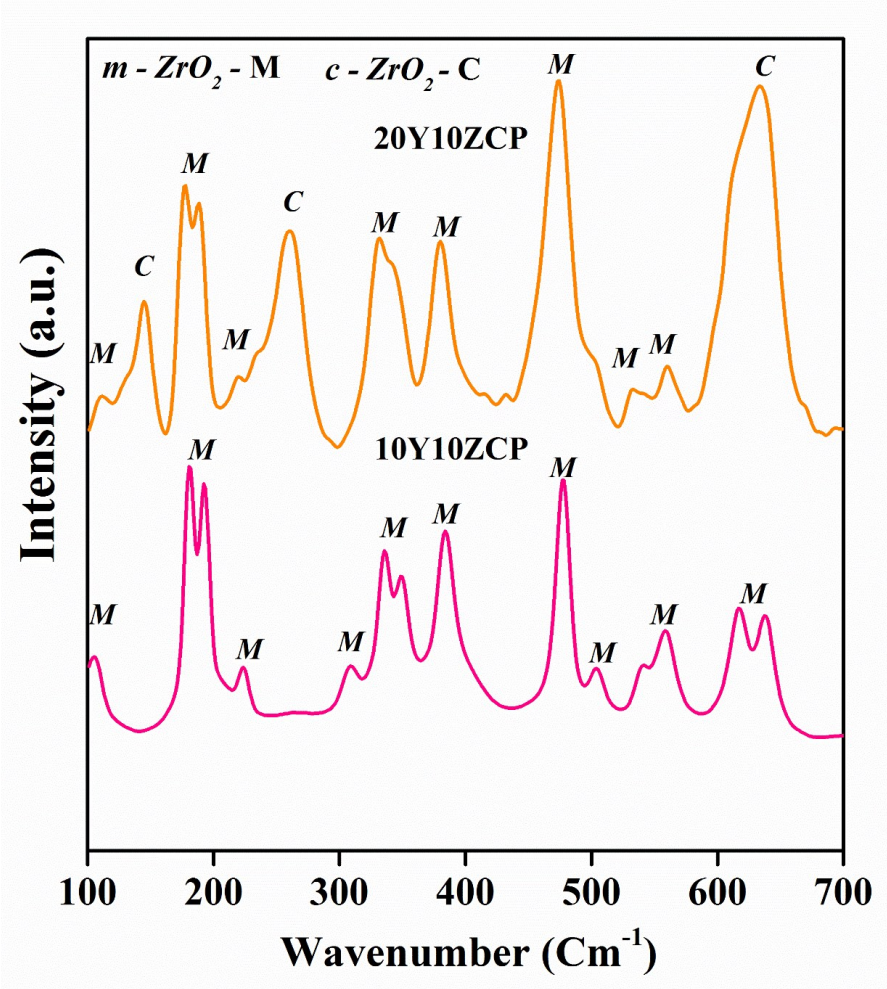
Supporting Information

Probing the combined additions of Ca^{2+} and PO_4^{3-} in yttria stabilized ZrO_2 polymorph. Structural, morphological and mechanical analysis

S. Kalaivani, V. Anamiga and S. Kannan*

Centre for Nanoscience and Technology,
Pondicherry University, Puducherry-605 014, INDIA

