Supplementary Information

The role of inter-particle heterogeneities in the selenization pathway of Cu-Zn-Sn-S nanoparticle thin films: A real-time study

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Table S1. Peak locations for fluorescence and diffraction signals in the EDXRD spectra presented in Figures 1 and 2 in the main text and S1 and S2 in this Supplementary Information. The two peaks observed at 8.6 keV and 9.7 keV for all samples in Figures S1 and S2 are ghost peaks of the Mo-Kβ peak, caused by the K and L absorption edges of the Ge in the detector, and thus are omitted from this table.

Photon Energy (keV)	Type of Signal	Source of Signal
11.1	Fluorescence	Se Kα
12.4	Fluorescence	Se Kβ
17.4	Fluorescence	Mo Kα
19.6	Fluorescence	Mo Kβ
22.4	Diffraction	CZTSe 101
25.2	Fluorescence	Sn Kα
28.5	Fluorescence	Sn Kβ
33.7	Diffraction	CuSe 101
34.3	Diffraction	$Cu_{2-\delta}Se$ 111
34.8	Diffraction	CZTSe 112
35.7	Diffraction	CuSe 102
36.6	Diffraction	CZTS 112
39.7	Diffraction	CuSe 006
51.4	Diffraction	Mo 110
56.1	Diffraction	$Cu_{2-\delta}Se$ 220
56.8	Diffraction	CZTSe 204
57.4	Diffraction	CuSe 110

