

## Wide-Surface Furnace for *In Situ* X-Ray Diffraction of Combinatorial Samples using a High-Throughput Approach

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### Supplementary Information

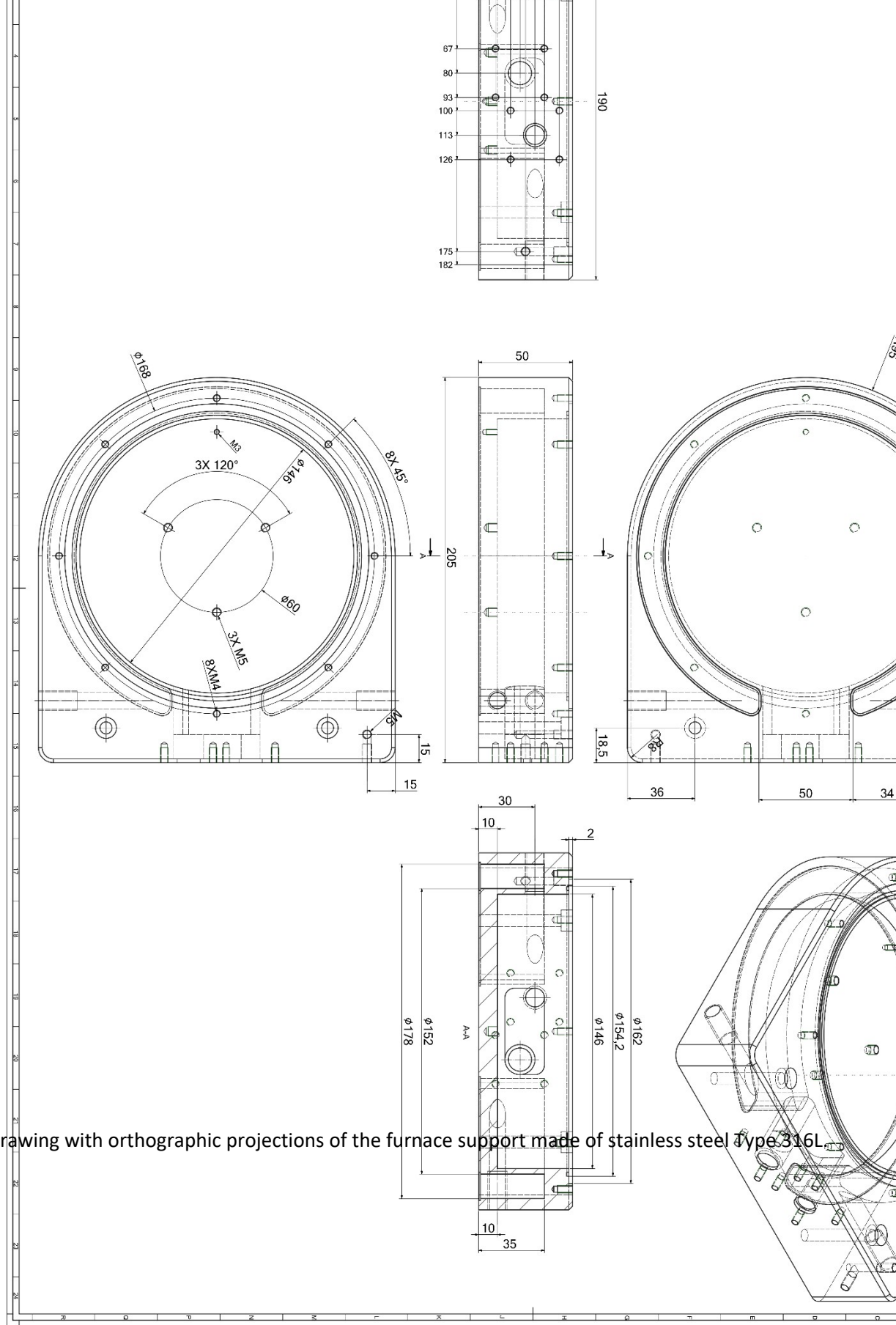
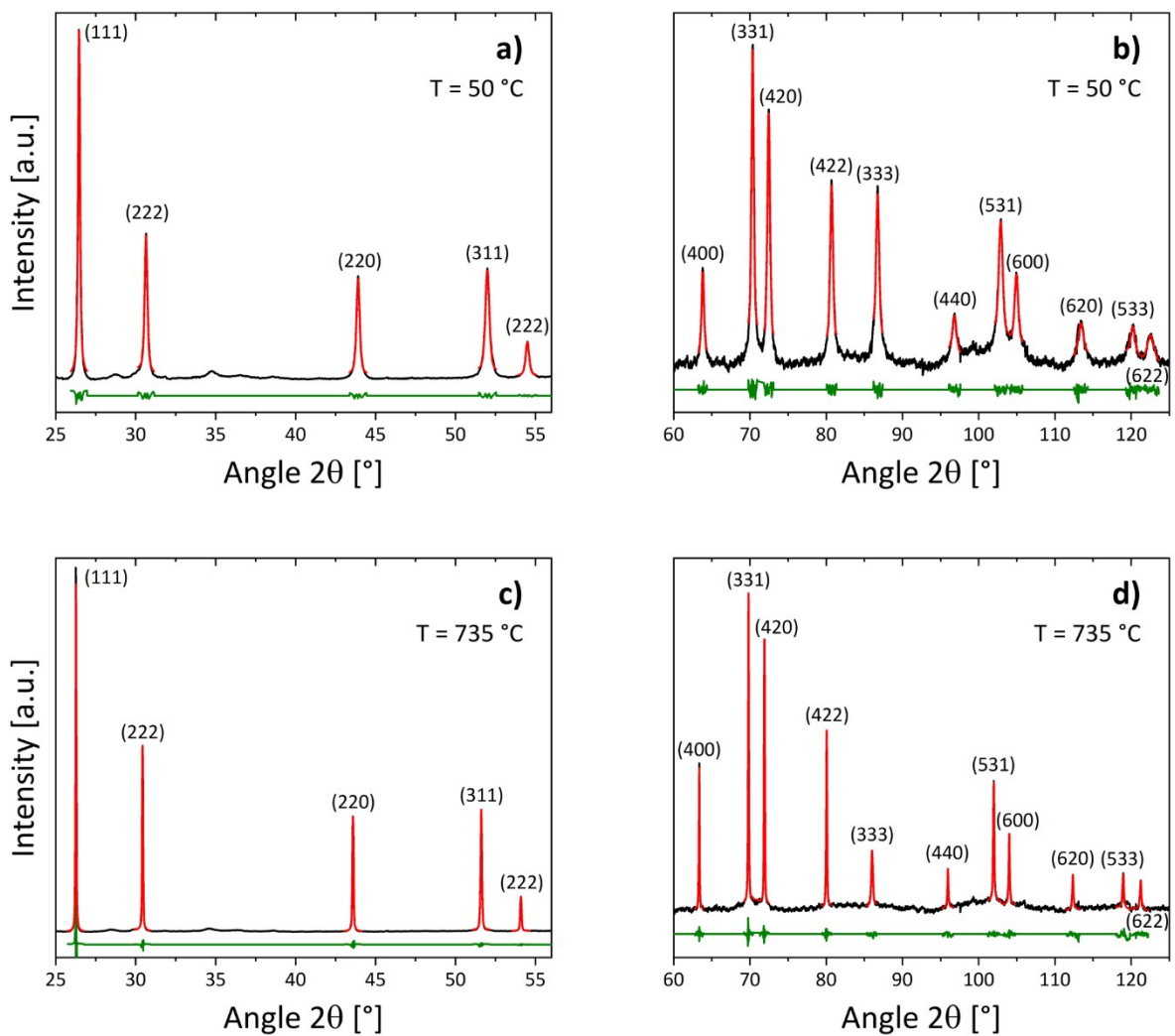


