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Modeling and Performance Optimization of $CH_3NH_3SnI_3$-Based Lead-Free Perovskite Solar Cells

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INTRODUCTION & AIM

The growing global demand for renewable energy requires the development of highly efficient and stable photovoltaic technologies. Perovskite solar cells (PSCs) have emerged as a next-generation solution due to their remarkable power conversion efficiencies exceeding 26%. Among them, lead-free tin-based perovskites ($CH_3NH_3SnI_3$) are of particular interest, offering an appropriate bandgap (~1.3 eV), high hole mobility, and environmentally friendly properties.

However, their performance is severely limited by fast Sn^{2+} oxidation, self-doping, intrinsic defects, and poor interfacial alignment. These challenges cause parasitic recombination losses, low open-circuit voltage, reduced carrier lifetimes, and most critically, strong hysteresis in J–V characteristics.

The aim of this study is to provide a comprehensive drift–diffusion modeling analysis of $CH_3NH_3SnI_3$ PSCs. We focus on the role of ion migration, trap-assisted recombination, and carrier lifetimes in determining device efficiency and hysteresis, aiming to identify pathways toward stable and high-performance lead-free photovoltaics.

METHOD

A planar $CH_3NH_3SnI_3$ perovskite solar cell was simulated with the architecture: Glass / ITO / TiO_2 (50 nm, ETL) / $CH_3NH_3SnI_3$ (500 nm, absorber) / MoO_3 (100 nm, HTL) / Au. To capture interfacial effects, 1 nm graded regions were introduced at both ETL/perovskite and HTL/perovskite interfaces, where band edges and dielectric properties were gradually varied.

The simulations were performed using the Driftfusion drift–diffusion solver, which couple electrostatics, electronic and ionic transport, and recombination. The model includes Poisson's equation, drift–diffusion continuity equations, and recombination processes:

$$\begin{aligned}
\nabla \cdot (\epsilon \nabla \Phi) &= -q\left(n - p + N_{\mathrm{a}}^{-} - N_{\mathrm{d}}^{+} - N_{\mathrm{ct}} + N_{\mathrm{an}} + n_{\mathrm{t}}^{-} - n_{\mathrm{t}}^{+}\right) \\
\nabla \cdot \{\mu_{\mathrm{n}} n(\nabla \Phi_{\mathrm{n}})\} &= G - R_{\mathrm{dir}} - R_{\mathrm{SRH}} \\
\nabla \cdot \left\{\mu_{\mathrm{p}} p\left(\nabla \Phi_{\mathrm{p}}\right)\right\} &= G - R_{\mathrm{dir}} - R_{\mathrm{SRH}} \\
\nabla \cdot \left\{\mu_{\mathrm{ct}} N_{\mathrm{ct}} \left(k_B \mathrm{T} \frac{\partial N_{\mathrm{ct}}}{\partial x}\right)\right\} &= 0 \\
\nabla \cdot \left\{\mu_{\mathrm{an}} N_{\mathrm{an}} \left(k_{\mathrm{B}} \mathrm{T} \frac{\partial N_{\mathrm{an}}}{\partial x}\right)\right\} &= 0
\end{aligned} \qquad (1)$$

where Φ is the electrostatic potential, n, p are carrier densities, μ mobilities, G optical generation, and Rrecombination. Direct bimolecular recombination is described by:

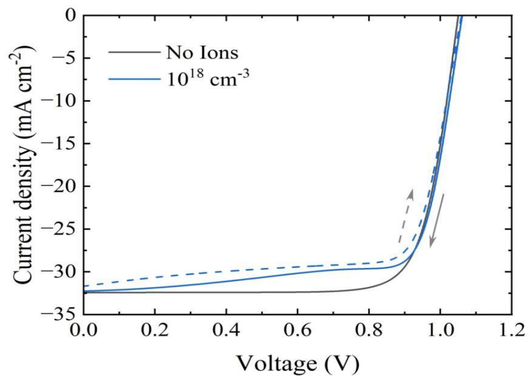
$$R_{dir} = B(np - n_i^2)$$

while trap-assisted Shockley–Read–Hall recombination was included to reproduce hysteresis in J–V curves.