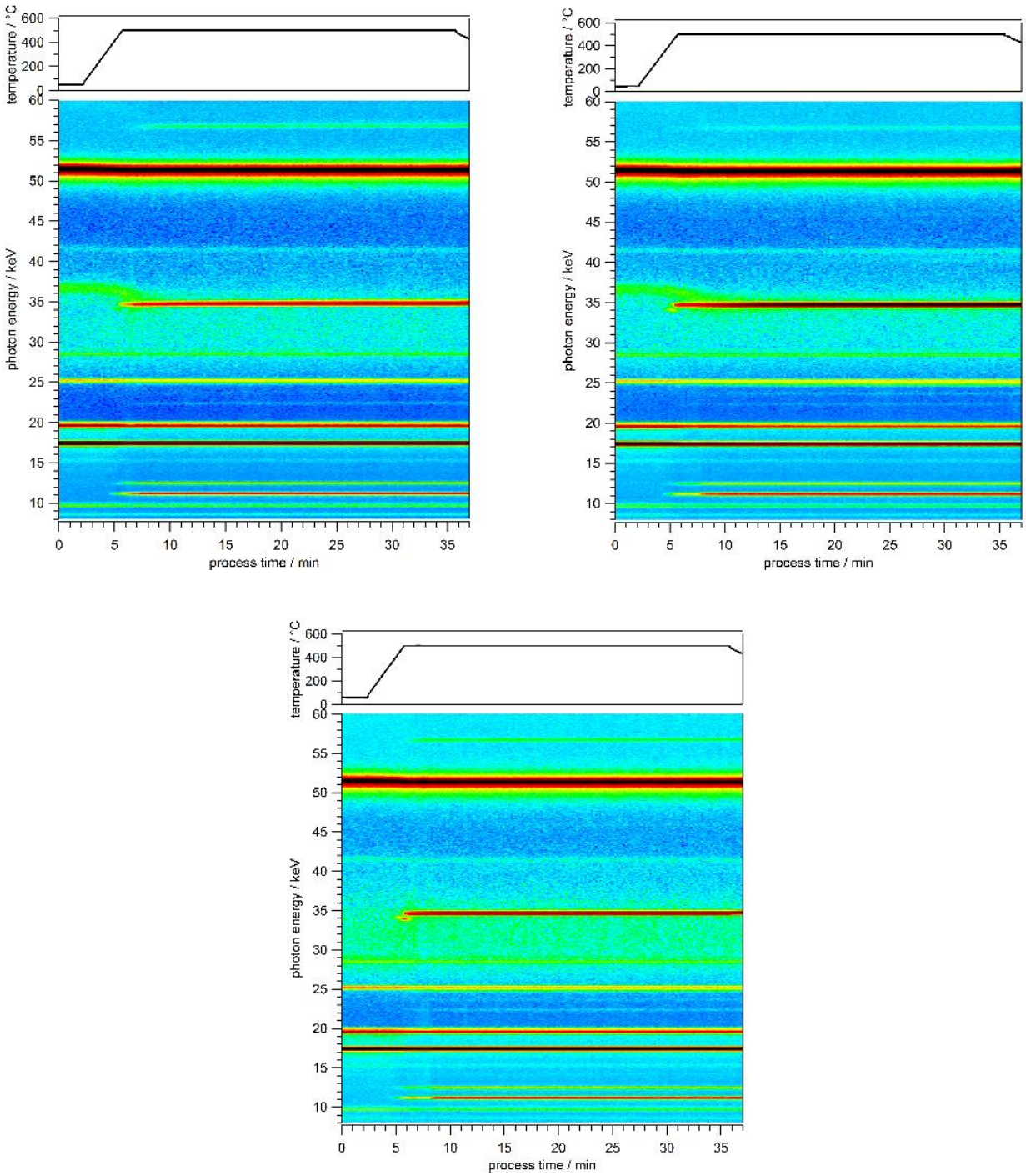

Figure S1. Full-range EDXRD data for fast heating of (a) large, (b) mixed, and (c) small particle films. See Table S1 for peak assignments.

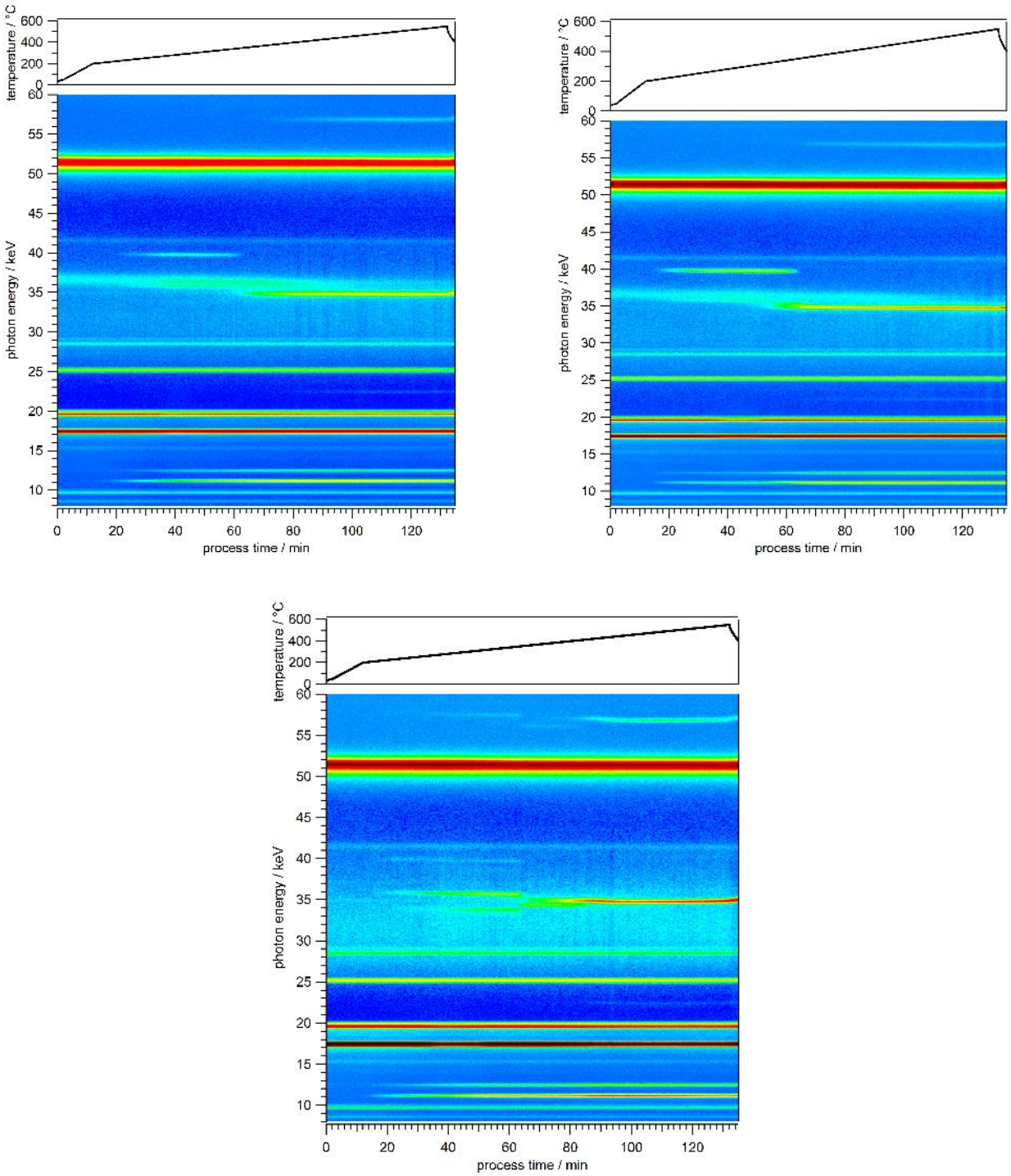

Figure S2. Full-range EDXRD data for slow heating of (a) large, (b) mixed, and (c) small particle films. See Table S1 for peak assignments.