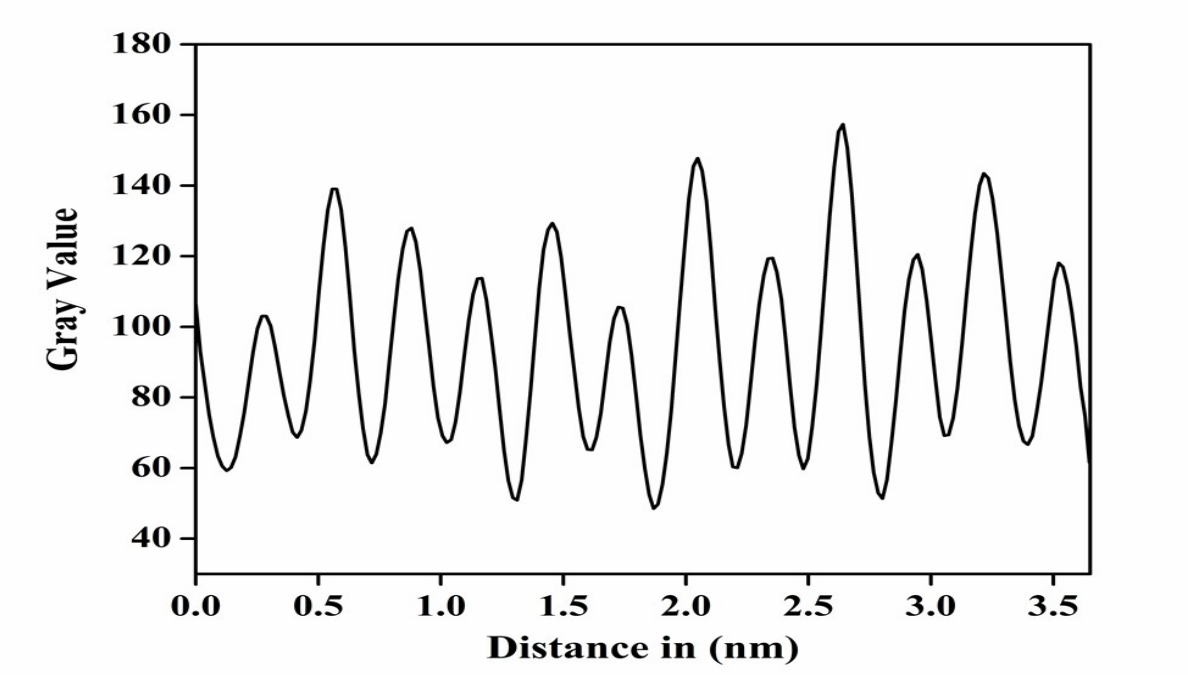


Supporting information S1 Raman spectra for 10 and 20 mol. % yttria stabilized zirconia with successive Ca^{2+} and PO_4^{3-}after heat treatment of 1400°C

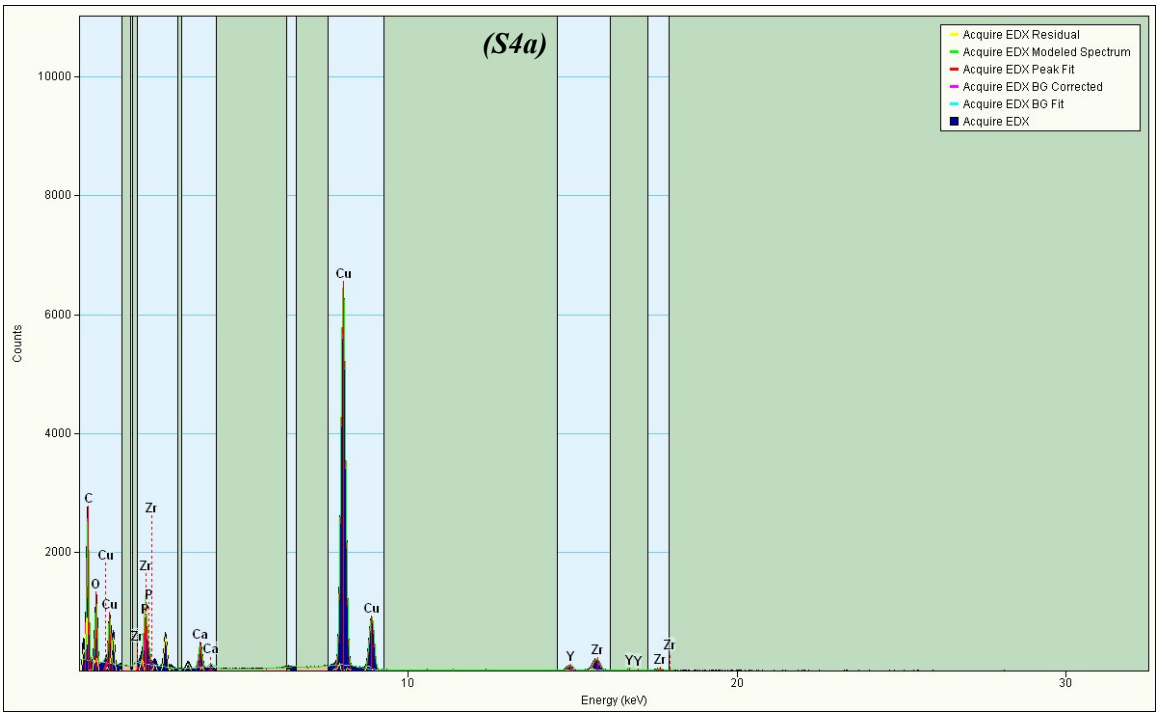
Supporting information S2 Phase, Atomic position of atoms and isothermal parameters obtained from refinement.

