Supplementary Materials for

High pO_2 Flux Growth and Characterization of $NdNiO_3$ Crystals

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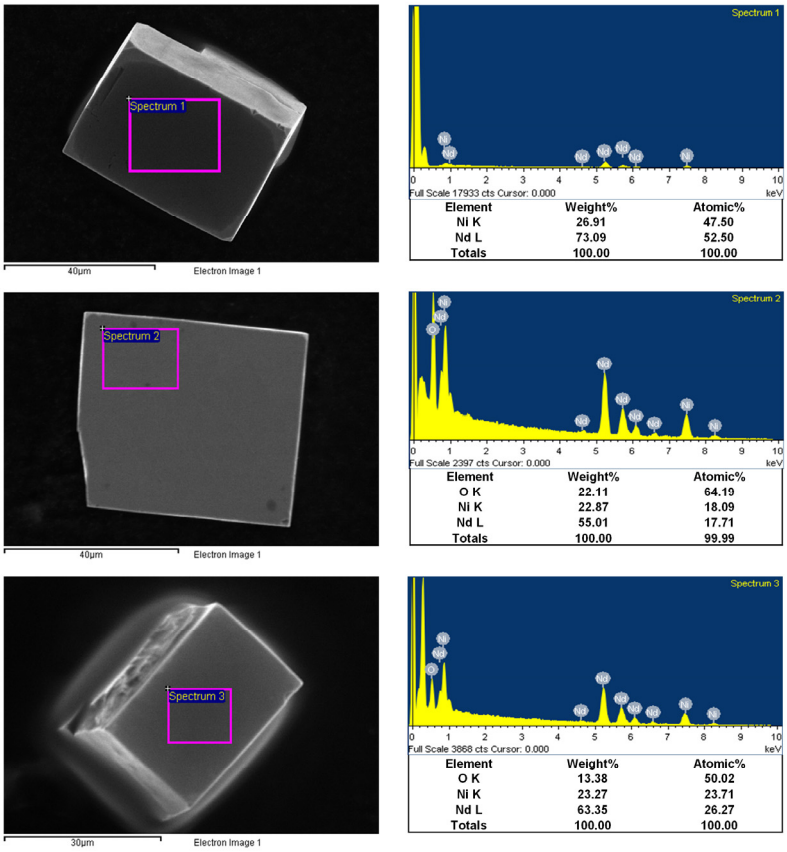

Figure S1. Elemental analysis for as-grown $NdNiO_3$ crystals.

