ELECTRONIC SUPPLEMENTARY INFORMATION FOR

From theory to experiment: $BaFe_{0.125}Co_{0.125}Zr_{0.75}O_{3-\delta}$, a highly promising cathode for intermediate temperature SOFCs

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SI1 – Synchrotron X-ray diffraction

Table SI1.1. Refined structural parameters obtained from synchrotron X-ray diffraction for $BaFe_{0.125}Co_{0.125}Zr_{0.75}O_{3-\delta}$ (BFCZO) at room temperature in the space group $Pm\bar{3}m$. Occupancy values for the BFCZO phase are fixed to the result obtained by neutron diffraction data. Information about the secondary phase, $BaZrO_3$ (BZO) is also added.

Phases	BFCZO	BZO
Lattice parameter, *a* / Å	4.1863(1)	4.1798(1)
Occ. Ba	0.3333	0.3333
Occ. Fe	0.042	0
Occ. Co	0.044	0
Occ. Zr	0.248	0.3333
Occ. O (1)	0.966	1
R_p **(%)**	3.77	
R_{wp} **(%)**	5.09	
R_{exp} **(%)**	1.49	
Bragg *R*-factor	3.33	1.2

SI2 – Neutron diffraction

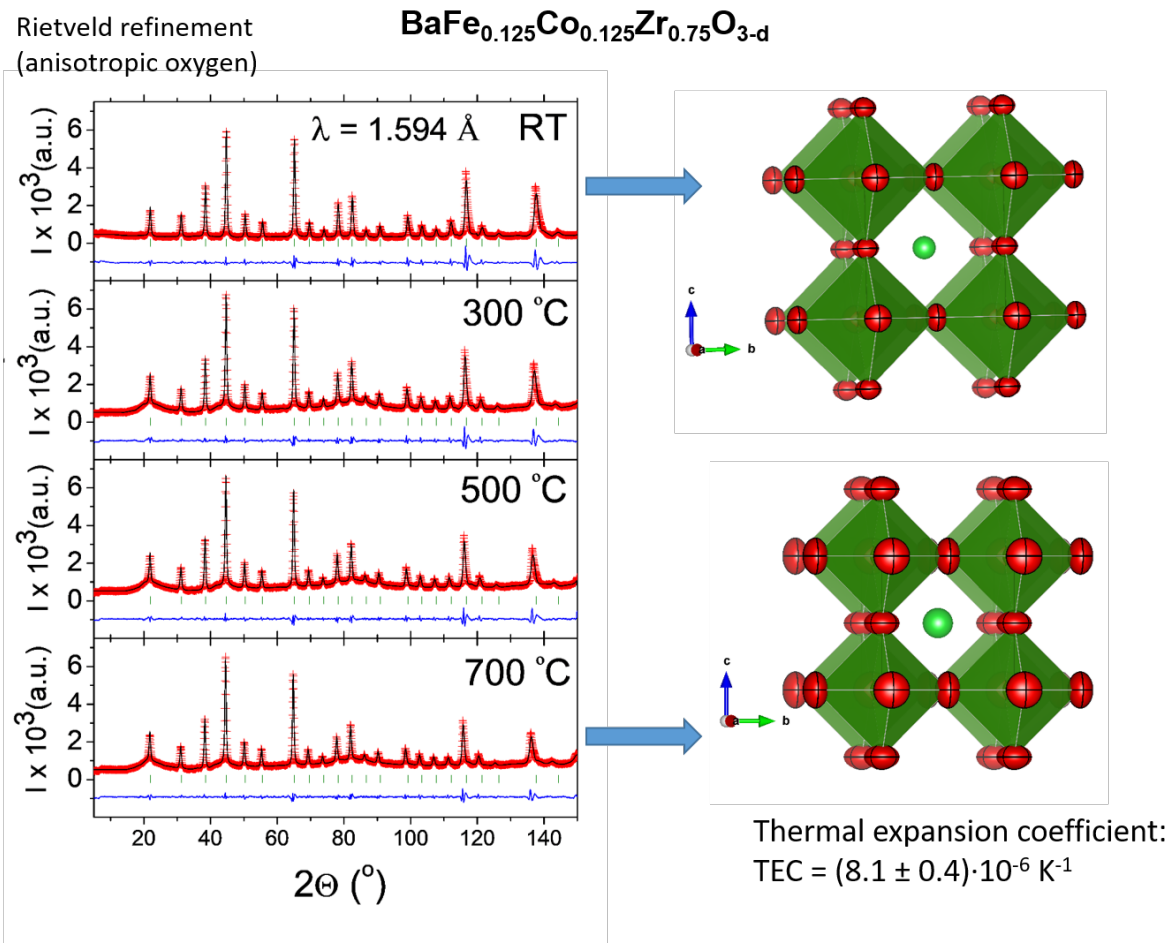

