materials

MDPI

Supplementary Data

Effect of Sr deficiency on electrical conductivity of Yb-doped strontium zirconate

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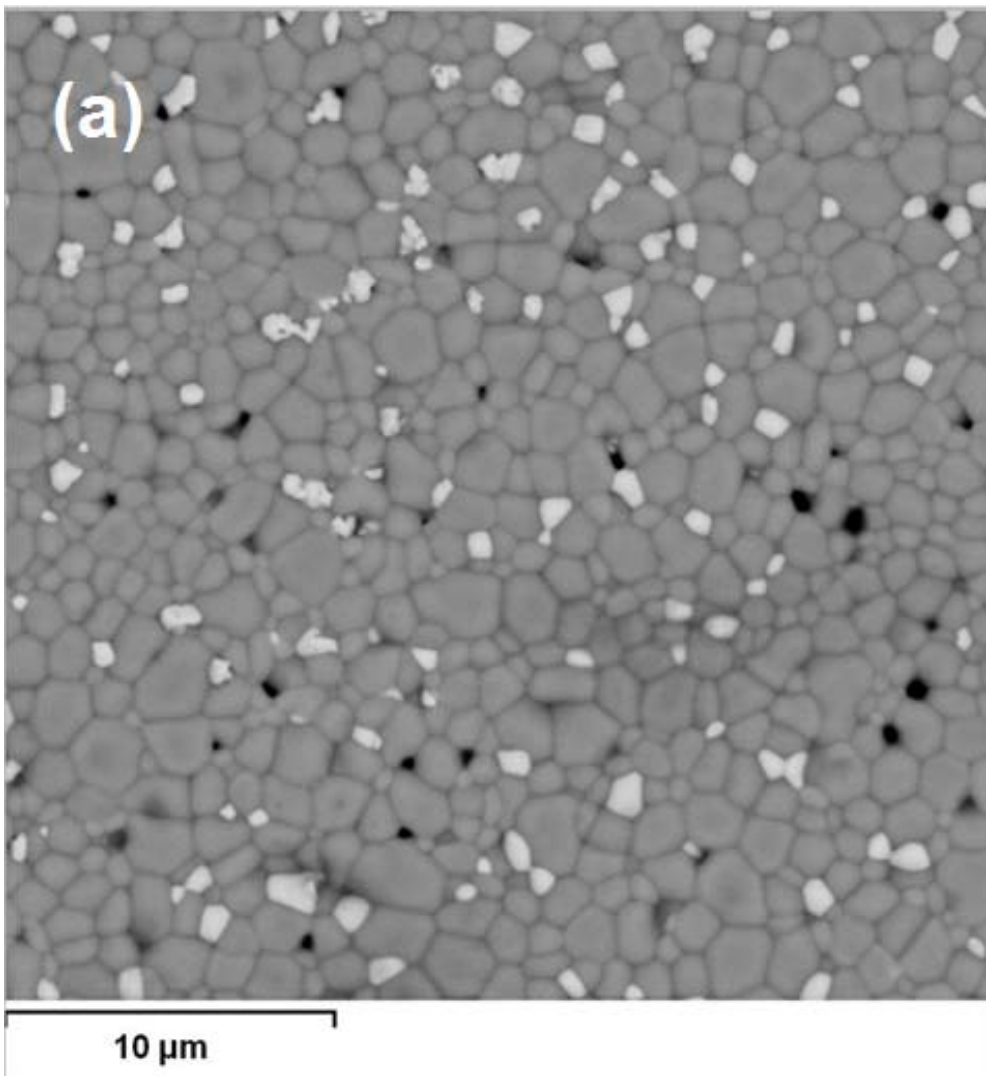