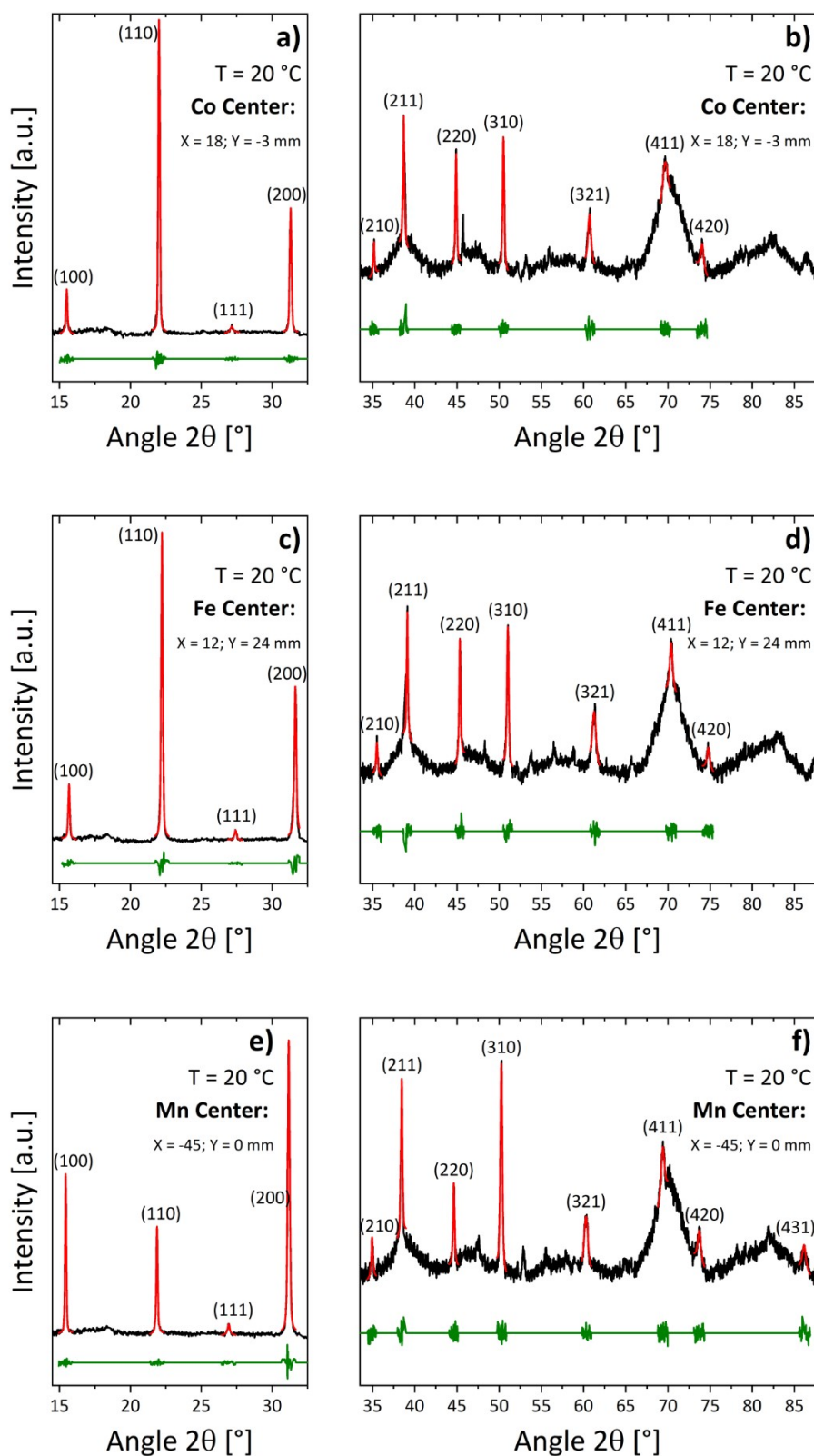
Figure S1 – Technical drawing with orthographic projections of the furnace support made of stainless steel Type 316L.

**Table S1** – Results of the peak fitting and minimization Matlab routine as platinum lattice parameters with standard deviations for heating and cooling measurements.

