

Understanding and Mitigating the Degradation of Perovskite

Solar Cells Based on a Nickel Oxide Hole Transport Material during Damp Heat Testing

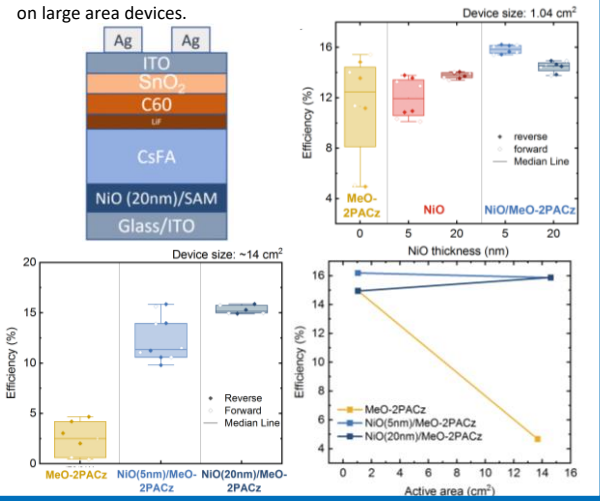
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Abstract: The development of stable, large-scale, processable materials is a prerequisite to industrialize perovskite solar cells (PSCs). Beyond the perovskite absorber itself, this prerequisite should also guide the development of the device-contacting layers. In this regard, the use of NiO_x as a hole transport material (HTM) offers several advantages as this inorganic p-type semiconductor can be deposited with high throughput on large flat or textured surfaces via sputtering, a well-established industrial method. However, NiO_x may trigger the degradation of PSCs when exposed to high temperature, light illumination, or humidity. A strong fill factor (FF) loss appears already after 100 hours of damp heat stressing, in conjunction with the appearance of a characteristic S-shaped J-V curve. This poster focuses on the understanding of this degradation.

High Eff vs. Upscaling: the choice of the HTM

- Best efficiencies on 1.04 cm²: MeO-2PACz.
- Better reproducibility over larger areas (15 cm²): NiO_x (continuous coverage).

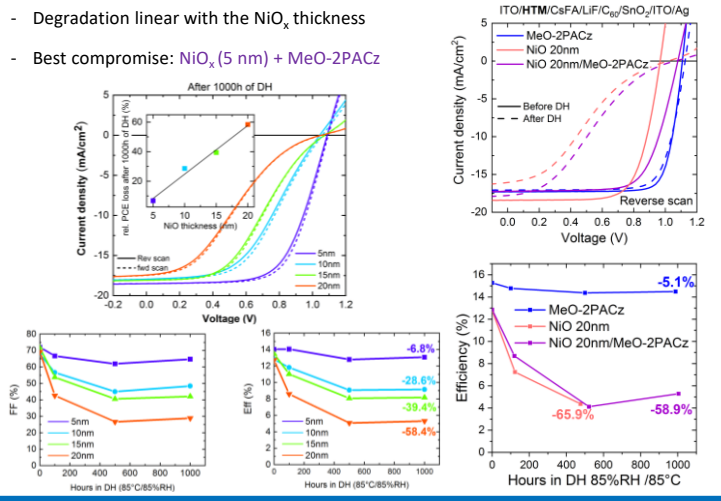
→ Bilayer NiO_x/MeO-2PACz: high efficiency and good reproducibility on large area devices.



NiO_x leads to the formation of a barrier at elevated T°

NiO_x-based PSCs show strong degradation under damp heat (DH) test (85°C / 85% relative humidity) regardless of the presence of the MeO-2PACz:

- Strong S-shape already visible after 100h of DH → FF and J_{sc} drop.
- Degradation linear with the NiO_x thickness
- Best compromise: NiO_x(5 nm) + MeO-2PACz



Understanding the degradation diagram

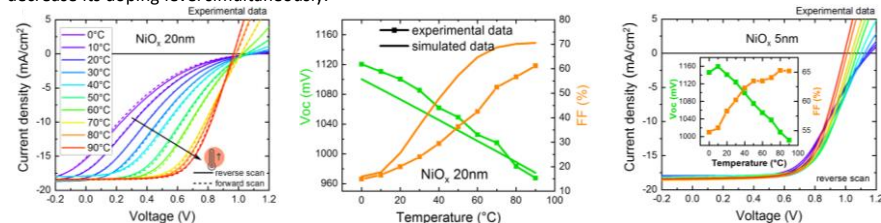
S-shape: barrier extraction?

- PLQY(V): the steeper the slope, the more efficient the carrier extraction.
 → Steeper slope for fresh NiO_x.
 → About aged NiO_x: lower PLQY (≈ 2x) across the whole voltage range for thicker NiO_x.

Formation of a barrier for hole extraction upon DH testing

- IV(T) and simulation on SCAPS software:

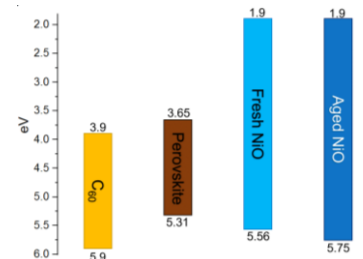
→ S-shape removes when temperature increases: barrier overcomes
 → to obtained at RT this characteristic S-shape on the simulated aged device and a good FF at 90°C: need to increase the NiO_x band-gap and decrease its doping level simultaneously.



Band diagram

	NiO _x fresh	NiO _x aged
Band gap (eV)	3.66	3.85
E(eV vs vacuum)	-4.56	-4.65
Doping concentration (1/cm ³)	1.01 x 10 ⁺²⁰	3.01 x 10 ⁺¹⁷

Values extracted from Tauc plot, EIS measurements and literature.



Conclusion

- NiO_x (20 nm) + MeO-2PACz bilayer: high efficiency, good reproducibility over large area (15 cm²).
- However, the thicker the NiO_x, the bigger the cell performances drop during the DH testing: band alignment mismatch between NiO_x and perovskite valence band + drop in NiO_x conductivity.
 → Formation of a barrier that scales with the thickness of the NiO_x layer.

- Best compromise: NiO_x (5 nm) + MeO-2PACz bilayer:
 - similar efficiencies on 1 cm² cells and on 14.6 cm² minimodules (16.2% and 14.4%, respectively),
 - superior stability: the bilayer devices retain >94% efficiency after 1000 h at 85°C, 85% R.H.