

SUPPLEMENTAL MATERIALS

for

High Temperature Thermo-Mechanical Properties of Praseodymium Doped Ceria Thin

Films Measured Two Ways

by

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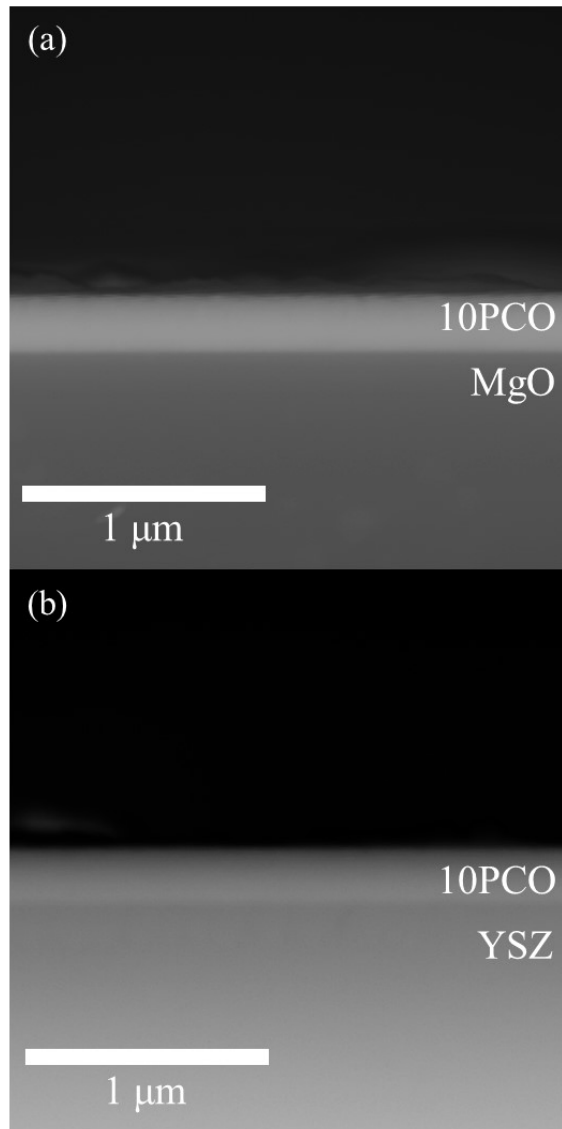


Figure S1. Representative Back Scattered Scanning Electron Microscopy (SEM) images of a) PCO|MgO and (b) PCO|YSZ samples showing that the film thickness was $\sim 235 \pm 2$ nm and 230 ± 5 nm, respectively.