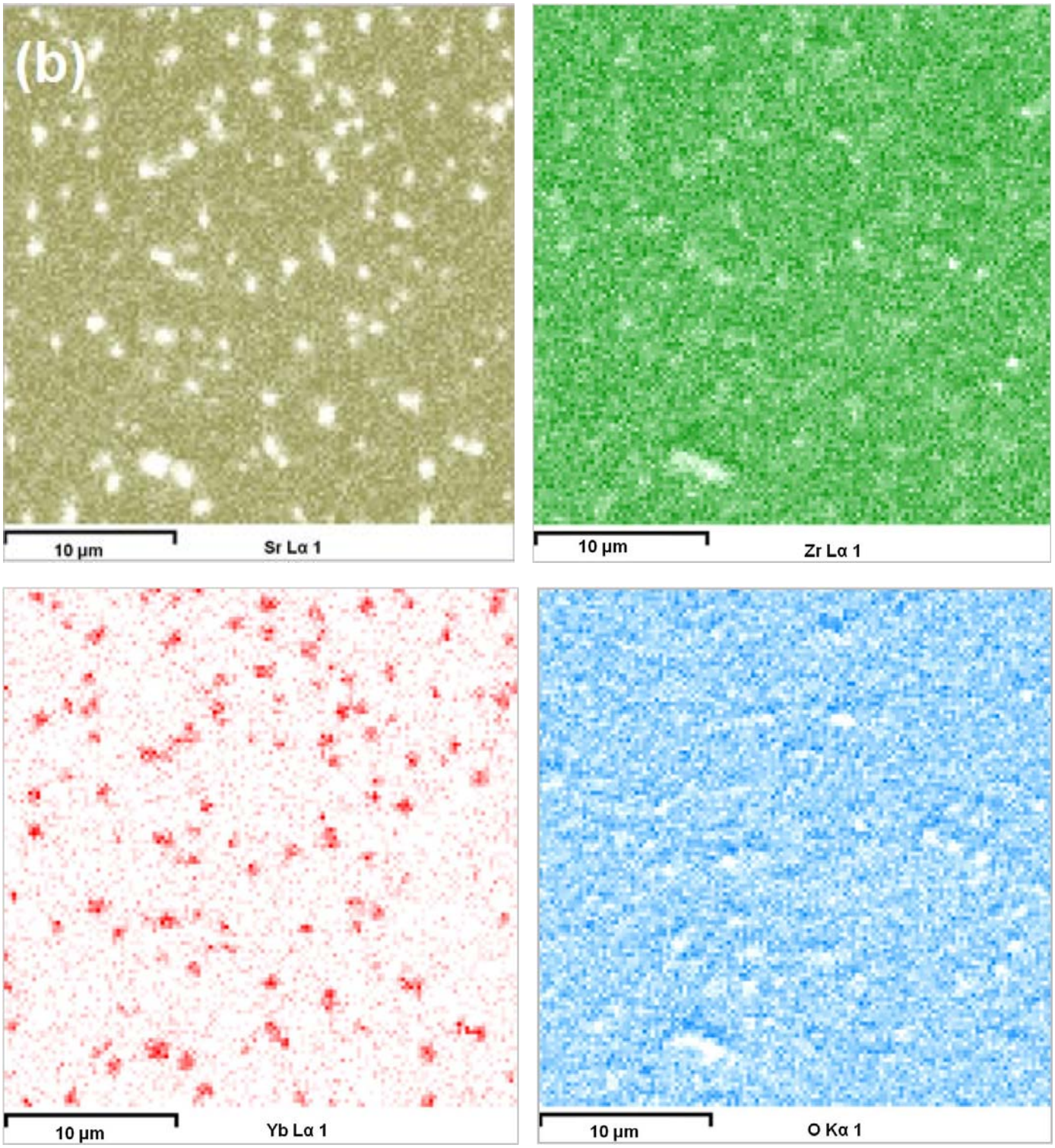
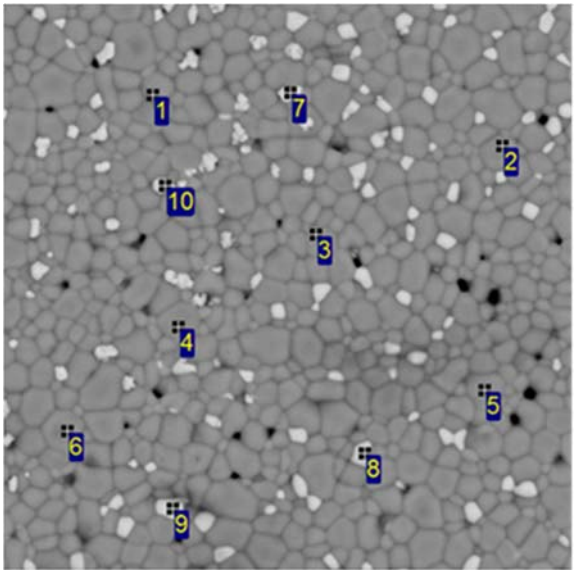


Figure S1. (a) Back scattered electron image of x = 0.94 sample and (b) corresponding EDX mapping images of Sr, Zr, Yb and O.

