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Modeling Ion Transport and Hysteresis Phenomenon in Perovskite Solar Cells Using Drift-Diffusion Simulation

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INTRODUCTION & AIM

Perovskite solar cells (PSCs) have already achieved efficiencies above 27%, making them competitive with silicon-based devices. Among them, $MAPbI_3$ is particularly attractive due to its strong light absorption, long carrier lifetime, and low fabrication cost, making it a promising material for next-generation photovoltaics. However, the main challenge is ion migration, which causes instability and hysteresis in current-voltage characteristics. To mitigate these issues, charge transport layers are employed: SnO_2 (ETL) with high electron mobility and NiOx (HTL) with strong hole conductivity and resistance to degradation. In this work, drift-diffusion modeling is applied to study the influence of carrier mobility, lifetime, and scan rate on hysteresis formation. The relevance of this research lies in the fact that understanding ion migration mechanisms and their numerical modeling is crucial for improving the stability and efficiency of PSCs.

METHOD

A modified one-dimensional drift-diffusion model Driftfusion [1] implemented in MATLAB was used to account for ion migration, carrier lifetime, mobility, and interband recombination rate.

A constant mobility model is used for the perovskite and transport layers; ions are immobile in transport layers, and transport is described by drift and diffusion, with equations below

$$\begin{cases} \nabla\cdot(\epsilon\nabla\Phi) = -q\left(n - p + N_a^- - N_d^+ - N_{ct} + N_{an} + n_t^- - n_t^+\right) \\ \nabla\cdot\{\mu_n n(\nabla\Phi_n)\} = G - R_{dir} - R_{SRH} \\ \nabla\cdot\{\mu_p p(\nabla\Phi_p)\} = G - R_{dir} - R_{SRH} \\ \nabla\cdot\left\{\mu_{ct}N_{ct}\left(\kappa_B T\dfrac{\partial N_{ct}}{\partial x}\right)\right\} = 0 \\ \nabla\cdot\left\{\mu_{an}N_{an}\left(\kappa_B T\dfrac{\partial N_{an}}{\partial x}\right)\right\} = 0 \end{cases}$$

Radiative (bimolecular) recombination of electrons and holes is taken into account through R_{dir}

$$R_{dir} = k_{dir}(np - n_i^2).$$

To account for carrier trapping by defects and traps, Shockley-Read-Hall (SRH) recombination is used, expressed as follows [2,3]:

$$R_{SRH} = \frac{np - n_i^2}{\left(n + N_c\exp\left(\frac{E_t - E_c}{k_B T}\right)\right)\tau_p + \left(p + N_V\exp\left(\frac{E_V - E_t}{k_B T}\right)\right)\tau_n}.$$

The capture time is determined using the trap capture coefficient $C_{n,p}$ and the trap density as follows:

$$\tau_{n,p} = \frac{1}{N_t C_{n,p}}.$$

To calculate the hysteresis index (HI) for all current-voltage (J-V) curves, the power conversion efficiency (PCE) values from forward and reverse scans are used [4], as follows:

$$HI = \frac{PCE_{(reverse)} - PCE_{(forward)}}{PCE_{(reverse)}}.$$

RESULTS & DISCUSSION

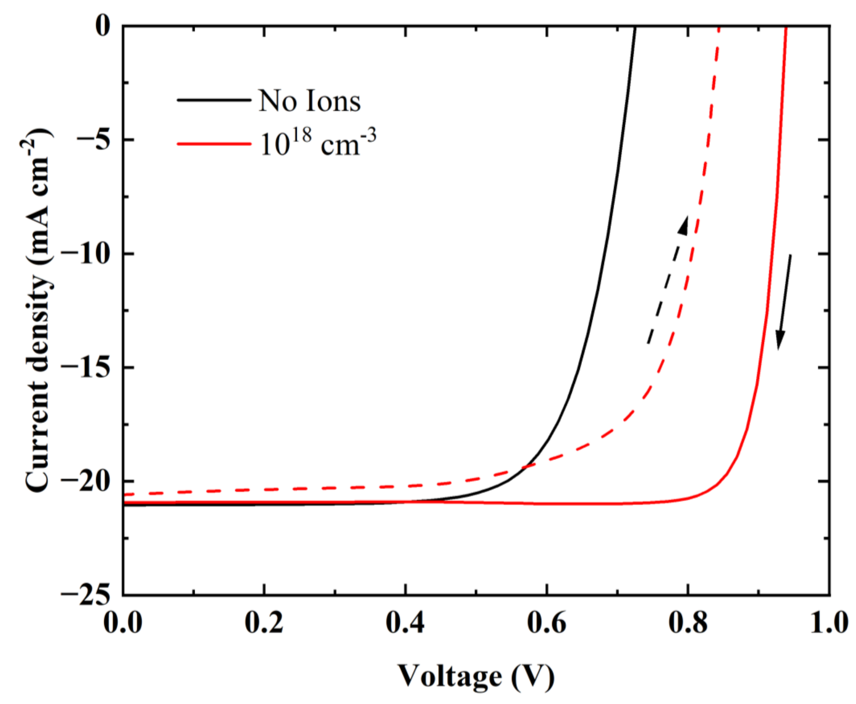

Figure 2. Simulated J–V curves of $MAPbI_3$ PSCs with different intrinsic ion densities.