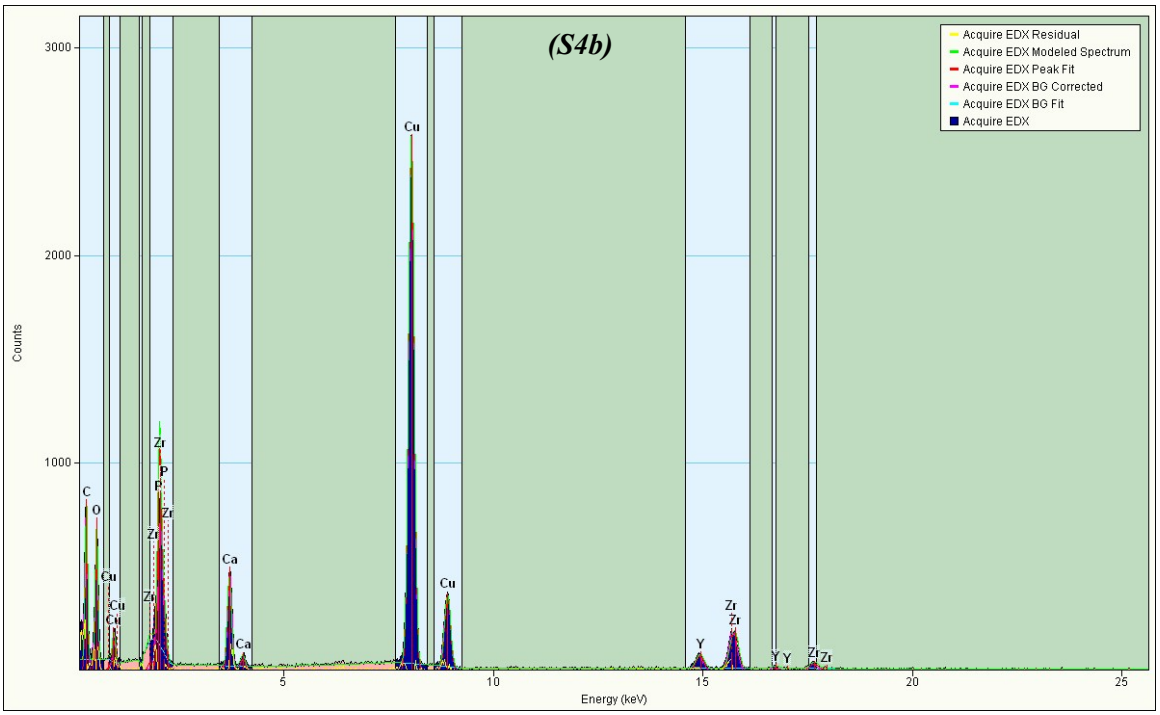
Sample Code	Phase	Atoms	Atomic coordinates			Wyckoff Position	U_{iso} (Å^2)
5ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.017(6)
		O	0.2500	0.2500	0.2500	8c	0.045(2)
10ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.013(4)
		O	0.2500	0.2500	0.2500	8c	0.043(2)
15ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.158(1)
		O	0.2500	0.2500	0.2500	8c	0.044(3)
20ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.015(4)
		O	0.2500	0.2500	0.2500	8c	0.040(1)
25ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.014(4)
		O	0.2500	0.2500	0.2500	8c	0.034(3)
	$Ca_3(PO_4)_2$	Ca1	-0.3064	-0.1522	0.1643	18b	0.024(1)
		Ca2	-0.3576	-0.1616	-0.0432	18b	0.009(3)
		Ca3	-0.2114	-0.0920	0.0543	18b	0.017(5)
		Ca4	0.0000	0.0000	-0.0658	6a	0.036(4)
		Ca5	0.0000	0.0000	-0.2709	6a	0.013(2)
		P1	0.0000	0.0000	-0.1297	6a	0.159(1)
		P2	-0.2927	-0.0873	-0.1189	18b	0.046(3)
		P3	-0.3119	-0.1210	-0.2507	18b	0.030(2)
		O1	-0.2085	-0.0776	-0.0845	18b	0.089(4)
		O2	-0.2678	-0.1605	-0.1448	18b	0.064(4)
		O3	-0.2748	0.0869	-0.1559	18b	0.011(2)
		O4	-0.4392	-0.2097	-0.1574	18b	0.030(2)
		O5	-0.5353	-0.1197	-0.2041	18b	0.091(4)
		O6	-0.4063	-0.3461	-0.2332	18b	0.215(6)
		O7	0.1559	-0.0683	-0.1920	18b	0.019(5)
		O8	-0.4076	0.0180	-0.2449	18b	0.318(3)
		O9	0.0716	-0.0627	-0.0197	18b	0.036(2)
		O10	0.0000	0.0000	0.1503	6a	0.107(6)
30ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.019(4)
		O	0.2500	0.2500	0.2500	8c	0.042(2)
	$Ca_3(PO_4)_2$	Ca1	-0.2816	-0.1432	0.1629	18b	0.014(3)
		Ca2	-0.3569	-0.1406	-0.0407	18b	0.009(2)
		Ca3	-0.2659	-0.1260	0.0577	18b	0.011(4)
		Ca4	0.0000	0.0000	-0.0718	6a	0.089(5)
		Ca5	0.0000	0.0000	-0.2600	6a	0.042(2)
		P1	0.0000	0.0000	0.0012	6a	0.012(5)
		P2	-0.2978	-0.1237	-0.1319	18b	0.050(3)
		P3	-0.3027	-0.2001	-0.2334	18b	0.014(2)