Table S1. Elemental composition (at.%) of the surface of of x = 0.94 sample after polishing and thermal etching (1400 °C, 4 h) from EDX data



Point	O	Sr	Zr	Yb
1	61.83	18.54	18.86	0.77
2	57.66	20.70	20.86	0.78
3	57.90	20.49	20.73	0.88
4	56.58	20.93	21.14	0.72
5	57.21	20.71	21.05	0.81
6	56.62	21.21	21.39	0.78
Average values for points 1–6 (main phase)				
	58.00	**20.43**	**20.67**	**0.79**
7	59.57	8.94	18.09	13.39
8	62.21	4.68	17.56	15.54
9	57.23	4.33	20.14	18.30
10	58.67	7.78	18.38	15.16
Average values for points 7–10 (secondary phase)				
	59.42	**6.43**	**18.54**	**15.60**

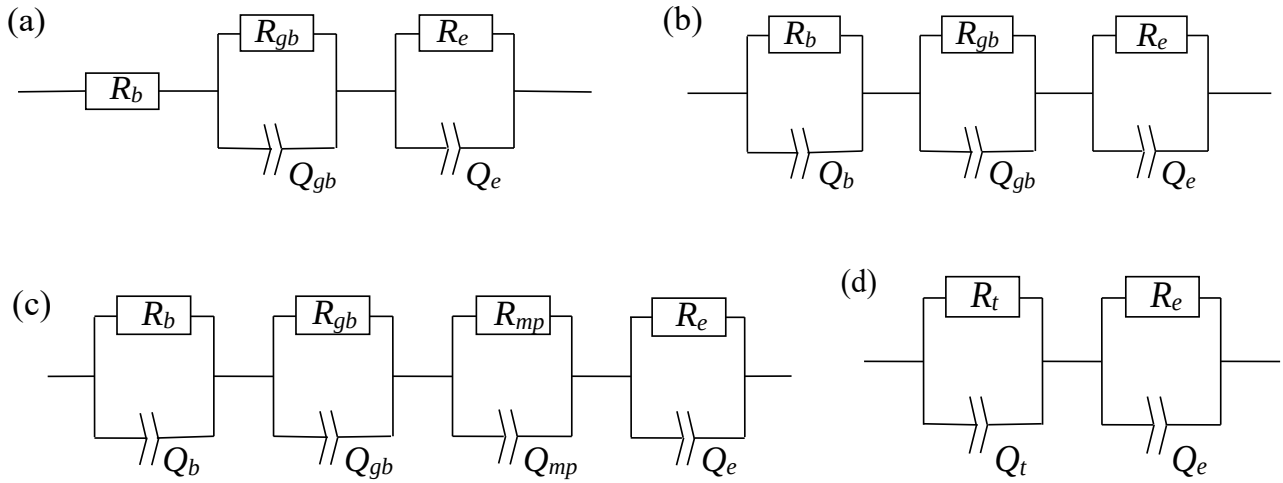
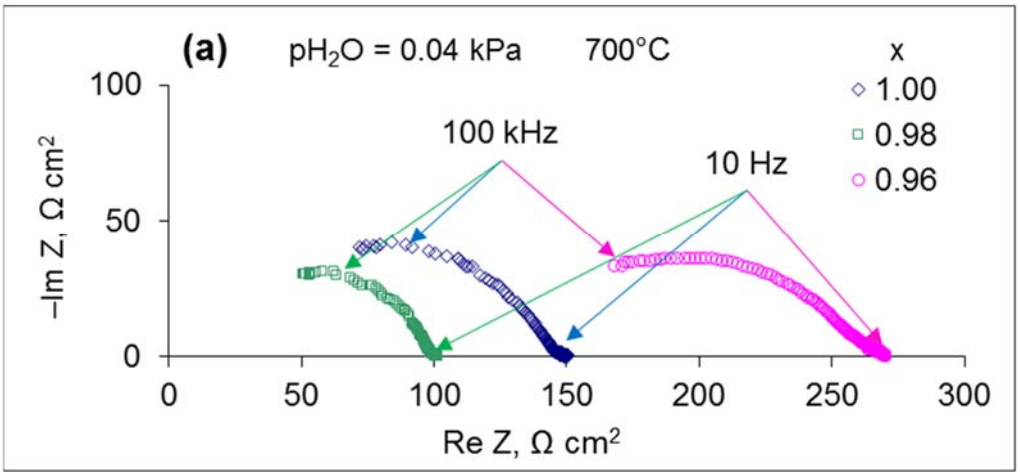
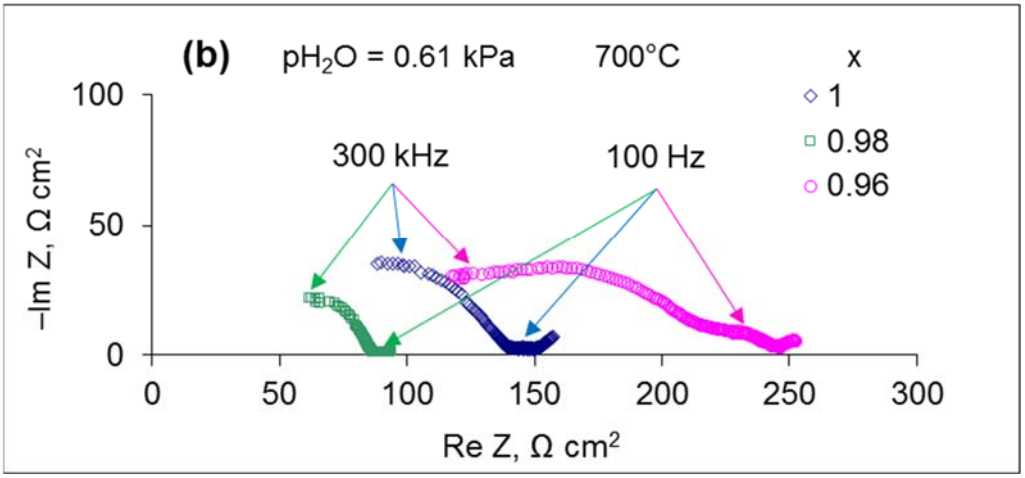
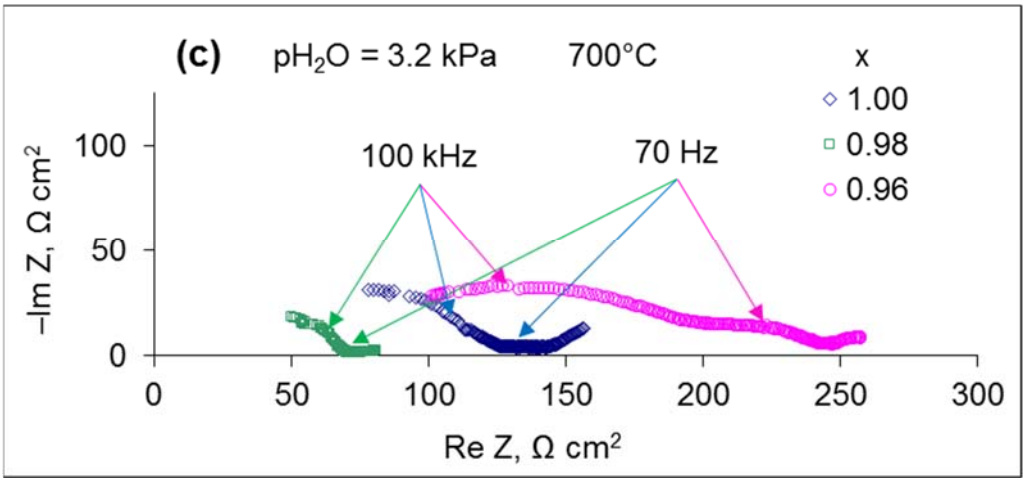
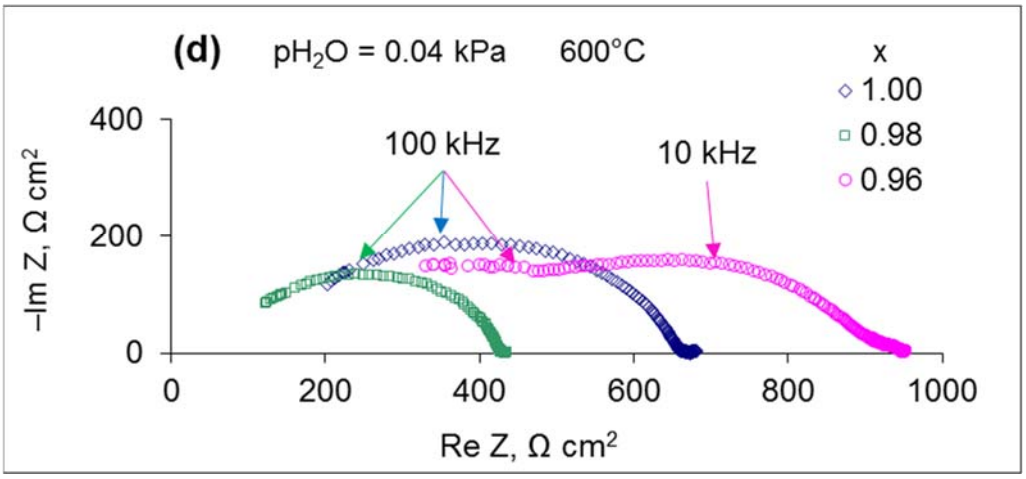