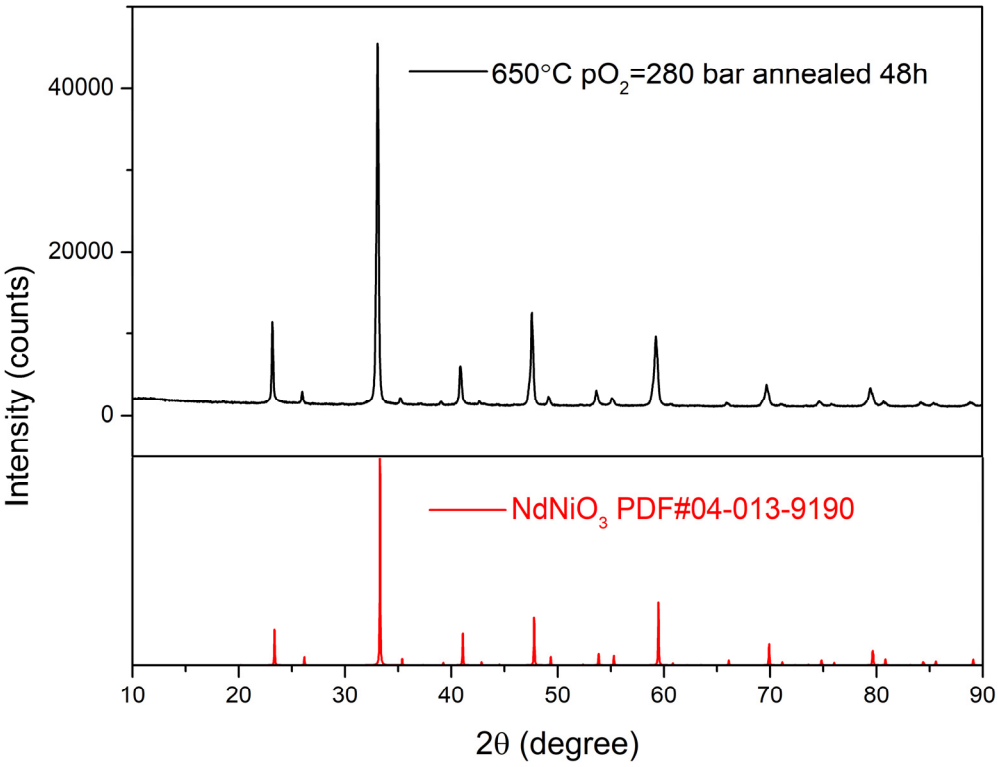

Figure S2. In-house X-ray powder diffraction for annealed $NdNiO_3$ sample.

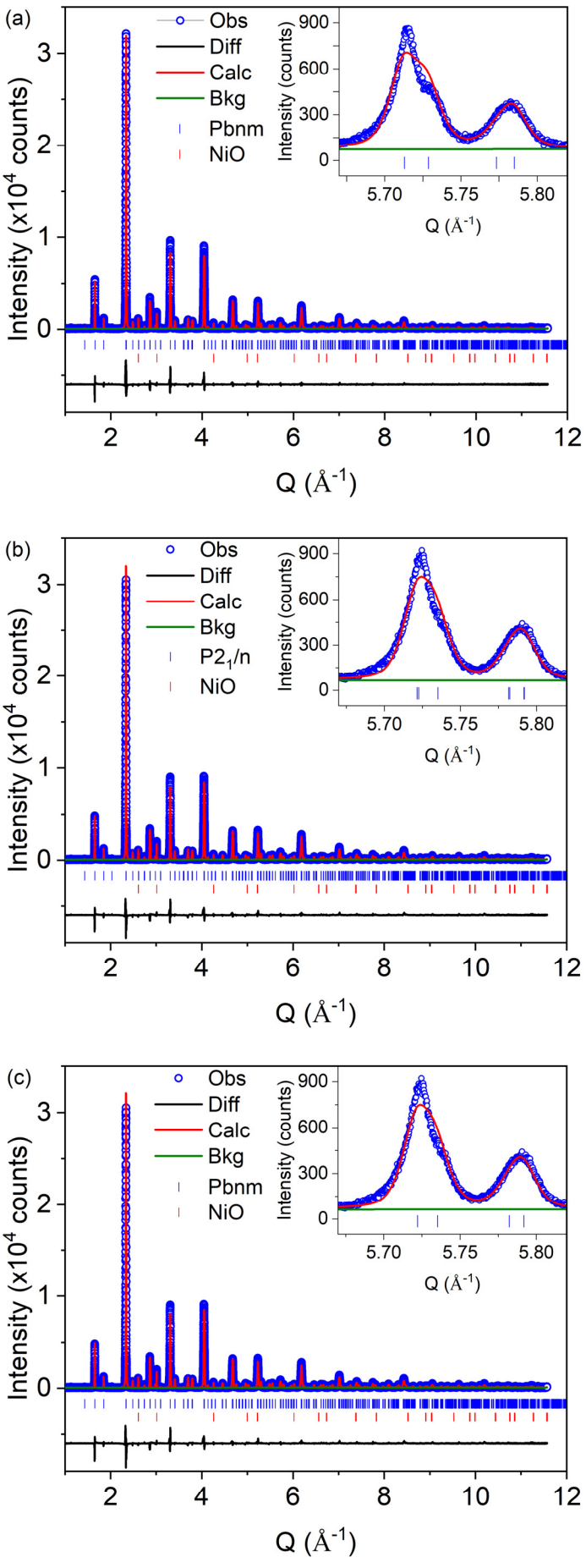
(a)
Obs
Diff
Calc
Bkg
Pbnm
NiO
Intensity (x10^4 counts)
Q (Å^{-1})
Intensity (counts)
(b)
Obs
Diff
Calc
Bkg
P2$_1$/n
NiO
Intensity (x10^4 counts)
Q (Å^{-1})
Intensity (counts)
(c)
Obs
Diff
Calc
Bkg
Pbnm
NiO
Intensity (x10^4 counts)
Q (Å^{-1})
Intensity (counts)