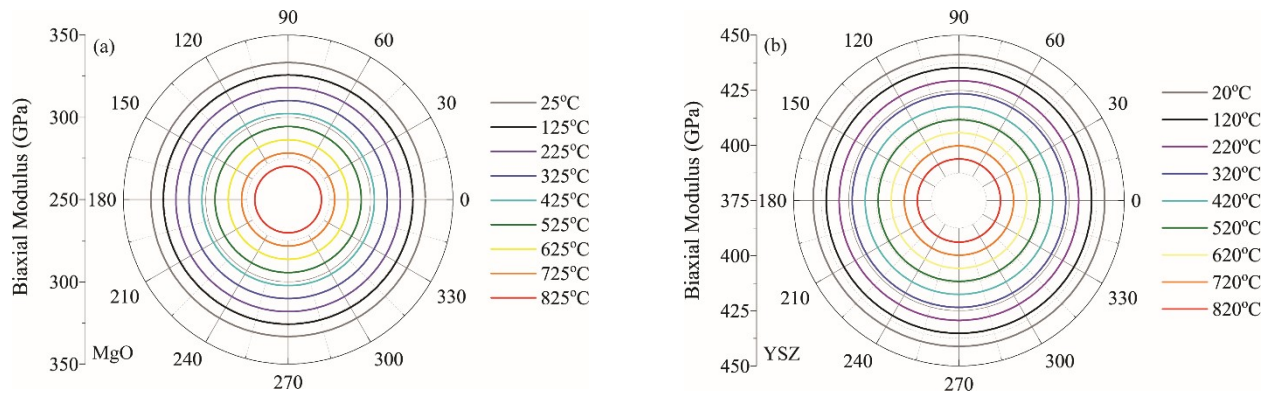


Figure S2. Biaxial moduli as a function of temperature in the a) (100) MgO plane and b) (100) $(Y_2O_3)_{0.095}(ZrO_2)_{0.905}$ plane calculated from literature data.^{1, 2} Note, the radius of each circle corresponds to the value of the biaxial modulus displayed on the y-axis.

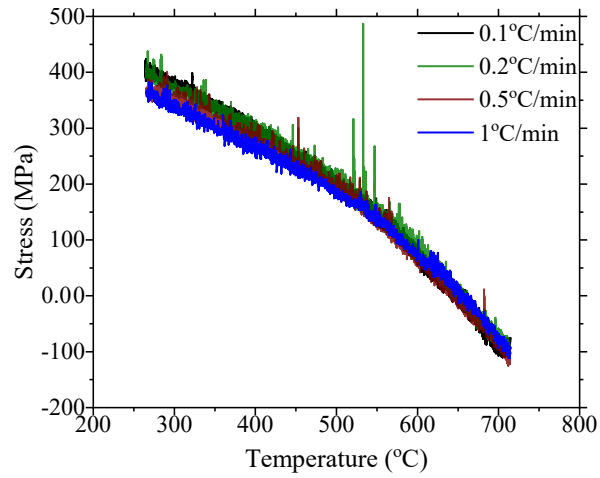


Figure S3. The effect of cooling rate on the stress vs. temperature measurements of representative 10PCO|YSZ samples. Note, samples tested with either 0.1 or 0.2 °C/min cooling rates were identical and hence both considered to be in thermal equilibrium from 280-700°C (since the additional time at each temperature with a slower 0.1 °C/min cooling rate had no effect on the stress-temperature trajectory).

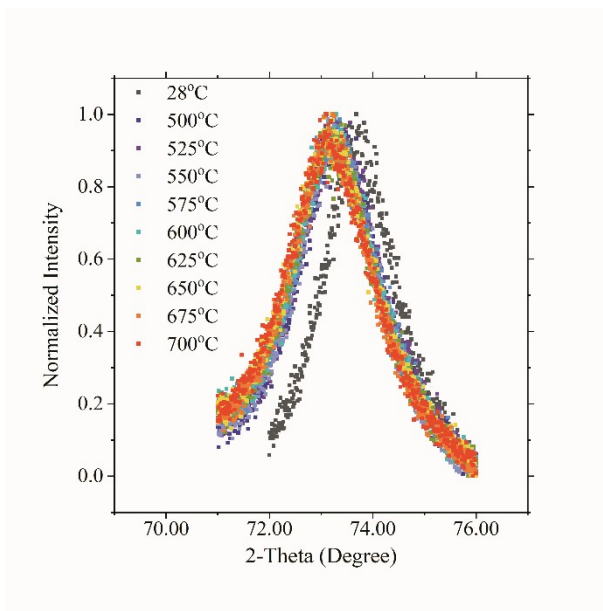


Figure S4. X-ray diffraction measurements of the (400) peak of the single crystal $(Y_2O_3)_{0.095}(ZrO_2)_{0.905}$ (YSZ) substrates used here. Note, the YSZ (200) peak was not used for these measurements because of overlap with XRD peaks from the overlying PCO film.

