

Supporting Information

Redox behavior of the SOFC electrode candidate $\text{NdBaMn}_2\text{O}_{5+\delta}$ investigated by high-temperature *in situ* neutron diffraction: first real-time characterisation of an $\text{LnBaMn}_2\text{O}_{5.5}$ intermediate phase

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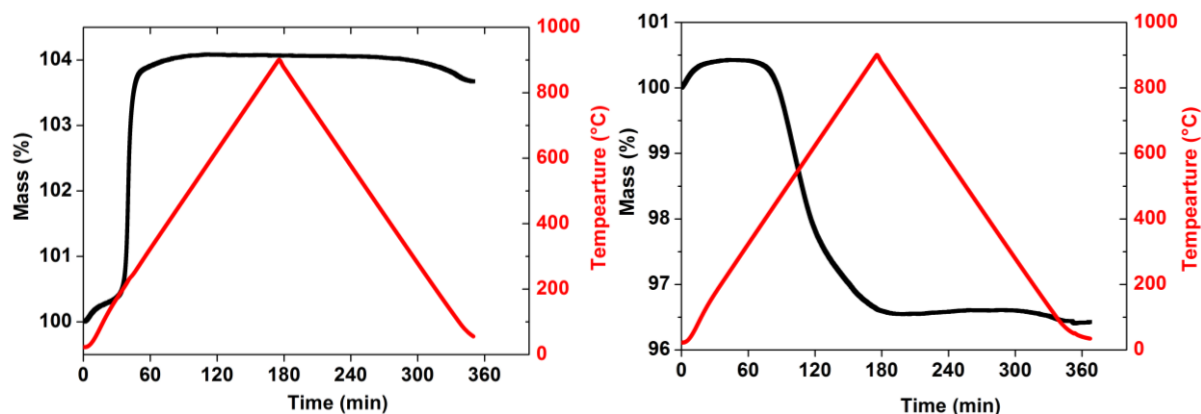


Figure S1. TGA of $\text{NdBaMn}_2\text{O}_{5+\delta}$ (left) under air (flow rate 40 mL min^{-1}) and (right) subsequent cycle under 5% H_2/N_2 (flow rate 20 mL min^{-1}); heating and cooling rates are $5 \text{ }^\circ\text{C min}^{-1}$.

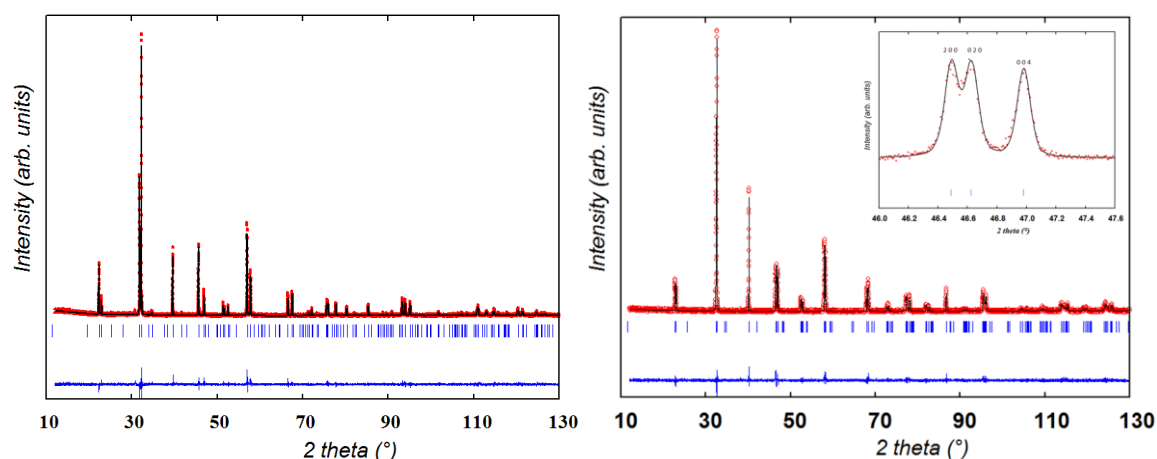


Figure S2. Rietveld refinement plot of the X-ray diffraction data of (let) as-prepared $\text{NdBaMn}_2\text{O}_5$, S.G. $P4/nmm$ and (right) $\text{NdBaMn}_2\text{O}_6$ (S.G. $Pmmm$) part of which is expanded in the inset to highlight the (200/020) doublet.

Table S1. Refined lattice parameters, coordinates, site occupancies and isotropic thermal vibration parameters B_{iso} (\AA^2) for NdBaMn₂O₅ at 800 °C (NPD, three-phase refinement, cycle 3) in the space group $P4/mmm$; the occupancy of O1 was fixed at 0, B_{iso} for O2 and O3 were constrained to be equal.

Atom		
	a (\AA)	4.0028(2)
	c (\AA)	7.8471(6)
	wt. %	39
Nd	B_{iso}	1.57(7)
Ba	B_{iso}	1.56(9)
Mn	z	0.2435(9)
	B_{iso}	1.7(1)
O3	z	0.1961(4)
	B_{iso} (O)	2.98(6)
	χ^2	1.11
	R_{B} %	3.8

Table S2. Refined lattice parameters, coordinates, site occupancies and isotropic vibration parameters B_{iso} (\AA^2) for NdBaMn₂O₆ at 800 °C (NPD, three-phase refinement, cycle 3) in the space group $Pmmm$, the occupation for the O sites was fixed at 1, B_{iso} for the oxygen sites were constrained to be equal, z coordinate for O2 and O3 were constrained to be equal.

Atom		
	a (\AA)	3.9445(2)
	b (\AA)	3.9458(4)
	c (\AA)	7.8239(5)
	wt. %	36
Nd	B_{iso}	1.57(7)
Ba	B_{iso}	1.56(9)
Mn	z	0.248(1)
	B_{iso}	1.00(6)
O3, O4	z	0.2285(5)
	B_{iso} (O)	2.45(4)
	χ^2	1.11
	R_{B} %	2.6

Table S3. Refined lattice parameters, coordinates, site occupancies and isotropic thermal vibration parameters B_{iso} (\AA^2) for $\text{NdBaMn}_2\text{O}_5$ at 65 °C (NPD, two-phase refinement, cycle 3) in the space group $P4/nmm$; B_{iso} for the O sites were constrained to be equal and the occupancy of O2 and O3 has been fixed at 1.

Atom		
	a (\AA)	5.6164(1)
	c (\AA)	7.7495(3)
	wt. %	68
Nd	B_{iso}	0.49(2)
Ba	B_{iso}	0.56(4)
Mn1	z	0.2676(9)
	B_{iso}	0.3(1)
Mn2	z	0.748(1)
	B_{iso}	0.4(1)
O1	occ	0.02(1)
O2	z	0.0078(9)
O3	x	0.4923(3)
	z	0.3084(1)
	B_{iso} (O)	0.88(2)
	χ^2	1.16
	R_{B} %	2.7