Stability in Metal Halide Perovskite Solar Cells – A Matter of Mixing

Laura E. Mundt

Laura T. Schelhas

Applied Energy Division, Energy Sciences, SLAC National Accelerator Laboratory

Contact: lmundt@slac.Stanford.edu

Renewable Energy

https://youtu.be/iwNDPFi_mTM

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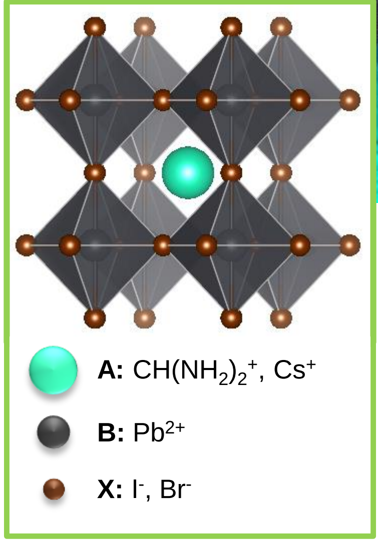
Introduction

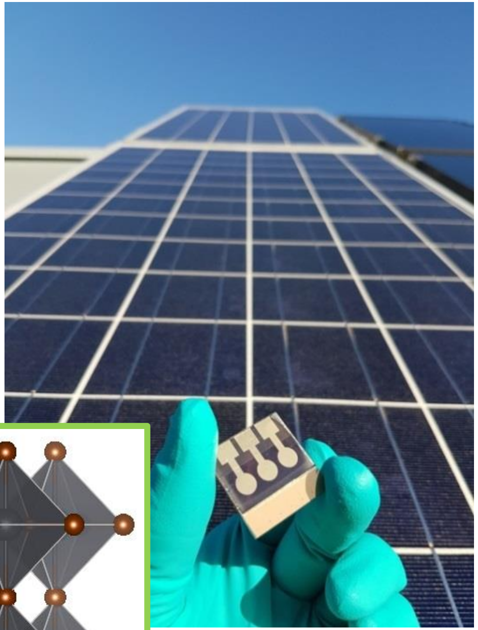
Game changer in photovoltaic (PV) technology:
Metal halide perovskite solar cells

- Materials based on crystal structure with ABX_3 formula
- High energy conversion efficiency through desirable optical and electrical properties
- Solution processing enables low-cost production

Goal: compete with Silicon PV for 30 year stability

- Device performance degradation remains a challenge
- Mixing ions in crystal lattice helps stabilize structure





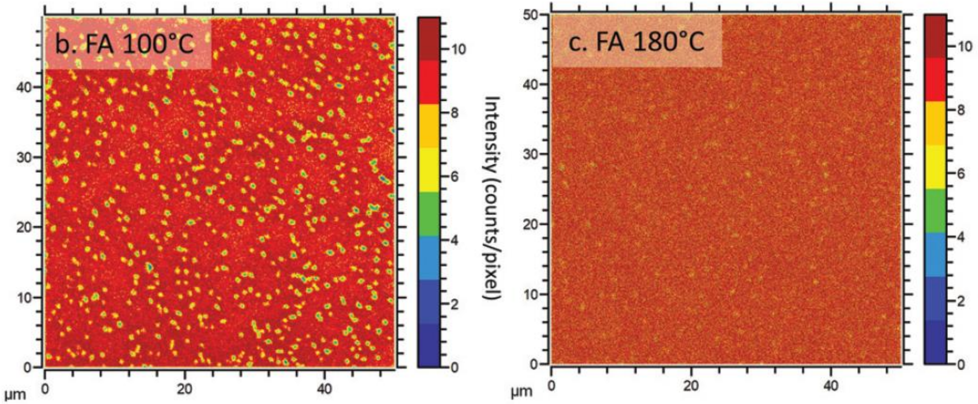
Lab-scale metal halide perovskite solar cell in front of Silicon solar panel

Objective

- If we want to improve the **stability**, we need to understand the **failure mechanisms**
- Previous results[1] suggest:

1) local heterogeneity depends on **annealing temperature** of perovskite thin film

2) **local heterogeneity** drives **phase segregation** and causes **device failure**



Time-of-Flight Secondary Ion Mass Spectroscopy (ToF SIMS) of perovskite films containing $CH(NH_2)_2^+$ (FA), Cs, Pb and I, annealed at 100°C (left) and 180°C (right), showing the local distribution of FA.[1]

Hypothesis: **Higher annealing temperatures** promotes mixing, which prevents **phase segregation** and leads to **improved stability**

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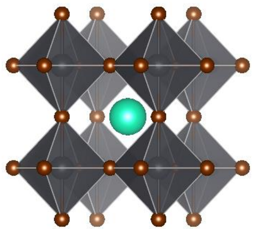
[1]Schelhas et al., EES 2019

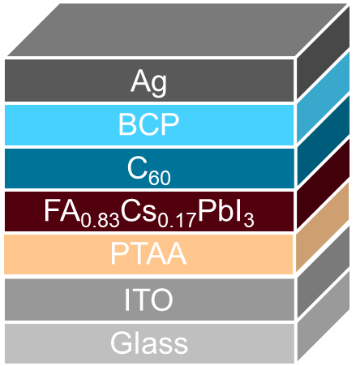
Methods – Samples

State-of-the-art perovskite solar cell with **mixed A-site**

$FA_{0.83}Cs_{0.17}PbI_3$

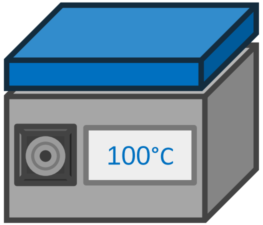


83% $CH(NH_2)_2^+$ ("FA")
17% Cs^+

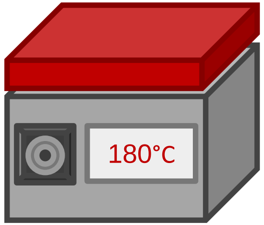


Chose **two annealing temperatures** for the perovskite absorber

low annealing temperature



high annealing temperature



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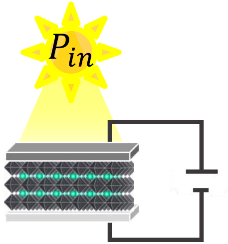
Methods – IV & XRD

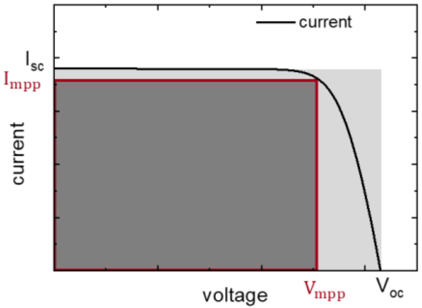
Figures of merit: **Photovoltaic performance** (efficiency, η) and **crystal structure**

conventionally measured separately

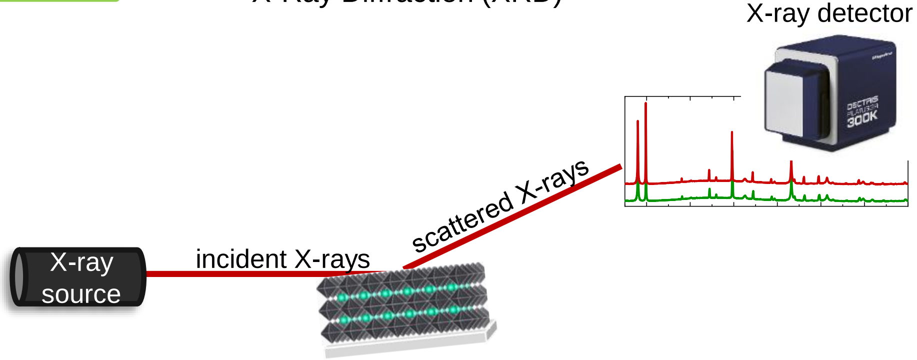
Current (I) – Voltage (V) characteristics



$$\eta = \frac{V_{mpp} * I_{mpp}}{P_{in}} = \frac{V_{oc} * I_{sc} * FF}{P_{in}}$$