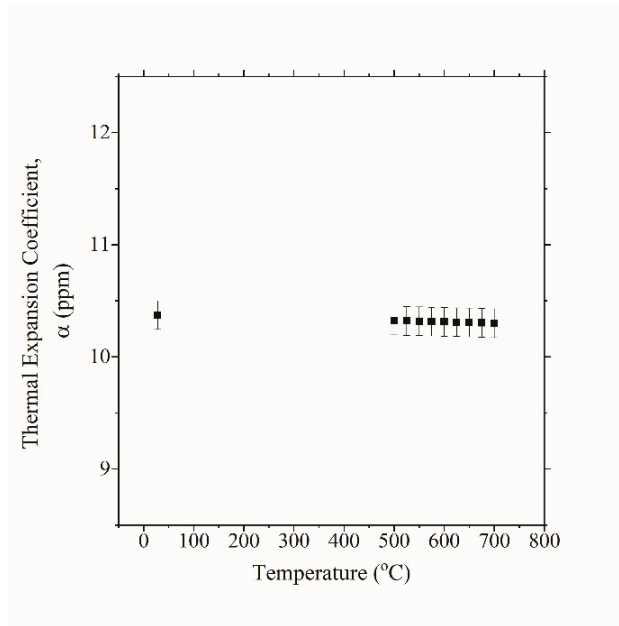
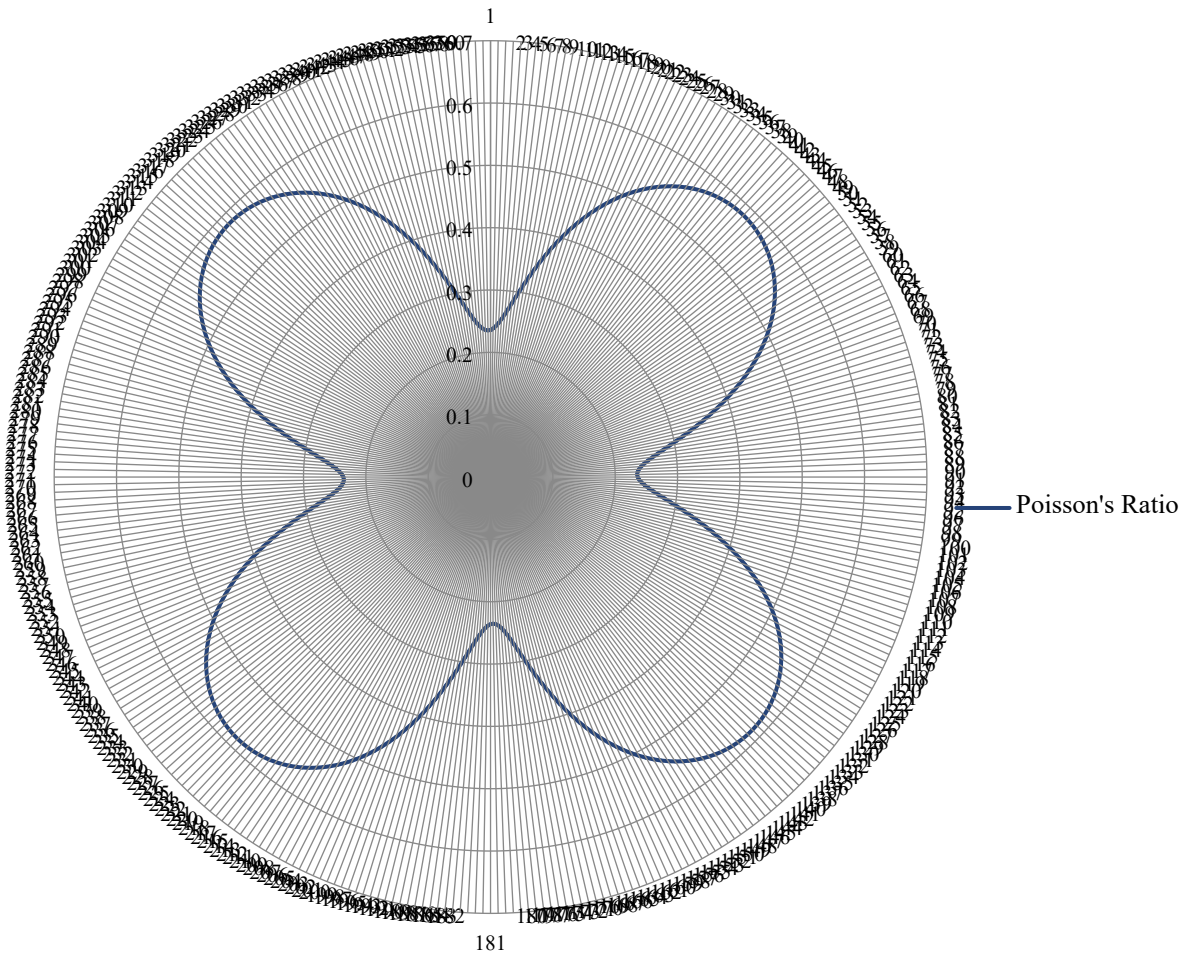