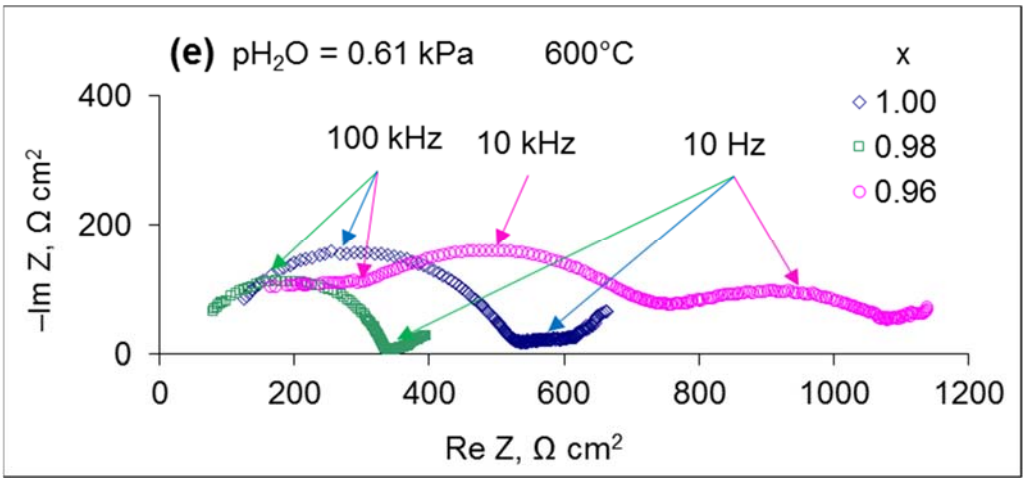
Figure S2. Equivalent circuits used for deconvolution of impedance spectra for: (**a**) x = 0.98 and 1.00 at 550–800 °C; (**b**) x = 0.98 and 1.00 at 500 °C and below; (**c**) x = 0.96 at 350 °C and below; (**d**) x = 0.94. R_t denotes the total resistance of a sample; R_b, R_{gb}, R_{mp} and R_e are the grain interior, grain boundary, minor phase and electrode resistances, respectively; Q_b, Q_{gb}, Q_{mp} and Q_e are the constant phase element associated with the grain interior, grain boundary, minor phase and electrode responses; Q_t is the constant phase element related with the total response of a sample.