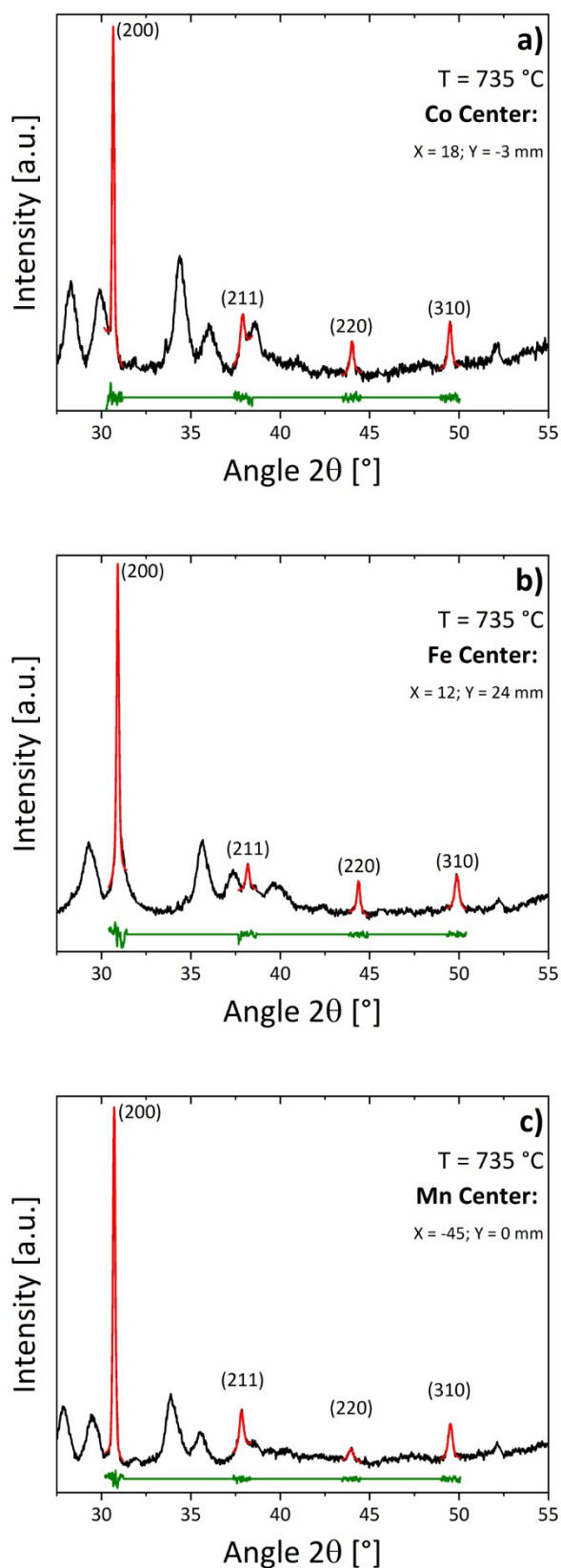
Temperature [°C]	Ramp	Pt Lattice Parameter [Å]
20	Heating	3.9222 ± 0.0004
50	Heating	3.9232 ± 0.0001
100	Heating	3.9250 ± 0.0003
150	Heating	3.9266 ± 0.0003
200	Heating	3.9287 ± 0.0003
250	Heating	3.9306 ± 0.0002
300	Heating	3.9323 ± 0.0002
350	Heating	3.9343 ± 0.0001
400	Heating	3.9360 ± 0.0001
450	Heating	3.9382 ± 0.0002
500	Heating	3.9402 ± 0.0001
550	Heating	3.9422 ± 0.0001
600	Heating	3.9443 ± 0.0001
650	Heating	3.9465 ± 0.0001
700	Heating	3.9486 ± 0.0001
750	Heating	3.9508 ± 0.0001
800	Heating	3.9532 ± 0.0001
850	Heating	3.9554 ± 0.0001
600	Cooling	3.9446 ± 0.0001
400	Cooling	3.9364 ± 0.0001
200	Cooling	3.9284 ± 0.0001
50	Cooling	3.9227 ± 0.0001



**Figure S2.** XRD diffractograms collected in the center (coordinates:  $X = 0$ ;  $Y = 0$  mm) of the Pt-coated Si(100) wafer inside the furnace mounted at the DiffAbs beamline of the Soleil synchrotron. The measurements are performed using the PEEK dome at 50 °C (a and b) and 735 °C (c and d) with experimental data (black line), fitted curves (red line), and the residuals (green line). The Miller indices of the first 16 reflections are reported. The scale is different among all 4 panels.