Fig SI2.1. Anisotropic atomic displacement analysis of oxygen atoms from Neutron powder diffraction data: Illustration of the perovskite crystal structure including 95% probability displacement ellipsoids for room temperature and 700 °C data.

SI3 –X-ray thermodiffraction and Thermal Expansion Coefficient (TEC)

X-ray thermodiffraction was performed from room temperature to 1100 °C on a PANalytical modelo X'Pert PRO diffractometer using Cu radiation.

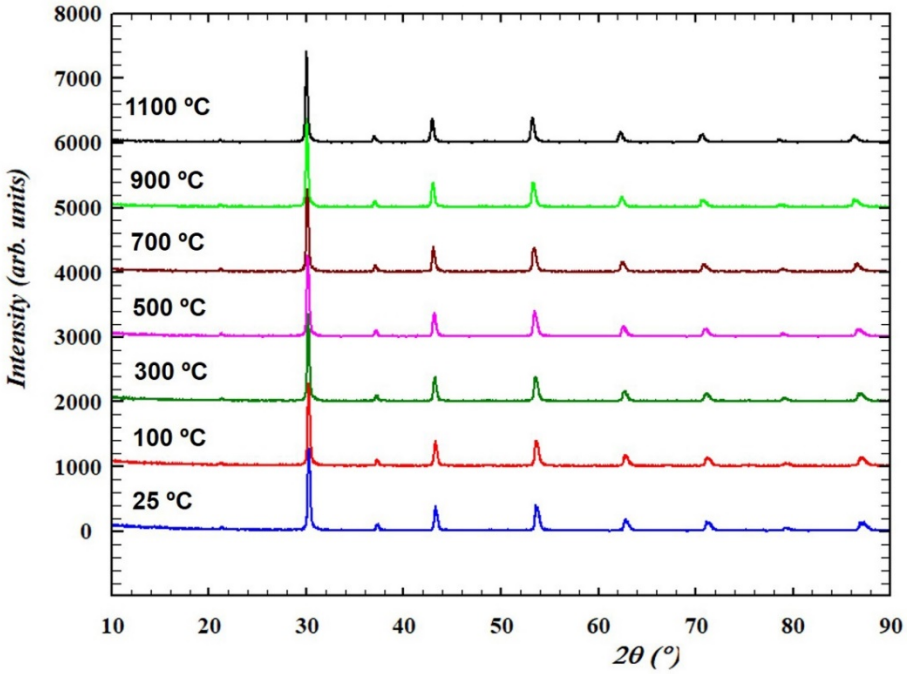

Figure SI3.1. X-ray thermodiffraction of $BaFe_{0.125}Co_{0.125}Zr_{0.75}O_{3-\delta}$

Table SI3.1. Temperature dependence of the cell parameters obtained from Le Bail analysis.

T (°C)	*a* (Å)
25	4.1878(1)
100	4.1916(1)
300	4.1980(1)
500	4.2051(1)
700	4.2098(1)
900	4.2181(1)
1100	4.2245(1)

The thermal expansion coefficient was determined using the lattice parameters at different temperatures by the expression:

$$TEC = \frac{{}^{(a_{T2}-a_{T1})}/_{a_{T1}}}{\Delta T}$$

where a_{Tx} is the lattice parameter at a selected temperature and ΔT corresponds to the difference of temperature. A TEC value of 8.0 x 10^{-6} K^{-1} is found from room temperature to 1100 °C.