Figure S3. (a) Synchrotron x-ray high-resolution powder diffraction pattern for as-grown $NdNiO_3$ at 295 K with Rietveld refinement using the orthorhombic *Pbnm* symmetry; **(b)** Synchrotron x-ray high-resolution powder diffraction pattern for $NdNiO_3$ at 100 K with Rietveld refinement using the monoclinic $P2_1/n$ symmetry; **(c)** Synchrotron x-ray high-resolution powder diffraction pattern for $NdNiO_3$ at 100 K with Rietveld refinement using the orthorhombic *Pbnm* symmetry. Insets are observed and calculated intensities in the Q range of 5.67-5.82 $Å^{-1}$, corresponding to the orthorhombic (404)/(044)/(423)/(243) region (from left to right) or the monoclinic $(40\bar{4})$/(404)/(044)/ $(42\bar{3})$/(423)/$(24\bar{3})$/(243) region (from left to right). The X-axis Q is $Q=2\pi/d=4\pi\sin\theta/\lambda$, where d is the d-spacing, λ is wavelength. Obs: observed intensity; Diff: difference; Calc: calculated intensity; Bkg: background.

Table S1. Unit cell parameters and atomic coordinates for $NdNiO_3$ at 300 K as obtained from Rietveld refinement to an in-house X-ray powder diffraction pattern.

Chemical formula: $NdNiO_3$					
Source: X-ray powder diffraction, instrument: Bruker D2, λ=1.5418 Å					
Formular weight (g/mol)		250.9315			
Temperature (K)		300	Fit reliability factors		
Crystal system		Orthorhombic	R_p		4.16%
Space group		*Pbnm*	R_{wp}		6.52%
a (Å)		5.4019(3)	R_{Bragg}		4.39%
b (Å)		5.3697(3)	Goodness-of-fit χ^2		3.26
c (Å)		7.6009(5)			
Unit cell vol. V (Å^3)		220.48(2)			
Z		4			
Density (g/cm^3)		7.5596(8)			
Starting model of $NdNiO_3$ was from the PDF4+ database (ID: 04-006-7145).					
Atomic positions	*x*	*y*	*z*	s.o.f	B_{eq} (Å^2)
Nd	0.9919(8)	0.0296(3)	0.25	1	0.61
Ni	0.5000	0	0	1	0.51
O1	0.027(7)	0.492(3)	0.25	1	0.76
O2	0.671(2)	0.266(3)	0.016(3)	1	0.88

Table S2. Unit cell parameters and atomic coordinates for $NdNiO_3$ at 295 K as obtained from Rietveld refinement to a synchrotron X-ray high-resolution powder diffraction pattern.

Chemical formula: $NdNiO_3$					
Source: Synchrotron X-ray high-resolution powder diffraction, instrument: 11-BM, APS, λ=0.458961 Å					
Formular weight (g/mol)	250.9315				
Temperature (K)	295	Fit reliability factors			
Crystal system	Orthorhombic	R_p		10.69%	
Space group	*Pbnm*	R_{wp}		14.88%	
a (Å)	5.39347(7)	R_{Bragg}		4.515%	
b (Å)	5.37116(6)	Goodness-of-fit χ^2		2.34	
c (Å)	7.60367(10)				
Unit cell vol. V (Å^3)	220.272(5)				
Z	4				
Density (g/cm^3)	7.56668(17)				
Starting model of $NdNiO_3$ was from the PDF4+ database (ID: 04-006-7145). Phase fraction: 96.01(4)%wt.					
Atomic positions	x	y	z	s.o.f	B_{eq} (Å^2)
Nd	0.99558(14)	0.03169(5)	0.25	1	0.310(6)
Ni	0.5000	0	0	1	0.200(9)
O1	0.0525(10)	0.4914(6)	0.25	1	0.20(13)
O2	0.7068(8)	0.2776(8)	0.0394(6)	1	0.29(7)
Starting model of NiO was from the PDF4+ database (ID: 04-013-0889) and atomic coordinates were not refined. Phase fraction: 3.99(4)%wt					
Space group	$R\bar{3}m$				
a (Å)	2.95592(5)				
c (Å)	7.2305(2)				
Atomic positions	*x*	*y*	*z*	s.o.f	B_{eq} (Å^2)
Ni	0	0	0	1	0.14
O	0	0	0.5	1	0.18

Table S3. Unit cell parameters and atomic coordinates for $NdNiO_3$ at 100 K as obtained from Rietveld refinement (using *Pbnm*) to a synchrotron X-ray high-resolution powder diffraction pattern.