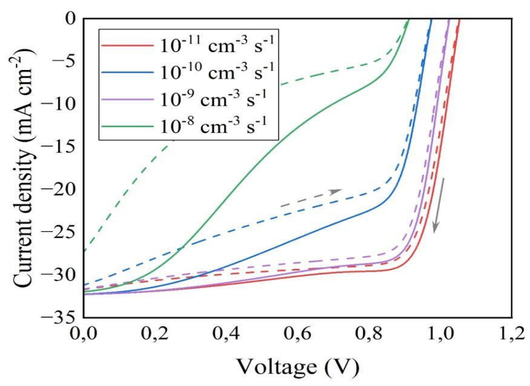
Key parameters varied were carrier mobility and lifetime, ionic density and mobility, trap density, and surface recombination velocity. Device stability was quantified by the Hysteresis Index (HI), comparing forward and reverse J–V scans.

RESULTS & DISCUSSION

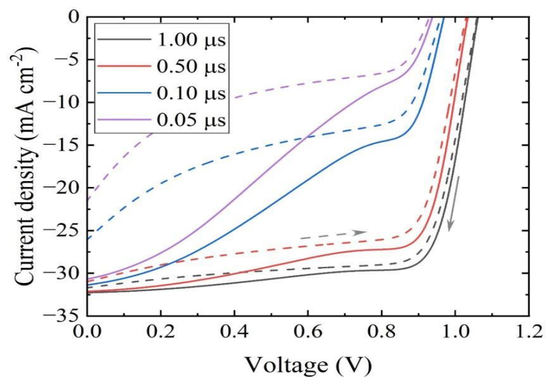
Ion migration induces hysteresis but has only a moderate effect on PCE at realistic concentrations. At ionic density $10^{18}\ cm^{-3}$,HI ≈ 0.039 while PCE remains ~26%. (Fig. 1)



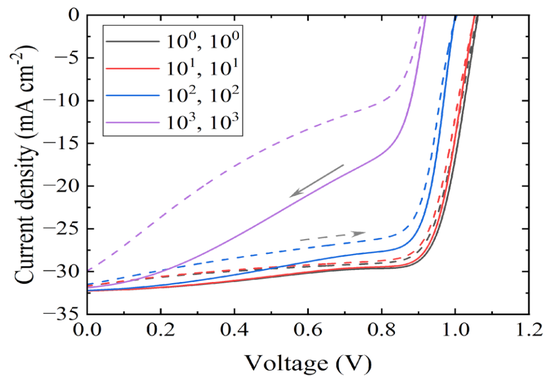
Bimolecular recombination rate is a key limiting factor. Reducing it from 10^{-8} to $10^{-11}\ cm^3 s^{-1}$ increases efficiency from 4.3% → 24.9% and reduces hysteresis. (Fig.2)



Carrier lifetime strongly governs stability.
Short lifetimes ($\tau < 0.1\ \mu s$) lead to severe hysteresis, V_{oc} drop to 0.94 V, and PCE collapse to ~5%. (Fig.3)



Surface recombination significantly degrades device quality. At $S_n = S_p = 10^3\ cm/s$, efficiency falls below 9% and S-shaped J–V curves appear. (Fig.4)



CONCLUSION

- Recombination rates strongly correlate with photovoltaic performance.
- Hysteresis is governed by ion relaxation and scan rate interplay.
- High surface recombination significantly reduces device efficiency.
- Longer carrier lifetimes improve stability and reduce hysteresis.
- Controlling recombination, ion migration, and interfaces is essential for stable Sn-based PSCs.

FUTURE WORK / REFERENCES

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