SI4 – Impedance Spectroscopy of the cells (Heating and cooling)

Table SI4.1. Area specific polarization resistance (ASRp) and ohmic resistance (ASRs) for the symmetrical cells tested in stagnant air in a 2-electrode configuration (heating process).

T (°C)	500	550	600	650	700	750	800
BFCZO Cell							
ASR_p ($\Omega \cdot cm^2$)	7.19	3.39	1.47	0.66	0.33	0.22	0.13
ASR_s ($\Omega \cdot cm^2$)	7.21	4.85	3.37	2.50	1.97	1.48	1.18
BFCZO-GDC cell							
ASR_p ($\Omega \cdot cm^2$)	5.89	2.13	0.83	0.33	0.13	0.08	0.05
ASR_s ($\Omega \cdot cm^2$)	7.64	4.82	3.28	2.35	1.78	1.31	1.02

BFCZO cell:

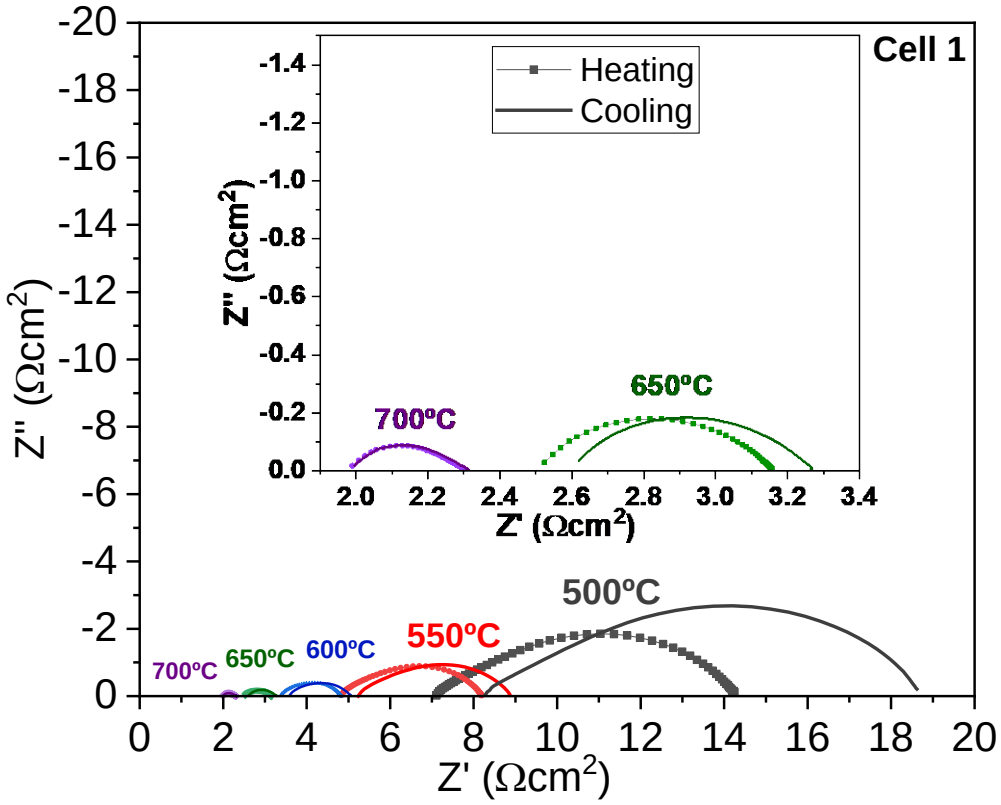

Fig SI4.1. Impedance spectroscopy data from a BFCZO symmetrical cell in a 2-electrode configuration from 500 °C to 700 °C during heating and cooling. Insets show the spectra at 650 °C and 700 °C zoomed in.

