Electronic Supplementary Material (ESI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2016

Supporting Information

Critical Kinetic Control of Non-stoichiometric Intermediate Phase Transformation for Efficient Perovskite Solar Cells

Yaoguang Rong[a†], Swaminathan Venkatesan[a†], Rui Guo[b], Yanan Wang[a], Jiming Bao[a], Wenzhi Li[b], Zhiyong Fan[c], Yan Yao[a,d]*

[a.] Department of Electrical & Computer Engineering and Materials Science and Engineering Program, University of Houston, Houston, Texas 77204, USA.
[b.] Department of Physics, Florida International University, Miami, FL 33199, USA.
[c.] Department of Electronic and Computer Engineering, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR, China.
[d.] Texas Center for Superconductivity at the University of Houston, Houston, Texas 77204, USA
† These authors contributed equally to the work.

Table S1. Photovoltaic performance at different temperature and time.

		1 min	5 min	10 min	15 min	30 min	60 min
70°C	V_{oc} (V)	0.95	0.98	0.98	0.96	0.90	0.93
	J_{sc} (mA cm^{-2})	13.36	13.60	13.88	15.76	16.76	11.78
	FF (%)	63.63	69.99	75.80	76.39	69.95	74.64
	PCE (%)	8.07	9.29	10.33	11.60	10.50	8.14
80°C	V_{oc} (V)	0.98	0.96	0.91	0.95	0.93	0.93
	J_{sc} (mA cm^{-2})	14.41	15.52	16.52	15.87	17.04	13.50
	FF (%)	74.11	79.16	76.60	75.77	73.60	70.27
	PCE (%)	10.49	11.84	11.55	11.40	11.72	8.83
90°C	V_{oc} (V)	0.96	1.00	1.01	0.96	0.842	0.83
	J_{sc} (mA cm^{-2})	19.27	19.84	18.23	18.25	17.15	15.80
	FF (%)	71.62	77.30	78.61	76.40	65.07	67.38
	PCE (%)	13.22	15.29	14.56	13.36	9.41	8.88
100°C	V_{oc} (V)	0.96	0.92	0.85	0.88	0.80	0.67
	J_{sc} (mA cm^{-2})	14.37	18.25	15.9	14.07	15.70	15.68
	FF (%)	75.27	75.5	74.7	68.09	66.27	64.20
	PCE (%)	10.42	12.6	10.04	8.42	8.28	6.73

Table S2. Calculations of the intermediate phase fraction in the composite thin film annealed at different temperature.

XRD results

Annealing condition	Intermediate phase (220) peak area	PbI_2 peak area	Perovskite (110) peak area	Intermediate phase fraction
Non-annealed	67905	0	0	1
70°C	45405	0	108113	0.296
80°C	24562	0	105083	0.189
90°C	24444	0	108607	0.184
100°C	11340	15732	109549	0.083

EDX results

Annealing condition	S atom concentration	Pb atom concentration	Cl/I atom concentration	Intermediate phase fraction
Non-annealed	/	/	/	1
70°C	5.02	14.17	43.01	0.274
80°C	3.86	14.5	43.91	0.181
90°C	3.22	12.44	37.45	0.174
100°C	2.22	15.07	45.47	0.086

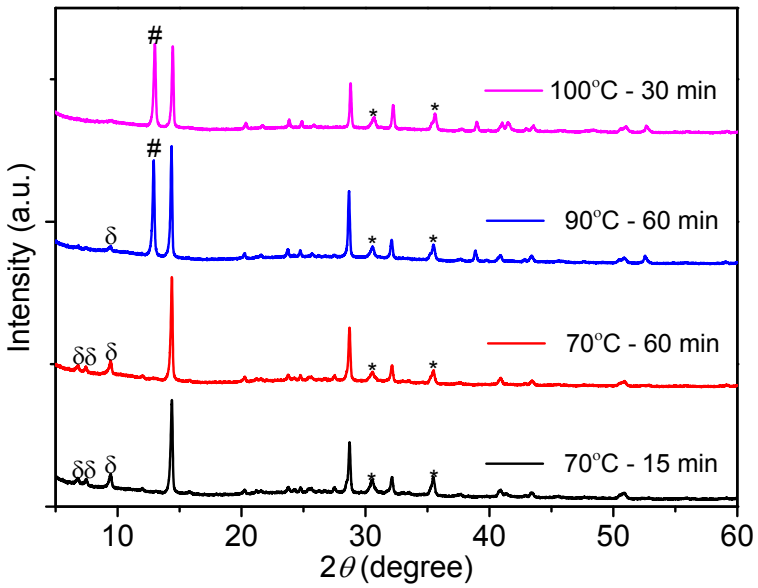

Figure S1. XRD spectra of intermediate phase films annealed at 70°C for 15 and 60 minutes, 90°C for 60 minutes and 100°C for 30 minutes. δ, * and # represent peaks for intermediate phase, ITO and PbI_2 respectively.

