

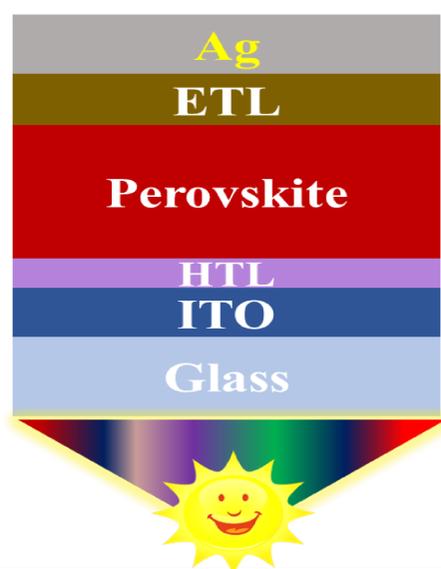
National Institute for Materials Science, Tsukuba, Japan; Indian Institute of Technology Bombay, Mumbai, India

Introduction

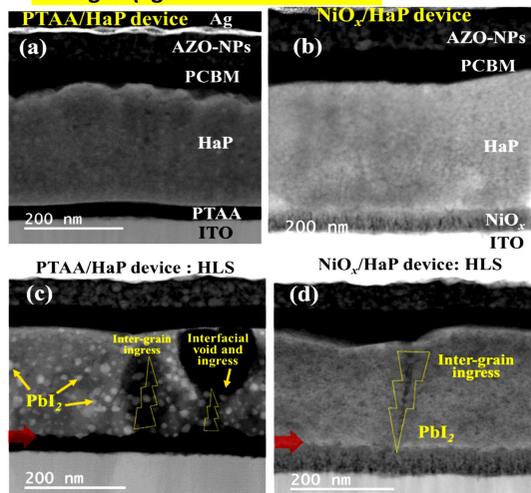
The Power conversion efficiency (PCE) of a Perovskite solar cell (PSC) declines during operation with time. The cause of the deterioration of perovskite solar cells is the instability of the perovskite crystal, induced by external factors, such as humidity, heat, light, and electric field. To understand the degradation, a simulation based on an analytical and numerical model is performed.

- In analytical model-based simulation, degradation is considered a function of surface recombination velocity.
- In numerical simulation based on the drift diffusion model, the degradation is considered as a function of ion density.

Device Structure and Ageing



STEM cross-sectional images of fresh (a, b) and aged (light and thermal stress)

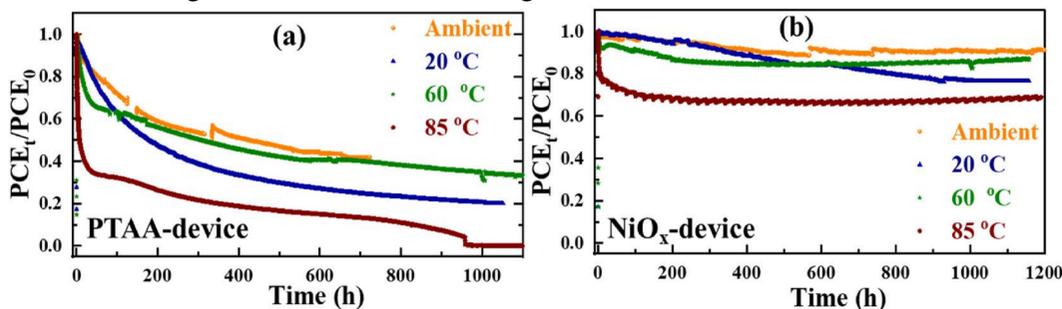


Results and Discussion

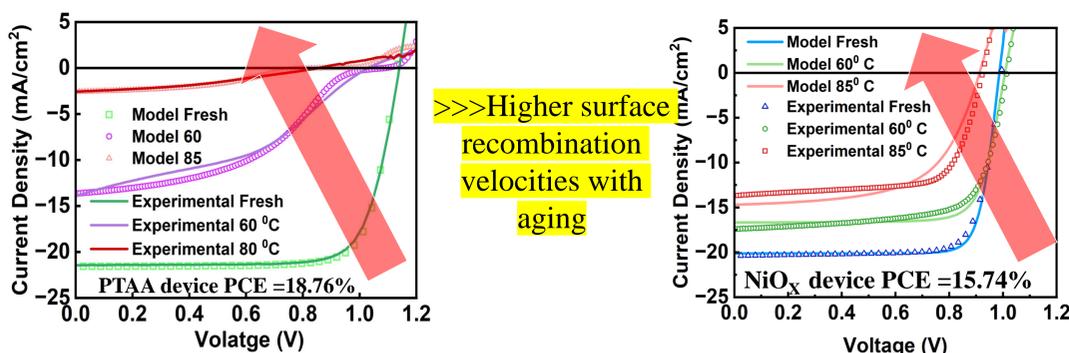
Devices using PTAA as the HTL achieved a higher initial efficiency compared to NiO_x, but PTAA device degraded significantly more with increasing temperature