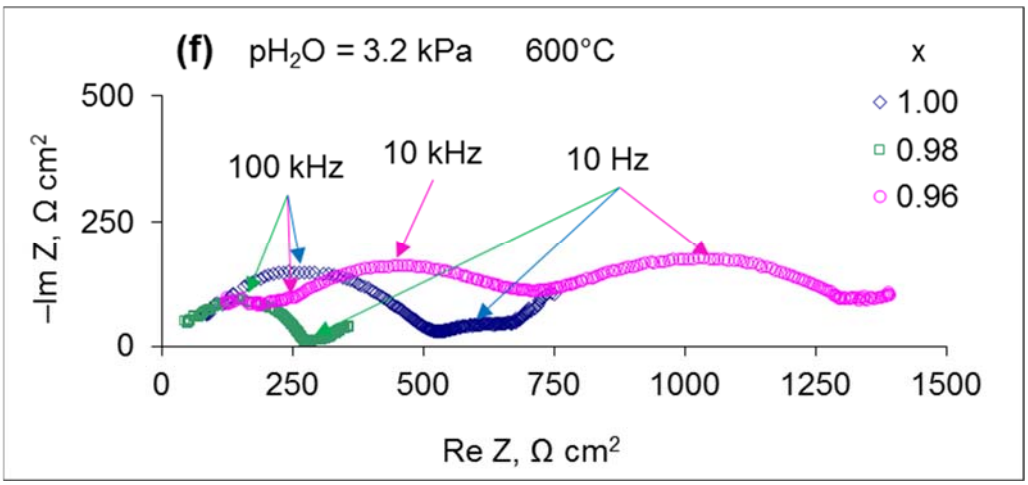

(a)
pH2O = 0.04 kPa
700°C
x
1.00
0.98
0.96
100 kHz
10 Hz
–Im Z, Ω cm2
Re Z, Ω cm2
0
50
100
150
200
250
300

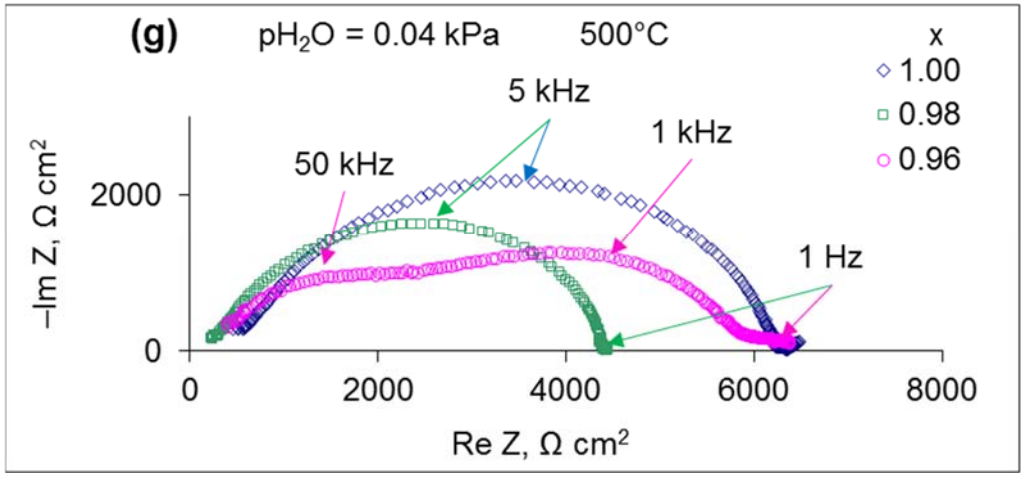

(b)
pH2O = 0.61 kPa
700°C
x
1
0.98
0.96
300 kHz
100 Hz
–Im Z, Ω cm2
Re Z, Ω cm2
0
50
100
150
200
250
300

