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Size-dependent phase transitions in nanostructured zirconia-scandia solid solutions

-Supporting information-

Crystallite sizes and phases of the powders at room temperature

In this study, the average crystallite size (nm) of the studied powders were determined by using the Scherrer equation $D = 0.9\lambda/(B \cos \theta)$, where D is the crystallite size, λ is the wavelength of the radiation, B is the corrected peak width at half-maximum intensity, and θ is the peak position. We have use the calculated FWHM determined by the fitting of the 111 peak of the cubic phase measured at high temperature (approximately 650ºC).

Table S1. Weight fractions of the different phases at room temperature for all the compositions and average crystallite sizes studied in this work.

Sc_2O_3 content (mol%)	Calcinations temperature (ºC)	Average crystallite size <D> (nm)	Present phases at room temperature (Weigh %)*
10	935	35	c (50) + β (50)
	1000	60	c (22) + β (78)
	1200	100	c (15) + β (85)
12	935	35	c (39) + β (40) + γ (21)
	1000	60	c (23) + β (55) + γ (22)
	1200	90	β (84) + γ (16)
14	935	40	c (40) + γ (60)
	1000	65	β (13) + γ (87)
	1200	105	β (12) + γ (88)

*Characterized in previous work, for more details see reference.[20]

Crystallite size distribution analysis

In order to estimate the size distribution of the powder calcined at different temperature we have used the line broadening analysis proposed by Pielaszek.[26] This method has been thought as an extension of the classical Scherrer equation. Measurement of two widths of the same peak (at 1/5 and 4/5 of the peak maximum), allows for two parameters to be distinguished: the average grain size and dispersion of sizes, σ. The derivation of the $FW_{\frac{1}{5}/\frac{4}{4}}M$ method can be found elsewhere.[26] Figure S1 shows the results of the analysis applied to ZrO_2- 10%Sc_2O_3 nanopowders calcined at different temperature. Although in these work we focused in samples with average crystallite size above 25 nm, smaller sizes have been included in the plot with the purpose of comparison.

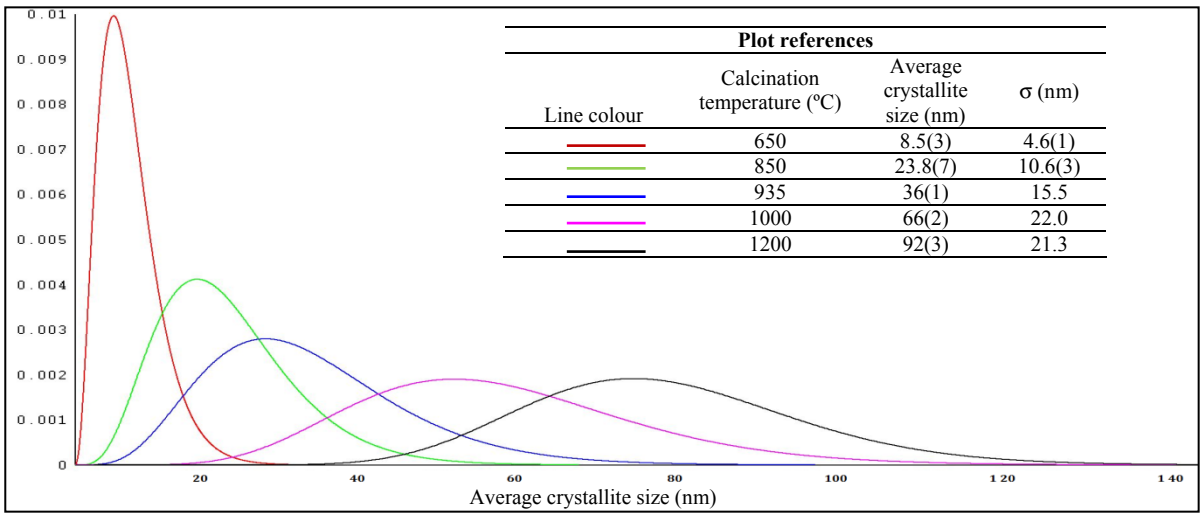

Figure S1: Crystallite size distribution functions for ZrO_2-10%Sc_2O_3 nanopowders calcined at different temperature. References to the graphic curves include the calculated average crystallite size and dispersion, σ.