J-V curves of $MAPbI_3$ PSCs show that ion-mediated recombination reduces efficiency from 16.94% to 12.31% and induces pronounced hysteresis (HI = 0.27).

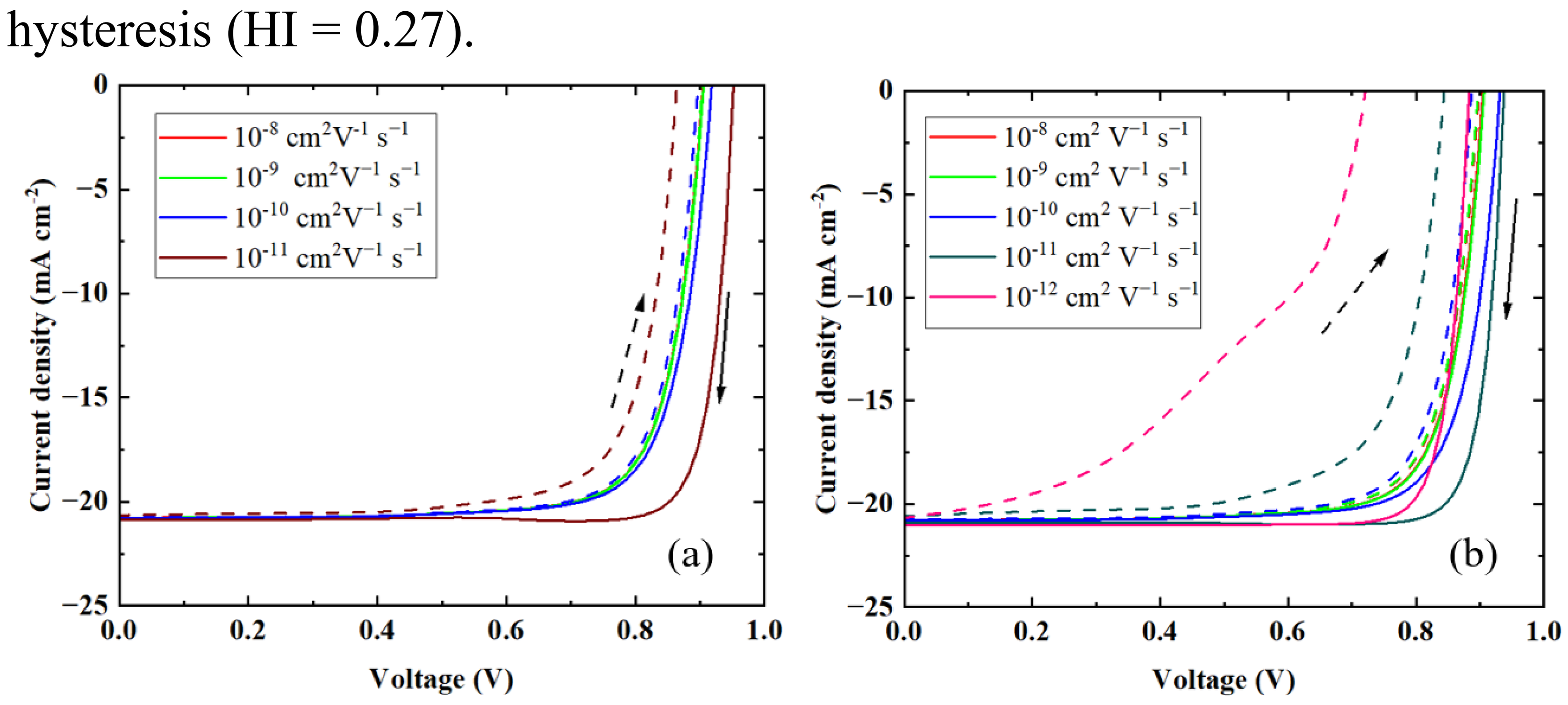

Figure 1. J–V curves of $MAPbI_3$ with varying ion mobility: (a) equal cation/anion mobilities, (b) varying anion mobility with fixed cation mobility (10^{-12} cm²/V·s).

At high symmetric ion mobility, the device is stable (V_{oc}=0.912 V, J_{sc}=20.77 mA/cm², FF≈0.77, PCE=14.7%, PCE=14.7%, HI≈0), whereas at low or asymmetric mobility it shows higher efficiency (PCE up to 15.9%) but strong hysteresis (HI up to 0.59) and instability.

CONCLUSION

Numerical modeling showed that the efficiency and stability of $MAPbI_3$-based perovskite solar cells depend on carrier lifetime, mobility, recombination rates, ion mobility, and voltage scan rate. The best performance is achieved with long carrier lifetimes, balanced mobilities, and minimal recombination. High and symmetric ion mobility ensures stable operation with negligible hysteresis, while low or asymmetric mobility leads to strong distortions and instability. These results highlight the need for precise engineering optimization to suppress ion-related instabilities and maximize device efficiency.

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