		O1	-0.1779	-0.0654	-0.0989	18b	0.063(3)
		O2	-0.2530	-0.2481	-0.1428	18b	0.090(8)
		O3	-0.2598	0.0809	-0.1603	18b	0.065(2)
		O4	-0.4757	-0.2671	-0.1508	18b	0.057(4)
		O5	-0.4052	-0.0386	-0.2404	18b	0.089(1)
		O6	-0.4453	-0.1918	-0.2160	18b	0.011(6)
		O7	0.0357	-0.1377	-0.1878	18b	0.018(4)
		O8	-0.4123	0.2420	-0.2699	18b	0.067(2)
		O9	0.0386	-0.0967	-0.0303	18b	0.061(1)
		O10	0.0000	0.0000	0.0652	6a	0.102(5)
40ZCP	*c*-ZrO_2	Zr	0.0000	0.0000	0.0000	4a	0.014(4)
		O	0.2500	0.2500	0.2500	8c	0.035(2)
	$Ca_3(PO_4)_2$	Ca1	-0.2732	-0.1389	0.1678	18b	0.024(7)
		Ca2	-0.3817	-0.1740	-0.0318	18b	0.002(4)
		Ca3	-0.2713	-0.1422	0.0627	18b	0.019(2)
		Ca4	0.0000	0.0000	-0.0827	6a	0.059(6)
		Ca5	0.0000	0.0000	-0.2660	6a	0.014(4)
		P1	0.0000	0.0000	-0.0057	6a	0.072(3)
		P2	-0.3150	-0.1430	-0.1325	18b	0.044(2)
		P3	-0.3522	-0.1595	-0.2349	18b	0.108(1)
		O1	-0.2635	-0.0847	-0.0878	18b	0.034(5)
		O2	-0.2064	-0.1939	-0.1401	18b	0.039(2)
		O3	-0.4736	0.0025	-0.1483	18b	0.018(2)
		O4	-0.4757	-0.2308	-0.1350	18b	0.021(1)
		O5	-0.4002	-0.0422	-0.2177	18b	0.033(5)
		O6	-0.4207	-0.3007	-0.2128	18b	0.013(2)
		O7	0.0874	-0.0929	-0.2203	18b	0.031(5)
		O8	-0.3642	-0.1697	-0.2706	18b	0.023(6)
		O9	0.0037	-0.1447	-0.0163	18b	0.074(3)
		O10	0.0000	0.0000	0.0238	6a	0.054(1)



Supporting information S3 Gray value Vs Distance of TE Micrograph of 5ZCP **(Fig7d).**





Supporting information S4 EDX spectra recorded from TEM for 5ZCP **(S4a)** and 40ZCP **(S4b)** samples after sintering at 1400 °C