Figure S5. The (100) $(\text{Y}_2\text{O}_3)_{0.095}(\text{ZrO}_2)_{0.905}$ (YSZ) thermal expansion coefficients extracted by 1) linearly fitting the change in lattice parameter with temperature shown in Figure S4, and 2) plugging the analytical derivative of that fit and the 25°C lattice parameter indicated in Figure S4 into Equation 1 of the main manuscript. The error bars were calculated from the standard deviation in the linear fit to the YSZ lattice constant vs temperature data.

Room Temperature Poisson's Ratio for CeO₂ in the (001) Plane



Young's Modulus and Biaxial Modulus in GPa for CeO₂ in the (001) Plane

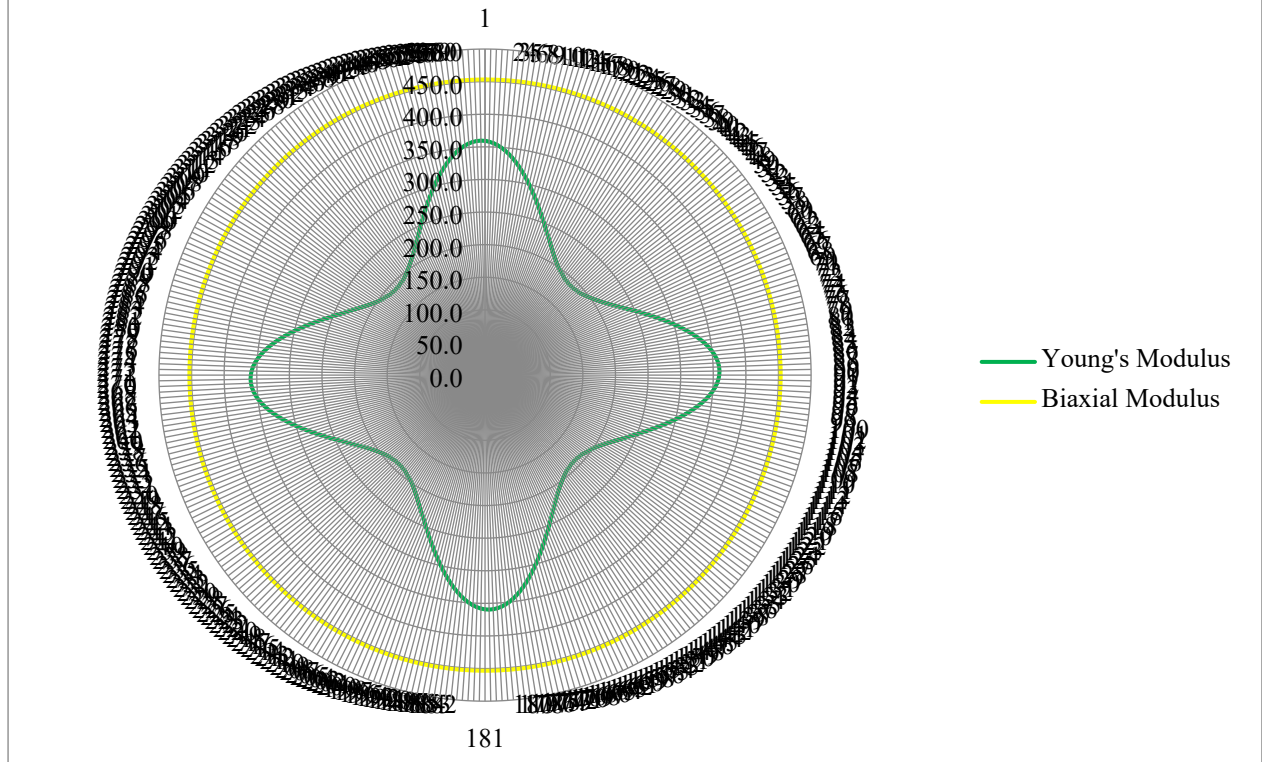


Figure S6. Directional dependence of the room temperature Poisson's Ratio, Young's Modulus, and Biaxial Modulus in the (100) plane of CeO₂ calculated from the C_{ij} values of Nakajima *et al.*³ The moduli values in the figures are in GPa.