Operational stability of PSCs with PTAA

>>> faster degradation under heat and light stress



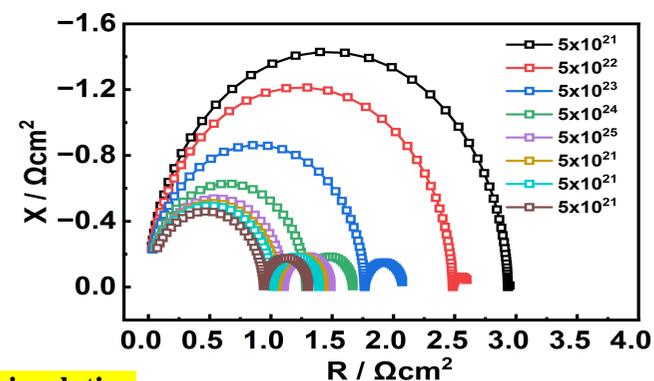
>>> Analysis of aged J-V curves using an analytical model



>>> Higher surface recombination velocities with aging

Drift diffusion simulation

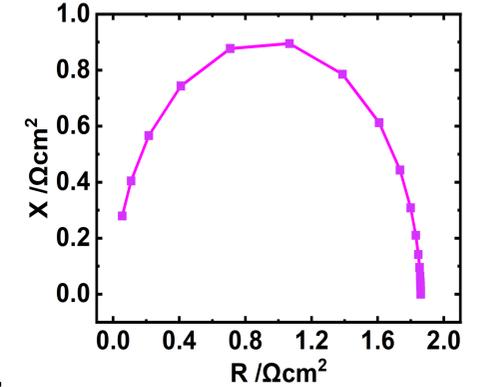
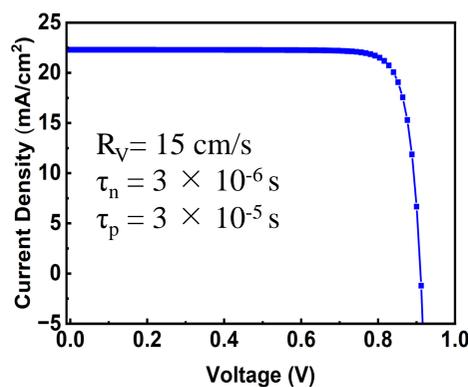
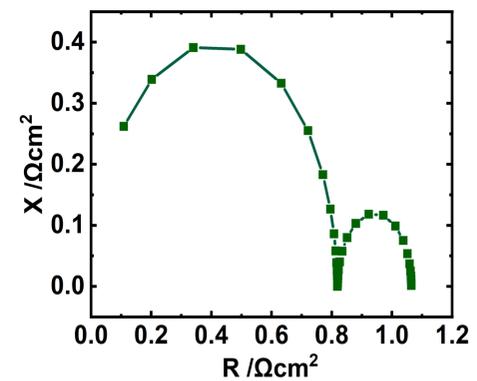
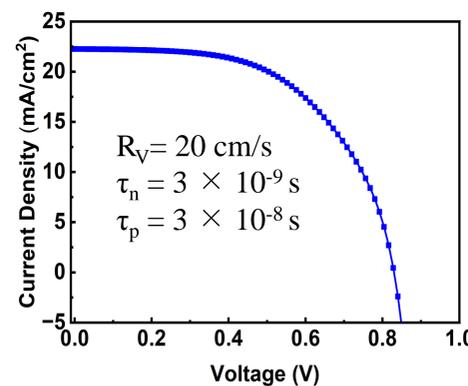
>>> Impedance spectra showing the effect of the Effective valence band DoS in HTL. The negative hook indicates strong ionic interactions with the surface.



Drift diffusion simulation

JV characteristics/ corresponding impedance spectra.

>>> A reduction in recombination velocity and an increase in carrier lifetimes suggest improved charge carrier dynamics



Conclusion

- Surface recombination leads to charge carrier loss, accelerating cell degradation over time and with temperature.
- Impedance spectra show that higher-frequency components play a larger role in degraded solar cells.
- Low ion density minimizes low-frequency contributions in impedance spectra.
- Impedance changes reveal how ion density impacts charge transport and recombination in PSCs.

References

1. D. B. Khadka, et al. *ACS Appl Energy Mater.* **2021**, 4, 11121–11132.
2. C. C. Boyd, et al. *Chem Rev.* **2019**, 119, 3418–3451.
3. X. Sun, et al. **2015**, 5, 1389–1394.
4. A. Matsushita, et al. *Solar Energy Materials and Solar Cells.* **2021**, 220, 110854.
5. W. Clarke, et al. *J Comput Electron.* **2023**, 22, 364–382
6. D. B. Khadka, et al. *Solar Energy Materials and Solar Cells.* **2022**, 246, 111899.
7. M. Diethelm, et al. *Energy Environ Sci.* **2025**, 18, 1385–1397.
8. D. B. Khadka et al. *J. Mater. Chem. C.* **6**, 162, 2018.