The ion migration in methylammonium lead halide perovskite ($CH_3NH_3PbI_3$) is described by drift-diffusion model. The ion migration and accumulation induce the electric field compensation and result in the J-V hysteresis. We examined the J-V hysteresis dependent on various factors: ion diffusion coefficient, preset voltage time, and voltage scan rate.

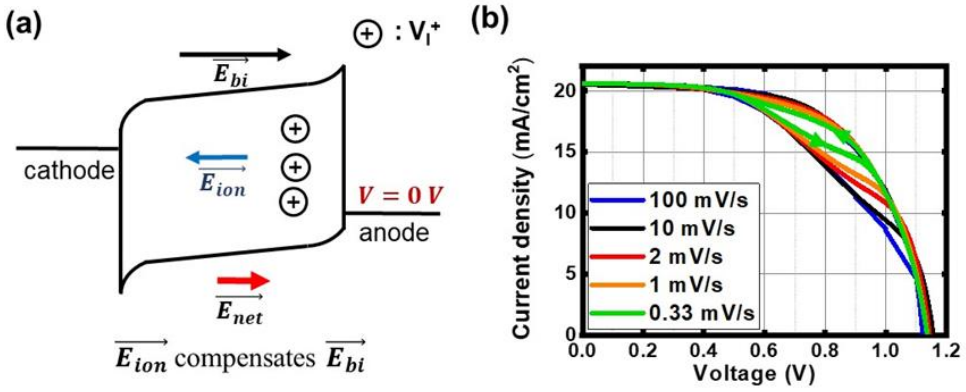

Figure 1. (a) A scheme of PSCs with the compensation of built-in electric field due to the ion migration. The cations represent the iodine vacancies and they transport to the anode side due to the built-in electric field. **(b)** The J-V hysteresis dependent on the voltage scan rate.

Keywords
Lead halide perovskite, Simulation, Silvaco, Ion migration, Drift-diffusion model

Reference

[1] B. Lei *et al.*, "High-performance CH3NH3PbI3 perovskite solar cells fabricated under ambient conditions with high relative humidity", *Jpn. J. Appl. Phys.*, vol. 54, no. 10, 2015.
[2] B. Yu *et al.*, "Charge carrier lifetimes exceeding 15 μs in methylammonium lead iodide single crystals", *J. Phys. Chem.*, vol. 7, no. 5, 2016.
[3] "NREL efficiency chart." [Online]. Available: https://www.nrel.gov/pv/cell-efficiency.html.
[4] M. Grätzel *et al.*, "Understanding the rate-dependent J-V hysteresis, slow time component, and aging in $CH_3NH_3PbI_3$ perovskite solar cells: The role of a compensated electric field", *Energy Environ. Sci.*, vol. 8, no. 3, 2015.
[5] Y. Zhao *et al.*, "Anomalously large interface charge in polarity-switchable photovoltaic devices: An indication of mobile ions in organic-inorganic halide perovskites,", *Energy Environ. Sci.*, vol. 8, no. 4, 2015.