Crystal lattice parameters
X-Ray Diffraction (XRD)



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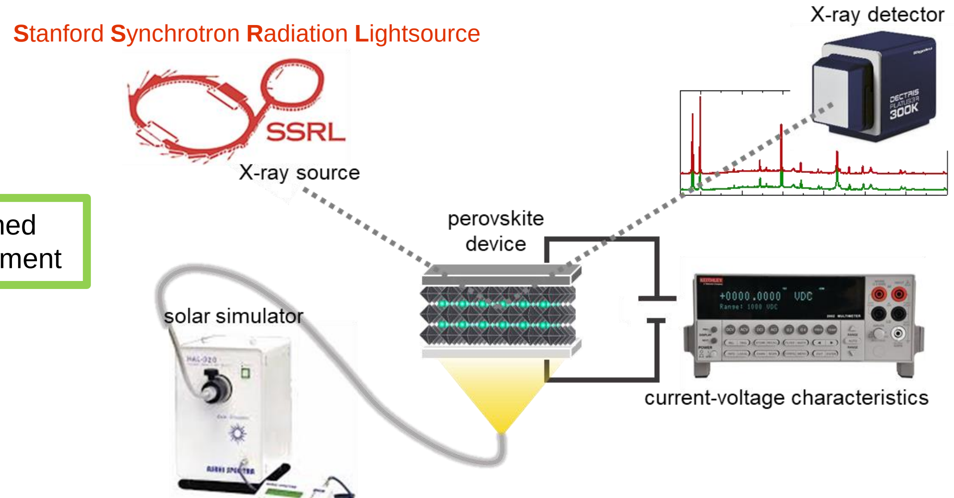
Methods – *operando* XRD

Synchrotron Radiation,
high energy and **flux** enables:

1) Rapid data collection (short integration times)
2) Penetration of active layer through the top metal electrode

combined measurement



Schematic *operando* XRD setup

➢ **Operando XRD**

In situ characterization of device **efficiency and crystal structure** under electrical load

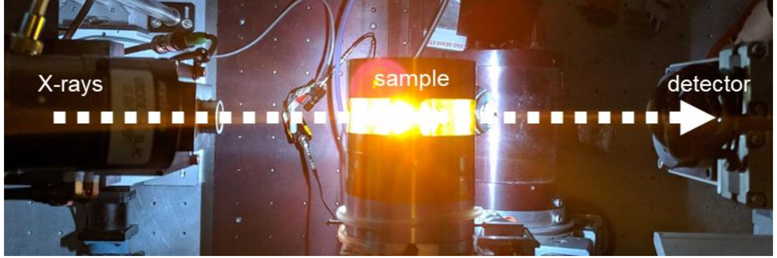
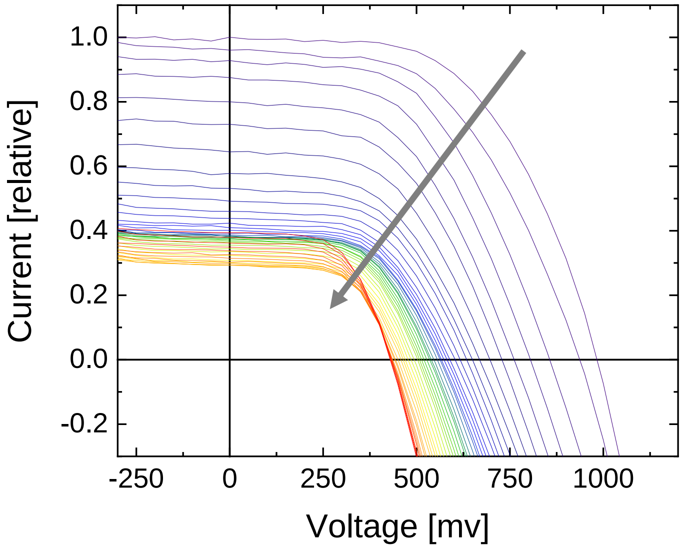


