

Supplementary materials

Proton Conductivity in Multi-component ABO₄-type Oxides

Ashraf A.A. Elameen et al.

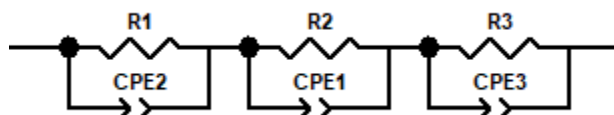


Figure S1. Electrochemical equivalent circuit used for fit an impedance spectra.

Comment: The C1, C2 and C3 parameters, listed in Tables S1-5 were calculated based on the CPE parameter obtained as a result of the fit. The used formula was:

$$C = ((CPE)^{\frac{1}{n}} R^{n-1}) \frac{L}{S} \quad (1)$$

where *CPE* is a constant phase element capacitance from fit, *n* is an admittance factor, *L* denotes a sample thickness, *S* is an area of electrode.

Table S1. Parameters of the electrochemical equivalent system obtained as a result of fitting of

SAMPLE A7NbO ₄ – DRY AIR							
T (°C)	R _{TOT} (x10 ⁵ Ω)	R ₁ (x10 ⁵ Ω)	R ₂ (x10 ⁵ Ω)	R ₃ (x10 ⁵ Ω)	C ₁ (x10 ⁻¹¹ F/cm)	C ₂ (x10 ⁻⁹ F/cm)	C ₃ (x10 ⁻¹¹ F/cm)
800	4.41	1.58	1.05	1.79	3.21	1.25	1.02
750	8.32	2.14	1.95	4.24	6.28	1.55	0.92
700	1.79	4.98	3.92	8.98	6.03	1.23	0.92
650	39.8	15.4	10.7	13.7	2.86	0.63	1.11
600	97.7	23.6	26.8	47.3	6.85	0.76	0.96

impedance spectra for sample A7NbO₄ measured in dry air.

Table S2. Parameters of the electrochemical equivalent system obtained as a result of fitting of impedance spectra for sample A7NbO₄ measured in wet air.

SAMPLE A7NbO ₄ – WET AIR							
T (°C)	R _{TOT} (x10 ⁵ Ω)	R ₁ (x10 ⁵ Ω)	R ₂ (x10 ⁵ Ω)	R ₃ (x10 ⁵ Ω)	C ₁ (x10 ⁻¹² F/cm)	C ₂ (x10 ⁻⁹ F/cm)	C ₃ (x10 ⁻¹⁰ F/cm)
800	2.40	1.56	4.72	0.38	7.97	9.40	2.12

750	3.81	2.49	0.716	0.61	7.96	6.49	1.97
700	6.48	4.02	1.26	1.20	8.17	3.23	1.06
650	11.5	2.65	2.44	6.41	14.6	1.47	14.9

Table S3. Parameters of the electrochemical equivalent system obtained as a result of fitting of impedance spectra for sample A6NbO4 measured in dry air.

SAMPLE A6NbO4 – DRY AIR							
T (°C)	R _{TOT} (x10 ⁵ Ω)	R ₁ (x10 ⁵ Ω)	R ₂ (x10 ⁵ Ω)	R ₃ (x10 ⁵ Ω)	C ₁ (x10 ⁻⁹ F/cm)	C ₂ (x10 ⁻¹² F/cm)	C ₃ (x10 ⁻¹¹ F/cm)
800	2.87	0.762	1.30	0.808	1.75	7.75	3.85
750	6.39	1.60	2.94	1.85	1.29	7.54	4.11
700	14.2	3.50	5.81	4.86	0.93	7.90	3.22
650	38.3	10.5	16.5	11.3	0.49	8.36	3.95

Table S4. Parameters of the electrochemical equivalent system obtained as a result of fitting of impedance spectra for sample A6NbO4 measured in wet air.

SAMPLE A6NbO4 – WET AIR							
T (°C)	R _{TOT} (x10 ⁵ Ω)	R ₁ (x10 ⁵ Ω)	R ₂ (x10 ⁵ Ω)	R ₃ (x10 ⁵ Ω)	C ₁ (x10 ⁻⁹ F/cm)	C ₂ (x10 ⁻⁹ F/cm)	C ₃ (x10 ⁻¹¹ F/cm)
800	1.89	3.93	1.21	0.29	5.53	6.72	15.9
750	3.03	7.32	1.75	0.54	3.46	6.97	9.23
700	5.10	1.05	3.20	0.85	3.43	6.83	1.21
650	8.62	1.92	3.77	2.94	1.54	8.34	2.63
600	15.0	3.27	5.42	6.27	1.23	10.4	1.79

Table S5. Parameters of the electrochemical equivalent system obtained as a result of fitting of impedance spectra for sample A5NbO4 measured in dry air.

SAMPLE A5NbO4 – DRY AIR							
T (°C)	R _{TOT} (x10 ⁵ Ω)	R ₁ (x10 ⁵ Ω)	R ₂ (x10 ⁵ Ω)	R ₃ (x10 ⁵ Ω)	C ₁ (x10 ⁻¹⁰ F/cm)	C ₂ (x10 ⁻⁹ F/cm)	C ₃ (x10 ⁻¹¹ F/cm)
800	2.54	0.513	0.45	1.58	10.9	1.32	1.83
750	5.50	1.27	1.04	3.19	5.69	1.43	1.84
700	12.30	3.10	2.07	7.11	3.73	1.44	1.74
650	28.90	9.88	3.73	15.30	1.57	1.83	1.64
600	80.40	23.90	17.90	38.60	2.04	1.47	2.27

Table S6. Parameters of the electrochemical equivalent system obtained as a result of fitting of impedance spectra for sample A5NbO4 measured in wet air.

SAMPLE A5NbO4 – WET AIR							
T (°C)	R_{TOT} (x10⁵ Ω)	R₁ (x10⁵ Ω)	R₂ (x10⁵ Ω)	R₃ (x10⁵ Ω)	C₁ (x10⁻¹⁰ F/cm)	C₂ (x10⁻⁹ F/cm)	C₃ (x10⁻¹¹ F/cm)
800	1.86	0.28	0.60	0.97	32.5	1.48	2.72
750	3.34	0.61	0.73	2.00	9.72	1.69	2.01
700	5.72	1.29	0.839	3.59	4.30	1.93	1.66
650	9.29	2.82	1.09	5.39	1.18	1.98	1.45
600	19.3	3.48	3.08	12.7	7.01	2.00	1.64