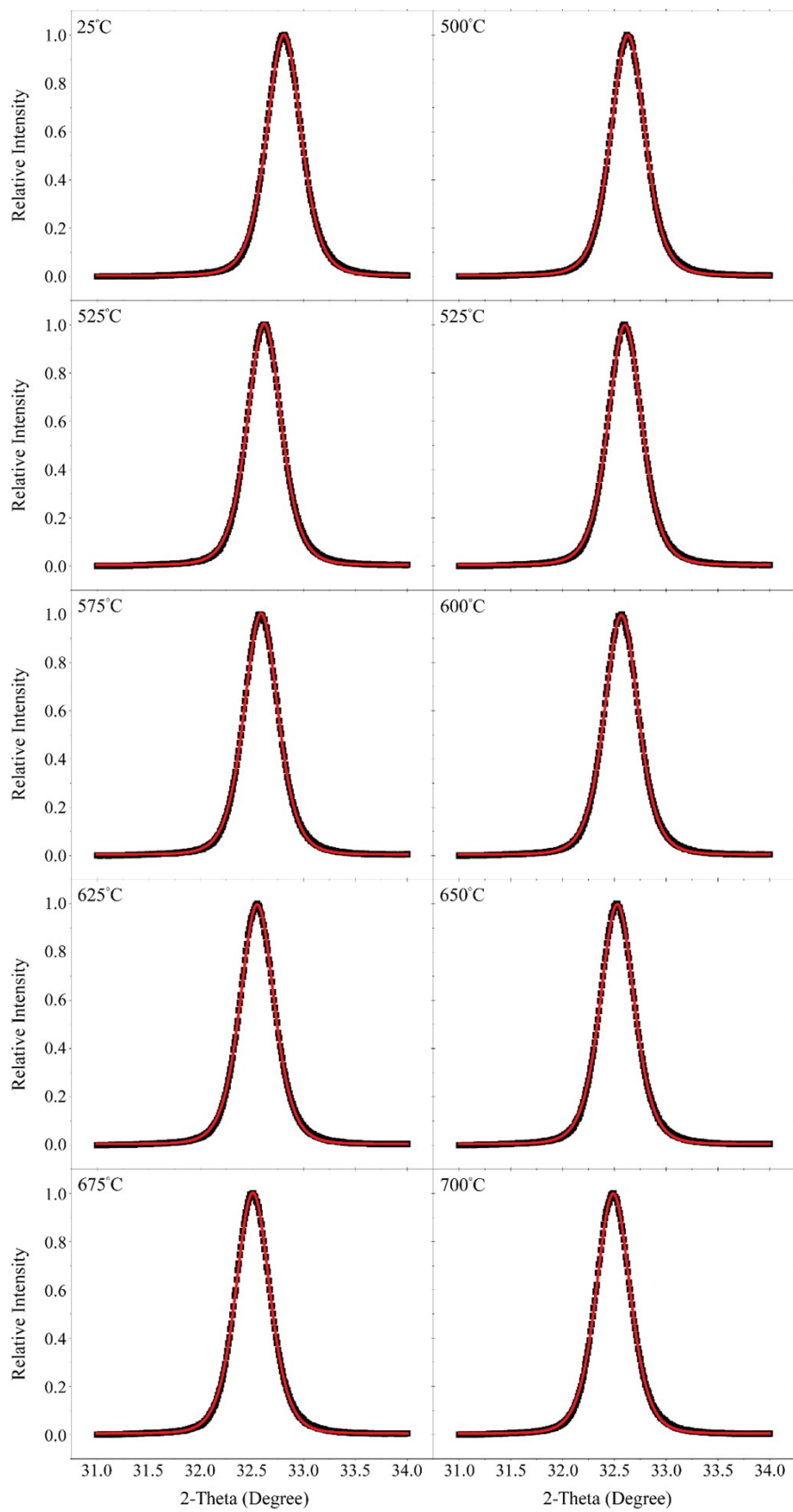


Figure S7. Pearson VII function fits to the (200) 10PCO peak at