Photo of experimental setup at beamline 2-1 at SSRL

Results – *in situ* IV

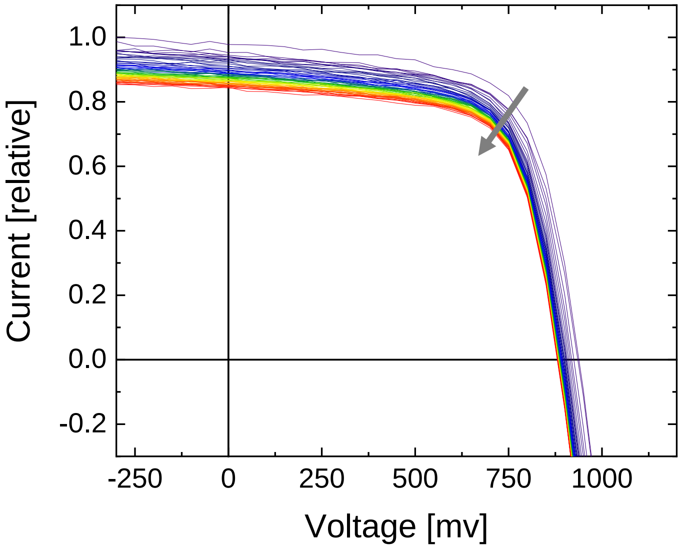
low annealing temperature

- *in situ* IV over 11h shows loss in V_{oc} and I_{sc}
- severe device degradation



high annealing temperature

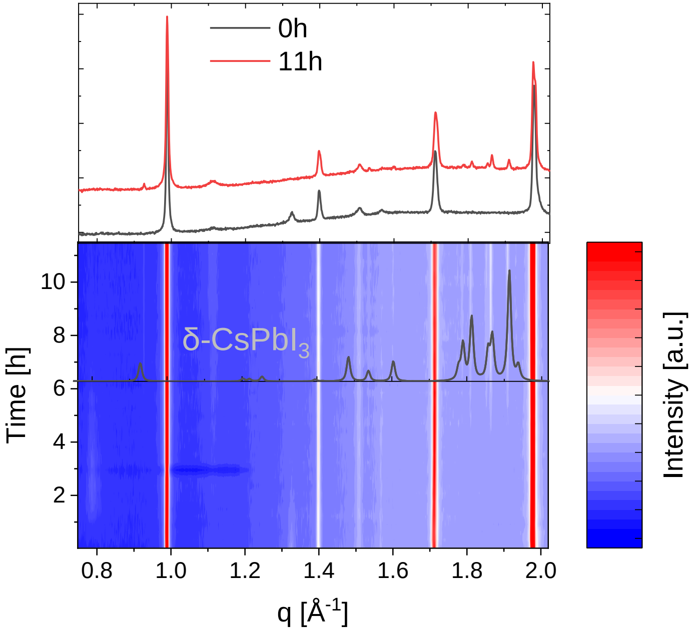
- *in situ* IV over 19 h shows improved stability compared to lower annealed device