**Figure S3.** XRD diffractograms collected in the Co (a and b, sample coordinates:  $X = 18; Y = -3\text{ mm}$ ), Fe (c and d, sample coordinates:  $X = 12; Y = 24\text{ mm}$ ), and Mn (e and f, sample coordinates:  $X = -45; Y = 0\text{ mm}$ ) of the combinatorial  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{1-x-y}\text{Fe}_x\text{Mn}_y\text{O}_{3-\delta}$  (LSCFM) library at the DiffAbs beamline of the Soleil synchrotron at room temperature ( $20\text{ }^{\circ}\text{C}$ ) without the PEEK dome with experimental data (black line), fitted curves (red line), and the residuals (green line). The Miller indices of the first 12 reflections are reported. The scale is different among all 6 panels.

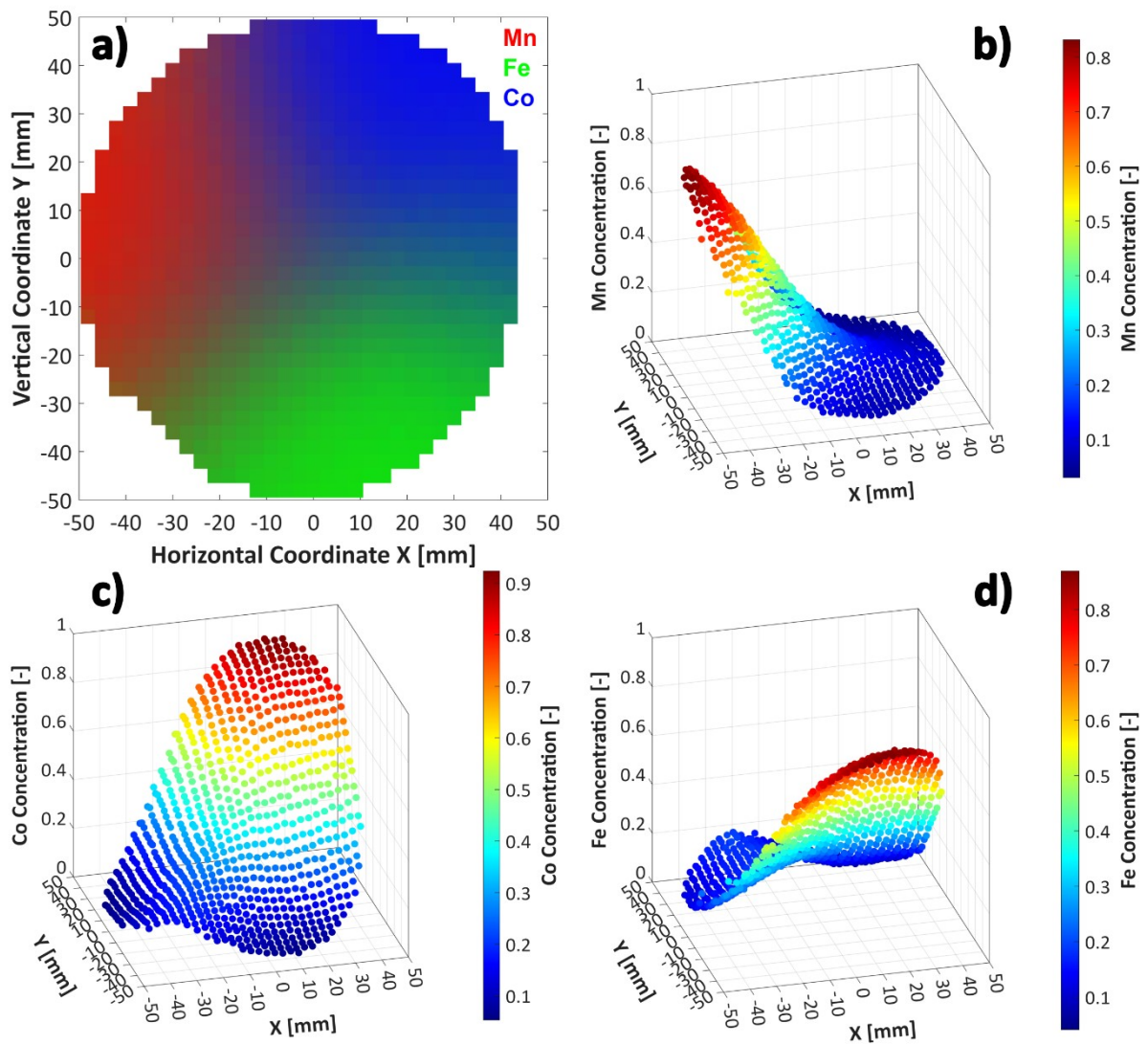


**Figure S4.** XRD diffractograms collected in the Co (a, sample coordinates:  $X = 18; Y = -3\text{ mm}$ ), Fe (b, sample coordinates:  $X = 12; Y = 24\text{ mm}$ ), and Mn (c, sample coordinates:  $X = -45; Y = 0\text{ mm}$ ) of the combinatorial  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{1-x-y}\text{Fe}_x\text{Mn}_y\text{O}_{3-\delta}$  (LSCFM) library inside the furnace mounted at the DiffAbs beamline of the Soleil synchrotron. The measurements are performed using the PEEK dome at  $735\text{ }^\circ\text{C}$

with experimental data (black line), fitted curves (red line), and the residuals (green line). The Miller indices of the 4 fitted reflections of LSCFM are reported. The extra peaks are related to the PEEK polymer reflections, which strongly