various temperatures.

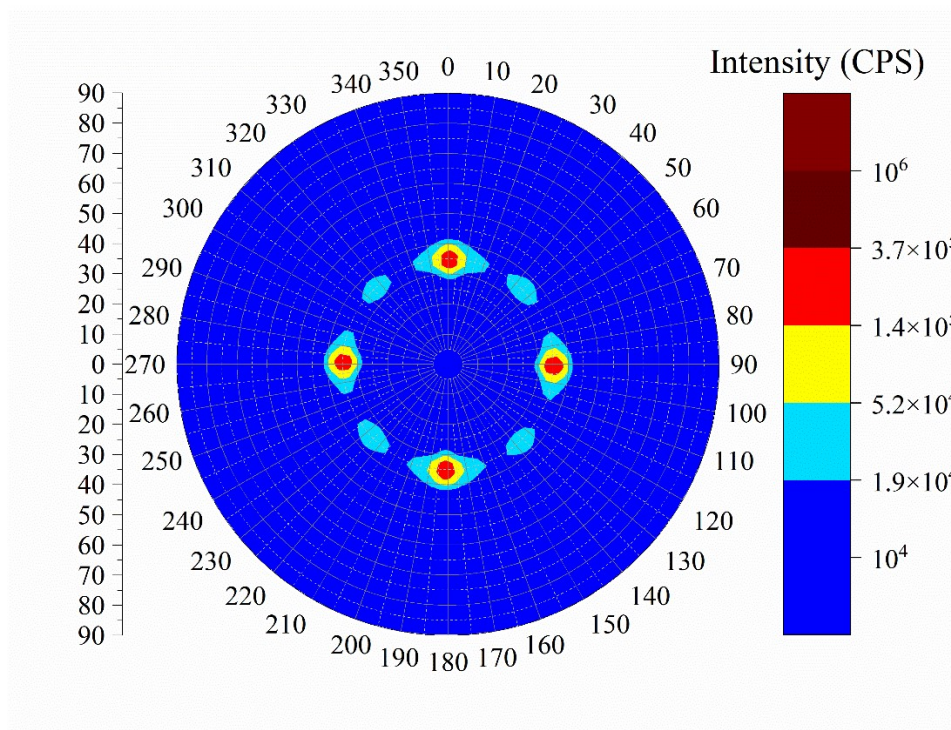
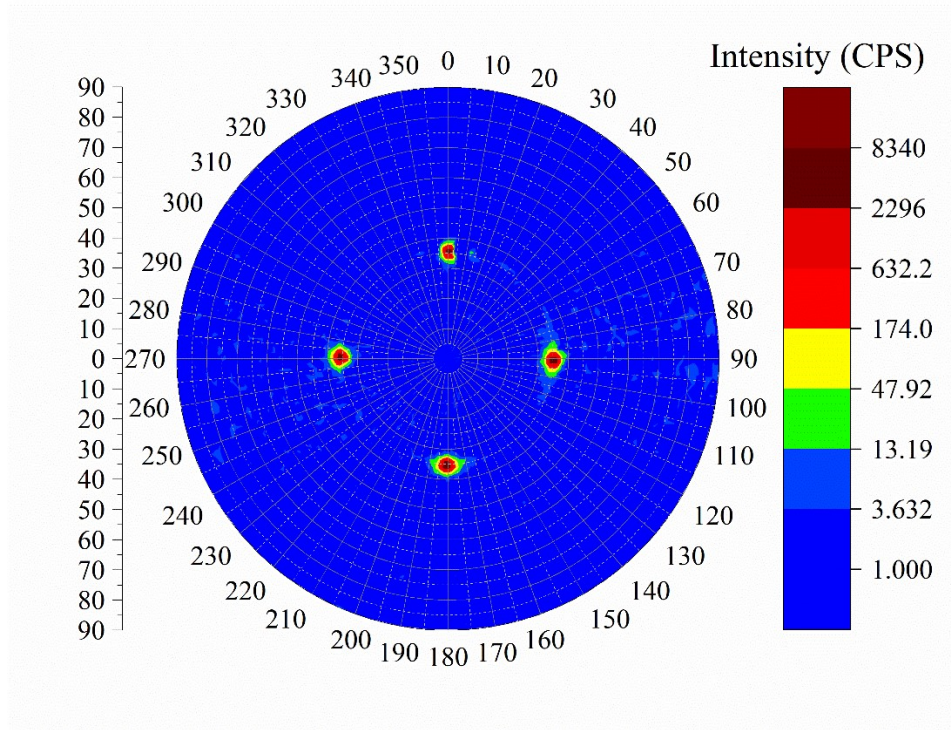