Results – *operando* XRD

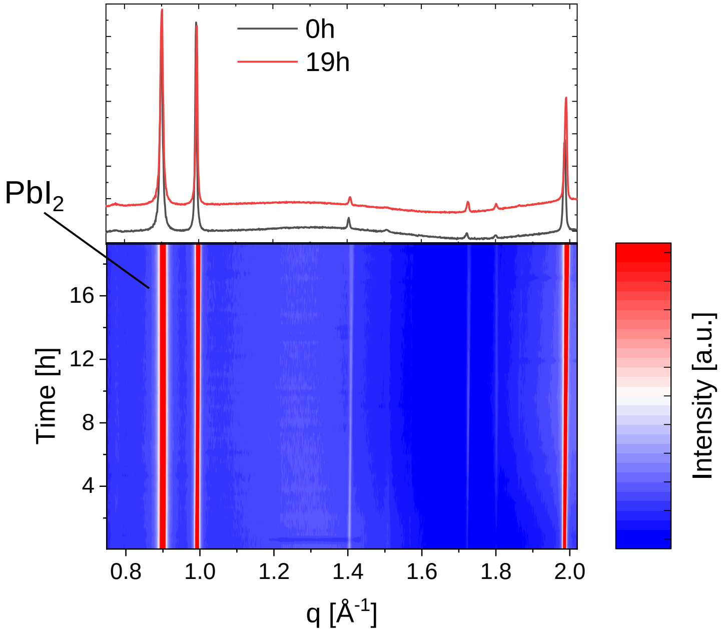
low annealing temperature

- secondary phase formation, δ-$CsPbI_3$



high annealing temperature

- no structural changes observed



Conclusions

Confirmed hypothesis:

- **Secondary phase formation** for lower annealed device
- New phase identified as hexagonal δ-$CsPbI_3$, which is photo-inactive
- Lower-annealed device shows severe loss in V_{oc} and I_{sc}, resulting in lower efficiency η
- **No structural changes** and **improved device stability** for higher annealed sample

Future work- The thermodynamic limits of mixing

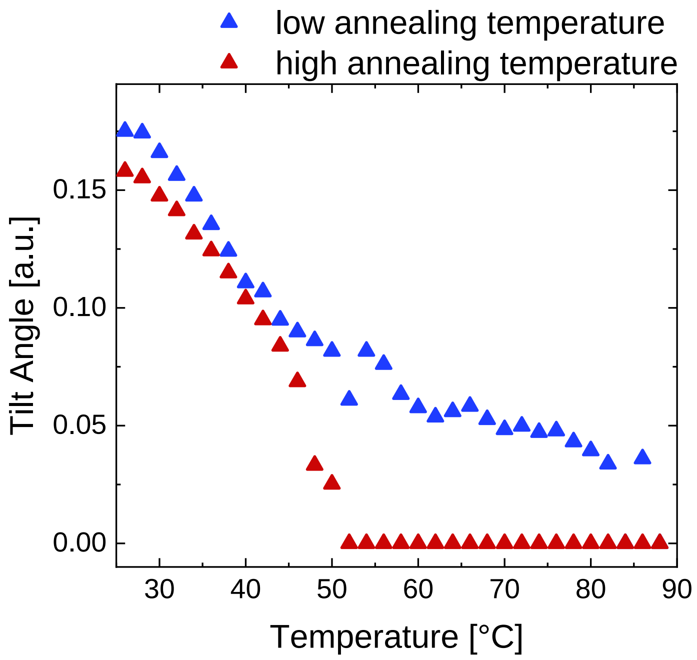
Previously probed heterogeneity length scales in micrometer range

<u>Hypothesis:</u>

Small length scale heterogeneities also have detrimental impact on structural stability

But how to probe if there is no secondary phase?

- Demonstrate manifestation of nanoscale heterogeneities in **"smearing"** of tetragonal to cubic **phase transition**
- Octahedral tilt angle as measure for "smearing" (tilt angle 0° = cubic lattice)



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References

L. T. Schelhas, Z. Li, J. A. Christians, A. Goyal, P. Kairys, S. P. Harvey, D. H. Kim, K. H. Stone, J. M. Luther, K. Zhu, V. Stevanovic, J. J. Berry, *Energy Environ. Sci.* **2019**, *12*, 1341.

Acknowledgments

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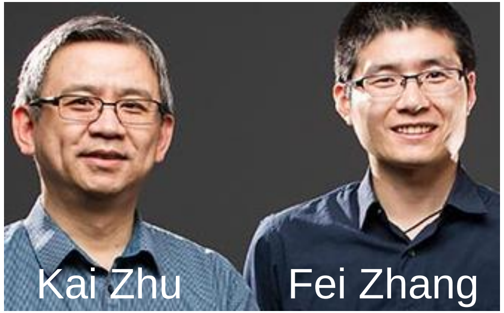

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