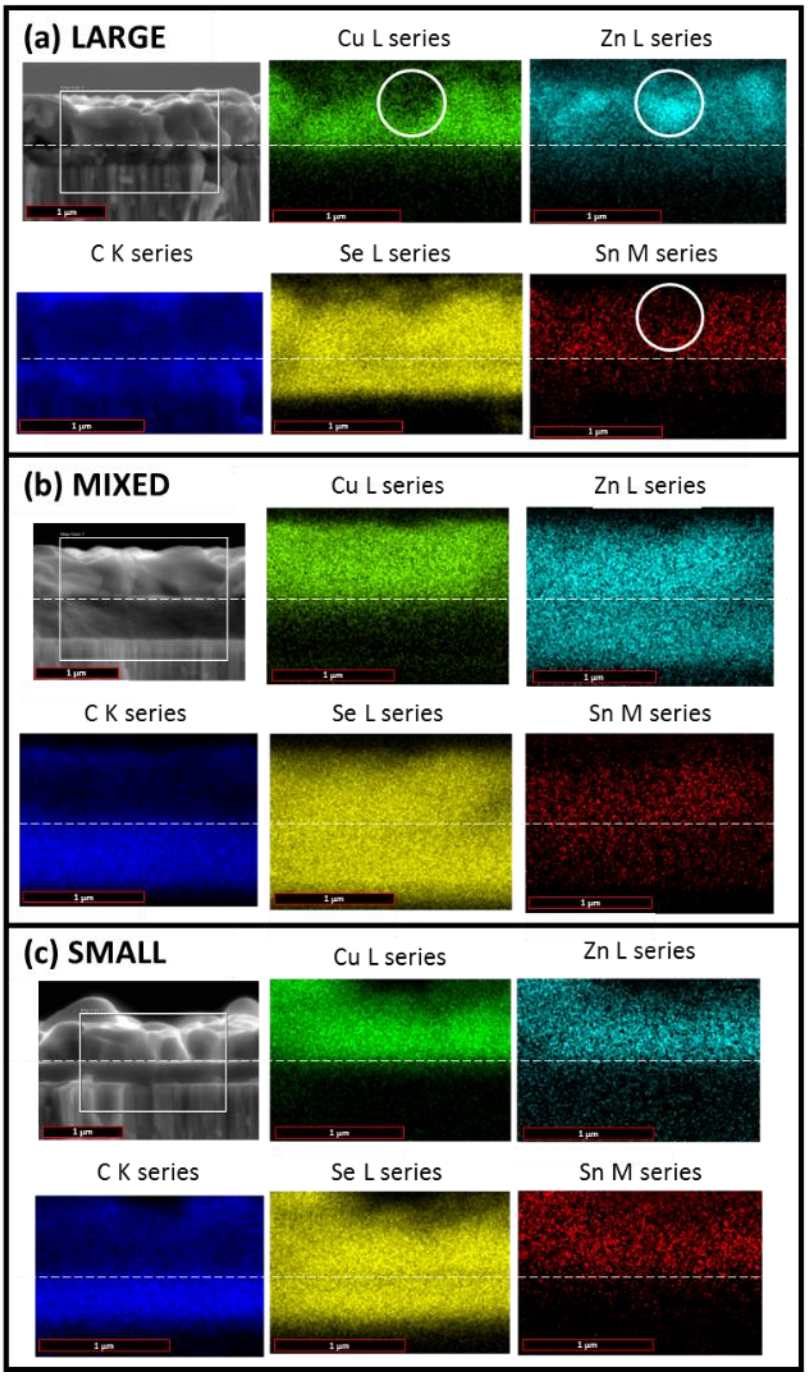

Figure S3. SEM-EDS compositional maps for cross sections of (a) large, (b) mixed, and (c) small precursor films after fast heating. The horizontal dashed lines represent the interface between the large-grain and fine-grain layers. The circles on the Cu, Zn, and Sn maps of the selenized large particle film demonstrated a segregated Zn-rich region.