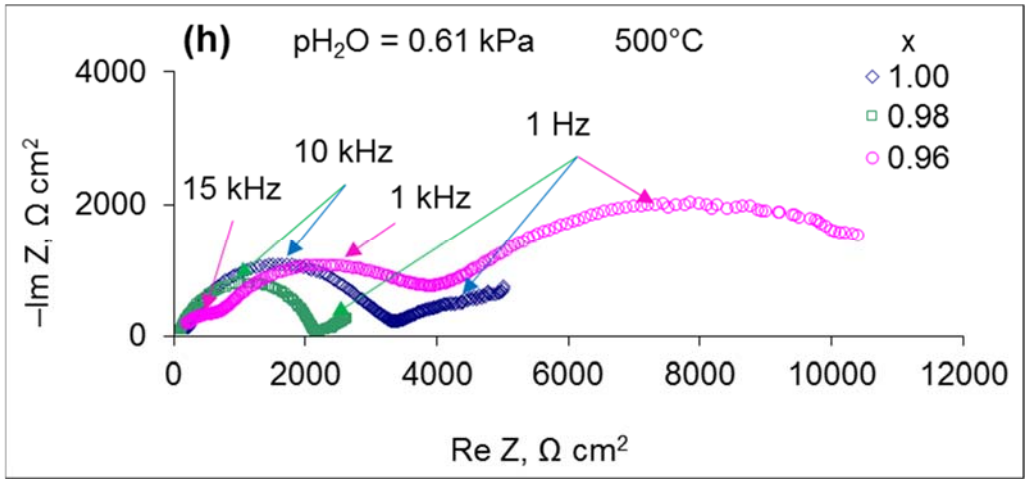

(c)
pH2O = 3.2 kPa
700°C
x
1.00
0.98
0.96
100 kHz
70 Hz
–Im Z, Ω cm2
Re Z, Ω cm2
0
50
100
150
200
250
300

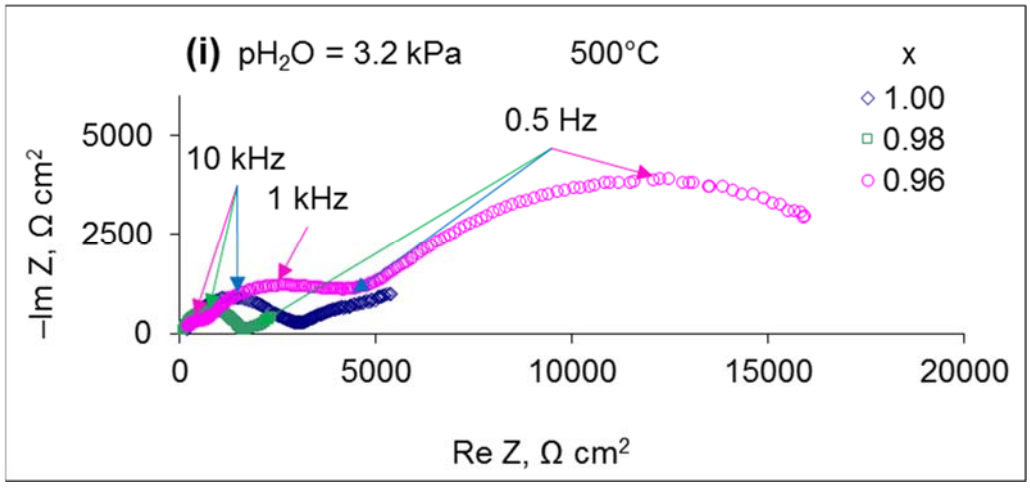

(d) pH2O = 0.04 kPa 600°C
x
1.00
0.98
0.96
100 kHz
10 kHz
400
200
0
–Im Z, Ω cm2
0
200
400
600
800
1000
Re Z, Ω cm2


(e) pH2O = 0.61 kPa 600°C
x
1.00
0.98
0.96
100 kHz
10 kHz
10 Hz
400
200
0
–Im Z, Ω cm2
0
200
400
600
800
1000
1200
Re Z, Ω cm2


(f) pH2O = 3.2 kPa 600°C
x
1.00
0.98
0.96
100 kHz
10 kHz
10 Hz
500
250
0
–Im Z, Ω cm2
0
250
500
750
1000
1250
1500
Re Z, Ω cm2


(g)
pH2O = 0.04 kPa
500°C
x
1.00
0.98
0.96
5 kHz
1 kHz
50 kHz
1 Hz
2000
0
0
2000
4000
6000
8000
–Im Z, Ω cm2
Re Z, Ω cm2


(h)
pH2O = 0.61 kPa
500°C
x
1.00
0.98
0.96
1 Hz
10 kHz
15 kHz
1 kHz
4000
2000
0
0
2000
4000
6000
8000
10000
12000
–Im Z, Ω cm2
Re Z, Ω cm2


(i)
pH2O = 3.2 kPa
500°C
x
1.00
0.98
0.96
0.5 Hz
10 kHz
1 kHz
5000
2500
0
0
5000
10000
15000
20000
–Im Z, Ω cm2
Re Z, Ω cm2