Figure S8. Representative pole figure of a 10PCO|YSZ sample (top) and a 10PCO|MgO sample (bottom).

2. Error Analysis

The strain vs. temperature data was fitted by:

$$\varepsilon_z = Ae^{BT} \quad [S1]$$

The first-order derivatives of the strain values with respect to temperature can be expressed as:

$$y = \frac{\partial \varepsilon_z}{\partial T} = AB e^{BT} \quad [S2]$$

The error of the fitting can be expressed as:⁴

$$\delta y = \sqrt{(Be^{BT} * \delta A)^2 + ((Ae^{BT} + AB^2 e^{BT}))^2} \quad [S3]$$

According to Equation S3, the error of thermo-expansion coefficient is:

$$\delta \alpha_{tc} = \frac{1 - \nu}{1 + \nu} \sqrt{(\delta y)^2 + \left(\frac{2\nu}{1 - \nu} \delta \alpha_s\right)^2} \quad [S4]$$

Reference

1. D. G. Isaak, O. L. Anderson and T. Goto, *Physics and Chemistry of Minerals*, 1989, **16**, 704-713.
2. P. J. Botha, J. C. H. Chiang, J. D. Comins, P. M. Mjwara and P. E. Ngoepe, *Journal of Applied Physics*, 1993, **73**, 7268-7274.
3. A. Nakajima, A. Yoshihara and M. Ishigame, *Physical Review B*, 1994, **50**, 13297-13307.
4. I. Hughes and T. Hase, *Measurements and Their Uncertainties: A Practical Guide to Modern Error Analysis*, Oxford University Press 2010.