The influence of stabiliser concentration on the formation of In₂O₃ thin films Supplementary Information

Aysha A. Riaz,¹ Curran Kalha,¹ Maria Basso,² Máté Füredi,³ and Anna Regoutz^{1,*}

 ¹Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, United Kingdom.
²Department of Industrial Engineering, University of Padova and INSTM, Via Marzolo 9, Padova 35131, Italy.
³Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, United Kingdom. (Dated: October 4, 2024)

^{*} a.regoutz@ucl.ac.uk



FIG. S1. Images of the solutions for the four MEA stabiliser ratios including 0:1, 0.25:1, 0.50:1, and 1:1 going from left to right and for 0, 2, and 24 h going from top to bottom.



FIG. S2. UV-Vis absorbance data of nitrate absorption for the four MEA stabiliser ratios including 0:1, 0.25:1, 0.50:1, and 1:1. Green lines are marked to show shifts in peaks between the solution without stabiliser and other solutions containing stabiliser.



FIG. S3. IR spectra collected for a solution of monoethanolamine (MEA) and 2-methoxyethanol (2ME) at 0 hours and 24 hours and pure 2ME as a reference. The amount of stabiliser used was equivalent to a 1:1 ratio of MEA:In. The MEA with 2ME spectra completely overlap with the 2ME reference suggesting the stabiliser is undetectable through IR at this concentration.

TABLE S1. Summary of peak positions and assignments for IR data collected for all four solutions at 0, 2, and 24 h.

Wavenumber (cm ⁻¹)	Assignment	
3526	O-H (H ₂ O)	
3226	$O-H(In(OH)_3)$	
2967	C-H (Solvent)	
1647	$O-H (In(OH)_3)$	
1516	N–O (Precursor)	
1296	N–O (Precursor)	
951	C–H (Solvent)	
414	In–O $(In(OH)_3/In_2O_3)$	



FIG. S4. Enlarged section of the IR spectrum of the 0.25:1 MEA:In stabiliser solution to highlight the shift in the C-H peak over time.



FIG. S5. IR spectra collected for precipitates from the 1:1, 0.50:1, and 0.25:1 solutions after 24 hours.



FIG. S6. XPS core level spectra for the deposits of the MEA stabiliser ratios (0.25, 0.50, and 1) solutions collected after 24 hours, including (a) In 3*d*, (b) O 1*s*, (c) N 1*s*, and (d) C 1*s*. Spectra are normalised to the respective areas of the In $3d_{5/2}$ peak.



FIG. S7. XPS survey spectra of films deposited after 24 hours from solutions with the four MEA stabiliser ratios (0, 0.25, 0.50, and 1). Spectra are normalised 0:1 and stacked. All major core and Auger-Meitner lines are labelled.



FIG. S8. Complete set of core level spectra (In 3*d*, O 1*s*, N 1*s*, and C 1*s*) for films deposited from solutions with the four MEA stabiliser ratios (0, 0.25, 0.50, and 1) after 0, 2, and 24 h compared to an annealed film.



FIG. S9. Representative XPS peak fit of the O 1s spectrum for the 0:1 MEA stabiliser ratio at 24 hours. The spectrum can be fitted with three distinct chemical state peaks, associated with the SiO_2 , OH, and In–O environments.



FIG. S10. XPS survey spectra of thin films deposited from solutions using the 0.50:1 MEA stabiliser ratio after 0, 2, and 24 h compared to an annealed film. Spectra are normalised 0:1 and stacked. All major core and Auger-Meitner lines are labelled.

TABLE S2. Ratio of hydroxide to oxide content, excluding SiO_2 contribution, found through peak fitting for all samples.

Hydroxide:Oxide Ratio					
Time	0:1	0.25:1	0.50:1	1:1	
0 h	47.6 : 52.4	47.9 : 52.1	45.0 : 55.0	47.9 : 52.1	
2 h	53.7:46.3	45.9 : 54.1	42.7 : 57.3	44.2 : 55.8	
24 h	58.3:41.6	72.0 : 28.0	100.0:0.0	100.0:0.0	
Annealed	30.1 : 69.9	34.0 : 66.0	28.8:71.2	37.6 : 62.4	



FIG. S11. Ellipsometry fits of Delta (top) and Psi (bottom) for the four MEA stabiliser ratios (0, 0.25, 0.50, and 1) fitted with the Sellmeier and Lorentz dispersion laws using SEA software.



FIG. S12. GI-XRD data of 0.5:1 ratio In_2O_3 annealed thin film samples with 1 dip and 13 dips. The main reflections are labelled. The narrow reflection labelled with an asterisk is associated with the 311 reflection of the Si substrate (Weiss, C. (2017). New Silicon Nanocrystal Materials for Photovoltaic Applications. PhD Thesis. Friedrich Schiller University Jena.).