Chemical formula: $NdNiO_3$					
Source: Synchrotron X-ray high-resolution powder diffraction, instrument: 11-BM, APS, λ= 0.458956 Å					
Formular weight (g/mol)	250.9315				
Temperature (K)	100	Fit reliability factors			
Crystal system	Orthorhombic	R_p		11.80%	
Space group	*Pbnm*	R_{wp}		16.25%	
a (Å)	5.38439(8)	R_{Bragg}		6.630%	
b (Å)	5.36601(6)	Goodness-of-fit χ^2		2.52	
c (Å)	7.59296(12)				
Unit cell vol. V (Å^3)	219.381(5)				
Z	4				
Density (g/cm^3)	7.59741(19)				
Starting model of $NdNiO_3$ was from the PDF4+ database (ID: 04-006-7145). Phase fraction: 95.78(4)%wt.					
Atomic positions	x	y	z	s.o.f	B_{eq} (Å^2)
Nd	0.9973(2)	0.03332(6)	0.25	1	0.200(6)
Ni	0.5000	0	0	1	0.200(9)
O1	0.0567(12)	0.4909(7)	0.25	1	0.20(14)
O2	0.7126(9)	0.2780(9)	0.0407(6)	1	0.20(7)
Starting model of NiO was from the PDF4+ database (ID: 04-013-0889) and atomic coordinates were not refined. Phase fraction: 4.22(4)%%wt.					
Space group	$R\bar{3}m$				
a (Å)	2.95194(4)				
c (Å)	7.21816(18)				
Atomic positions	*x*	*y*	*z*	s.o.f	B_{eq} (Å^2)
Ni	0	0	0	1	0.14
O	0	0	0.5	1	0.18

Table S4. Unit cell parameters and atomic coordinates for $NdNiO_3$ at 100 K as obtained from Rietveld refinement (using $P2_1/n$) to a synchrotron X-ray high-resolution powder diffraction pattern.

Chemical formula: $NdNiO_3$					
Source: Synchrotron X-ray high-resolution powder diffraction, instrument: 11-BM, APS, λ= 0.458956 Å					
Formular weight (g/mol)	250.9315				
Temperature (K)	100	Fit reliability factors			
Crystal system	Monoclinic	R_p			11.69%
Space group	$P2_1/n$	R_{wp}			16.19%
a (Å)	5.38464(8)	R_{Bragg}			6.302%
b (Å)	5.36604(6)	Goodness-of-fit χ^2			2.51
c (Å)	7.59258(12)				
β(°)	90.010(10)				
Unit cell vol. V (Å^3)	219.381(5)				
Z	4				
Density (g/cm^3)	7.59740(19)				
Starting model of $NdNiO_3$ was from the PDF4+ database (ID: 04-016-9612). Phase fraction: 95.79(4)%wt.					
Atomic positions	x	y	z	s.o.f	B_{eq} (Å^2)
Nd	0.9978(2)	0.03317(5)	0.2498(6)	1	0.2
Ni1	0.5000	0	0	1	0.2
Ni2	0.5000	0	0.5000	1	0.2
O1	0.0558(17)	0.4920(6)	0.245(3)	1	0.2
O2	0.684(2)	0.266(3)	0.0319(16)	1	0.2
O3	0.2360(19)	0.215(3)	0.955(2)	1	0.2
Starting model of NiO was from the PDF4+ database (ID: 04-013-0889) and atomic coordinates were not refined. Phase fraction: 4.21(4)%wt.					
Space group	$R\bar{3}m$				
a (Å)	2.95194(4)				
c (Å)	7.21808(18)				
Atomic positions	x	y	z	s.o.f	B_{eq} (Å^2)
Ni	0	0	0	1	0.14
O	0	0	0.5	1	0.18