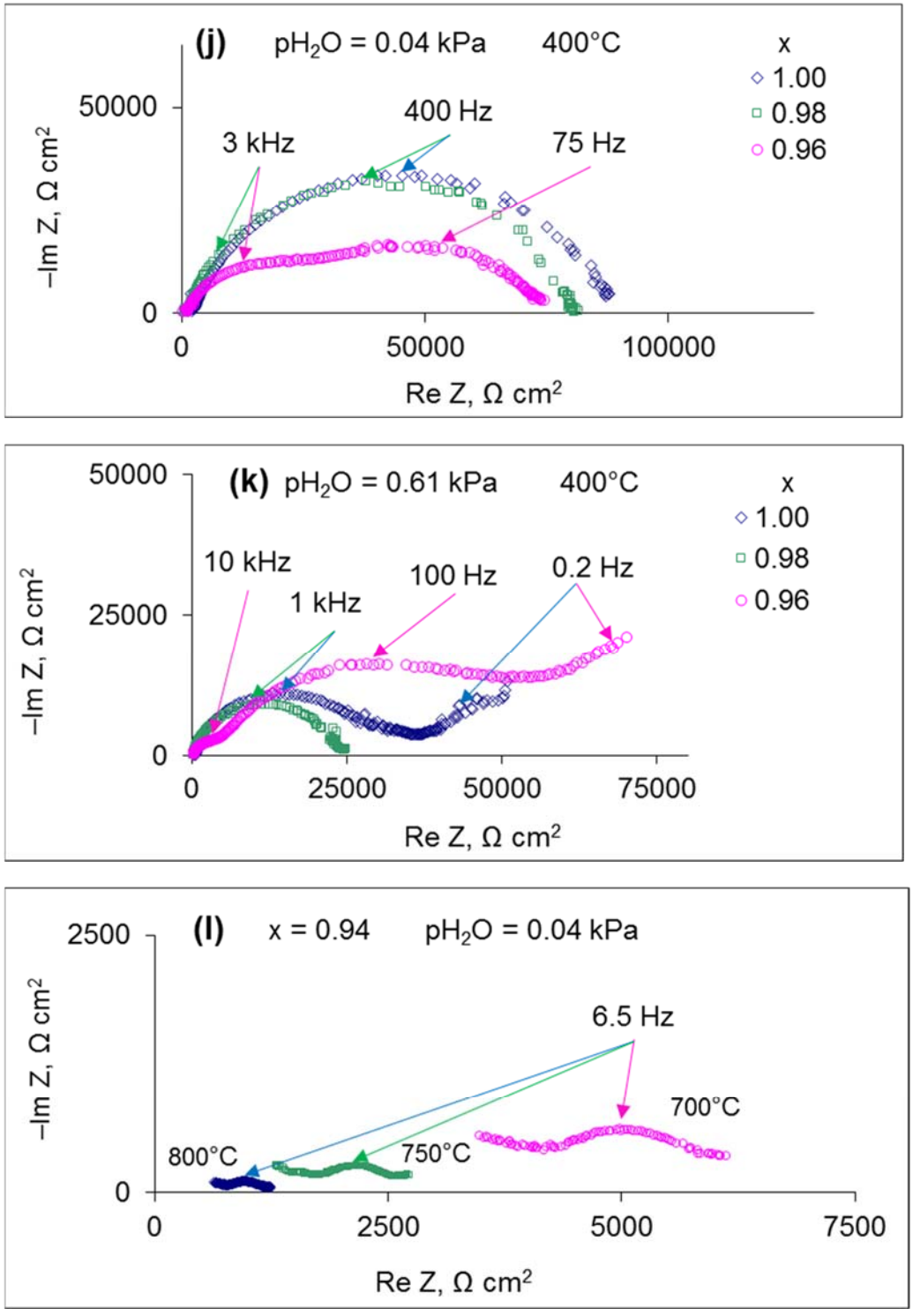


Figure S3. Impedance spectra of the samples with x = 0.96–1.00 measured in air at 700 °C (a–c), 600 °C (d–f), 500 °C (g–i) and 400 °C (j,k); at pH_2O = 0.04 kPa (a,d,g,j), 0.61 kPa (b,e,h,k) and 3.2 kPa (c,f,i); and the spectra of the x = 0.94 sample at pH_2O = 0.04 kPa (l).