shift due to the variation of the contact point between the beam and the dome. The main PEEK reflections are not visible because they are at lower angular positions: the (110) at  $\approx 14^\circ 2\theta$ , (113) at  $\approx 15^\circ 2\theta$ , (220) at  $\approx 17^\circ 2\theta$ , and (213) at  $\approx 21^\circ 2\theta$ . The scale is different among all 3 panels.

**Table S2** – Results of the *in situ* XRD high-temperature measurements on the Pt-coated wafer: Pt lattice parameter is expressed in Å, while the temperatures are in °C.

Setpoint temperature	Thermocouple temperature	Dome temperature	Pt lattice parameter	Minimum temperature	Mean temperature	Maximum temperature
20	20.0	20.0	3.9219	6.6	19.0	31.0
50	43.6	24.7	3.9223	17.1	31.0	44.9
100	84.7	28.1	3.9237	54.6	70.7	83.8
200	168.1	37.3	3.9268	139.3	154.3	165.1
250	208.9	42.5	3.9287	192.0	204.8	217.8
300	249.1	48.5	3.9304	239.2	251.0	265.1
350	288.6	52.5	3.9321	284.0	296.0	309.0
400	327.2	59.3	3.9338	324.1	338.8	353.6
450	365.2	67.2	3.9355	357.2	381.8	398.5
500	402.8	71.0	3.9371	395.7	422.2	443.1
550	439.3	86.3	3.9390	430.3	468.6	493.0
600	476.6	113.5	3.9405	467.2	505.9	530.7
650	509.7	107.5	3.9421	500.7	545.3	578.1
700	545.7	133.3	3.9439	543.6	586.7	625.3
735	570.5	139.4	3.9451	571.4	616.3	652.8



**Figure S5.** Element concentration measured by X-ray fluorescence (XRF) results reported as the RGB plot (a) with Mn in red, Fe in green, and Co in blue. The same results are presented as single element 3D distributions for Mn (b), Co (c), and Fe (d).