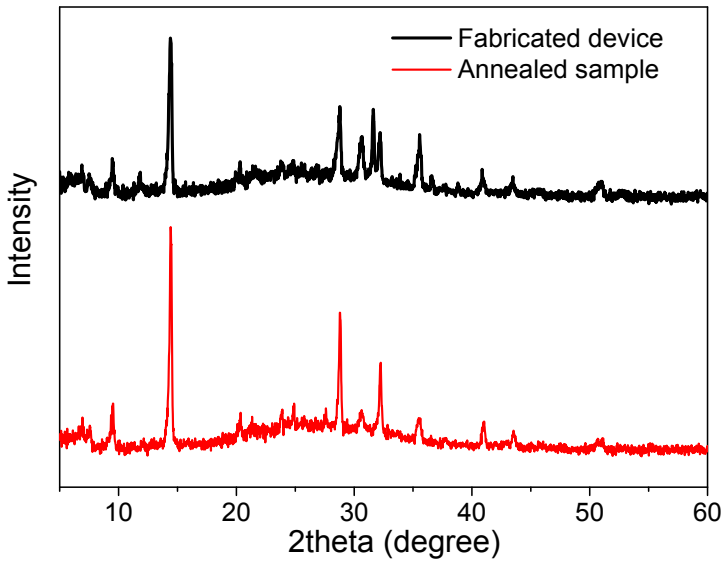

Figure S2. XRD results of an annealed (90°C 5 min) perovskite film on PEDOT:PSS coated ITO glass substrate, and a ITO/PEDOT:PSS/Perovskite/PCBM/BCP/Al device (90°C 5 min) after light soaking for 2 hours. Both samples contain peaks corresponding to the intermediate phase.

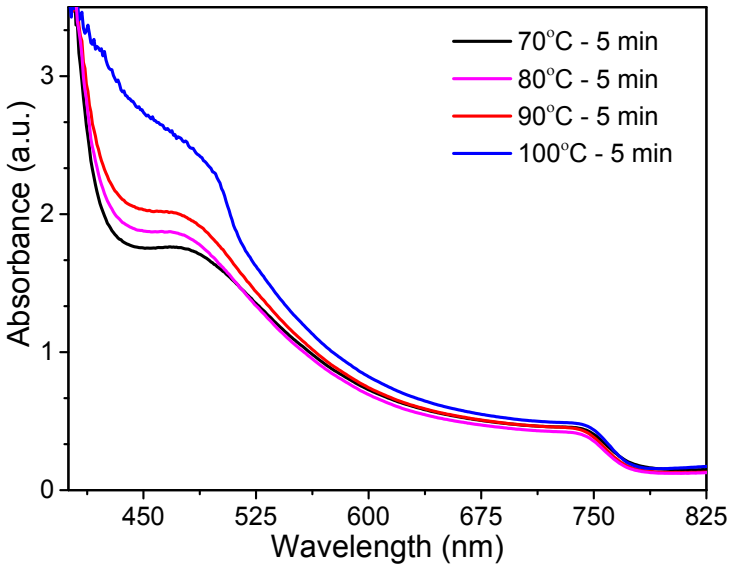

Figure S3. UV-Visible spectra of the intermediate phase films annealed at 80°C for 5 min, 90°C for 1 min, 90°C for 5 min and 100°C for 5 min.