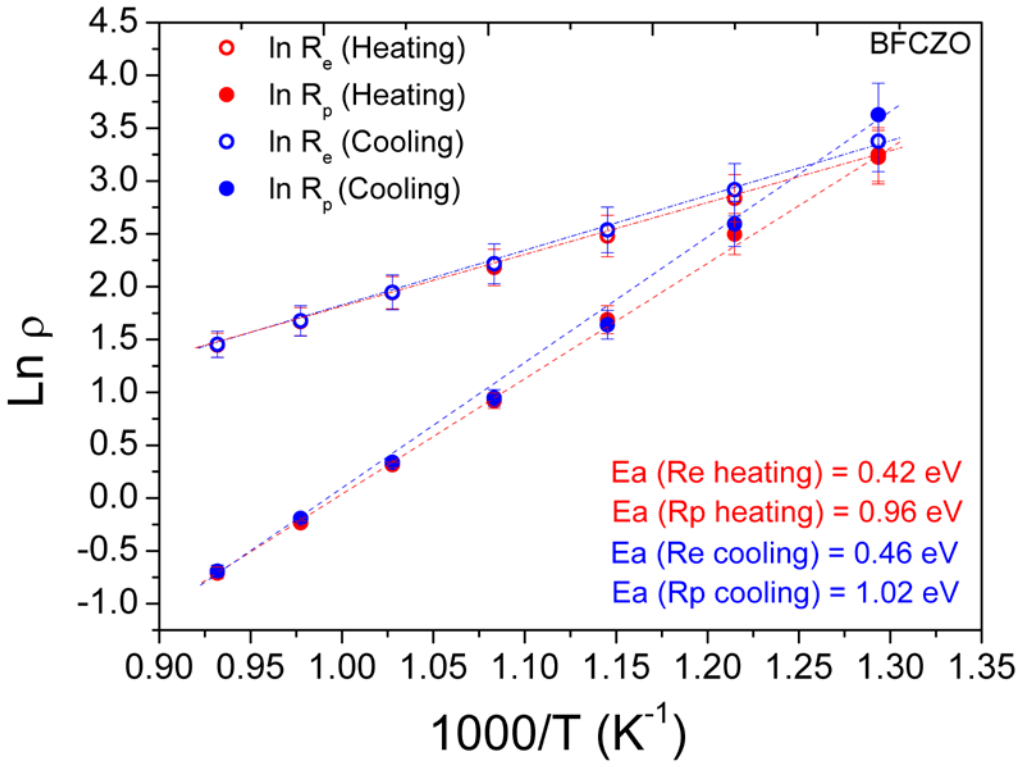

Figure SI4.2. Temperature dependence of the resistivity for BFCZO cell during heating and cooling processes.

BFCZO-GDC cell:

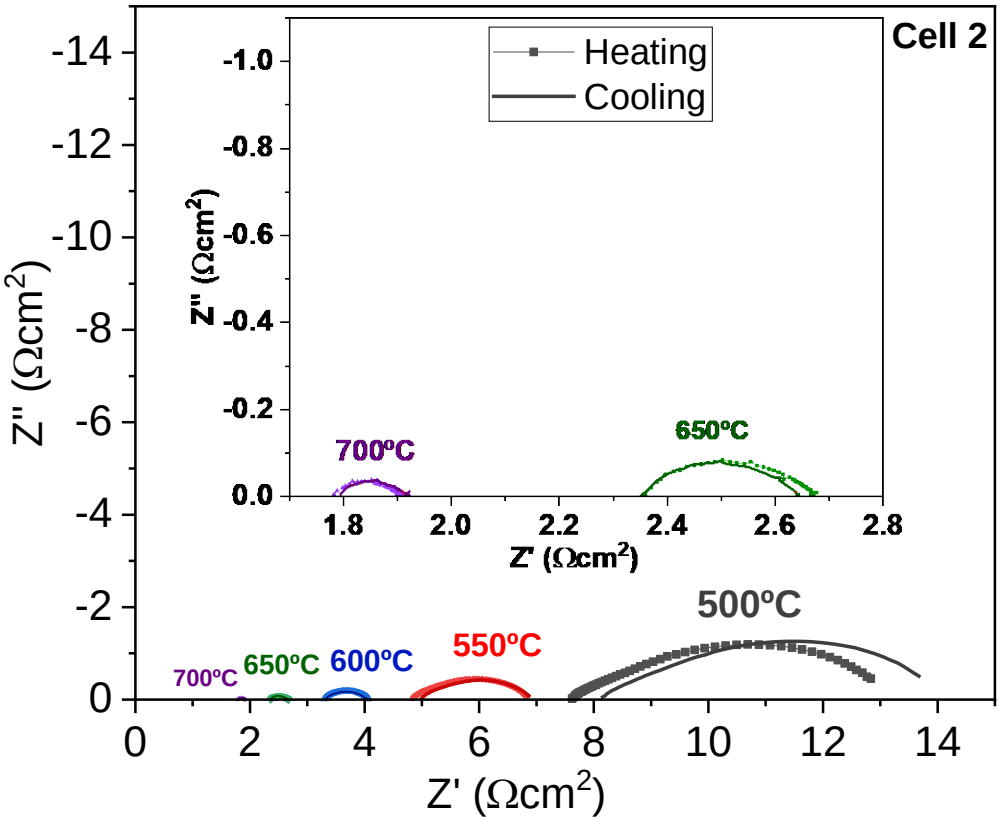

Fig SI4.3. Impedance spectroscopy data from a BFCZO-GDC symmetrical cell in a 2-electrode configuration from 500 °C to 700 °C during heating and cooling. Insets show the spectra at 650 °C and 700 °C zoomed in.

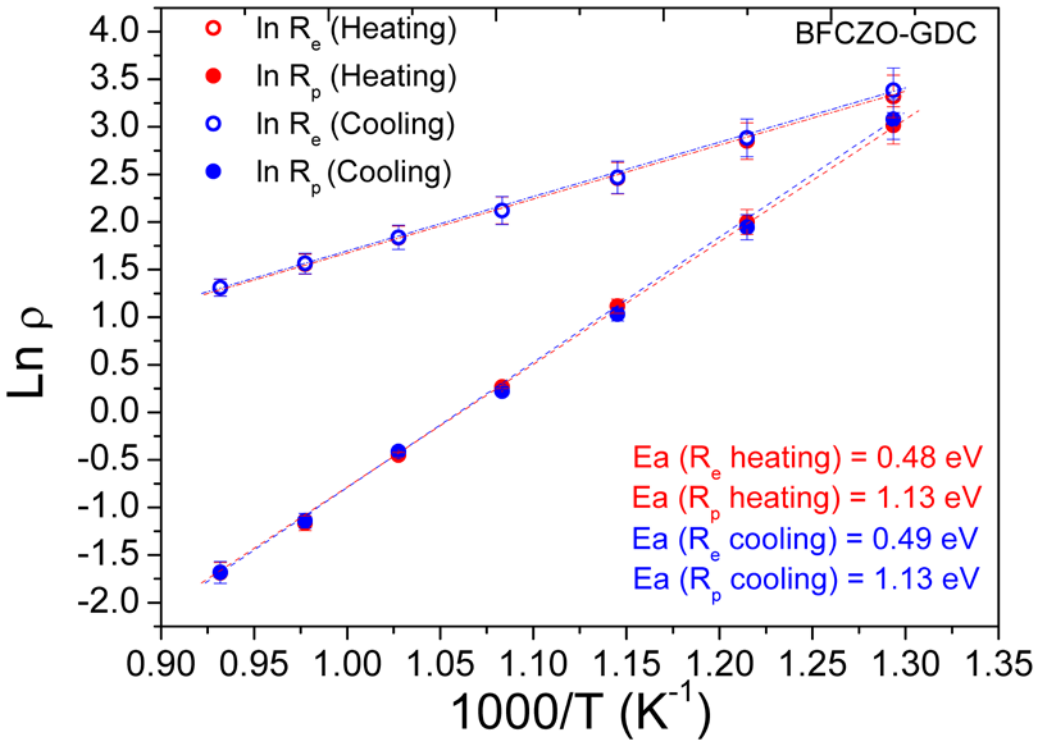

Figure SI4.4. Temperature dependence of the resistivity for BFCZO-GDC cell during heating and cooling processes.