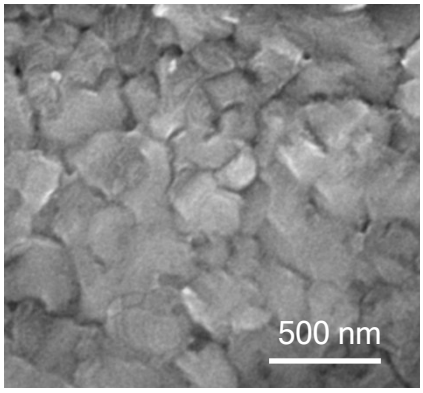

Figure S4. High-magnification SEM image of the perovskite film annealed at 90°C for 5 min.

(a) (b)

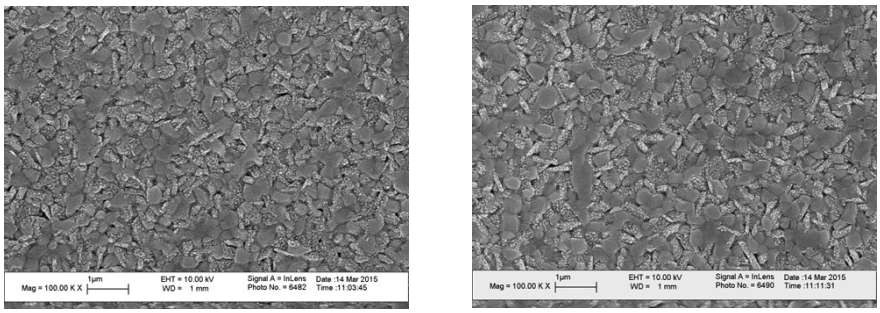

Figure S5. SEM images of perovskite films annealed at 100°C for 15 min (a) and 30 min (b).

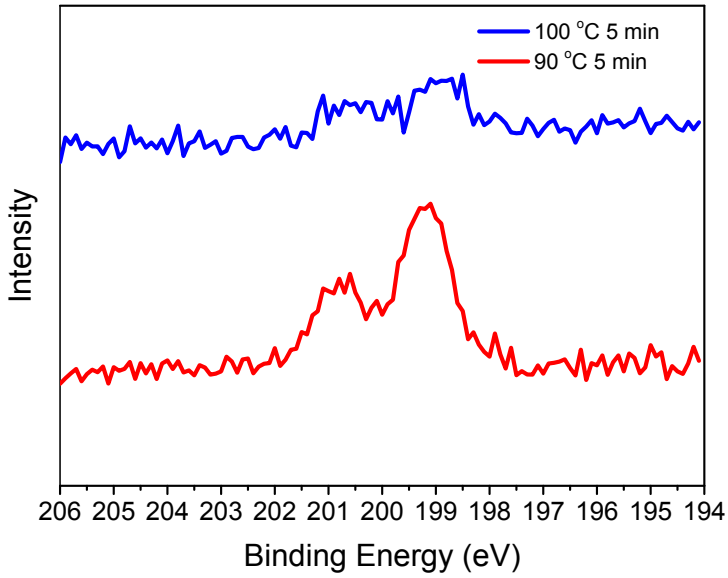

Figure S6. XPS Cl 2p spectra showing 90°C 5 min sample (bottom) containing Cl. However, 100°C 5 min annealed perovskite films (top) without Cl.

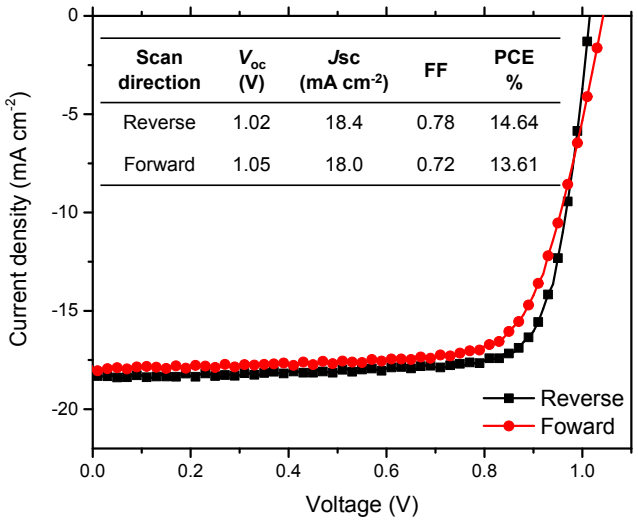

Figure S7. *J-V* curves for 90°C for 5 min annealed device under reverse scan (open circuit → short circuit) and forward scan (short circuit → open circuit) under AM 1.5G illumination.